**Supplementary Information**

**Structure of Amido-Pyridinium Betaines: Persistent Intermolecular C-H**···**N Hydrogen Bonding in Solution**

Robert J. Thatcher, David G. Johnson, John M. Slattery\* and Richard E. Douthwaite\*

Fitting of NMR data 5

Fig. S1 VT NMR of 1 in thf-d8 (13.5 mM) 6

Fig. S3. Van’t Hoff plot for 1 in thf-d8. 7

Fig. S4 VT NMR of 2 in thf-d8 (120 mM) 8

Fig. S5 VT NMR of 2 in thf-d8 (7.8 mM) 8

Fig. S6 Van’t Hoff plot for 2 in thf-d8. 9

Computational Supplementary Information 10

Visualisation 10

Isomers of 1 and [1]2 10

Structural comparison for [1]2 and [2]2 11

Tables of energies for each computational methodology 12

Summary of calculated NMR data for 1, 2, [1]2 and [2]2 14

Summary of selected NBO data for [1]2 and [2]2 26

Optimised structures of norharman (1) and BETAINE (2) complexes with CH2Cl2 28

Energies, optimised structures and vibrational frequencies for dichloromethane complexes 29

Norharman Iso1.CH2Cl2 29

Norharman Iso2.CH2Cl2 32

BETAINE.CH2Cl2 Isomer2 36

Energies, optimised structures and vibrational frequencies for norharman motif (compounds 1 and [1]2) 40

Norharman monomer\_iso1 40

Norharman monomer\_iso2 44

Norharman dimer\_iso1 47

Norharman dimer\_iso2 52

Energies, optimised structures and vibrational frequencies for betaine motif (compounds 2 and [2]2) 57

BETAINE monomer\_iso1 57

BETAINE dimer\_iso1 60

BETAINE monomer\_iso2 64

BETAINE\_dimer\_iso2 68

NMR chemical shift calculations – norharman motif (compounds 1 and [1]2) 74

Norharman monomer\_iso 1 (gas-phase) - BP86/IGLO-III level 74

Norharman monomer\_iso 1 (gas-phase) – PBE0/IGLO-III level 77

Norharman monomer\_iso 1 (IEFPCM solvent = tetrahydrofuran) - BP86/IGLO-III level 80

Norharman monomer\_iso 1 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level 84

Norharman monomer\_iso 2 (gas-phase) - BP86/IGLO-III level 87

Norharman monomer\_iso2 (gas-phase) – PBE0/IGLO-III level 91

Norharman monomer\_iso2 (IEFPCM solvent = tetrahydrofuran) - BP86/IGLO-III level 94

Norharman monomer\_iso2 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level 97

Norharman dimer\_iso 1 (gas-phase) - BP86/IGLO-III level 101

Norharman dimer\_iso 1 (gas-phase) – PBE0/IGLO-III level 108

Norharman dimer\_iso 1 (IEFPCM solvent = tetrahydrofuran) - BP86/IGLO-III level 114

Norharman dimer\_iso 1 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level 121

Norharman dimer\_iso 2 (gas-phase) - BP86/IGLO-III level 128

Norharman dimer\_iso 2 (gas-phase) – PBE0/IGLO-III level 134

Norharman dimer\_iso 2 (IEFPCM solvent = tetrahydrofuran) - BP86/IGLO-III level 141

Norharman dimer\_iso 2 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level 148

NMR chemical shift calculations – BETAINE motif (compounds 2 and[2]2) 154

BETAINE monomer\_iso1 (gas-phase) - BP86/IGLO-III level 154

BETAINE monomer\_iso1 (gas-phase) – PBE0/IGLO-III level 158

BETAINE monomer\_iso1 (IEFPCM solvent = tetrahydrofuran) – BP86/IGLO-III level 162

BETAINE monomer\_iso1 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level 165

BETAINE dimer\_iso1 (gas-phase) - BP86/IGLO-III level 169

BETAINE dimer\_iso1 (gas-phase) – PBE0/IGLO-III level 176

BETAINE dimer\_iso1 (IEFPCM solvent = tetrahydrofuran) – BP86/IGLO-III level 183

BETAINE dimer\_iso1 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level 190

BETAINE monomer\_iso2 (gas-phase) - BP86/IGLO-III level 197

BETAINE monomer\_iso2 (gas-phase) – PBE0/IGLO-III level 201

BETAINE monomer\_iso2 (IEFPCM solvent = tetrahydrofuran) – BP86/IGLO-III level 205

BETAINE monomer\_iso2 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level 208

BETAINE dimer\_iso2 (gas-phase) - BP86/IGLO-III level 212

BETAINE dimer\_iso2 (gas-phase) – PBE0/IGLO-III level 219

BETAINE dimer\_iso2 (IEFPCM solvent = tetrahydrofuran) – BP86/IGLO-III level 226

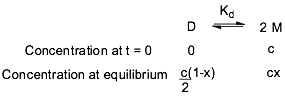
BETAINE dimer\_iso2 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level 233

References 241

**VT NMR:** NMR data were acquired in tubes sealed with a Young’s Teflon stopcock. Samples were prepared by extracting (*via* microsyringe) a known volume from thf-d8 stock solutions of **1** (26.9 mM (3.4 mg in 0.6 mL)) and **2** (120 mM (15.3 mg in 0.6 mL)) and adding additional thf-d8 to a total volume of 0.6 mL. Compound **1** is less soluble than **2** in thf and the most concentrated samples were chosen to avoid precipitation at low temperature. Spectra were referenced to the downfield residual proton signals of thf-d8. Data was acquired for three concentrations of **1** and **2** on a Bruker AV500 and the temperature was calibrated using methanol in toluene-d8. Before data acquisition samples were equilibrated at each temperature for 10-30 min.

# Fitting of NMR data

Dissociation of dimer to monomer[[1](#_ENREF_1)]



Equilibrium constant of dissociation



Rearranging for x



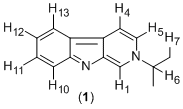
Under fast exchange the observed chemical shift of H(1) (obs) is a number weighted average of the dimer (D) and monomer (M) chemical shift.



Substitution for x



Simultaneous fitting of plots of obs vs T at several concentrations allows Kd, M, and D to be determined. Fitting was performed to minimize the difference between observed and predicted obs across all the data simultaneously. Sφ and Hφ were extracted from the Van’t Hoff plots using the standard equations.

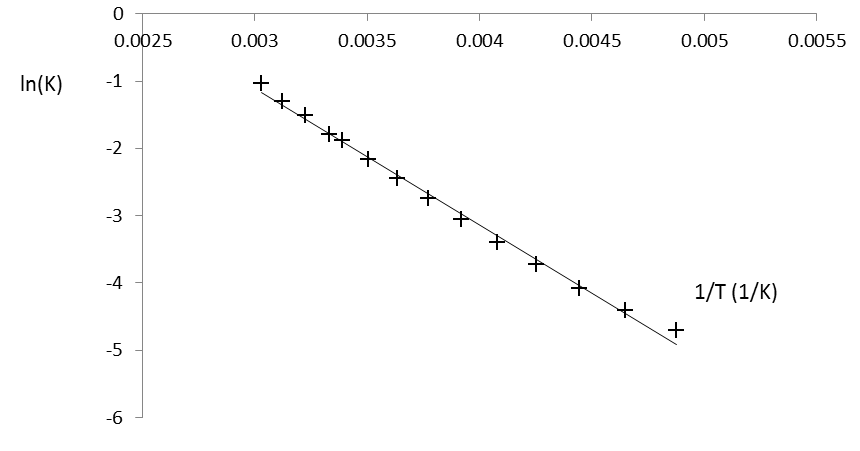




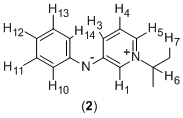
# Fig. S1 VT NMR of 1 in thf-d8 (13.5 mM)



Fig. S2 VT NMR of **1** in thf-d8 (7.2 mM)



# Fig. S3. Van’t Hoff plot for 1 in thf-d8.

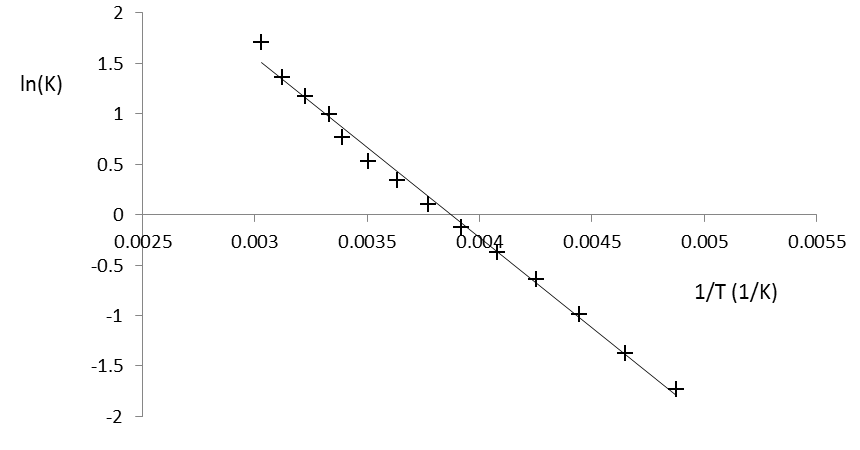




# Fig. S4 VT NMR of 2 in thf-d8 (120 mM)



# Fig. S5 VT NMR of 2 in thf-d8 (7.8 mM)



# Fig. S6 Van’t Hoff plot for 2 in thf-d8.

# Computational Supplementary Information

|  |
| --- |
|  |
| [1]2\_iso2 |
|  |
| [2]2\_iso2 (monomer numbered from C1 to H32) |

Fig. S7 Numbering schemes used for **1**, **[1]2**, **2** and **[2]2**.

## Visualisation

Structures were visualised and modified using Facio,[[2](#_ENREF_2)] Jmol,[[3](#_ENREF_3)] gOpenMol and Gaussview.

## Isomers of 1 and [1]2

Two isomers were optimised for both **1** and **2** and their dimers, where the methyl substituents of the iPr groups point towards (iso1) or away from (iso2) the nitrogen atom of the five-membered ring. Both are observed in the X-ray crystal structure of **[1]2**, but only the isomer related to iso2 is seen in the X-ray crystal structure of **[2]2**. Energetically there is little or no difference between these for **1**, but there is a significant stabilization of **[2]2\_iso2**, presumably for steric reasons.

## Structural comparison for [1]2 and [2]2



See figure S7 for numbering scheme. All distances in Å.

## Tables of energies for each computational methodology

Enthalpies, entropies and free energies are shown relative to the monomeric form of each system (relative to isomer 2 of **1**).

### Dimerisation of 1







Note: Basis set superposition errors were calculated based on isomer 2.

### Dimerisation of 2







Note: Basis set superposition errors were calculated based on isomer 2.

## Summary of calculated NMR data for 1, 2, [1]2 and [2]2

















Betaine monomer Iso1 (gas-phase)

Betaine monomer Iso2 (gas-phase)



Betaine monomer Iso1 (thf)

Betaine monomer Iso2 (thf)



Betaine Dimer Iso1 (gas-phase)

Betaine Dimer Iso2 (gas-phase) 

Betaine Dimer Iso1 (thf) 

Betaine Dimer Iso2 (thf) 

## Summary of selected NBO data for [1]2 and [2]2

### [1]2 isomer 1



### [1]2 isomer 2



Atom numbering as shown in figure S7

### [2]2 isomer1

### 

### [2]2 isomer2



Atom numbering as shown in figure S7

# Optimised structures of norharman (1) and BETAINE (2) complexes with CH2Cl2

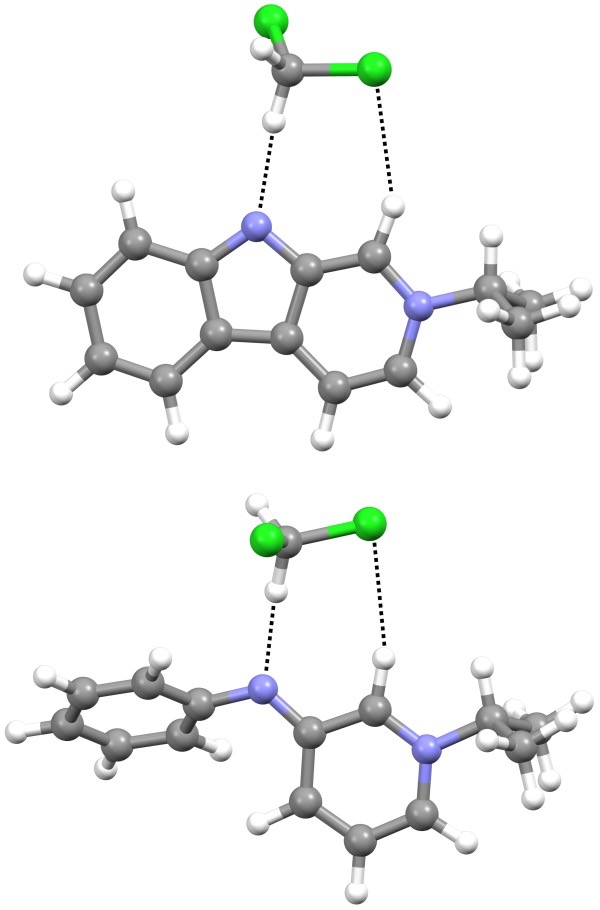


Fig. S8. Optimised structures of **1**.CH2Cl2 and **2**.CH2Cl2 (at the (RI-)PBE0/def2-TZVPP level), where each substrate forms two hydrogen bonding interactions (C-H…N and C-H…Cl) to a molecule of CH2Cl2 to form a 7-membered ring structure. The C-H…N bonds in these structures (3.25 and 3.23 Å for the C-N distances respectively) are significantly shorter than those found in [**1**]2 and [**2**]2 (3.40 and 3.46 Å at the same level of theory). This suggests a relatively strong interaction that is potentially sufficient to inhibit dimerisation, which is consistent with the experimental observation that the NMR of **1** and **2** in dcm-d2 is temperature insensitive.

# Energies, optimised structures and vibrational frequencies for dichloromethane complexes

## Norharman Iso1.CH2Cl2

bp86 energy (au): -1610.4585694500

Zero point energy (au): 0.2719714

Entropy (kJ mol^-1): 0.62860

Chemical potential (kJ mol^-1): 578.55

XYZ coordinates:

35

C -2.38520 3.25216 -0.09388

C -1.05073 2.85340 -0.15712

C -0.74641 1.47263 -0.05590

C -1.80731 0.48869 0.10933

C -3.15827 0.92538 0.17210

C -3.42612 2.28959 0.07031

C 0.45733 0.70457 -0.07145

N -1.34364 -0.80069 0.19067

H -3.96754 0.18930 0.30290

H -4.47140 2.63969 0.11859

C 1.83744 0.95021 -0.18955

C 0.00176 -0.68288 0.08555

C 0.95333 -1.70966 0.11514

H 2.24354 1.96714 -0.31200

C 2.72608 -0.12194 -0.15046

N 2.27878 -1.41898 -0.00004

H 3.81460 0.00138 -0.23474

H 0.66548 -2.76540 0.23270

C 3.27347 -2.53815 0.03729

H -2.64497 4.32087 -0.16963

H -0.24860 3.60071 -0.28266

C 3.22791 -3.27194 1.38557

H 4.25970 -2.03773 -0.05408

C 3.09282 -3.47429 -1.16667

H 2.26898 -3.81605 1.52663

H 3.35642 -2.56259 2.23100

H 4.05026 -4.01863 1.43138

H 2.12610 -4.02079 -1.11976

H 3.90903 -4.22912 -1.17870

H 3.13005 -2.90854 -2.12235

H -3.15435 -4.14404 -0.19940

C -2.47116 -3.81936 0.60653

H -2.14938 -2.75471 0.49412

Cl -0.99574 -4.86778 0.47984

Cl -3.31825 -4.01244 2.16677

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 7.36 0.73634 YES YES

8 a 25.99 0.12019 YES YES

9 a 35.91 1.99433 YES YES

10 a 39.37 0.31542 YES YES

11 a 56.20 0.58491 YES YES

12 a 60.89 0.49302 YES YES

13 a 73.94 0.14874 YES YES

14 a 133.80 1.58234 YES YES

15 a 145.62 0.12294 YES YES

16 a 148.09 0.28304 YES YES

17 a 172.53 19.46968 YES YES

18 a 223.93 6.03242 YES YES

19 a 236.56 0.22387 YES YES

20 a 263.42 0.01106 YES YES

21 a 269.70 2.42767 YES YES

22 a 277.80 0.16782 YES YES

23 a 311.93 0.27300 YES YES

24 a 315.92 2.07723 YES YES

25 a 390.36 1.23221 YES YES

26 a 415.16 5.97354 YES YES

27 a 443.83 2.26560 YES YES

28 a 462.02 4.86516 YES YES

29 a 484.07 0.30295 YES YES

30 a 534.82 0.54153 YES YES

31 a 558.52 0.13578 YES YES

32 a 564.42 1.47316 YES YES

33 a 578.92 2.00987 YES YES

34 a 622.52 7.06570 YES YES

35 a 648.81 10.07579 YES YES

36 a 654.47 47.71684 YES YES

37 a 704.66 99.77567 YES YES

38 a 716.21 7.45185 YES YES

39 a 721.72 9.64977 YES YES

40 a 729.91 55.08707 YES YES

41 a 746.35 2.66081 YES YES

42 a 762.98 6.16116 YES YES

43 a 786.19 0.41339 YES YES

44 a 852.90 0.61018 YES YES

45 a 862.96 5.21771 YES YES

46 a 866.11 14.12542 YES YES

47 a 878.21 1.55365 YES YES

48 a 899.28 1.63354 YES YES

49 a 911.93 1.50913 YES YES

50 a 916.81 0.40062 YES YES

pbe0\_def2-tzvpp energy (au): -1610.2951601390

Zero point energy (au): -1610.2951601390

Entropy (kJ mol^-1): 0.63956

Chemical potential (kJ mol^-1): 597.58

XYZ coordinates:

35

C -2.34234 3.19602 -0.09400

C -1.02773 2.80348 -0.14029

C -0.73097 1.43566 -0.05679

C -1.77617 0.46364 0.07264

C -3.11425 0.89502 0.11900

C -3.37404 2.24035 0.03595

C 0.46097 0.67829 -0.06580

N -1.32034 -0.81402 0.14009

H -3.91453 0.17238 0.22168

H -4.40120 2.58523 0.07170

C 1.82515 0.93188 -0.15559

C 0.01354 -0.69203 0.05963

C 0.95816 -1.70090 0.08739

H 2.22119 1.93499 -0.25152

C 2.70331 -0.12257 -0.11957

N 2.26455 -1.40453 0.00049

H 3.77351 0.00346 -0.18238

H 0.68655 -2.74326 0.17983

C 3.25579 -2.50241 0.03571

H -2.59815 4.24652 -0.15608

H -0.23667 3.53884 -0.23901

C 3.19180 -3.25081 1.35623

H 4.22338 -2.00334 -0.03407

C 3.09484 -3.41728 -1.16645

H 2.25027 -3.79134 1.46579

H 3.29811 -2.56905 2.20063

H 4.00112 -3.98104 1.40029

H 2.14682 -3.95636 -1.13360

H 3.89791 -4.15579 -1.17267

H 3.13908 -2.85380 -2.09908

H -3.28916 -4.09767 -0.02759

C -2.50879 -3.79766 0.66346

H -2.18082 -2.76728 0.50399

Cl -1.12023 -4.87125 0.37589

Cl -3.13666 -3.95338 2.30210

Vibrational Spectrum (first 50 lines):

$vibrational spectrum

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 3.75 0.94982 YES YES

8 a 14.45 0.06467 YES YES

9 a 30.64 1.67029 YES YES

10 a 34.09 0.34415 YES YES

11 a 48.05 0.64269 YES YES

12 a 60.66 1.09074 YES YES

13 a 65.73 0.09162 YES YES

14 a 136.47 1.83875 YES YES

15 a 143.57 4.69318 YES YES

16 a 150.51 0.21702 YES YES

17 a 159.56 16.36171 YES YES

18 a 226.65 4.78617 YES YES

19 a 228.82 0.91993 YES YES

20 a 255.69 0.05794 YES YES

21 a 282.04 0.05215 YES YES

22 a 284.07 1.58421 YES YES

23 a 319.12 0.32482 YES YES

24 a 322.59 2.05797 YES YES

25 a 401.11 2.16528 YES YES

26 a 426.04 6.86342 YES YES

27 a 457.24 0.90638 YES YES

28 a 470.17 6.79232 YES YES

29 a 495.62 0.04479 YES YES

30 a 553.30 1.09239 YES YES

31 a 571.39 0.06216 YES YES

32 a 579.72 1.68824 YES YES

33 a 596.36 2.15875 YES YES

34 a 650.08 7.16570 YES YES

35 a 671.73 4.59007 YES YES

36 a 708.66 27.79304 YES YES

37 a 745.24 2.19146 YES YES

38 a 750.35 28.92406 YES YES

39 a 755.98 122.93909 YES YES

40 a 766.71 40.16722 YES YES

41 a 773.03 3.42121 YES YES

42 a 782.61 9.45212 YES YES

43 a 803.37 3.03198 YES YES

44 a 873.47 1.83814 YES YES

45 a 892.57 7.86879 YES YES

46 a 907.71 1.70948 YES YES

47 a 912.46 14.54030 YES YES

48 a 933.84 0.32709 YES YES

49 a 935.78 0.15587 YES YES

50 a 940.26 1.24261 YES YES

## Norharman Iso2.CH2Cl2

bp86 energy (au): -1610.4578974970

Zero point energy (au): 0.2717473

Entropy (kJ mol^-1): 0.63948

Chemical potential (kJ mol^-1): 575.04

XYZ coordinates:

35

C -2.38755 3.23753 -0.09785

C -1.05261 2.84204 -0.16928

C -0.74301 1.46379 -0.05042

C -1.79905 0.47978 0.14065

C -3.15058 0.91326 0.21315

C -3.42377 2.27477 0.09324

C 0.46204 0.69840 -0.07019

N -1.33127 -0.80690 0.23320

H -3.95588 0.17687 0.36452

H -4.46937 2.62271 0.14838

C 1.83974 0.94734 -0.20865

C 0.01259 -0.68809 0.11014

C 0.96894 -1.71158 0.13782

H 2.23973 1.96460 -0.34734

C 2.73328 -0.12026 -0.17017

N 2.29256 -1.41756 -0.00066

H 3.81830 0.01311 -0.27126

H 0.69203 -2.76987 0.26710

C 3.28851 -2.53407 0.03810

H -2.65143 4.30413 -0.18770

H -0.25436 3.58982 -0.31528

C 4.04427 -2.65202 -1.29345

H 2.67265 -3.44738 0.16690

C 4.21609 -2.40771 1.25505

H 4.71046 -1.78053 -1.47522

H 3.33784 -2.73670 -2.14685

H 4.68039 -3.56345 -1.27956

H 4.88413 -1.52242 1.17869

H 4.86002 -3.31088 1.32818

H 3.63048 -2.32401 2.19559

H -3.23088 -4.08103 -0.26116

C -2.54365 -3.80126 0.55805

H -2.19471 -2.74245 0.48421

Cl -1.09178 -4.87334 0.40401

Cl -3.40715 -4.02565 2.10706

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 5.44 0.70113 YES YES

8 a 19.44 0.02252 YES YES

9 a 30.13 1.76802 YES YES

10 a 33.16 0.21094 YES YES

11 a 49.68 0.04007 YES YES

12 a 62.73 1.63495 YES YES

13 a 69.52 0.21818 YES YES

14 a 123.79 1.38218 YES YES

15 a 144.68 0.17629 YES YES

16 a 161.61 0.01354 YES YES

17 a 171.51 20.83177 YES YES

18 a 221.77 0.02013 YES YES

19 a 241.69 1.15557 YES YES

20 a 257.62 1.64659 YES YES

21 a 269.31 1.73325 YES YES

22 a 274.39 0.01724 YES YES

23 a 282.19 7.00581 YES YES

24 a 309.83 0.40368 YES YES

25 a 390.09 1.13119 YES YES

26 a 398.66 2.84516 YES YES

27 a 439.20 2.60451 YES YES

28 a 462.20 4.31381 YES YES

29 a 494.97 3.20354 YES YES

30 a 537.93 0.59134 YES YES

31 a 551.32 2.57484 YES YES

32 a 564.37 1.45402 YES YES

33 a 590.09 0.44764 YES YES

34 a 622.40 7.75902 YES YES

35 a 656.05 9.28686 YES YES

36 a 660.59 40.29237 YES YES

37 a 702.24 90.58397 YES YES

38 a 709.67 22.31978 YES YES

39 a 716.51 7.21759 YES YES

40 a 729.79 55.60430 YES YES

41 a 747.51 3.88574 YES YES

42 a 762.71 6.18078 YES YES

43 a 785.98 0.47784 YES YES

44 a 852.91 0.64553 YES YES

45 a 860.41 4.64385 YES YES

46 a 863.73 11.82537 YES YES

47 a 874.73 1.42055 YES YES

48 a 901.42 1.31514 YES YES

49 a 911.82 0.94011 YES YES

50 a 912.27 1.85490 YES YES

pbe0\_def2-tzvpp energy (au): -1610.2947225960

Zero point energy (au): 0.2807245

Entropy (kJ mol^-1): 0.63528

Chemical potential (kJ mol^-1): 598.90

XYZ coordinates:

35

C -2.33781 3.18463 -0.09730

C -1.02371 2.79311 -0.16113

C -0.72256 1.42825 -0.04891

C -1.76318 0.45895 0.12835

C -3.10085 0.88933 0.19250

C -3.36508 2.23149 0.07956

C 0.46982 0.67188 -0.06546

N -1.30385 -0.81580 0.21780

H -3.89698 0.16839 0.33218

H -4.39185 2.57607 0.12824

C 1.83157 0.92428 -0.19409

C 0.02767 -0.69477 0.10380

C 0.97518 -1.70215 0.13204

H 2.22275 1.92569 -0.32306

C 2.71257 -0.12682 -0.15621

N 2.27909 -1.40647 0.00381

H 3.77902 0.00493 -0.24959

H 0.71259 -2.74483 0.25462

C 3.26692 -2.50607 0.04047

H -2.59679 4.23290 -0.18124

H -0.23658 3.52700 -0.29532

C 4.01673 -2.61174 -1.27647

H 2.66773 -3.40845 0.16941

C 4.19253 -2.36889 1.23721

H 4.65891 -1.74595 -1.44612

H 3.32617 -2.69848 -2.11591

H 4.65258 -3.49794 -1.26195

H 4.83799 -1.49336 1.14967

H 4.83407 -3.24865 1.30289

H 3.62536 -2.28770 2.16497

H -3.32279 -4.03956 -0.18902

C -2.58406 -3.78497 0.56335

H -2.23061 -2.75496 0.47318

Cl -1.19482 -4.86561 0.31706

Cl -3.32074 -4.00270 2.14968

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 6.62 0.85540 YES YES

8 a 16.75 0.08584 YES YES

9 a 28.44 1.63087 YES YES

10 a 37.01 0.00289 YES YES

11 a 43.08 0.14738 YES YES

12 a 61.98 0.38495 YES YES

13 a 64.69 1.73486 YES YES

14 a 127.34 1.56143 YES YES

15 a 142.23 5.71602 YES YES

16 a 158.43 16.62692 YES YES

17 a 164.87 0.10969 YES YES

18 a 225.44 0.00508 YES YES

19 a 244.07 0.85013 YES YES

20 a 265.17 1.65793 YES YES

21 a 280.36 0.00287 YES YES

22 a 283.65 0.34651 YES YES

23 a 287.69 7.79134 YES YES

24 a 316.55 0.39787 YES YES

25 a 400.51 2.08142 YES YES

26 a 408.41 3.43173 YES YES

27 a 453.44 1.48904 YES YES

28 a 469.13 6.02996 YES YES

29 a 509.71 4.04059 YES YES

30 a 552.11 0.43877 YES YES

31 a 569.25 2.94490 YES YES

32 a 579.74 1.69426 YES YES

33 a 608.33 0.26168 YES YES

34 a 651.16 7.32485 YES YES

35 a 680.11 2.27969 YES YES

36 a 711.10 25.59754 YES YES

37 a 733.42 4.07467 YES YES

38 a 750.11 28.27193 YES YES

39 a 755.95 126.26279 YES YES

40 a 769.35 40.04903 YES YES

41 a 774.97 3.97000 YES YES

42 a 783.45 6.84251 YES YES

43 a 804.98 4.20185 YES YES

44 a 874.21 1.70295 YES YES

45 a 890.02 6.08565 YES YES

46 a 904.90 2.08965 YES YES

47 a 905.16 13.92319 YES YES

48 a 933.76 0.31317 YES YES

49 a 935.35 0.77491 YES YES

50 a 944.90 1.61068 YES YES

## BETAINE.CH2Cl2 Isomer2

bp86 energy (au): -1611.6180439970

Zero point energy (au): 0.2916496

Entropy (kJ mol^-1): 0.67589

Chemical potential (kJ mol^-1): 620.25

XYZ coordinates:

37

C 0.10023 -0.06284 -4.01540

C 1.46621 0.04329 -4.70672

C -0.98347 0.81031 -4.66176

H -1.94887 0.71325 -4.12064

H -1.14200 0.48172 -5.71173

H -0.69848 1.88438 -4.68329

C 0.60493 1.47888 -2.14003

H 0.81997 2.22198 -2.91683

C 0.69556 1.73085 -0.75896

H 0.98787 2.74204 -0.43194

C 0.41976 0.74476 0.17915

H 0.48207 0.97351 1.25372

C 0.01500 -0.59060 -0.23697

C -0.06034 -0.75658 -1.67124

H -0.37256 -1.72457 -2.09256

C -0.17595 -1.65504 1.89899

C -1.23807 -2.15772 2.70101

H -2.17766 -2.44386 2.20021

C -1.09997 -2.28528 4.08981

H -1.94563 -2.67157 4.68453

C 0.10337 -1.93060 4.72812

H 0.21129 -2.03752 5.82005

C 1.17102 -1.44976 3.94890

H 2.12903 -1.18568 4.42969

C 1.03808 -1.31068 2.55891

H 1.89689 -0.96369 1.95977

N 0.21985 0.23009 -2.54633

N -0.33858 -1.62228 0.51692

H 1.37361 -0.30187 -5.75901

H 2.22078 -0.59500 -4.19896

H 1.84538 1.08807 -4.72563

H -0.23316 -1.11929 -4.05791

H -1.25682 -3.32623 -0.29140

C -1.77008 -4.21284 -0.74290

H -1.40510 -5.17522 -0.34053

Cl -1.40190 -4.21564 -2.51580

Cl -3.52229 -4.09577 -0.39925

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 5.96 0.11221 YES YES

8 a 18.13 0.57309 YES YES

9 a 21.50 0.09878 YES YES

10 a 32.53 1.49777 YES YES

11 a 41.79 0.39007 YES YES

12 a 45.90 0.46779 YES YES

13 a 58.36 0.67000 YES YES

14 a 71.47 1.00397 YES YES

15 a 88.25 0.39656 YES YES

16 a 130.73 0.39893 YES YES

17 a 168.55 13.89729 YES YES

18 a 175.25 5.38860 YES YES

19 a 178.51 8.32296 YES YES

20 a 226.23 0.03434 YES YES

21 a 236.19 1.69916 YES YES

22 a 246.56 0.53338 YES YES

23 a 268.78 1.67543 YES YES

24 a 274.22 1.48093 YES YES

25 a 332.16 2.15959 YES YES

26 a 344.19 2.64243 YES YES

27 a 387.58 4.49999 YES YES

28 a 410.79 0.14237 YES YES

29 a 440.50 3.83485 YES YES

30 a 471.22 3.90321 YES YES

31 a 506.10 12.72181 YES YES

32 a 548.48 0.62807 YES YES

33 a 585.46 1.62460 YES YES

34 a 592.24 4.51029 YES YES

35 a 607.24 0.53814 YES YES

36 a 634.08 6.52097 YES YES

37 a 643.75 36.69892 YES YES

38 a 660.34 52.52242 YES YES

39 a 686.23 4.94191 YES YES

40 a 696.50 45.21566 YES YES

41 a 699.03 72.92030 YES YES

42 a 713.09 4.74995 YES YES

43 a 761.35 17.08783 YES YES

44 a 797.25 25.36074 YES YES

45 a 816.34 7.72362 YES YES

46 a 826.97 12.47551 YES YES

47 a 841.15 4.24653 YES YES

48 a 868.67 2.94196 YES YES

49 a 887.53 5.01022 YES YES

50 a 912.69 0.92983 YES YES

pbe0\_def2-tzvpp energy (au): -1611.4558993010

Zero point energy (au): 0.3015266

Entropy (kJ mol^-1): 0.66356

Chemical potential (kJ mol^-1): 648.66

XYZ coordinates:

37

C 0.09074 -0.05828 -3.96847

C 1.43893 0.06737 -4.65500

C -0.98027 0.81525 -4.59659

H -1.92813 0.71649 -4.06680

H -1.13303 0.50727 -5.63177

H -0.69304 1.86769 -4.60085

C 0.59889 1.44512 -2.10821

H 0.81017 2.18011 -2.86641

C 0.69724 1.67971 -0.74496

H 0.99535 2.66720 -0.41536

C 0.42203 0.70068 0.17526

H 0.49567 0.91574 1.23259

C 0.00802 -0.60833 -0.24387

C -0.06926 -0.75828 -1.66217

H -0.37578 -1.70503 -2.08542

C -0.17930 -1.64638 1.86326

C -1.23273 -2.09918 2.66905

H -2.16922 -2.36207 2.19039

C -1.08983 -2.20376 4.04215

H -1.92570 -2.55054 4.63931

C 0.11031 -1.87193 4.65665

H 0.22188 -1.95879 5.73036

C 1.16947 -1.43868 3.87081

H 2.11996 -1.19307 4.33159

C 1.03080 -1.32593 2.49721

H 1.87642 -1.01400 1.89457

N 0.21180 0.22003 -2.51576

N -0.34731 -1.63496 0.48882

H 1.34587 -0.25902 -5.69163

H 2.18854 -0.55548 -4.16595

H 1.79536 1.09840 -4.66120

H -0.23269 -1.09816 -4.02122

H -1.26767 -3.39955 -0.28335

C -1.75708 -4.26431 -0.74224

H -1.48716 -5.20201 -0.26888

Cl -1.22532 -4.35734 -2.43520

Cl -3.50393 -4.06297 -0.60671

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 11.04 0.80374 YES YES

8 a 18.58 0.13317 YES YES

9 a 29.48 1.23221 YES YES

10 a 30.93 0.06327 YES YES

11 a 39.34 0.46166 YES YES

12 a 44.49 0.51953 YES YES

13 a 56.74 0.76703 YES YES

14 a 68.47 1.39356 YES YES

15 a 88.36 0.54821 YES YES

16 a 135.06 0.30919 YES YES

17 a 157.47 25.75155 YES YES

18 a 176.21 1.54386 YES YES

19 a 181.77 1.03259 YES YES

20 a 227.80 0.01147 YES YES

21 a 242.93 1.43805 YES YES

22 a 249.33 0.67675 YES YES

23 a 278.95 0.89675 YES YES

24 a 284.09 1.46070 YES YES

25 a 343.20 1.78786 YES YES

26 a 354.06 3.00994 YES YES

27 a 400.00 4.31075 YES YES

28 a 422.33 0.08797 YES YES

29 a 459.24 4.39801 YES YES

30 a 486.19 4.10533 YES YES

31 a 520.03 16.94166 YES YES

32 a 566.40 0.30128 YES YES

33 a 604.27 1.58808 YES YES

34 a 613.98 7.10253 YES YES

35 a 626.72 0.49546 YES YES

36 a 657.39 5.67341 YES YES

37 a 695.31 45.90443 YES YES

38 a 710.51 29.81512 YES YES

39 a 717.71 29.96042 YES YES

40 a 729.25 3.90754 YES YES

41 a 740.65 3.81023 YES YES

42 a 753.52 104.53827 YES YES

43 a 789.27 23.44801 YES YES

44 a 827.99 26.94256 YES YES

45 a 851.43 5.61975 YES YES

46 a 863.05 17.61393 YES YES

47 a 883.42 2.23323 YES YES

48 a 898.45 3.50830 YES YES

49 a 924.88 5.06797 YES YES

50 a 938.05 0.71165 YES YES

# Energies, optimised structures and vibrational frequencies for norharman motif (compounds 1 and [1]2)

## Norharman monomer\_iso1

bp86 energy (au): -650.9643798716

Zero point energy (au): 0.2423222

Entropy (kJ mol^-1): 0.47665

Chemical potential (kJ mol^-1): 531.34

XYZ coordinates:

30

C -2.39650 3.20435 -0.14670

C -1.06039 2.80971 -0.19239

C -0.75401 1.42899 -0.09061

C -1.81476 0.43907 0.05965

C -3.16807 0.87497 0.10344

C -3.43798 2.23802 0.00036

C 0.44846 0.66246 -0.09573

N -1.35924 -0.85132 0.14511

H -3.97435 0.13284 0.21719

H -4.48464 2.58632 0.03278

C 1.82849 0.90770 -0.20039

C -0.01608 -0.72944 0.05430

C 0.93995 -1.75298 0.08961

H 2.23677 1.92481 -0.31620

C 2.71701 -0.16486 -0.15833

N 2.26849 -1.46363 -0.01571

H 3.80612 -0.04184 -0.23504

H 0.65379 -2.80819 0.20313

C 3.26923 -2.57410 0.03952

H -2.65839 4.27257 -0.22419

H -0.25900 3.56011 -0.30567

C 3.26776 -3.25048 1.41851

H 4.24932 -2.07239 -0.09793

C 3.07427 -3.56133 -1.12034

H 2.31444 -3.78852 1.61254

H 3.41761 -2.50458 2.22812

H 4.09284 -3.99365 1.47351

H 2.12307 -4.12867 -1.02715

H 3.90646 -4.29858 -1.12645

H 3.07131 -3.03337 -2.09795

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 29.68 0.39533 YES YES

8 a 59.40 1.07608 YES YES

9 a 132.60 1.55272 YES YES

10 a 145.87 0.23994 YES YES

11 a 146.59 1.29110 YES YES

12 a 220.22 2.33875 YES YES

13 a 231.93 0.22180 YES YES

14 a 258.86 0.03342 YES YES

15 a 276.16 0.16995 YES YES

16 a 308.33 0.38644 YES YES

17 a 314.75 0.69519 YES YES

18 a 386.66 1.96356 YES YES

19 a 415.32 4.45515 YES YES

20 a 438.74 2.25110 YES YES

21 a 461.22 5.05586 YES YES

22 a 482.79 0.15655 YES YES

23 a 534.63 0.42330 YES YES

24 a 553.37 0.07817 YES YES

25 a 563.03 1.47773 YES YES

26 a 576.96 1.21329 YES YES

27 a 619.43 7.83168 YES YES

28 a 648.11 2.82494 YES YES

29 a 704.08 8.93332 YES YES

30 a 719.54 5.34922 YES YES

31 a 728.34 52.48107 YES YES

32 a 741.10 4.04424 YES YES

33 a 760.94 5.72275 YES YES

34 a 784.28 0.58971 YES YES

35 a 836.01 15.55961 YES YES

36 a 853.58 2.44808 YES YES

37 a 857.85 3.01472 YES YES

38 a 877.60 1.02077 YES YES

39 a 896.58 2.36941 YES YES

40 a 913.26 0.66935 YES YES

41 a 924.46 0.10924 YES YES

42 a 930.71 0.24269 YES YES

43 a 932.57 2.06827 YES YES

44 a 964.40 0.10967 YES YES

45 a 994.58 26.42228 YES YES

46 a 998.94 1.61306 YES YES

47 a 1068.06 1.95036 YES YES

48 a 1100.96 14.33713 YES YES

49 a 1113.07 4.04491 YES YES

50 a 1121.30 74.11751 YES YES

pbe0\_def2-tzvpp energy (au): -650.8875648006

Zero point energy (au): 0.2502544

Entropy (kJ mol^-1): 0.47002

Chemical potential (kJ mol^-1): 553.22

XYZ coordinates:

30

C -2.35257 3.15595 -0.15326

C -1.03803 2.76455 -0.20067

C -0.73866 1.39854 -0.09116

C -1.78247 0.42642 0.06733

C -3.12148 0.85875 0.11153

C -3.38317 2.20117 0.00190

C 0.45142 0.64133 -0.09491

N -1.33133 -0.84923 0.15983

H -3.91762 0.13420 0.23019

H -4.41052 2.54621 0.03473

C 1.81447 0.88861 -0.20537

C -0.00157 -0.72858 0.06439

C 0.94369 -1.73666 0.10267

H 2.21264 1.88820 -0.32738

C 2.69109 -0.16726 -0.15927

N 2.25096 -1.44652 -0.00774

H 3.76070 -0.04557 -0.23904

H 0.67097 -2.77541 0.22140

C 3.24331 -2.54059 0.04355

H -2.61031 4.20477 -0.23503

H -0.24902 3.49928 -0.31988

C 3.22604 -3.22856 1.39816

H 4.20746 -2.04522 -0.07963

C 3.05132 -3.50945 -1.11081

H 2.28749 -3.75941 1.56540

H 3.36204 -2.50883 2.20591

H 4.03471 -3.95918 1.44824

H 2.11115 -4.05597 -1.02413

H 3.86124 -4.24051 -1.11203

H 3.05804 -2.98700 -2.06792

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 35.05 0.53701 YES YES

8 a 61.65 1.12735 YES YES

9 a 135.78 1.87825 YES YES

10 a 149.76 1.48387 YES YES

11 a 149.79 0.14259 YES YES

12 a 223.07 1.87143 YES YES

13 a 228.26 0.78866 YES YES

14 a 254.83 0.04897 YES YES

15 a 280.80 0.17968 YES YES

16 a 316.96 0.54565 YES YES

17 a 321.25 0.85348 YES YES

18 a 399.15 2.89993 YES YES

19 a 426.05 5.71634 YES YES

20 a 453.94 1.09641 YES YES

21 a 470.25 6.98553 YES YES

22 a 494.71 0.08654 YES YES

23 a 553.05 1.00722 YES YES

24 a 567.86 0.02650 YES YES

25 a 578.87 1.56064 YES YES

26 a 595.31 1.37290 YES YES

27 a 647.88 8.13935 YES YES

28 a 669.94 3.01031 YES YES

29 a 744.16 4.80978 YES YES

30 a 748.79 25.38112 YES YES

31 a 759.98 53.50957 YES YES

32 a 768.95 4.97284 YES YES

33 a 782.59 8.46431 YES YES

34 a 799.35 3.01768 YES YES

35 a 875.25 1.48184 YES YES

36 a 888.50 5.28810 YES YES

37 a 891.97 20.42676 YES YES

38 a 907.12 0.73080 YES YES

39 a 934.36 1.53363 YES YES

40 a 937.66 0.83030 YES YES

41 a 956.82 0.53656 YES YES

42 a 957.62 0.28829 YES YES

43 a 969.38 2.08016 YES YES

44 a 992.76 0.20056 YES YES

45 a 1028.23 19.03328 YES YES

46 a 1033.55 6.87123 YES YES

47 a 1105.77 0.62841 YES YES

48 a 1142.92 21.37365 YES YES

49 a 1152.31 11.51887 YES YES

50 a 1160.44 50.79455 YES YES

## Norharman monomer\_iso2

bp86 energy (au): -650.9644200146

Zero point energy (au): 0.2422089

Entropy (kJ mol^-1): 0.47639

Chemical potential (kJ mol^-1): 531.20

XYZ coordinates:

30

C -2.40135 3.20135 -0.16178

C -1.06464 2.80910 -0.20986

C -0.75470 1.43032 -0.09331

C -1.81282 0.44038 0.07385

C -3.16689 0.87382 0.11925

C -3.44025 2.23492 0.00171

C 0.44912 0.66573 -0.09647

N -1.35449 -0.84789 0.17139

H -3.97085 0.13123 0.24551

H -4.48741 2.58150 0.03522

C 1.82852 0.91180 -0.21179

C -0.01201 -0.72462 0.07115

C 0.94657 -1.74572 0.10890

H 2.23369 1.92876 -0.33947

C 2.72039 -0.15782 -0.16523

N 2.27453 -1.45579 -0.00786

H 3.80699 -0.02635 -0.25048

H 0.67055 -2.80344 0.23158

C 3.26777 -2.57217 0.03357

H -2.66576 4.26806 -0.25053

H -0.26562 3.55993 -0.33640

C 4.02070 -2.69748 -1.29931

H 2.65178 -3.48511 0.16750

C 4.19973 -2.44543 1.24748

H 4.68245 -1.82413 -1.48765

H 3.31177 -2.78792 -2.15005

H 4.66014 -3.60669 -1.28262

H 4.87306 -1.56489 1.16453

H 4.83874 -3.35191 1.32412

H 3.61727 -2.35155 2.18905

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 32.96 0.02682 YES YES

8 a 59.60 1.87295 YES YES

9 a 122.94 1.46510 YES YES

10 a 144.51 1.35058 YES YES

11 a 160.65 0.02370 YES YES

12 a 221.26 0.02999 YES YES

13 a 240.81 0.33552 YES YES

14 a 257.26 1.65949 YES YES

15 a 274.04 0.01510 YES YES

16 a 280.65 2.33683 YES YES

17 a 306.34 0.46655 YES YES

18 a 387.87 1.89515 YES YES

19 a 398.94 2.45565 YES YES

20 a 434.40 2.69325 YES YES

21 a 461.23 4.34565 YES YES

22 a 494.41 1.74843 YES YES

23 a 533.43 0.40050 YES YES

24 a 550.15 1.60296 YES YES

25 a 563.39 1.45343 YES YES

26 a 589.40 0.26726 YES YES

27 a 619.65 8.39342 YES YES

28 a 655.60 1.72383 YES YES

29 a 705.61 7.96672 YES YES

30 a 707.35 5.77446 YES YES

31 a 728.30 53.76970 YES YES

32 a 742.81 5.02979 YES YES

33 a 760.93 5.33060 YES YES

34 a 784.51 0.71420 YES YES

35 a 835.47 15.07679 YES YES

36 a 853.59 2.39775 YES YES

37 a 856.22 2.97816 YES YES

38 a 872.42 0.52288 YES YES

39 a 899.50 1.72223 YES YES

40 a 911.13 1.01554 YES YES

41 a 924.45 0.10451 YES YES

42 a 928.40 0.16303 YES YES

43 a 945.54 3.97250 YES YES

44 a 964.19 0.10383 YES YES

45 a 994.79 23.97642 YES YES

46 a 998.97 1.91939 YES YES

47 a 1046.05 2.77144 YES YES

48 a 1100.75 28.81305 YES YES

49 a 1111.52 36.92888 YES YES

50 a 1125.40 6.82598 YES YES

pbe0\_def2-tzvpp energy (au): -650.8875172471

Zero point energy (au): 0.2501017

Entropy (kJ mol^-1): 0.47155

Chemical potential (kJ mol^-1): 552.49

XYZ coordinates:

30

C -2.35030 3.15859 -0.16729

C -1.03565 2.76701 -0.20970

C -0.73626 1.40188 -0.08806

C -1.78065 0.43150 0.07800

C -3.11962 0.86439 0.11941

C -3.38128 2.20560 -0.00316

C 0.45314 0.64363 -0.08926

N -1.33003 -0.84366 0.17759

H -3.91570 0.14091 0.24479

H -4.40858 2.55111 0.02584

C 1.81676 0.88854 -0.20548

C -0.00038 -0.72414 0.07768

C 0.94457 -1.73328 0.11267

H 2.21457 1.88780 -0.33198

C 2.69317 -0.16683 -0.16084

N 2.25221 -1.44532 -0.00543

H 3.76085 -0.04013 -0.24639

H 0.67707 -2.77407 0.23211

C 3.23437 -2.54799 0.03190

H -2.60797 4.20654 -0.26006

H -0.24672 3.50075 -0.33562

C 3.98440 -2.65849 -1.28492

H 2.63210 -3.44833 0.16108

C 4.16160 -2.41701 1.22826

H 4.62763 -1.79378 -1.45600

H 3.29349 -2.74430 -2.12412

H 4.61881 -3.54586 -1.26969

H 4.81161 -1.54528 1.13999

H 4.79826 -3.30054 1.29440

H 3.59553 -2.33125 2.15631

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 32.44 0.08442 YES YES

8 a 59.97 2.12670 YES YES

9 a 126.18 1.75611 YES YES

10 a 146.90 1.42572 YES YES

11 a 163.24 0.04018 YES YES

12 a 218.94 0.01551 YES YES

13 a 239.26 0.36371 YES YES

14 a 264.51 1.75704 YES YES

15 a 279.65 0.01807 YES YES

16 a 283.95 2.83083 YES YES

17 a 313.97 0.64799 YES YES

18 a 398.92 2.86305 YES YES

19 a 406.77 2.98958 YES YES

20 a 450.09 1.68597 YES YES

21 a 468.97 6.14697 YES YES

22 a 506.38 3.00868 YES YES

23 a 549.06 0.26832 YES YES

24 a 567.74 2.00520 YES YES

25 a 579.36 1.54695 YES YES

26 a 605.72 0.22619 YES YES

27 a 648.74 8.38989 YES YES

28 a 677.71 1.66254 YES YES

29 a 731.70 5.44991 YES YES

30 a 748.78 30.24222 YES YES

31 a 762.17 48.38969 YES YES

32 a 771.07 5.96644 YES YES

33 a 782.92 7.59680 YES YES

34 a 800.70 3.28483 YES YES

35 a 875.19 1.11811 YES YES

36 a 886.72 4.38283 YES YES

37 a 888.25 20.64296 YES YES

38 a 901.94 0.46056 YES YES

39 a 930.56 0.68302 YES YES

40 a 941.76 1.99893 YES YES

41 a 955.94 0.10828 YES YES

42 a 956.99 0.44252 YES YES

43 a 982.98 4.49515 YES YES

44 a 992.72 0.20217 YES YES

45 a 1028.61 14.08836 YES YES

46 a 1033.97 7.85868 YES YES

47 a 1080.51 6.79710 YES YES

48 a 1142.43 44.43802 YES YES

49 a 1148.04 28.82746 YES YES

50 a 1161.44 5.49256 YES YES

## Norharman dimer\_iso1

bp86 energy (au): -1301.9519619700

Zero point energy (au): 0.4867615

Entropy (kJ mol^-1): 0.78241

Chemical potential (kJ mol^-1): 1120.93

XYZ coordinates:

60

C -0.83884 6.42163 -0.00968

C 0.41820 5.81877 -0.03724

C 0.49749 4.40486 -0.02273

C -0.70462 3.58743 0.01971

C -1.97151 4.23247 0.04810

C -2.02107 5.62609 0.03288

C 1.57129 3.46389 -0.04102

N -0.44400 2.23652 0.02727

H -2.89594 3.63596 0.08254

H -3.00213 6.13114 0.05492

C 2.97528 3.52339 -0.07999

C 0.91375 2.15372 -0.00810

C 1.70868 0.99554 -0.01510

H 3.52195 4.47971 -0.10629

C 3.69924 2.33587 -0.08531

N 3.06601 1.11185 -0.05303

H 4.79726 2.30615 -0.11493

H 1.29436 -0.03153 0.00900

C 3.90359 -0.13274 -0.05758

H -0.92560 7.52058 -0.02036

H 1.33360 6.43386 -0.06954

C 3.70624 -0.92042 1.24525

H 4.94903 0.23885 -0.09316

C 3.63298 -0.96211 -1.32080

H 2.67843 -1.33859 1.30791

H 3.89395 -0.27675 2.13194

H 4.42375 -1.76913 1.27721

H 2.60350 -1.38144 -1.31119

H 4.34819 -1.81205 -1.36605

H 3.76960 -0.34737 -2.23696

C 0.83907 -6.42149 -0.00810

C -0.41796 -5.81869 -0.03746

C -0.49733 -4.40478 -0.02365

C 0.70471 -3.58725 0.01928

C 1.97161 -4.23223 0.04906

C 2.02124 -5.62587 0.03508

C -1.57119 -3.46387 -0.04255

N 0.44400 -2.23636 0.02647

H 2.89599 -3.63565 0.08396

H 3.00230 -6.13087 0.05874

C -2.97516 -3.52343 -0.08174

C -0.91373 -2.15366 -0.00938

C -1.70872 -0.99554 -0.01597

H -3.52178 -4.47978 -0.10845

C -3.69919 -2.33595 -0.08658

N -3.06604 -1.11191 -0.05373

H -4.79721 -2.30628 -0.11601

H -1.29437 0.03150 0.00862

C -3.90373 0.13261 -0.05690

H 0.92588 -7.52046 -0.01766

H -1.33330 -6.43383 -0.07046

C -3.70588 0.91923 1.24649

H -4.94914 -0.23905 -0.09231

C -3.63380 0.96302 -1.31958

H -2.67811 1.33753 1.30901

H -3.89304 0.27476 2.13272

H -4.42352 1.76778 1.27954

H -2.60431 1.38231 -1.31018

H -4.34901 1.81301 -1.36373

H -3.77093 0.34904 -2.23617

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 12.14 2.30486 YES YES

8 a 24.92 0.24130 YES YES

9 a 44.50 0.03113 YES YES

10 a 51.62 5.56460 YES YES

11 a 55.07 0.60836 YES YES

12 a 60.23 2.90797 YES YES

13 a 61.88 0.03133 YES YES

14 a 61.96 0.09835 YES YES

15 a 65.60 0.00779 YES YES

16 a 71.89 0.33650 YES YES

17 a 134.87 0.00426 YES YES

18 a 135.55 3.01181 YES YES

19 a 152.94 0.28770 YES YES

20 a 153.11 0.00174 YES YES

21 a 154.46 0.04896 YES YES

22 a 155.27 8.16231 YES YES

23 a 225.06 0.00032 YES YES

24 a 226.22 6.74647 YES YES

25 a 271.01 0.00362 YES YES

26 a 272.56 0.00164 YES YES

27 a 286.41 0.11158 YES YES

28 a 288.24 0.30500 YES YES

29 a 300.49 1.19128 YES YES

30 a 302.24 0.02710 YES YES

31 a 309.82 0.07276 YES YES

32 a 315.22 0.30570 YES YES

33 a 317.43 0.00042 YES YES

34 a 318.99 2.59017 YES YES

35 a 395.97 0.01370 YES YES

36 a 396.17 2.47686 YES YES

37 a 415.43 11.99843 YES YES

38 a 417.14 0.00291 YES YES

39 a 448.18 4.87388 YES YES

40 a 450.80 0.00980 YES YES

41 a 462.25 0.00647 YES YES

42 a 462.31 7.47761 YES YES

43 a 484.50 0.00007 YES YES

44 a 486.64 2.61567 YES YES

45 a 536.23 1.53639 YES YES

46 a 536.34 0.00122 YES YES

47 a 558.75 0.00024 YES YES

48 a 560.58 0.47901 YES YES

49 a 566.27 2.97827 YES YES

50 a 567.10 0.00092 YES YES

pbe0\_def2-tzvpp energy (au): -1301.7974863620

Zero point energy (au): 0.5024354

Entropy (kJ mol^-1): 0.77630

Chemical potential (kJ mol^-1): 1162.29

XYZ coordinates:

60

C -0.81693 6.35052 -0.01142

C 0.42121 5.75597 -0.03325

C 0.49793 4.35757 -0.02438

C -0.68503 3.55152 0.00672

C -1.93961 4.18950 0.02930

C -1.98628 5.56250 0.01986

C 1.56179 3.42791 -0.03837

N -0.42926 2.21538 0.01145

H -2.85030 3.60513 0.05455

H -2.94967 6.05987 0.03711

C 2.95006 3.49163 -0.06652

C 0.91597 2.13705 -0.01491

C 1.70334 0.99554 -0.02004

H 3.48582 4.43232 -0.08521

C 3.66404 2.32151 -0.07012

N 3.04034 1.11404 -0.04708

H 4.74287 2.29276 -0.09122

H 1.30026 -0.01397 -0.00206

C 3.87110 -0.11273 -0.04971

H -0.90307 7.43007 -0.01783

H 1.32143 6.36051 -0.05666

C 3.65912 -0.90215 1.23051

H 4.89927 0.25249 -0.07372

C 3.61015 -0.93161 -1.30203

H 2.64702 -1.30743 1.27780

H 3.83587 -0.27883 2.10842

H 4.35928 -1.73866 1.26063

H 2.59724 -1.33770 -1.30079

H 4.30870 -1.76914 -1.33945

H 3.75295 -0.32890 -2.20028

C 0.81602 -6.35111 -0.01155

C -0.42200 -5.75632 -0.03327

C -0.49846 -4.35790 -0.02391

C 0.68468 -3.55215 0.00745

C 1.93913 -4.19034 0.02971

C 1.98555 -5.56334 0.01992

C -1.56208 -3.42796 -0.03825

N 0.42928 -2.21599 0.01194

H 2.84990 -3.60609 0.05499

H 2.94882 -6.06092 0.03725

C -2.95037 -3.49128 -0.06648

C -0.91591 -2.13725 -0.01470

C -1.70293 -0.99545 -0.01995

H -3.48640 -4.43179 -0.08524

C -3.66398 -2.32095 -0.07034

N -3.03998 -1.11362 -0.04715

H -4.74280 -2.29190 -0.09149

H -1.29938 0.01394 -0.00194

C -3.87052 0.11330 -0.04981

H 0.90195 -7.43068 -0.01804

H -1.32234 -6.36069 -0.05685

C -3.65893 0.90230 1.23075

H -4.89874 -0.25174 -0.07427

C -3.60905 0.93234 -1.30190

H -2.64670 1.30718 1.27869

H -3.83635 0.27873 2.10836

H -4.35881 1.73905 1.26081

H -2.59603 1.33815 -1.30036

H -4.30739 1.77004 -1.33939

H -3.75180 0.32976 -2.20026

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 8.00 3.01010 YES YES

8 a 21.84 0.03218 YES YES

9 a 45.47 0.00503 YES YES

10 a 49.84 0.26772 YES YES

11 a 53.34 6.24173 YES YES

12 a 59.81 2.46225 YES YES

13 a 62.08 0.03518 YES YES

14 a 64.35 0.00453 YES YES

15 a 79.25 0.00298 YES YES

16 a 84.22 0.72244 YES YES

17 a 137.14 0.00427 YES YES

18 a 138.94 3.48169 YES YES

19 a 155.45 0.36124 YES YES

20 a 155.86 0.01047 YES YES

21 a 157.40 0.01709 YES YES

22 a 158.64 7.36501 YES YES

23 a 229.33 0.00170 YES YES

24 a 230.28 7.55056 YES YES

25 a 264.21 0.04603 YES YES

26 a 264.83 0.00199 YES YES

27 a 285.74 0.00131 YES YES

28 a 286.73 1.42180 YES YES

29 a 286.88 0.17130 YES YES

30 a 287.43 0.01940 YES YES

31 a 318.28 0.01111 YES YES

32 a 322.85 0.46476 YES YES

33 a 325.59 0.00193 YES YES

34 a 326.16 2.39290 YES YES

35 a 406.75 0.21831 YES YES

36 a 407.25 3.99146 YES YES

37 a 425.86 13.15262 YES YES

38 a 427.15 0.00344 YES YES

39 a 462.57 2.33451 YES YES

40 a 464.27 0.00558 YES YES

41 a 469.24 0.03919 YES YES

42 a 471.03 10.91260 YES YES

43 a 497.19 0.00036 YES YES

44 a 498.62 1.67363 YES YES

45 a 554.58 2.50703 YES YES

46 a 554.71 0.20208 YES YES

47 a 572.83 0.00004 YES YES

48 a 574.88 0.42229 YES YES

49 a 581.83 3.41948 YES YES

50 a 582.36 0.02961 YES YES

## Norharman dimer\_iso2

bp86 energy (au): -1301.9519870850

Zero point energy (au): 0.4860864

Entropy (kJ mol^-1): 0.80969

Chemical potential (kJ mol^-1): 1112.43

XYZ coordinates:

60

C -0.94159 6.38046 -0.03753

C 0.31606 5.77835 -0.07481

C 0.39818 4.36463 -0.04731

C -0.80591 3.54943 0.01821

C -2.07306 4.19306 0.05639

C -2.12423 5.58627 0.02816

C 1.47048 3.42051 -0.06953

N -0.54847 2.20127 0.03599

H -2.99643 3.59357 0.11001

H -3.10459 6.09210 0.05807

C 2.87624 3.46770 -0.12674

C 0.80812 2.11485 -0.01502

C 1.59652 0.95291 -0.01941

H 3.42845 4.42030 -0.16947

C 3.59518 2.27624 -0.12989

N 2.95247 1.05713 -0.07688

H 4.69181 2.24502 -0.17371

H 1.19570 -0.07938 0.02057

C 3.75385 -0.20954 -0.08403

H -1.02837 7.47931 -0.05797

H 1.22981 6.39498 -0.12464

C 4.53012 -0.36252 -1.39935

H 2.98869 -1.01231 -0.03365

C 4.64309 -0.30647 1.16330

H 5.33232 0.40063 -1.50704

H 3.84924 -0.28360 -2.27372

H 5.01151 -1.36397 -1.42998

H 5.45169 0.45750 1.16559

H 5.12605 -1.30717 1.19580

H 4.04244 -0.18601 2.09019

C 0.94177 -6.38033 -0.03704

C -0.31588 -5.77827 -0.07501

C -0.39807 -4.36454 -0.04780

C 0.80598 -3.54930 0.01783

C 2.07314 -4.19288 0.05663

C 2.12437 -5.58610 0.02889

C -1.47041 -3.42046 -0.07029

N 0.54849 -2.20112 0.03522

H 2.99648 -3.59334 0.11041

H 3.10473 -6.09190 0.05940

C -2.87616 -3.46772 -0.12738

C -0.80811 -2.11477 -0.01601

C -1.59656 -0.95286 -0.02055

H -3.42832 -4.42034 -0.17000

C -3.59514 -2.27630 -0.13053

N -2.95250 -1.05716 -0.07780

H -4.69178 -2.24514 -0.17399

H -1.19578 0.07945 0.01949

C -3.75397 0.20945 -0.08429

H 1.02858 -7.47919 -0.05705

H -1.22958 -6.39493 -0.12521

C -4.53186 0.36222 -1.39866

H -2.98881 1.01227 -0.03488

C -4.64168 0.30645 1.16411

H -5.33423 -0.40088 -1.50524

H -3.85210 0.28314 -2.27389

H -5.01325 1.36368 -1.42883

H -5.45005 -0.45776 1.16758

H -5.12485 1.30703 1.19703

H -4.03982 0.18633 2.09026

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 7.90 2.85847 YES YES

8 a 18.65 0.08382 YES YES

9 a 35.81 0.00514 YES YES

10 a 36.43 3.16231 YES YES

11 a 38.05 4.63732 YES YES

12 a 38.21 0.02114 YES YES

13 a 54.87 0.01824 YES YES

14 a 61.63 0.05148 YES YES

15 a 62.94 0.09179 YES YES

16 a 66.33 2.73810 YES YES

17 a 124.69 0.01192 YES YES

18 a 124.91 2.59468 YES YES

19 a 145.40 3.61180 YES YES

20 a 152.76 0.00025 YES YES

21 a 163.57 0.00417 YES YES

22 a 165.21 0.02239 YES YES

23 a 225.60 0.01537 YES YES

24 a 225.66 0.01126 YES YES

25 a 243.50 0.82232 YES YES

26 a 243.56 0.40470 YES YES

27 a 257.85 0.00042 YES YES

28 a 258.30 3.34185 YES YES

29 a 274.31 0.00188 YES YES

30 a 275.16 0.00832 YES YES

31 a 284.08 0.00585 YES YES

32 a 285.30 15.12293 YES YES

33 a 306.88 0.11528 YES YES

34 a 313.32 0.21239 YES YES

35 a 393.82 0.03689 YES YES

36 a 394.98 2.00845 YES YES

37 a 398.98 5.34738 YES YES

38 a 399.33 0.00119 YES YES

39 a 443.24 5.71101 YES YES

40 a 446.61 0.02521 YES YES

41 a 462.34 6.90311 YES YES

42 a 463.32 0.00204 YES YES

43 a 495.75 5.92039 YES YES

44 a 496.14 0.00399 YES YES

45 a 539.64 0.00000 YES YES

46 a 540.41 0.03088 YES YES

47 a 551.53 2.93963 YES YES

48 a 552.50 0.00150 YES YES

49 a 566.67 2.98464 YES YES

50 a 567.63 0.00331 YES YES

pbe0\_def2-tzvpp energy (au): -1301.7968766680

Zero point energy (au): 0.5016917

Entropy (kJ mol^-1): 0.81032

Chemical potential (kJ mol^-1): 1151.73

XYZ coordinates:

60

C -0.90899 6.32963 -0.06463

C 0.32707 5.73037 -0.08790

C 0.39972 4.33166 -0.06199

C -0.78950 3.53404 -0.01205

C -2.04139 4.17599 0.01214

C -2.08299 5.54856 -0.01455

C 1.45765 3.39358 -0.07401

N -0.54338 2.19867 0.00660

H -2.95377 3.59251 0.05286

H -3.04341 6.05147 0.00368

C 2.84859 3.43772 -0.11514

C 0.80070 2.11091 -0.02993

C 1.57622 0.96168 -0.02890

H 3.39479 4.37208 -0.14921

C 3.55155 2.26070 -0.11267

N 2.91281 1.06107 -0.07040

H 4.62928 2.22496 -0.14347

H 1.18003 -0.04984 0.00380

C 3.70045 -0.19325 -0.06843

H -0.99029 7.40944 -0.08392

H 1.22866 6.33214 -0.12569

C 4.49981 -0.33402 -1.35194

H 2.94720 -0.98236 -0.03695

C 4.56204 -0.28985 1.17840

H 5.28512 0.42050 -1.42916

H 3.85324 -0.25281 -2.22622

H 4.97833 -1.31418 -1.37339

H 5.34688 0.46901 1.19188

H 5.04540 -1.26742 1.20888

H 3.95872 -0.18089 2.08016

C 0.91093 -6.32836 -0.06212

C -0.32536 -5.72969 -0.08858

C -0.39875 -4.33099 -0.06371

C 0.79001 -3.53284 -0.01195

C 2.04215 -4.17416 0.01518

C 2.08446 -5.54673 -0.01001

C -1.45710 -3.39336 -0.07687

N 0.54321 -2.19759 0.00631

H 2.95416 -3.59020 0.05740

H 3.04506 -6.04918 0.01129

C -2.84798 -3.43809 -0.11889

C -0.80085 -2.11041 -0.03162

C -1.57684 -0.96151 -0.02986

H -3.39372 -4.37266 -0.15390

C -3.55151 -2.26141 -0.11557

N -2.91338 -1.06148 -0.07174

H -4.62925 -2.22617 -0.14657

H -1.18097 0.05012 0.00382

C -3.70170 0.19242 -0.06682

H 0.99277 -7.40814 -0.08066

H -1.22656 -6.33191 -0.12765

C -4.50265 0.33514 -1.34909

H -2.94885 0.98191 -0.03471

C -4.56189 0.28611 1.18122

H -5.28724 -0.42005 -1.42711

H -3.85700 0.25661 -2.22430

H -4.98228 1.31480 -1.36777

H -5.34638 -0.47312 1.19401

H -5.04558 1.26342 1.21438

H -3.95746 0.17545 2.08205

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 5.14 3.37386 YES YES

8 a 14.09 0.01191 YES YES

9 a 33.19 0.59815 YES YES

10 a 35.81 7.34197 YES YES

11 a 38.49 0.00361 YES YES

12 a 39.37 0.00845 YES YES

13 a 39.92 0.05426 YES YES

14 a 60.28 0.05440 YES YES

15 a 61.63 0.02633 YES YES

16 a 65.26 3.02870 YES YES

17 a 128.20 0.00725 YES YES

18 a 128.54 3.11478 YES YES

19 a 149.20 3.80377 YES YES

20 a 155.19 0.00022 YES YES

21 a 162.86 0.00397 YES YES

22 a 166.77 0.07097 YES YES

23 a 224.62 0.00134 YES YES

24 a 224.81 0.00468 YES YES

25 a 242.21 0.52660 YES YES

26 a 242.25 0.70232 YES YES

27 a 265.18 0.00048 YES YES

28 a 265.63 3.16372 YES YES

29 a 280.08 0.00191 YES YES

30 a 281.04 0.02870 YES YES

31 a 288.87 0.00409 YES YES

32 a 290.03 16.53968 YES YES

33 a 315.26 0.06044 YES YES

34 a 319.27 0.43845 YES YES

35 a 402.08 0.02472 YES YES

36 a 404.57 3.95399 YES YES

37 a 408.09 6.03735 YES YES

38 a 408.28 0.00470 YES YES

39 a 457.24 2.73226 YES YES

40 a 457.86 0.01190 YES YES

41 a 467.84 0.00835 YES YES

42 a 468.34 10.97386 YES YES

43 a 509.16 6.69410 YES YES

44 a 509.17 0.12416 YES YES

45 a 554.47 0.00034 YES YES

46 a 555.11 0.04904 YES YES

47 a 569.70 4.20923 YES YES

48 a 570.63 0.00151 YES YES

49 a 581.90 3.42980 YES YES

50 a 582.01 0.06173 YES YES

# Energies, optimised structures and vibrational frequencies for betaine motif (compounds 2 and [2]2)

## BETAINE monomer\_iso1

bp86 energy (au): -652.1244957980

Zero point energy (au): 0.2620419

Entropy (kJ mol^-1): 0.51636

Chemical potential (kJ mol^-1): 575.32

XYZ coordinates:

32

C 0.09151 -0.06465 -4.04092

C -1.35541 -0.38077 -4.44309

C 1.09368 -1.14573 -4.46667

H 2.12455 -0.88295 -4.14607

H 1.08787 -1.24042 -5.57403

H 0.83726 -2.13957 -4.04039

C 0.56864 1.46533 -2.16137

H 0.78702 2.20305 -2.94359

C 0.65052 1.72116 -0.77799

H 0.93748 2.73478 -0.45289

C 0.37520 0.73631 0.15872

H 0.43439 0.96427 1.23401

C -0.02637 -0.60623 -0.25538

C -0.09299 -0.77051 -1.69256

H -0.40031 -1.74547 -2.09583

C -0.20171 -1.68148 1.86512

C -1.25983 -2.17616 2.67899

H -2.20460 -2.45093 2.18200

C -1.10946 -2.31224 4.06515

H -1.95314 -2.69199 4.66725

C 0.10566 -1.97767 4.69306

H 0.22434 -2.09317 5.78306

C 1.17071 -1.50696 3.90399

H 2.13745 -1.25777 4.37563

C 1.02382 -1.35627 2.51671

H 1.87957 -1.01424 1.90999

N 0.19139 0.21358 -2.56816

N -0.37824 -1.63662 0.49006

H -1.42403 -0.45704 -5.54992

H -2.04764 0.42072 -4.10681

H -1.70245 -1.34553 -4.01437

H 0.38609 0.89116 -4.52074

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 27.50 0.04149 YES YES

8 a 44.15 1.88633 YES YES

9 a 45.83 0.27265 YES YES

10 a 79.06 0.78604 YES YES

11 a 125.72 0.50126 YES YES

12 a 152.85 1.46052 YES YES

13 a 166.25 1.36147 YES YES

14 a 223.76 0.01556 YES YES

15 a 235.75 1.43739 YES YES

16 a 251.28 0.02440 YES YES

17 a 305.84 0.42543 YES YES

18 a 329.46 2.53676 YES YES

19 a 337.75 1.74999 YES YES

20 a 387.09 6.18221 YES YES

21 a 410.43 0.47647 YES YES

22 a 436.08 3.93816 YES YES

23 a 473.26 2.23210 YES YES

24 a 503.83 11.13745 YES YES

25 a 548.62 0.94542 YES YES

26 a 570.71 0.41514 YES YES

27 a 587.60 9.28332 YES YES

28 a 604.94 0.60418 YES YES

29 a 622.80 25.80360 YES YES

30 a 623.74 7.13763 YES YES

31 a 679.08 10.00342 YES YES

32 a 694.02 26.24277 YES YES

33 a 709.47 5.59886 YES YES

34 a 760.64 18.23652 YES YES

35 a 793.91 23.78885 YES YES

36 a 809.66 17.74237 YES YES

37 a 812.82 0.61409 YES YES

38 a 824.02 6.42352 YES YES

39 a 876.21 1.85054 YES YES

40 a 881.64 3.66599 YES YES

41 a 911.77 12.10039 YES YES

42 a 913.18 2.20183 YES YES

43 a 931.87 0.46155 YES YES

44 a 939.53 0.61917 YES YES

45 a 952.46 0.05195 YES YES

46 a 961.89 0.24007 YES YES

47 a 975.71 2.17041 YES YES

48 a 1006.80 51.79902 YES YES

49 a 1021.28 10.21368 YES YES

50 a 1064.32 7.06866 YES YES

pbe0\_def2-tzvpp energy (au): -652.0483109060

Zero point energy (au): 0.2707962

Entropy (kJ mol^-1): 0.50957

Chemical potential (kJ mol^-1): 599.26

XYZ coordinates:

32

C 0.08928 -0.05938 -3.99378

C -1.34261 -0.37841 -4.38546

C 1.07513 -1.13011 -4.42556

H 2.08928 -0.88015 -4.11217

H 1.06218 -1.21527 -5.51294

H 0.81665 -2.10549 -4.01123

C 0.56669 1.42938 -2.12761

H 0.77665 2.16161 -2.88988

C 0.65355 1.66608 -0.76114

H 0.93846 2.65751 -0.43135

C 0.38450 0.68537 0.15572

H 0.44956 0.90008 1.21374

C -0.01432 -0.63354 -0.26455

C -0.08491 -0.77994 -1.68535

H -0.38573 -1.73183 -2.09759

C -0.19316 -1.68394 1.82993

C -1.23778 -2.16695 2.63055

H -2.16087 -2.45573 2.14205

C -1.09738 -2.27859 4.00253

H -1.92684 -2.64973 4.59432

C 0.09415 -1.92758 4.62446

H 0.20497 -2.02310 5.69759

C 1.14606 -1.46705 3.84484

H 2.09074 -1.20699 4.30998

C 1.00806 -1.34366 2.47192

H 1.84929 -1.00955 1.87491

N 0.19293 0.19968 -2.53664

N -0.35989 -1.66302 0.45886

H -1.41310 -0.44811 -5.47184

H -2.02608 0.40050 -4.04571

H -1.67020 -1.33112 -3.96740

H 0.37576 0.88504 -4.45820

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 28.71 0.07825 YES YES

8 a 45.14 2.35285 YES YES

9 a 46.41 0.37830 YES YES

10 a 83.13 1.00354 YES YES

11 a 130.22 0.46209 YES YES

12 a 155.83 1.23890 YES YES

13 a 169.23 1.82378 YES YES

14 a 219.06 0.01700 YES YES

15 a 244.36 1.16210 YES YES

16 a 247.82 0.05258 YES YES

17 a 311.49 0.47701 YES YES

18 a 339.96 2.91070 YES YES

19 a 346.54 1.97487 YES YES

20 a 397.57 6.17268 YES YES

21 a 422.12 0.21973 YES YES

22 a 456.59 4.21420 YES YES

23 a 486.28 1.82544 YES YES

24 a 518.65 15.28934 YES YES

25 a 564.32 0.75438 YES YES

26 a 590.05 0.50683 YES YES

27 a 610.70 10.74148 YES YES

28 a 625.38 0.57001 YES YES

29 a 648.54 1.80813 YES YES

30 a 677.15 45.81639 YES YES

31 a 714.08 35.37081 YES YES

32 a 716.69 1.37131 YES YES

33 a 737.76 8.45327 YES YES

34 a 789.46 22.85308 YES YES

35 a 825.30 23.93641 YES YES

36 a 847.52 7.60403 YES YES

37 a 856.83 20.42281 YES YES

38 a 869.48 1.35059 YES YES

39 a 906.23 1.82332 YES YES

40 a 921.00 4.39299 YES YES

41 a 933.84 0.67416 YES YES

42 a 946.38 19.62954 YES YES

43 a 959.32 0.53861 YES YES

44 a 978.93 0.30164 YES YES

45 a 987.44 0.23906 YES YES

46 a 997.00 0.38413 YES YES

47 a 1015.30 2.54550 YES YES

48 a 1045.07 76.18379 YES YES

49 a 1056.35 14.58156 YES YES

50 a 1101.16 7.90153 YES YES

## BETAINE dimer\_iso1

bp86 energy (au): -1304.2674071500

Zero point energy (au): 0.5260638

Entropy (kJ mol^-1): 0.86061

Chemical potential (kJ mol^-1): 1209.08

XYZ coordinates:

64

C 0.92613 2.71015 -2.54302

C -0.39270 2.56863 -3.31279

C 1.86581 1.51178 -2.71386

H 2.79524 1.64490 -2.11837

H 2.14759 1.42386 -3.78503

H 1.37217 0.56118 -2.41679

C 0.83610 4.26863 -0.63602

H 1.22254 5.00255 -1.35449

C 0.50053 4.56351 0.69515

H 0.61243 5.60212 1.04725

C 0.03572 3.57532 1.55333

H -0.23997 3.82925 2.58838

C -0.09993 2.19882 1.10564

C 0.19576 1.99790 -0.29651

H 0.00862 1.01297 -0.76498

C -0.77435 1.25063 3.18111

C -2.03698 0.82303 3.67868

H -2.79682 0.50095 2.94764

C -2.31474 0.81677 5.05357

H -3.30771 0.48649 5.40474

C -1.34226 1.22751 5.98439

H -1.56113 1.21900 7.06486

C -0.08488 1.64817 5.51325

H 0.69250 1.96769 6.22920

C 0.19708 1.66363 4.13831

H 1.19285 1.98194 3.78577

N 0.65237 2.98991 -1.08832

N -0.51320 1.15297 1.81568

H -0.18022 2.47315 -4.39917

H -1.04033 3.45922 -3.16008

H -0.94685 1.65810 -3.00084

H 1.45072 3.62211 -2.89704

C 0.92603 -2.71068 2.54311

C -0.39298 -2.56896 3.31252

C 1.86580 -1.51242 2.71433

H 2.79543 -1.64562 2.11916

H 2.14722 -1.42459 3.78560

H 1.37235 -0.56178 2.41712

C 0.83685 -4.26883 0.63579

H 1.22284 -5.00291 1.35434

C 0.50213 -4.56346 -0.69565

H 0.61457 -5.60193 -1.04800

C 0.03749 -3.57517 -1.55383

H -0.23739 -3.82886 -2.58916

C -0.09896 -2.19889 -1.10577

C 0.19619 -1.99815 0.29652

H 0.00876 -1.01332 0.76508

C -0.77322 -1.25037 -3.18116

C -2.03601 -0.82347 -3.67889

H -2.79607 -0.50189 -2.94789

C -2.31348 -0.81697 -5.05383

H -3.30656 -0.48715 -5.40512

C -1.34049 -1.22673 -5.98455

H -1.55907 -1.21792 -7.06508

C -0.08292 -1.64664 -5.51326

H 0.69487 -1.96533 -6.22915

C 0.19873 -1.66239 -4.13825

H 1.19462 -1.98019 -3.78558

N 0.65271 -2.99024 1.08829

N -0.51257 -1.15301 -1.81562

H -0.18077 -2.47424 4.39902

H -1.04104 -3.45911 3.15909

H -0.94650 -1.65791 3.00097

H 1.45035 -3.62276 2.89723

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 10.81 1.00494 YES YES

8 a 26.88 0.44177 YES YES

9 a 31.91 0.79278 YES YES

10 a 35.69 0.04143 YES YES

11 a 40.83 1.51000 YES YES

12 a 43.11 0.16431 YES YES

13 a 48.25 0.00047 YES YES

14 a 49.14 0.39990 YES YES

15 a 67.90 5.53842 YES YES

16 a 68.42 3.35527 YES YES

17 a 72.02 0.00893 YES YES

18 a 73.58 0.19338 YES YES

19 a 82.93 0.33847 YES YES

20 a 88.49 8.55017 YES YES

21 a 129.27 0.43437 YES YES

22 a 129.82 0.00233 YES YES

23 a 156.23 4.32006 YES YES

24 a 159.77 0.50602 YES YES

25 a 167.65 1.58480 YES YES

26 a 175.79 2.10046 YES YES

27 a 235.37 0.07178 YES YES

28 a 235.72 0.65825 YES YES

29 a 240.93 0.48209 YES YES

30 a 241.54 1.45890 YES YES

31 a 278.58 0.51988 YES YES

32 a 279.15 0.02465 YES YES

33 a 305.90 0.76819 YES YES

34 a 306.07 0.38593 YES YES

35 a 331.02 4.97557 YES YES

36 a 331.05 2.55436 YES YES

37 a 350.17 1.07404 YES YES

38 a 350.72 1.25797 YES YES

39 a 397.33 10.63165 YES YES

40 a 401.76 4.83640 YES YES

41 a 412.93 0.22355 YES YES

42 a 413.00 0.38006 YES YES

43 a 450.10 1.38357 YES YES

44 a 452.91 5.33056 YES YES

45 a 474.73 2.55621 YES YES

46 a 474.89 0.21838 YES YES

47 a 502.91 6.28744 YES YES

48 a 502.94 14.78817 YES YES

49 a 552.82 2.30452 YES YES

50 a 553.63 0.35003 YES YES

pbe0\_def2-tzvpp energy (au): -1304.1163962130

Zero point energy (au): 0.5437512

Entropy (kJ mol^-1): 0.85014

Chemical potential (kJ mol^-1): 1256.53

XYZ coordinates:

64

C 0.70075 2.69739 -2.45647

C -0.64146 2.41259 -3.10351

C 1.70975 1.58411 -2.66672

H 2.64928 1.80403 -2.15691

H 1.91087 1.48394 -3.73400

H 1.32021 0.62842 -2.31339

C 0.77119 4.23394 -0.57056

H 1.11247 4.95137 -1.29869

C 0.55805 4.51690 0.76829

H 0.73296 5.52724 1.11625

C 0.12891 3.54855 1.63923

H -0.04699 3.79518 2.67754

C -0.10605 2.20570 1.19476

C 0.10281 2.01129 -0.20480

H -0.10612 1.05002 -0.66239

C -0.69029 1.30531 3.27783

C -1.92456 0.98203 3.85752

H -2.74307 0.71633 3.19859

C -2.10112 1.00092 5.23121

H -3.07080 0.75081 5.64710

C -1.05107 1.33648 6.07555

H -1.18957 1.34845 7.14964

C 0.18099 1.65425 5.51957

H 1.01479 1.91162 6.16370

C 0.36071 1.64120 4.14575

H 1.33289 1.87646 3.72621

N 0.52234 2.98349 -1.00770

N -0.53134 1.18492 1.90587

H -0.50592 2.28029 -4.17754

H -1.33791 3.23635 -2.94004

H -1.07651 1.49304 -2.71242

H 1.10577 3.62445 -2.86493

C 0.70019 -2.69249 2.45694

C -0.64241 -2.40902 3.10377

C 1.70785 -1.57777 2.66574

H 2.64853 -1.79876 2.15848

H 1.90669 -1.47389 3.73308

H 1.31843 -0.62357 2.30823

C 0.76921 -4.23138 0.57288

H 1.10977 -4.94828 1.30188

C 0.55581 -4.51564 -0.76565

H 0.73003 -5.52645 -1.11261

C 0.12776 -3.54778 -1.63771

H -0.04883 -3.79577 -2.67557

C -0.10585 -2.20413 -1.19489

C 0.10299 -2.00850 0.20447

H -0.10571 -1.04681 0.66119

C -0.68899 -1.30640 -3.27910

C -1.92225 -0.98112 -3.85979

H -2.73988 -0.71062 -3.20172

C -2.09935 -1.00542 -5.23333

H -3.06864 -0.75502 -5.64994

C -1.05054 -1.34753 -6.07659

H -1.18956 -1.36405 -7.15055

C 0.18108 -1.66544 -5.51972

H 1.01411 -1.92729 -6.16304

C 0.36128 -1.64714 -4.14603

H 1.33296 -1.88329 -3.72582

N 0.52170 -2.98013 1.00847

N -0.53023 -1.18371 -1.90725

H -0.50718 -2.27560 4.17770

H -1.33758 -3.23397 2.94090

H -1.07885 -1.49052 2.71186

H 1.10651 -3.61863 2.86621

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 7.66 1.23450 YES YES

8 a 28.61 0.85868 YES YES

9 a 31.22 0.44888 YES YES

10 a 35.05 0.02016 YES YES

11 a 40.97 0.33458 YES YES

12 a 41.61 1.41575 YES YES

13 a 49.79 0.03994 YES YES

14 a 52.58 0.98578 YES YES

15 a 68.54 2.75591 YES YES

16 a 68.99 4.10764 YES YES

17 a 73.77 0.00902 YES YES

18 a 79.67 0.10191 YES YES

19 a 90.52 8.10169 YES YES

20 a 90.92 1.64624 YES YES

21 a 132.11 0.43400 YES YES

22 a 135.11 0.02929 YES YES

23 a 163.34 0.15377 YES YES

24 a 164.08 3.66203 YES YES

25 a 172.35 1.45616 YES YES

26 a 179.57 2.02458 YES YES

27 a 235.11 0.95720 YES YES

28 a 236.72 0.00405 YES YES

29 a 245.57 0.38445 YES YES

30 a 246.83 0.50184 YES YES

31 a 267.56 1.49123 YES YES

32 a 269.85 0.11706 YES YES

33 a 312.86 0.45731 YES YES

34 a 312.97 2.21129 YES YES

35 a 345.45 4.64303 YES YES

36 a 345.98 1.05963 YES YES

37 a 356.31 2.00314 YES YES

38 a 356.83 1.46242 YES YES

39 a 411.31 10.79614 YES YES

40 a 414.96 4.80881 YES YES

41 a 423.94 0.27488 YES YES

42 a 424.10 0.50625 YES YES

43 a 468.01 2.08554 YES YES

44 a 469.11 4.84374 YES YES

45 a 488.20 2.41043 YES YES

46 a 488.51 0.02461 YES YES

47 a 517.66 21.54513 YES YES

48 a 517.86 6.29538 YES YES

49 a 571.32 1.70733 YES YES

50 a 572.26 0.38206 YES YES

## BETAINE monomer\_iso2

bp86 energy (au): -652.1244117202

Zero point energy (au): 0.2620303

Entropy (kJ mol^-1): 0.52031

Chemical potential (kJ mol^-1): 574.17

XYZ coordinates:

32

C 0.08671 -0.06662 -4.03942

C 1.45731 0.04829 -4.72059

C -0.99736 0.79853 -4.69635

H -1.96670 0.69562 -4.16326

H -1.14397 0.47077 -5.74842

H -0.71925 1.87435 -4.71308

C 0.57522 1.47552 -2.16339

H 0.79613 2.21724 -2.93970

C 0.66064 1.72804 -0.77981

H 0.95338 2.73982 -0.45422

C 0.38288 0.74430 0.15782

H 0.44567 0.97176 1.23284

C -0.02552 -0.59538 -0.25690

C -0.09595 -0.75766 -1.69413

H -0.40758 -1.72941 -2.10383

C -0.20376 -1.67690 1.86026

C -1.26196 -2.17515 2.67185

H -2.20655 -2.44789 2.17348

C -1.11173 -2.31738 4.05737

H -1.95554 -2.69959 4.65775

C 0.10361 -1.98622 4.68671

H 0.22243 -2.10696 5.77617

C 1.16869 -1.51200 3.89974

H 2.13564 -1.26562 4.37244

C 1.02164 -1.35431 2.51329

H 1.87731 -1.00904 1.90843

N 0.19123 0.22586 -2.57077

N -0.38067 -1.62700 0.48557

H 1.37653 -0.29981 -5.77298

H 2.21278 -0.58194 -4.20416

H 1.82816 1.09590 -4.73847

H -0.23743 -1.12613 -4.08625

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 16.15 0.00963 YES YES

8 a 38.48 0.22062 YES YES

9 a 52.65 2.23718 YES YES

10 a 76.29 0.82349 YES YES

11 a 128.99 0.40233 YES YES

12 a 167.11 1.52922 YES YES

13 a 173.55 1.26291 YES YES

14 a 225.96 0.03973 YES YES

15 a 234.93 2.48588 YES YES

16 a 246.45 0.19670 YES YES

17 a 272.58 0.24250 YES YES

18 a 331.37 2.50439 YES YES

19 a 342.41 1.04085 YES YES

20 a 386.72 6.46953 YES YES

21 a 410.24 0.53189 YES YES

22 a 433.26 3.81479 YES YES

23 a 469.26 2.14259 YES YES

24 a 504.55 10.93370 YES YES

25 a 546.65 0.63563 YES YES

26 a 583.34 4.64870 YES YES

27 a 587.38 4.67638 YES YES

28 a 605.30 0.67377 YES YES

29 a 625.17 5.62250 YES YES

30 a 629.66 29.96303 YES YES

31 a 680.21 9.17584 YES YES

32 a 693.97 26.91227 YES YES

33 a 709.32 3.12741 YES YES

34 a 758.65 18.91295 YES YES

35 a 791.49 25.77473 YES YES

36 a 811.28 13.34923 YES YES

37 a 814.24 7.22753 YES YES

38 a 824.74 4.86143 YES YES

39 a 866.15 3.96104 YES YES

40 a 880.97 4.06579 YES YES

41 a 911.76 0.91162 YES YES

42 a 928.77 22.06978 YES YES

43 a 932.32 0.34516 YES YES

44 a 939.57 1.04165 YES YES

45 a 951.73 0.06440 YES YES

46 a 961.92 0.29315 YES YES

47 a 975.71 2.21646 YES YES

48 a 1009.21 47.33291 YES YES

49 a 1021.30 10.88061 YES YES

50 a 1044.34 6.00950 YES YES

pbe0\_def2-tzvpp energy (au): -652.0481778399

Zero point energy (au): 0.2708269

Entropy (kJ mol^-1): 0.51283

Chemical potential (kJ mol^-1): 598.40

XYZ coordinates:

32

C 0.08272 -0.07190 -3.99535

C 1.43172 0.06314 -4.67912

C -0.99234 0.79421 -4.62750

H -1.94118 0.68915 -4.10065

H -1.13904 0.48713 -5.66395

H -0.71258 1.84836 -4.62839

C 0.57884 1.43234 -2.13562

H 0.79032 2.16716 -2.89353

C 0.67267 1.66736 -0.77022

H 0.96496 2.65707 -0.44170

C 0.40243 0.68927 0.15006

H 0.47430 0.90517 1.20725

C -0.00609 -0.62654 -0.26780

C -0.08277 -0.77320 -1.68897

H -0.39020 -1.72240 -2.10413

C -0.19202 -1.67861 1.82530

C -1.23929 -2.16217 2.62202

H -2.16073 -2.45032 2.13022

C -1.10358 -2.27473 3.99433

H -1.93496 -2.64632 4.58302

C 0.08586 -1.92412 4.62040

H 0.19299 -2.02008 5.69382

C 1.14062 -1.46381 3.84455

H 2.08372 -1.20421 4.31307

C 1.00731 -1.33948 2.47127

H 1.85070 -1.00535 1.87745

N 0.19682 0.20468 -2.54321

N -0.35605 -1.65588 0.45388

H 1.34384 -0.26418 -5.71582

H 2.18480 -0.55315 -4.18707

H 1.78066 1.09657 -4.68444

H -0.23246 -1.11416 -4.05119

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 18.64 0.02759 YES YES

8 a 37.63 0.39304 YES YES

9 a 53.72 2.77364 YES YES

10 a 80.06 1.05115 YES YES

11 a 132.45 0.35951 YES YES

12 a 170.03 2.00848 YES YES

13 a 178.48 1.16623 YES YES

14 a 224.46 0.00110 YES YES

15 a 241.37 1.42019 YES YES

16 a 247.95 1.02708 YES YES

17 a 277.03 0.34118 YES YES

18 a 341.74 2.10286 YES YES

19 a 350.97 1.56038 YES YES

20 a 397.44 5.58723 YES YES

21 a 421.96 0.22195 YES YES

22 a 454.16 4.02692 YES YES

23 a 483.26 2.61502 YES YES

24 a 519.65 14.27349 YES YES

25 a 563.15 0.43743 YES YES

26 a 601.82 2.20920 YES YES

27 a 610.98 8.66631 YES YES

28 a 625.68 0.60788 YES YES

29 a 651.33 2.88255 YES YES

30 a 682.19 47.28820 YES YES

31 a 714.45 35.92718 YES YES

32 a 719.82 0.90881 YES YES

33 a 738.09 5.20038 YES YES

34 a 786.88 24.94171 YES YES

35 a 822.92 26.20997 YES YES

36 a 847.11 7.71722 YES YES

37 a 856.57 20.03880 YES YES

38 a 870.73 1.24045 YES YES

39 a 896.24 4.55598 YES YES

40 a 921.18 4.45353 YES YES

41 a 932.90 0.85322 YES YES

42 a 959.28 0.34279 YES YES

43 a 963.12 34.03530 YES YES

44 a 978.92 0.35385 YES YES

45 a 987.29 0.33112 YES YES

46 a 996.54 0.42602 YES YES

47 a 1015.35 2.49275 YES YES

48 a 1049.28 57.92850 YES YES

49 a 1056.71 20.91402 YES YES

50 a 1079.97 7.33648 YES YES

## BETAINE\_dimer\_iso2

bp86 energy (au): -1304.2721332640

Zero point energy (au): 0.5259837

Entropy (kJ mol^-1): 0.86795

Chemical potential (kJ mol^-1): 1207.06

XYZ coordinates:

64

C 0.07760 2.57491 -2.69042

C 1.47070 2.77579 -3.29874

C -1.02729 3.34337 -3.42555

H -2.01251 3.19210 -2.93444

H -1.10049 2.95941 -4.46558

H -0.82302 4.43547 -3.47780

C 0.32458 4.19864 -0.83149

H 0.50901 4.94020 -1.61782

C 0.31743 4.49070 0.54141

H 0.49278 5.53217 0.85682

C 0.09019 3.49856 1.48904

H 0.07426 3.75361 2.55969

C -0.15244 2.12502 1.08649

C -0.14961 1.91466 -0.34363

H -0.34137 0.91091 -0.77508

C -0.28521 1.12130 3.24877

C -1.32905 0.60461 4.07012

H -2.25875 0.27606 3.57630

C -1.19244 0.52879 5.46406

H -2.02766 0.13600 6.06983

C -0.00827 0.95504 6.09494

H 0.09781 0.89357 7.19048

C 1.03839 1.46132 5.30143

H 1.97863 1.79169 5.77667

C 0.90678 1.54718 3.90738

H 1.74631 1.92442 3.29945

N 0.08236 2.91000 -1.22325

N -0.42792 1.08240 1.86825

H 1.46977 2.38970 -4.34041

H 2.23826 2.21100 -2.72748

H 1.76807 3.84730 -3.32919

H -0.16530 1.49468 -2.72775

C 0.07634 -2.57504 2.69036

C 1.46947 -2.77720 3.29821

C -1.02903 -3.34231 3.42601

H -2.01427 -3.19016 2.93523

H -1.10148 -2.95811 4.46599

H -0.82580 -4.43461 3.47837

C 0.32127 -4.19925 0.83156

H 0.50530 -4.94088 1.61792

C 0.31353 -4.49143 -0.54131

H 0.48773 -5.53313 -0.85665

C 0.08708 -3.49917 -1.48901

H 0.07057 -3.75436 -2.55962

C -0.15414 -2.12535 -1.08656

C -0.15091 -1.91490 0.34355

H -0.34168 -0.91088 0.77482

C -0.28626 -1.12143 -3.24882

C -1.32956 -0.60329 -4.06992

H -2.25880 -0.27370 -3.57591

C -1.19300 -0.52724 -5.46385

H -2.02780 -0.13328 -6.06944

C -0.00939 -0.95472 -6.09497

H 0.09662 -0.89314 -7.19051

C 1.03673 -1.46248 -5.30170

H 1.97654 -1.79381 -5.77711

C 0.90514 -1.54859 -3.90767

H 1.74428 -1.92701 -3.29994

N 0.08029 -2.91034 1.22324

N -0.42864 -1.08247 -1.86829

H 1.46932 -2.39089 4.33981

H 2.23740 -2.21330 2.72655

H 1.76578 -3.84900 3.32877

H -0.16550 -1.49456 2.72762

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 11.76 1.41649 YES YES

8 a 24.71 0.05356 YES YES

9 a 28.45 0.00010 YES YES

10 a 30.97 0.62357 YES YES

11 a 38.43 0.54123 YES YES

12 a 39.33 1.07372 YES YES

13 a 45.87 1.04983 YES YES

14 a 53.29 0.10490 YES YES

15 a 54.54 0.67184 YES YES

16 a 54.96 0.61938 YES YES

17 a 71.02 2.42995 YES YES

18 a 72.42 7.92896 YES YES

19 a 85.08 5.22974 YES YES

20 a 90.14 0.06968 YES YES

21 a 132.38 0.53329 YES YES

22 a 133.72 0.13179 YES YES

23 a 176.50 0.38993 YES YES

24 a 177.09 9.81546 YES YES

25 a 177.85 0.05004 YES YES

26 a 187.59 0.18672 YES YES

27 a 231.29 0.13503 YES YES

28 a 231.80 0.49504 YES YES

29 a 235.34 3.15703 YES YES

30 a 236.17 0.17504 YES YES

31 a 249.47 0.68067 YES YES

32 a 250.11 0.03394 YES YES

33 a 273.04 0.01014 YES YES

34 a 273.17 2.68717 YES YES

35 a 333.04 1.68835 YES YES

36 a 333.13 2.02385 YES YES

37 a 346.75 3.27553 YES YES

38 a 347.92 0.38158 YES YES

39 a 392.88 22.01708 YES YES

40 a 396.54 1.32175 YES YES

41 a 412.39 0.04406 YES YES

42 a 412.47 0.08158 YES YES

43 a 448.56 2.69558 YES YES

44 a 452.63 5.99588 YES YES

45 a 471.35 2.06130 YES YES

46 a 471.37 2.13352 YES YES

47 a 503.40 0.44307 YES YES

48 a 503.95 27.50030 YES YES

49 a 549.52 0.69711 YES YES

50 a 550.10 0.00564 YES YES

pbe0\_def2-tzvpp energy (au): -1304.1207260210

Zero point energy (au): 0.5434798

Entropy (kJ mol^-1): 0.86262

Chemical potential (kJ mol^-1): 1252.79

XYZ coordinates:

64

C -0.08015 2.48008 -2.60253

C 1.26871 2.56206 -3.29219

C -1.14248 3.33164 -3.27239

H -2.09123 3.26930 -2.73796

H -1.29813 2.96414 -4.28737

H -0.84755 4.38073 -3.33601

C 0.42705 4.06760 -0.80467

H 0.63502 4.77037 -1.59406

C 0.52793 4.35813 0.54397

H 0.82351 5.35849 0.83482

C 0.25773 3.41131 1.50333

H 0.33247 3.66968 2.55106

C -0.14785 2.08990 1.13586

C -0.23779 1.88014 -0.27262

H -0.53191 0.91735 -0.67957

C -0.27948 1.12451 3.28294

C -1.29680 0.67499 4.14070

H -2.24930 0.40312 3.69981

C -1.10117 0.58681 5.50889

H -1.91300 0.24537 6.14190

C 0.11853 0.93540 6.07476

H 0.27122 0.86523 7.14458

C 1.14004 1.37459 5.24211

H 2.10340 1.64052 5.66368

C 0.94895 1.47032 3.87375

H 1.76686 1.79066 3.23825

N 0.04090 2.82617 -1.16170

N -0.49300 1.08836 1.92036

H 1.17070 2.16625 -4.30375

H 2.01190 1.96077 -2.76784

H 1.63238 3.58922 -3.36083

H -0.40599 1.44093 -2.60725

C -0.07854 -2.47962 2.60257

C 1.27134 -2.56462 3.28994

C -1.14161 -3.32871 3.27434

H -2.09130 -3.26382 2.74189

H -1.29425 -2.96109 4.28973

H -0.84919 -4.37855 3.33706

C 0.42230 -4.06850 0.80424

H 0.62949 -4.77171 1.59343

C 0.52121 -4.35933 -0.54449

H 0.81416 -5.36039 -0.83559

C 0.25247 -3.41185 -1.50358

H 0.32570 -3.67038 -2.55138

C -0.14977 -2.08953 -1.13577

C -0.23794 -1.87948 0.27277

H -0.52963 -0.91605 0.68000

C -0.27969 -1.12412 -3.28276

C -1.29615 -0.67364 -4.14103

H -2.24852 -0.40051 -3.70061

C -1.09989 -0.58613 -5.50918

H -1.91110 -0.24402 -6.14263

C 0.11959 -0.93635 -6.07450

H 0.27274 -0.86674 -7.14429

C 1.14026 -1.37654 -5.24133

H 2.10347 -1.64371 -5.66244

C 0.94852 -1.47164 -3.87304

H 1.76575 -1.79296 -3.23714

N 0.03951 -2.82614 1.16160

N -0.49337 -1.08740 -1.92023

H 1.17610 -2.16850 4.30163

H 2.01503 -1.96519 2.76417

H 1.63270 -3.59264 3.35802

H -0.40208 -1.43976 2.60775

Vibrational Spectrum (first 50 lines):

# mode symmetry wave number IR intensity selection rules

# cm\*\*(-1) km/mol IR RAMAN

1 0.00 0.00000 - -

2 0.00 0.00000 - -

3 0.00 0.00000 - -

4 0.00 0.00000 - -

5 0.00 0.00000 - -

6 0.00 0.00000 - -

7 a 10.49 1.23808 YES YES

8 a 22.95 0.41661 YES YES

9 a 30.25 0.00766 YES YES

10 a 32.24 0.06412 YES YES

11 a 33.16 0.11481 YES YES

12 a 35.89 0.66601 YES YES

13 a 40.13 1.50801 YES YES

14 a 49.76 0.07921 YES YES

15 a 50.51 1.38128 YES YES

16 a 55.00 1.16501 YES YES

17 a 67.58 7.42819 YES YES

18 a 75.54 2.68195 YES YES

19 a 87.83 5.69122 YES YES

20 a 91.24 0.00001 YES YES

21 a 136.03 0.24398 YES YES

22 a 136.09 0.48707 YES YES

23 a 180.66 4.81755 YES YES

24 a 182.05 0.06380 YES YES

25 a 182.64 6.80001 YES YES

26 a 189.10 0.42687 YES YES

27 a 226.39 0.05061 YES YES

28 a 226.69 0.02209 YES YES

29 a 240.73 0.29657 YES YES

30 a 241.02 2.02237 YES YES

31 a 247.82 2.18227 YES YES

32 a 249.35 0.16176 YES YES

33 a 278.00 0.12123 YES YES

34 a 278.04 2.41277 YES YES

35 a 342.15 1.66868 YES YES

36 a 342.77 1.31456 YES YES

37 a 354.83 3.90130 YES YES

38 a 356.13 0.39210 YES YES

39 a 397.93 22.56426 YES YES

40 a 400.98 1.66903 YES YES

41 a 424.21 0.03541 YES YES

42 a 424.28 0.06470 YES YES

43 a 466.86 4.01191 YES YES

44 a 467.26 5.05488 YES YES

45 a 485.86 5.11590 YES YES

46 a 485.91 0.34243 YES YES

47 a 520.11 0.43734 YES YES

48 a 520.68 33.95357 YES YES

49 a 565.67 0.72508 YES YES

50 a 566.70 0.00204 YES YES

# NMR chemical shift calculations – norharman motif (compounds 1 and [1]2)

## Norharman monomer\_iso 1 (gas-phase) - BP86/IGLO-III level

30

C -4.35898 0.77297 0.00505

C -3.09426 1.35901 -0.00383

C -1.95326 0.51716 -0.00475

C -2.09779 -0.93433 0.00403

C -3.40260 -1.50063 0.01354

C -4.50449 -0.64795 0.01367

C -0.54374 0.73339 -0.01215

N -0.90419 -1.60909 0.00240

H -3.51918 -2.59621 0.02065

H -5.52098 -1.07741 0.02060

C 0.33191 1.83275 -0.02256

C 0.02507 -0.62755 -0.00670

C 1.41899 -0.76935 -0.00893

H -0.03205 2.87299 -0.02907

C 1.70731 1.60927 -0.02579

N 2.22678 0.32935 -0.01887

H 2.44482 2.42364 -0.03414

H 1.89990 -1.75774 -0.00154

C 3.71180 0.14984 -0.00639

H -5.26041 1.40785 0.00570

H -2.98676 2.45746 -0.01000

C 4.17908 -0.49385 1.30756

H 4.11708 1.18191 -0.04843

C 4.19526 -0.60145 -1.25520

H 3.81874 -1.54117 1.40420

H 3.81459 0.08208 2.18488

H 5.29006 -0.51381 1.34206

H 3.85423 -1.65930 -1.26134

H 5.30681 -0.60627 -1.28070

H 3.82915 -0.11155 -2.18275

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 52.2211 Anisotropy = 166.0909

XX= -9.2805 YX= 47.3142 ZX= 0.5336

XY= 51.5446 YY= 3.0017 ZY= 0.6448

XZ= 0.4653 YZ= 0.7460 ZZ= 162.9421

Eigenvalues: -52.9488 46.6638 162.9484

2 C Isotropic = 49.1794 Anisotropy = 169.6275

XX= 36.5604 YX= 3.0208 ZX= 0.5729

XY= 3.2915 YY= -51.2782 ZY= 1.0905

XZ= 0.6140 YZ= 1.0809 ZZ= 162.2559

Eigenvalues: -51.3967 36.6705 162.2644

3 C Isotropic = 46.6711 Anisotropy = 159.4952

XX= -9.1304 YX= -17.4232 ZX= 0.8609

XY= -8.4999 YY= -3.8491 ZY= 0.8804

XZ= 0.8037 YZ= 0.8299 ZZ= 152.9930

Eigenvalues: -19.7257 6.7379 153.0013

4 C Isotropic = 6.6503 Anisotropy = 158.6104

XX= -42.3284 YX= -1.4157 ZX= 0.7700

XY= 8.0977 YY= -50.1028 ZY= 0.8878

XZ= 0.6343 YZ= 0.9454 ZZ= 112.3820

Eigenvalues: -51.3436 -41.0961 112.3906

5 C Isotropic = 48.9090 Anisotropy = 154.8519

XX= 32.5624 YX= -19.9971 ZX= 0.6910

XY= -20.1454 YY= -37.9688 ZY= 1.2258

XZ= 0.6834 YZ= 1.1840 ZZ= 152.1333

Eigenvalues: -43.2897 37.8730 152.1436

6 C Isotropic = 41.1782 Anisotropy = 178.9406

XX= -43.5293 YX= -42.7038 ZX= 1.1670

XY= -44.2406 YY= 6.6034 ZY= 1.0699

XZ= 1.2127 YZ= 1.0689 ZZ= 160.4604

Eigenvalues: -68.6549 31.7174 160.4719

7 C Isotropic = 36.0100 Anisotropy = 178.4710

XX= -26.2490 YX= 9.7778 ZX= 0.7632

XY= 12.4234 YY= -20.7032 ZY= 0.9424

XZ= 0.8625 YZ= 0.8084 ZZ= 154.9821

Eigenvalues: -34.9178 -12.0429 154.9906

8 N Isotropic = -21.3709 Anisotropy = 345.9397

XX= -223.8614 YX= -27.1208 ZX= 2.0389

XY= -37.1832 YY= -49.4868 ZY= 1.6522

XZ= 2.5426 YZ= 1.5619 ZZ= 209.2354

Eigenvalues: -229.6155 -43.7528 209.2555

9 H Isotropic = 23.1025 Anisotropy = 6.5815

XX= 27.3688 YX= -0.5399 ZX= -0.0364

XY= -0.8813 YY= 23.3235 ZY= -0.0204

XZ= -0.0350 YZ= -0.0288 ZZ= 18.6150

Eigenvalues: 18.6147 23.2025 27.4901

10 H Isotropic = 23.4684 Anisotropy = 5.4944

XX= 24.4697 YX= -1.3989 ZX= -0.0156

XY= -1.6192 YY= 26.2757 ZY= -0.0302

XZ= -0.0117 YZ= -0.0307 ZZ= 19.6598

Eigenvalues: 19.6596 23.6143 27.1313

11 C Isotropic = 57.8266 Anisotropy = 157.2555

XX= 37.5675 YX= 25.6188 ZX= 0.2612

XY= 24.1900 YY= -26.7427 ZY= 1.2505

XZ= 0.1911 YZ= 1.1026 ZZ= 162.6551

Eigenvalues: -35.2647 46.0810 162.6636

12 C Isotropic = 22.4366 Anisotropy = 150.2013

XX= -17.2772 YX= 17.9507 ZX= 0.3249

XY= 7.5432 YY= -37.9731 ZY= 0.9604

XZ= 0.5564 YZ= 1.3839 ZZ= 122.5603

Eigenvalues: -44.0481 -11.2128 122.5709

13 C Isotropic = 48.4641 Anisotropy = 134.7981

XX= 26.0594 YX= 10.6802 ZX= -0.0057

XY= 14.0725 YY= -18.9859 ZY= 1.2183

XZ= -1.1052 YZ= 1.1210 ZZ= 138.3189

Eigenvalues: -22.1725 29.2353 138.3296

14 H Isotropic = 23.0348 Anisotropy = 7.1149

XX= 27.7005 YX= 1.3247 ZX= -0.0464

XY= -0.2561 YY= 24.0846 ZY= -0.0382

XZ= -0.0380 YZ= -0.0682 ZZ= 17.3193

Eigenvalues: 17.3188 24.0076 27.7780

15 C Isotropic = 55.4614 Anisotropy = 92.8432

XX= 51.0811 YX= -38.2171 ZX= 0.2186

XY= -38.0314 YY= -2.0404 ZY= 0.9015

XZ= -0.7744 YZ= 0.9675 ZZ= 117.3434

Eigenvalues: -21.9474 70.9747 117.3568

16 N Isotropic = 36.8619 Anisotropy = 222.8457

XX= -73.4138 YX= 14.9830 ZX= -0.0645

XY= 10.1620 YY= -1.4053 ZY= 1.5729

XZ= 1.2992 YZ= 2.1671 ZZ= 185.4049

Eigenvalues: -75.5461 0.7061 185.4257

17 H Isotropic = 23.8872 Anisotropy = 7.8922

XX= 26.4288 YX= -2.6309 ZX= 0.0062

XY= -2.3843 YY= 26.8354 ZY= -0.0776

XZ= 0.0002 YZ= -0.1529 ZZ= 18.3974

Eigenvalues: 18.3957 24.1173 29.1487

18 H Isotropic = 22.7800 Anisotropy = 11.1958

XX= 28.4311 YX= 3.8231 ZX= -0.1432

XY= 3.2686 YY= 23.3049 ZY= -0.0149

XZ= -0.0782 YZ= 0.0412 ZZ= 16.6040

Eigenvalues: 16.6026 21.4936 30.2439

19 C Isotropic = 106.6768 Anisotropy = 62.5454

XX= 148.3718 YX= 3.8951 ZX= -0.3951

XY= -4.3607 YY= 87.4432 ZY= 0.6804

XZ= 0.9052 YZ= 0.4453 ZZ= 84.2152

Eigenvalues: 84.1186 87.5380 148.3737

20 H Isotropic = 23.7945 Anisotropy = 5.3807

XX= 25.8896 YX= 1.4848 ZX= -0.0356

XY= 1.6103 YY= 25.7757 ZY= -0.0420

XZ= -0.0405 YZ= -0.0370 ZZ= 19.7181

Eigenvalues: 19.7178 24.2841 27.3816

21 H Isotropic = 22.8444 Anisotropy = 7.8856

XX= 28.0932 YX= -0.4613 ZX= -0.0448

XY= 0.0523 YY= 22.9042 ZY= -0.0319

XZ= -0.0509 YZ= -0.0222 ZZ= 17.5358

Eigenvalues: 17.5354 22.8963 28.1015

22 C Isotropic = 150.1636 Anisotropy = 37.5013

XX= 146.4826 YX= -3.9502 ZX= 8.4032

XY= -5.8286 YY= 138.8250 ZY= -12.5681

XZ= 15.2897 YZ= -10.2755 ZZ= 165.1833

Eigenvalues: 134.5376 140.7889 175.1645

23 H Isotropic = 26.6389 Anisotropy = 5.2152

XX= 27.7233 YX= 1.5035 ZX= -0.1390

XY= -0.4732 YY= 29.9989 ZY= -0.1802

XZ= -0.1267 YZ= -0.1949 ZZ= 22.1944

Eigenvalues: 22.1873 27.6136 30.1157

24 C Isotropic = 150.7318 Anisotropy = 36.4684

XX= 147.3423 YX= -4.8346 ZX= -8.1582

XY= -6.5318 YY= 140.8534 ZY= 14.3266

XZ= -12.8298 YZ= 11.9258 ZZ= 163.9997

Eigenvalues: 134.8393 142.3120 175.0440

25 H Isotropic = 29.1772 Anisotropy = 6.4262

XX= 28.1503 YX= 0.5421 ZX= 0.9400

XY= 1.2373 YY= 32.0271 ZY= -1.7785

XZ= 2.4821 YZ= -4.1390 ZZ= 27.3542

Eigenvalues: 24.8085 29.2618 33.4613

26 H Isotropic = 29.4106 Anisotropy = 7.7108

XX= 26.9680 YX= -1.0923 ZX= 0.3541

XY= -0.7662 YY= 27.4551 ZY= 1.3651

XZ= 2.9083 YZ= 2.3413 ZZ= 33.8088

Eigenvalues: 25.5338 28.1469 34.5511

27 H Isotropic = 29.5264 Anisotropy = 9.8083

XX= 34.5108 YX= -0.6128 ZX= 2.4482

XY= -1.0445 YY= 26.1932 ZY= -0.4020

XZ= 4.4126 YZ= -0.7769 ZZ= 27.8752

Eigenvalues: 25.9843 26.5296 36.0653

28 H Isotropic = 29.1159 Anisotropy = 6.5432

XX= 28.1524 YX= 0.3818 ZX= -1.0244

XY= 1.1040 YY= 32.4869 ZY= 1.4530

XZ= -2.3982 YZ= 3.7235 ZZ= 26.7085

Eigenvalues: 24.7095 29.1602 33.4781

29 H Isotropic = 29.5084 Anisotropy = 9.7262

XX= 34.5970 YX= -0.7045 ZX= -2.3788

XY= -1.2053 YY= 26.3001 ZY= 0.5950

XZ= -4.0438 YZ= 0.9473 ZZ= 27.6281

Eigenvalues: 25.8827 26.6499 35.9925

30 H Isotropic = 29.3934 Anisotropy = 7.7538

XX= 26.9549 YX= -1.0657 ZX= -0.2432

XY= -0.7307 YY= 27.1029 ZY= -0.7886

XZ= -2.7481 YZ= -1.6383 ZZ= 34.1223

Eigenvalues: 25.6892 27.9284 34.5626

## Norharman monomer\_iso 1 (gas-phase) – PBE0/IGLO-III level

30

C -4.35898 0.77297 0.00505

C -3.09426 1.35901 -0.00383

C -1.95326 0.51716 -0.00475

C -2.09779 -0.93433 0.00403

C -3.40260 -1.50063 0.01354

C -4.50449 -0.64795 0.01367

C -0.54374 0.73339 -0.01215

N -0.90419 -1.60909 0.00240

H -3.51918 -2.59621 0.02065

H -5.52098 -1.07741 0.02060

C 0.33191 1.83275 -0.02256

C 0.02507 -0.62755 -0.00670

C 1.41899 -0.76935 -0.00893

H -0.03205 2.87299 -0.02907

C 1.70731 1.60927 -0.02579

N 2.22678 0.32935 -0.01887

H 2.44482 2.42364 -0.03414

H 1.89990 -1.75774 -0.00154

C 3.71180 0.14984 -0.00639

H -5.26041 1.40785 0.00570

H -2.98676 2.45746 -0.01000

C 4.17908 -0.49385 1.30756

H 4.11708 1.18191 -0.04843

C 4.19526 -0.60145 -1.25520

H 3.81874 -1.54117 1.40420

H 3.81459 0.08208 2.18488

H 5.29006 -0.51381 1.34206

H 3.85423 -1.65930 -1.26134

H 5.30681 -0.60627 -1.28070

H 3.82915 -0.11155 -2.18275

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 55.6645 Anisotropy = 170.7390

XX= -6.0032 YX= 49.1795 ZX= 0.5370

XY= 53.8616 YY= 3.5126 ZY= 0.6664

XZ= 0.4773 YZ= 0.7615 ZZ= 169.4841

Eigenvalues: -52.9851 50.4881 169.4905

2 C Isotropic = 50.7915 Anisotropy = 176.9986

XX= 38.1893 YX= 5.3280 ZX= 0.5837

XY= 5.0160 YY= -54.5965 ZY= 1.1335

XZ= 0.6185 YZ= 1.1296 ZZ= 168.7818

Eigenvalues: -54.8893 38.4733 168.7906

3 C Isotropic = 51.2475 Anisotropy = 163.5792

XX= -7.1524 YX= -17.5463 ZX= 0.8843

XY= -9.1983 YY= 0.6032 ZY= 0.8986

XZ= 0.8236 YZ= 0.8542 ZZ= 160.2918

Eigenvalues: -17.2061 10.6484 160.3003

4 C Isotropic = 8.5002 Anisotropy = 168.7132

XX= -44.5434 YX= -2.5630 ZX= 0.8231

XY= 7.9173 YY= -50.9224 ZY= 0.9419

XZ= 0.6894 YZ= 1.0244 ZZ= 120.9665

Eigenvalues: -51.8996 -43.5754 120.9757

5 C Isotropic = 51.8667 Anisotropy = 160.5677

XX= 34.4768 YX= -22.8784 ZX= 0.7309

XY= -22.5630 YY= -37.7777 ZY= 1.2770

XZ= 0.7213 YZ= 1.2320 ZZ= 158.9011

Eigenvalues: -44.3382 41.0265 158.9119

6 C Isotropic = 43.0609 Anisotropy = 186.1810

XX= -43.9772 YX= -45.5338 ZX= 1.2136

XY= -47.2093 YY= 5.9905 ZY= 1.1242

XZ= 1.2613 YZ= 1.1177 ZZ= 167.1696

Eigenvalues: -71.6782 33.6795 167.1816

7 C Isotropic = 38.0904 Anisotropy = 186.3912

XX= -26.9628 YX= 9.3671 ZX= 0.8096

XY= 13.1420 YY= -21.1082 ZY= 0.9791

XZ= 0.8877 YZ= 0.8462 ZZ= 162.3424

Eigenvalues: -35.6646 -12.4153 162.3513

8 N Isotropic = -15.2418 Anisotropy = 351.4798

XX= -217.7239 YX= -27.9475 ZX= 2.0485

XY= -36.9286 YY= -47.0591 ZY= 1.6931

XZ= 2.5254 YZ= 1.6267 ZZ= 219.0576

Eigenvalues: -223.6961 -41.1074 219.0780

9 H Isotropic = 22.9531 Anisotropy = 6.8308

XX= 27.3547 YX= -0.6490 ZX= -0.0374

XY= -0.9295 YY= 23.4113 ZY= -0.0239

XZ= -0.0372 YZ= -0.0320 ZZ= 18.0933

Eigenvalues: 18.0929 23.2594 27.5069

10 H Isotropic = 23.3332 Anisotropy = 5.6720

XX= 24.5197 YX= -1.3842 ZX= -0.0171

XY= -1.6736 YY= 26.2135 ZY= -0.0319

XZ= -0.0134 YZ= -0.0325 ZZ= 19.2663

Eigenvalues: 19.2661 23.6190 27.1145

11 C Isotropic = 60.0679 Anisotropy = 163.4984

XX= 39.7935 YX= 26.0865 ZX= 0.2752

XY= 24.8442 YY= -28.6478 ZY= 1.3046

XZ= 0.2134 YZ= 1.1389 ZZ= 169.0580

Eigenvalues: -37.0889 48.2257 169.0669

12 C Isotropic = 25.2265 Anisotropy = 158.2298

XX= -17.2560 YX= 18.5690 ZX= 0.3523

XY= 7.4961 YY= -37.7665 ZY= 1.0034

XZ= 0.6056 YZ= 1.4317 ZZ= 130.7021

Eigenvalues: -44.0994 -10.9341 130.7131

13 C Isotropic = 48.6690 Anisotropy = 143.0928

XX= 25.1747 YX= 11.3842 ZX= -0.0052

XY= 13.9300 YY= -23.2208 ZY= 1.2945

XZ= -1.0488 YZ= 1.2367 ZZ= 144.0531

Eigenvalues: -26.3419 28.2847 144.0642

14 H Isotropic = 22.8507 Anisotropy = 7.3358

XX= 27.6728 YX= 1.3204 ZX= -0.0479

XY= -0.3183 YY= 24.0594 ZY= -0.0419

XZ= -0.0384 YZ= -0.0729 ZZ= 16.8198

Eigenvalues: 16.8192 23.9916 27.7412

15 C Isotropic = 56.6589 Anisotropy = 102.4342

XX= 51.1948 YX= -39.5874 ZX= 0.2720

XY= -39.1852 YY= -6.1534 ZY= 0.9998

XZ= -0.7567 YZ= 1.0710 ZZ= 124.9352

Eigenvalues: -26.2021 71.2304 124.9483

16 N Isotropic = 38.6831 Anisotropy = 236.8739

XX= -80.5880 YX= 16.8165 ZX= -0.1358

XY= 11.5229 YY= 0.0589 ZY= 1.6362

XZ= 1.2195 YZ= 2.2245 ZZ= 196.5784

Eigenvalues: -83.0053 2.4556 196.5991

17 H Isotropic = 23.7140 Anisotropy = 8.1225

XX= 26.4032 YX= -2.6096 ZX= 0.0061

XY= -2.3725 YY= 26.8511 ZY= -0.0845

XZ= -0.0027 YZ= -0.1577 ZZ= 17.8876

Eigenvalues: 17.8858 24.1272 29.1290

18 H Isotropic = 22.5489 Anisotropy = 11.5783

XX= 28.3662 YX= 3.9137 ZX= -0.1444

XY= 3.3756 YY= 23.2794 ZY= -0.0187

XZ= -0.0816 YZ= 0.0312 ZZ= 16.0012

Eigenvalues: 15.9999 21.3790 30.2678

19 C Isotropic = 114.2991 Anisotropy = 61.4367

XX= 155.2550 YX= 3.9013 ZX= -0.3915

XY= -4.3426 YY= 95.4060 ZY= 0.6539

XZ= 0.9095 YZ= 0.4208 ZZ= 92.2362

Eigenvalues: 92.1463 95.4941 155.2569

20 H Isotropic = 23.7219 Anisotropy = 5.5268

XX= 26.0725 YX= 1.3817 ZX= -0.0376

XY= 1.5755 YY= 25.7667 ZY= -0.0442

XZ= -0.0427 YZ= -0.0393 ZZ= 19.3266

Eigenvalues: 19.3262 24.4331 27.4064

21 H Isotropic = 22.6884 Anisotropy = 8.1427

XX= 28.1137 YX= -0.3577 ZX= -0.0468

XY= 0.1072 YY= 22.8667 ZY= -0.0348

XZ= -0.0536 YZ= -0.0250 ZZ= 17.0848

Eigenvalues: 17.0844 22.8639 28.1169

22 C Isotropic = 155.6309 Anisotropy = 36.0405

XX= 152.4999 YX= -3.9054 ZX= 7.8954

XY= -5.8723 YY= 144.3389 ZY= -12.0995

XZ= 14.7751 YZ= -9.7285 ZZ= 170.0537

Eigenvalues: 140.2712 146.9636 179.6578

23 H Isotropic = 26.6835 Anisotropy = 5.7922

XX= 27.7657 YX= 1.7515 ZX= -0.1518

XY= -0.2668 YY= 30.3398 ZY= -0.1988

XZ= -0.1384 YZ= -0.2125 ZZ= 21.9451

Eigenvalues: 21.9372 27.5683 30.5450

24 C Isotropic = 156.1712 Anisotropy = 35.0594

XX= 153.3030 YX= -4.7469 ZX= -7.6548

XY= -6.5540 YY= 146.2868 ZY= 13.8314

XZ= -12.3954 YZ= 11.3514 ZZ= 168.9239

Eigenvalues: 140.5435 148.4260 179.5442

25 H Isotropic = 29.1544 Anisotropy = 6.9450

XX= 27.9581 YX= 0.7086 ZX= 0.9122

XY= 1.3671 YY= 32.3415 ZY= -1.8963

XZ= 2.5335 YZ= -4.2630 ZZ= 27.1635

Eigenvalues: 24.5529 29.1259 33.7844

26 H Isotropic = 29.3988 Anisotropy = 8.0811

XX= 26.8404 YX= -1.2122 ZX= 0.2074

XY= -0.8705 YY= 27.3589 ZY= 1.6114

XZ= 2.9110 YZ= 2.5506 ZZ= 33.9972

Eigenvalues: 25.2894 28.1208 34.7862

27 H Isotropic = 29.5164 Anisotropy = 10.3515

XX= 34.8986 YX= -0.6655 ZX= 2.5418

XY= -1.0731 YY= 25.9860 ZY= -0.4023

XZ= 4.4622 YZ= -0.7801 ZZ= 27.6647

Eigenvalues: 25.7804 26.3515 36.4174

28 H Isotropic = 29.0923 Anisotropy = 7.0696

XX= 27.9530 YX= 0.5370 ZX= -1.0138

XY= 1.2236 YY= 32.8218 ZY= 1.5312

XZ= -2.4536 YZ= 3.7984 ZZ= 26.5022

Eigenvalues: 24.4598 29.0118 33.8054

29 H Isotropic = 29.4954 Anisotropy = 10.2777

XX= 34.9836 YX= -0.7545 ZX= -2.4665

XY= -1.2271 YY= 26.0873 ZY= 0.5976

XZ= -4.0922 YZ= 0.9512 ZZ= 27.4152

Eigenvalues: 25.6734 26.4655 36.3472

30 H Isotropic = 29.3764 Anisotropy = 8.1199

XX= 26.8230 YX= -1.1709 ZX= -0.0881

XY= -0.8206 YY= 26.9643 ZY= -1.0047

XZ= -2.7379 YZ= -1.8123 ZZ= 34.3420

Eigenvalues: 25.4482 27.8913 34.7897

## Norharman monomer\_iso 1 (IEFPCM solvent = tetrahydrofuran) - BP86/IGLO-III level

30

C -4.35898 0.77297 0.00505

C -3.09426 1.35901 -0.00383

C -1.95326 0.51716 -0.00475

C -2.09779 -0.93433 0.00403

C -3.40260 -1.50063 0.01354

C -4.50449 -0.64795 0.01367

C -0.54374 0.73339 -0.01215

N -0.90419 -1.60909 0.00240

H -3.51918 -2.59621 0.02065

H -5.52098 -1.07741 0.02060

C 0.33191 1.83275 -0.02256

C 0.02507 -0.62755 -0.00670

C 1.41899 -0.76935 -0.00893

H -0.03205 2.87299 -0.02907

C 1.70731 1.60927 -0.02579

N 2.22678 0.32935 -0.01887

H 2.44482 2.42364 -0.03414

H 1.89990 -1.75774 -0.00154

C 3.71180 0.14984 -0.00639

H -5.26041 1.40785 0.00570

H -2.98676 2.45746 -0.01000

C 4.17908 -0.49385 1.30756

H 4.11708 1.18191 -0.04843

C 4.19526 -0.60145 -1.25520

H 3.81874 -1.54117 1.40420

H 3.81459 0.08208 2.18488

H 5.29006 -0.51381 1.34206

H 3.85423 -1.65930 -1.26134

H 5.30681 -0.60627 -1.28070

H 3.82915 -0.11155 -2.18275

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 53.2093 Anisotropy = 166.2272

XX= -8.8345 YX= 46.8297 ZX= 0.5380

XY= 50.9116 YY= 4.4413 ZY= 0.6459

XZ= 0.4772 YZ= 0.7423 ZZ= 164.0211

Eigenvalues: -51.5160 47.1165 164.0274

2 C Isotropic = 48.6984 Anisotropy = 172.2264

XX= 34.2950 YX= 2.8439 ZX= 0.5899

XY= 3.3093 YY= -51.7074 ZY= 1.0984

XZ= 0.6205 YZ= 1.0922 ZZ= 163.5074

Eigenvalues: -51.8226 34.4017 163.5160

3 C Isotropic = 47.1280 Anisotropy = 159.4536

XX= -9.5364 YX= -17.1501 ZX= 0.8630

XY= -9.5909 YY= -2.5017 ZY= 0.8822

XZ= 0.8120 YZ= 0.8369 ZZ= 153.4220

Eigenvalues: -19.8526 7.8061 153.4304

4 C Isotropic = 8.5537 Anisotropy = 157.0376

XX= -39.7770 YX= -0.1983 ZX= 0.7505

XY= 9.0971 YY= -47.7989 ZY= 0.8747

XZ= 0.6296 YZ= 0.9455 ZZ= 113.2369

Eigenvalues: -49.7802 -37.8042 113.2454

5 C Isotropic = 50.9842 Anisotropy = 151.7607

XX= 36.3308 YX= -18.5550 ZX= 0.6646

XY= -19.1005 YY= -35.5261 ZY= 1.2070

XZ= 0.6602 YZ= 1.1643 ZZ= 152.1479

Eigenvalues: -40.1694 40.9639 152.1580

6 C Isotropic = 42.1935 Anisotropy = 179.3706

XX= -43.1222 YX= -41.5471 ZX= 1.1646

XY= -43.7080 YY= 7.9403 ZY= 1.0677

XZ= 1.2143 YZ= 1.0582 ZZ= 161.7625

Eigenvalues: -67.2901 32.0967 161.7739

7 C Isotropic = 36.5062 Anisotropy = 177.2080

XX= -27.3063 YX= 9.8377 ZX= 0.7666

XY= 10.4834 YY= -17.8113 ZY= 0.9344

XZ= 0.9147 YZ= 0.8026 ZZ= 154.6361

Eigenvalues: -33.7740 -11.3523 154.6448

8 N Isotropic = -2.8164 Anisotropy = 317.0073

XX= -181.1715 YX= -24.5809 ZX= 1.8355

XY= -31.8195 YY= -35.7812 ZY= 1.5387

XZ= 2.2620 YZ= 1.4785 ZZ= 208.5034

Eigenvalues: -186.4629 -30.5082 208.5218

9 H Isotropic = 23.1482 Anisotropy = 6.5567

XX= 27.4222 YX= -0.3996 ZX= -0.0371

XY= -0.8672 YY= 23.3883 ZY= -0.0208

XZ= -0.0353 YZ= -0.0299 ZZ= 18.6342

Eigenvalues: 18.6339 23.2914 27.5194

10 H Isotropic = 23.3975 Anisotropy = 5.4081

XX= 24.5099 YX= -1.3557 ZX= -0.0164

XY= -1.5377 YY= 26.1632 ZY= -0.0307

XZ= -0.0130 YZ= -0.0312 ZZ= 19.5193

Eigenvalues: 19.5190 23.6705 27.0029

11 C Isotropic = 56.7022 Anisotropy = 161.2188

XX= 34.4120 YX= 25.2027 ZX= 0.2861

XY= 22.0770 YY= -28.4783 ZY= 1.2796

XZ= 0.2299 YZ= 1.0975 ZZ= 164.1727

Eigenvalues: -36.3786 42.3037 164.1813

12 C Isotropic = 22.2057 Anisotropy = 150.5845

XX= -18.4591 YX= 12.2140 ZX= 0.3641

XY= 3.6058 YY= -37.5083 ZY= 0.9653

XZ= 0.5845 YZ= 1.3976 ZZ= 122.5847

Eigenvalues: -40.3701 -15.6081 122.5954

13 C Isotropic = 45.6499 Anisotropy = 140.1159

XX= 20.8596 YX= 9.5870 ZX= 0.0163

XY= 14.7041 YY= -22.9593 ZY= 1.2364

XZ= -1.1711 YZ= 1.2044 ZZ= 139.0493

Eigenvalues: -26.1112 24.0003 139.0605

14 H Isotropic = 22.8151 Anisotropy = 7.0402

XX= 27.4004 YX= 1.3737 ZX= -0.0464

XY= -0.1413 YY= 23.9889 ZY= -0.0400

XZ= -0.0385 YZ= -0.0686 ZZ= 17.0559

Eigenvalues: 17.0553 23.8813 27.5086

15 C Isotropic = 49.6858 Anisotropy = 104.8036

XX= 41.6940 YX= -36.3917 ZX= 0.2639

XY= -35.5986 YY= -12.1791 ZY= 0.9945

XZ= -0.7727 YZ= 1.0822 ZZ= 119.5424

Eigenvalues: -30.2050 59.7075 119.5549

16 N Isotropic = 25.2154 Anisotropy = 242.5597

XX= -88.7987 YX= 14.7661 ZX= -0.0786

XY= 9.8489 YY= -22.4554 ZY= 1.7462

XZ= 1.2190 YZ= 2.3498 ZZ= 186.9001

Eigenvalues: -91.0084 -20.2674 186.9219

17 H Isotropic = 23.4119 Anisotropy = 7.9298

XX= 26.0901 YX= -2.5903 ZX= 0.0065

XY= -2.4163 YY= 26.2947 ZY= -0.0790

XZ= 0.0001 YZ= -0.1538 ZZ= 17.8511

Eigenvalues: 17.8493 23.6880 28.6985

18 H Isotropic = 22.4960 Anisotropy = 11.3167

XX= 28.3534 YX= 3.7720 ZX= -0.1439

XY= 3.1910 YY= 22.8526 ZY= -0.0139

XZ= -0.0810 YZ= 0.0457 ZZ= 16.2821

Eigenvalues: 16.2806 21.1670 30.0405

19 C Isotropic = 105.9912 Anisotropy = 64.4492

XX= 148.9537 YX= 3.5087 ZX= -0.3508

XY= -4.2890 YY= 84.3840 ZY= 0.7534

XZ= 0.9319 YZ= 0.5295 ZZ= 84.6359

Eigenvalues: 83.8526 85.1636 148.9573

20 H Isotropic = 23.7121 Anisotropy = 5.2681

XX= 25.8243 YX= 1.3637 ZX= -0.0351

XY= 1.5242 YY= 25.7340 ZY= -0.0421

XZ= -0.0405 YZ= -0.0374 ZZ= 19.5781

Eigenvalues: 19.5777 24.3345 27.2242

21 H Isotropic = 22.6624 Anisotropy = 7.8075

XX= 27.8605 YX= -0.4389 ZX= -0.0445

XY= 0.0718 YY= 22.8189 ZY= -0.0329

XZ= -0.0506 YZ= -0.0233 ZZ= 17.3078

Eigenvalues: 17.3074 22.8124 27.8674

22 C Isotropic = 150.0556 Anisotropy = 37.8447

XX= 146.7817 YX= -3.6889 ZX= 8.5878

XY= -5.3540 YY= 138.8002 ZY= -12.9497

XZ= 15.8993 YZ= -11.0680 ZZ= 164.5848

Eigenvalues: 134.0639 140.8174 175.2854

23 H Isotropic = 26.3604 Anisotropy = 5.3654

XX= 27.3770 YX= 1.6263 ZX= -0.1450

XY= -0.4538 YY= 29.7971 ZY= -0.1802

XZ= -0.1323 YZ= -0.1940 ZZ= 21.9070

Eigenvalues: 21.8997 27.2441 29.9373

24 C Isotropic = 150.6984 Anisotropy = 36.8152

XX= 147.6992 YX= -4.5446 ZX= -8.3137

XY= -6.1137 YY= 140.9478 ZY= 14.6927

XZ= -13.4397 YZ= 12.6846 ZZ= 163.4480

Eigenvalues: 134.4763 142.3770 175.2418

25 H Isotropic = 29.2054 Anisotropy = 6.4918

XX= 28.0933 YX= 0.5887 ZX= 0.8929

XY= 1.2299 YY= 32.0923 ZY= -1.7559

XZ= 2.4436 YZ= -4.1710 ZZ= 27.4306

Eigenvalues: 24.8725 29.2104 33.5333

26 H Isotropic = 29.4063 Anisotropy = 7.7482

XX= 26.9337 YX= -1.0838 ZX= 0.3345

XY= -0.7518 YY= 27.4554 ZY= 1.3661

XZ= 2.9320 YZ= 2.3436 ZZ= 33.8299

Eigenvalues: 25.5263 28.1209 34.5718

27 H Isotropic = 29.3752 Anisotropy = 9.8910

XX= 34.4458 YX= -0.6056 ZX= 2.4493

XY= -0.9812 YY= 26.0092 ZY= -0.3827

XZ= 4.4082 YZ= -0.7563 ZZ= 27.6705

Eigenvalues: 25.8073 26.3491 35.9692

28 H Isotropic = 29.1380 Anisotropy = 6.6121

XX= 28.0908 YX= 0.4294 ZX= -0.9863

XY= 1.0993 YY= 32.5495 ZY= 1.4320

XZ= -2.3629 YZ= 3.7560 ZZ= 26.7738

Eigenvalues: 24.7646 29.1034 33.5461

29 H Isotropic = 29.3586 Anisotropy = 9.8155

XX= 34.5358 YX= -0.6937 ZX= -2.3765

XY= -1.1399 YY= 26.1121 ZY= 0.5736

XZ= -4.0492 YZ= 0.9264 ZZ= 27.4279

Eigenvalues: 25.7043 26.4693 35.9023

30 H Isotropic = 29.3895 Anisotropy = 7.7917

XX= 26.9225 YX= -1.0628 ZX= -0.2301

XY= -0.7231 YY= 27.1026 ZY= -0.7875

XZ= -2.7715 YZ= -1.6422 ZZ= 34.1434

Eigenvalues: 25.6758 27.9087 34.5840

## Norharman monomer\_iso 1 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level

30

C -4.35898 0.77297 0.00505

C -3.09426 1.35901 -0.00383

C -1.95326 0.51716 -0.00475

C -2.09779 -0.93433 0.00403

C -3.40260 -1.50063 0.01354

C -4.50449 -0.64795 0.01367

C -0.54374 0.73339 -0.01215

N -0.90419 -1.60909 0.00240

H -3.51918 -2.59621 0.02065

H -5.52098 -1.07741 0.02060

C 0.33191 1.83275 -0.02256

C 0.02507 -0.62755 -0.00670

C 1.41899 -0.76935 -0.00893

H -0.03205 2.87299 -0.02907

C 1.70731 1.60927 -0.02579

N 2.22678 0.32935 -0.01887

H 2.44482 2.42364 -0.03414

H 1.89990 -1.75774 -0.00154

C 3.71180 0.14984 -0.00639

H -5.26041 1.40785 0.00570

H -2.98676 2.45746 -0.01000

C 4.17908 -0.49385 1.30756

H 4.11708 1.18191 -0.04843

C 4.19526 -0.60145 -1.25520

H 3.81874 -1.54117 1.40420

H 3.81459 0.08208 2.18488

H 5.29006 -0.51381 1.34206

H 3.85423 -1.65930 -1.26134

H 5.30681 -0.60627 -1.28070

H 3.82915 -0.11155 -2.18275

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 56.6558 Anisotropy = 170.9290

XX= -5.7158 YX= 48.5938 ZX= 0.5430

XY= 53.0062 YY= 5.0812 ZY= 0.6680

XZ= 0.4911 YZ= 0.7579 ZZ= 170.6020

Eigenvalues: -51.4033 50.7624 170.6085

2 C Isotropic = 50.1171 Anisotropy = 179.9236

XX= 35.4161 YX= 4.9264 ZX= 0.6045

XY= 4.8804 YY= -55.1222 ZY= 1.1429

XZ= 0.6295 YZ= 1.1422 ZZ= 170.0573

Eigenvalues: -55.3924 35.6775 170.0662

3 C Isotropic = 51.7189 Anisotropy = 163.3440

XX= -7.6142 YX= -17.2849 ZX= 0.8865

XY= -10.4231 YY= 2.1645 ZY= 0.8991

XZ= 0.8335 YZ= 0.8565 ZZ= 160.6063

Eigenvalues: -17.4245 11.9663 160.6148

4 C Isotropic = 10.4728 Anisotropy = 166.8670

XX= -41.9127 YX= -1.0752 ZX= 0.8017

XY= 9.1025 YY= -48.3772 ZY= 0.9262

XZ= 0.6821 YZ= 1.0201 ZZ= 121.7083

Eigenvalues: -50.3001 -39.9989 121.7175

5 C Isotropic = 53.9889 Anisotropy = 157.5643

XX= 38.1850 YX= -21.2252 ZX= 0.7040

XY= -21.2857 YY= -35.2396 ZY= 1.2571

XZ= 0.6972 YZ= 1.2123 ZZ= 159.0211

Eigenvalues: -40.9583 43.8931 159.0317

6 C Isotropic = 43.8901 Anisotropy = 186.9427

XX= -43.8950 YX= -44.1261 ZX= 1.2114

XY= -46.4121 YY= 7.0587 ZY= 1.1225

XZ= 1.2631 YZ= 1.1079 ZZ= 168.5065

Eigenvalues: -70.3751 33.5267 168.5185

7 C Isotropic = 38.4359 Anisotropy = 185.1857

XX= -28.8010 YX= 9.1882 ZX= 0.8161

XY= 10.9188 YY= -17.7752 ZY= 0.9699

XZ= 0.9407 YZ= 0.8396 ZZ= 161.8840

Eigenvalues: -34.7543 -11.8310 161.8931

8 N Isotropic = 3.6538 Anisotropy = 321.8481

XX= -174.9287 YX= -25.7750 ZX= 1.8485

XY= -32.0848 YY= -32.3105 ZY= 1.5753

XZ= 2.2505 YZ= 1.5397 ZZ= 218.2005

Eigenvalues: -180.5870 -26.6708 218.2192

9 H Isotropic = 22.9925 Anisotropy = 6.7894

XX= 27.3970 YX= -0.4962 ZX= -0.0382

XY= -0.9057 YY= 23.4778 ZY= -0.0245

XZ= -0.0375 YZ= -0.0333 ZZ= 18.1026

Eigenvalues: 18.1023 23.3564 27.5187

10 H Isotropic = 23.2398 Anisotropy = 5.5841

XX= 24.5381 YX= -1.3385 ZX= -0.0180

XY= -1.5838 YY= 26.0818 ZY= -0.0325

XZ= -0.0147 YZ= -0.0329 ZZ= 19.0993

Eigenvalues: 19.0991 23.6577 26.9625

11 C Isotropic = 59.1048 Anisotropy = 167.1558

XX= 36.7752 YX= 25.6452 ZX= 0.2998

XY= 22.4672 YY= -29.9939 ZY= 1.3314

XZ= 0.2538 YZ= 1.1330 ZZ= 170.5331

Eigenvalues: -37.7639 44.5363 170.5420

12 C Isotropic = 25.0245 Anisotropy = 158.3889

XX= -18.4598 YX= 12.0085 ZX= 0.3957

XY= 2.9348 YY= -37.0727 ZY= 1.0090

XZ= 0.6356 YZ= 1.4466 ZZ= 130.6059

Eigenvalues: -39.7066 -15.8371 130.6171

13 C Isotropic = 45.7776 Anisotropy = 148.5344

XX= 19.6243 YX= 10.3082 ZX= 0.0160

XY= 14.6697 YY= -27.0803 ZY= 1.3124

XZ= -1.1094 YZ= 1.3222 ZZ= 144.7888

Eigenvalues: -30.2215 22.7538 144.8005

14 H Isotropic = 22.6207 Anisotropy = 7.2426

XX= 27.3516 YX= 1.3638 ZX= -0.0477

XY= -0.2017 YY= 23.9751 ZY= -0.0439

XZ= -0.0390 YZ= -0.0734 ZZ= 16.5355

Eigenvalues: 16.5349 23.8782 27.4491

15 C Isotropic = 50.7018 Anisotropy = 114.4119

XX= 41.5207 YX= -37.5657 ZX= 0.3125

XY= -36.6314 YY= -16.3793 ZY= 1.0887

XZ= -0.7541 YZ= 1.1724 ZZ= 126.9640

Eigenvalues: -34.4920 59.6210 126.9764

16 N Isotropic = 26.5871 Anisotropy = 257.2763

XX= -96.9684 YX= 16.5909 ZX= -0.1523

XY= 11.4055 YY= -21.3533 ZY= 1.8119

XZ= 1.1361 YZ= 2.4135 ZZ= 198.0830

Eigenvalues: -99.4766 -18.8667 198.1047

17 H Isotropic = 23.2090 Anisotropy = 8.1710

XX= 26.0309 YX= -2.5805 ZX= 0.0065

XY= -2.4106 YY= 26.2828 ZY= -0.0857

XZ= -0.0030 YZ= -0.1581 ZZ= 17.3133

Eigenvalues: 17.3115 23.6592 28.6563

18 H Isotropic = 22.2530 Anisotropy = 11.6807

XX= 28.2672 YX= 3.8583 ZX= -0.1447

XY= 3.2954 YY= 22.8204 ZY= -0.0177

XZ= -0.0839 YZ= 0.0354 ZZ= 15.6715

Eigenvalues: 15.6701 21.0488 30.0401

19 C Isotropic = 113.5955 Anisotropy = 63.4984

XX= 155.9238 YX= 3.5171 ZX= -0.3467

XY= -4.3339 YY= 92.3610 ZY= 0.7219

XZ= 0.9304 YZ= 0.5029 ZZ= 92.5017

Eigenvalues: 91.8110 93.0478 155.9278

20 H Isotropic = 23.6252 Anisotropy = 5.4033

XX= 25.9897 YX= 1.2552 ZX= -0.0371

XY= 1.4764 YY= 25.7194 ZY= -0.0443

XZ= -0.0426 YZ= -0.0397 ZZ= 19.1665

Eigenvalues: 19.1661 24.4821 27.2274

21 H Isotropic = 22.4780 Anisotropy = 8.0547

XX= 27.8451 YX= -0.3454 ZX= -0.0464

XY= 0.1202 YY= 22.7628 ZY= -0.0358

XZ= -0.0532 YZ= -0.0262 ZZ= 16.8260

Eigenvalues: 16.8256 22.7605 27.8478

22 C Isotropic = 155.6433 Anisotropy = 36.3162

XX= 152.8641 YX= -3.6727 ZX= 8.0217

XY= -5.4585 YY= 144.3823 ZY= -12.4278

XZ= 15.2498 YZ= -10.3826 ZZ= 169.6836

Eigenvalues: 139.9992 147.0767 179.8541

23 H Isotropic = 26.3844 Anisotropy = 5.9503

XX= 27.3890 YX= 1.8782 ZX= -0.1576

XY= -0.2447 YY= 30.1191 ZY= -0.1987

XZ= -0.1435 YZ= -0.2119 ZZ= 21.6450

Eigenvalues: 21.6370 27.1648 30.3513

24 C Isotropic = 156.2455 Anisotropy = 35.3393

XX= 153.7129 YX= -4.4880 ZX= -7.7537

XY= -6.1869 YY= 146.4317 ZY= 14.1503

XZ= -12.8769 YZ= 11.9826 ZZ= 168.5920

Eigenvalues: 140.3526 148.5790 179.8051

25 H Isotropic = 29.1749 Anisotropy = 7.0102

XX= 27.8947 YX= 0.7564 ZX= 0.8676

XY= 1.3611 YY= 32.4026 ZY= -1.8697

XZ= 2.4972 YZ= -4.2885 ZZ= 27.2274

Eigenvalues: 24.6074 29.0689 33.8484

26 H Isotropic = 29.4013 Anisotropy = 8.1248

XX= 26.8072 YX= -1.2016 ZX= 0.1815

XY= -0.8556 YY= 27.3684 ZY= 1.6159

XZ= 2.9254 YZ= 2.5630 ZZ= 34.0284

Eigenvalues: 25.2897 28.0965 34.8178

27 H Isotropic = 29.3569 Anisotropy = 10.4388

XX= 34.8302 YX= -0.6570 ZX= 2.5406

XY= -1.0150 YY= 25.7889 ZY= -0.3840

XZ= 4.4510 YZ= -0.7591 ZZ= 27.4518

Eigenvalues: 25.5920 26.1627 36.3162

28 H Isotropic = 29.1060 Anisotropy = 7.1379

XX= 27.8837 YX= 0.5856 ZX= -0.9777

XY= 1.2203 YY= 32.8786 ZY= 1.5054

XZ= -2.4207 YZ= 3.8242 ZZ= 26.5556

Eigenvalues: 24.5049 28.9485 33.8646

29 H Isotropic = 29.3373 Anisotropy = 10.3710

XX= 34.9182 YX= -0.7427 ZX= -2.4623

XY= -1.1665 YY= 25.8867 ZY= 0.5777

XZ= -4.0902 YZ= 0.9302 ZZ= 27.2070

Eigenvalues: 25.4848 26.2758 36.2513

30 H Isotropic = 29.3796 Anisotropy = 8.1634

XX= 26.7921 YX= -1.1650 ZX= -0.0683

XY= -0.8116 YY= 26.9724 ZY= -1.0071

XZ= -2.7527 YZ= -1.8254 ZZ= 34.3743

Eigenvalues: 25.4433 27.8736 34.8219

## Norharman monomer\_iso 2 (gas-phase) - BP86/IGLO-III level

30

C 4.29759 1.03877 0.00271

C 2.97776 1.48705 0.00141

C 1.93285 0.52847 -0.00060

C 2.23150 -0.89920 -0.00143

C 3.58922 -1.32355 -0.00022

C 4.59400 -0.35841 0.00202

C 0.50820 0.59286 -0.00163

N 1.11697 -1.69737 -0.00295

H 3.82157 -2.40043 -0.00105

H 5.65056 -0.67711 0.00337

C -0.48037 1.59252 -0.00101

C 0.08816 -0.82037 -0.00288

C -1.28282 -1.10913 -0.00371

H -0.22873 2.66559 0.00055

C -1.82455 1.22527 -0.00151

N -2.20408 -0.10301 -0.00250

H -2.63906 1.96137 -0.00045

H -1.66363 -2.14109 -0.00477

C -3.65815 -0.44995 0.00000

H 5.12631 1.76617 0.00437

H 2.75413 2.56783 0.00196

C -4.34368 0.03311 1.28681

H -3.67742 -1.55918 -0.00408

C -4.35165 0.04214 -1.27866

H -4.38446 1.14268 1.34577

H -3.81283 -0.34480 2.18669

H -5.38896 -0.34405 1.31688

H -4.39811 1.15176 -1.32573

H -5.39519 -0.34006 -1.30831

H -3.82289 -0.32353 -2.18493

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 52.0103 Anisotropy = 165.8980

XX= 1.1717 YX= -47.8664 ZX= -0.2465

XY= -51.7083 YY= -7.7493 ZY= -0.1991

XZ= -0.2567 YZ= -0.2094 ZZ= 162.6085

Eigenvalues: -53.2760 46.6980 162.6089

2 C Isotropic = 49.3143 Anisotropy = 169.3684

XX= 36.6008 YX= 6.0863 ZX= -0.1458

XY= 6.0376 YY= -50.8842 ZY= -0.1620

XZ= -0.1470 YZ= -0.2006 ZZ= 162.2262

Eigenvalues: -51.3024 37.0187 162.2265

3 C Isotropic = 46.7811 Anisotropy = 159.2282

XX= -11.4819 YX= 18.2243 ZX= -0.1442

XY= 7.5986 YY= -1.1079 ZY= -0.1236

XZ= -0.1534 YZ= -0.1335 ZZ= 152.9330

Eigenvalues: -20.2093 7.6193 152.9332

4 C Isotropic = 6.9977 Anisotropy = 159.9005

XX= -41.7017 YX= 2.2156 ZX= -0.1568

XY= -7.1516 YY= -50.9031 ZY= -0.1252

XZ= -0.1258 YZ= -0.1776 ZZ= 113.5977

Eigenvalues: -51.5234 -41.0816 113.5980

5 C Isotropic = 48.8953 Anisotropy = 155.1831

XX= 27.2988 YX= 27.3399 ZX= -0.1310

XY= 27.1471 YY= -32.9632 ZY= -0.1523

XZ= -0.1305 YZ= -0.0646 ZZ= 152.3505

Eigenvalues: -43.4534 37.7888 152.3507

6 C Isotropic = 41.4777 Anisotropy = 178.8541

XX= -51.8644 YX= 36.4259 ZX= -0.2829

XY= 37.8643 YY= 15.5841 ZY= -0.0643

XZ= -0.2522 YZ= -0.0630 ZZ= 160.7133

Eigenvalues: -68.3109 32.0301 160.7137

7 C Isotropic = 37.0749 Anisotropy = 177.2248

XX= -23.1906 YX= -7.0130 ZX= -0.0978

XY= -12.7580 YY= -20.8090 ZY= -0.1607

XZ= -0.1997 YZ= -0.2221 ZZ= 155.2244

Eigenvalues: -31.9571 -12.0429 155.2248

8 N Isotropic = -23.7049 Anisotropy = 348.6769

XX= -234.4286 YX= 5.4852 ZX= -0.3361

XY= 18.1061 YY= -45.4321 ZY= -0.1711

XZ= -0.3740 YZ= -0.1495 ZZ= 208.7459

Eigenvalues: -235.1622 -44.6989 208.7463

9 H Isotropic = 23.0835 Anisotropy = 6.5560

XX= 27.1232 YX= 0.9735 ZX= 0.0087

XY= 1.3026 YY= 23.5413 ZY= 0.0053

XZ= 0.0102 YZ= 0.0073 ZZ= 18.5859

Eigenvalues: 18.5859 23.2103 27.4542

10 H Isotropic = 23.4427 Anisotropy = 5.5473

XX= 24.1645 YX= 1.1481 ZX= 0.0038

XY= 1.3623 YY= 26.6116 ZY= 0.0081

XZ= 0.0088 YZ= 0.0062 ZZ= 19.5521

Eigenvalues: 19.5521 23.6352 27.1409

11 C Isotropic = 57.3592 Anisotropy = 160.9328

XX= 41.3984 YX= -18.5624 ZX= -0.0567

XY= -15.8665 YY= -33.9682 ZY= -0.2345

XZ= -0.0047 YZ= -0.3225 ZZ= 164.6473

Eigenvalues: -37.7144 45.1442 164.6477

12 C Isotropic = 23.0054 Anisotropy = 147.6000

XX= -14.2545 YX= -16.7851 ZX= -0.0987

XY= -5.0870 YY= -38.1345 ZY= -0.1093

XZ= -0.0722 YZ= -0.0742 ZZ= 121.4053

Eigenvalues: -42.3860 -10.0032 121.4054

13 C Isotropic = 44.2296 Anisotropy = 96.4814

XX= 44.2160 YX= -9.9946 ZX= -0.0105

XY= -7.9145 YY= -20.0776 ZY= -0.1381

XZ= 0.0848 YZ= -0.0767 ZZ= 108.5504

Eigenvalues: -21.3016 45.4398 108.5505

14 H Isotropic = 22.9292 Anisotropy = 7.5127

XX= 27.9320 YX= -0.9107 ZX= 0.0036

XY= 0.5997 YY= 23.6892 ZY= 0.0038

XZ= 0.0011 YZ= 0.0049 ZZ= 17.1664

Eigenvalues: 17.1664 23.6835 27.9376

15 C Isotropic = 60.4122 Anisotropy = 130.2207

XX= 32.0938 YX= 34.7092 ZX= 0.0586

XY= 37.3441 YY= 1.9170 ZY= -0.1432

XZ= 0.1164 YZ= -0.2149 ZZ= 147.2257

Eigenvalues: -22.0535 56.0640 147.2259

16 N Isotropic = 37.1062 Anisotropy = 222.7682

XX= -71.2559 YX= -23.8023 ZX= 0.1765

XY= -14.6300 YY= -3.0436 ZY= -0.1580

XZ= 0.0936 YZ= -0.1730 ZZ= 185.6181

Eigenvalues: -76.2968 1.9971 185.6184

17 H Isotropic = 23.8000 Anisotropy = 9.8195

XX= 26.6862 YX= 4.1790 ZX= 0.0121

XY= 2.9963 YY= 26.8298 ZY= 0.0051

XZ= 0.0023 YZ= 0.0048 ZZ= 17.8840

Eigenvalues: 17.8840 23.1697 30.3464

18 H Isotropic = 22.8477 Anisotropy = 9.2807

XX= 27.6179 YX= -2.4854 ZX= -0.0026

XY= -2.9248 YY= 23.8705 ZY= 0.0107

XZ= -0.0092 YZ= 0.0138 ZZ= 17.0548

Eigenvalues: 17.0548 22.4536 29.0349

19 C Isotropic = 105.7347 Anisotropy = 64.2087

XX= 141.2573 YX= 23.6161 ZX= -0.0097

XY= 16.0082 YY= 94.6452 ZY= -0.0587

XZ= -0.1633 YZ= -0.1087 ZZ= 81.3017

Eigenvalues: 81.3011 87.3625 148.5406

20 H Isotropic = 23.8355 Anisotropy = 5.3732

XX= 26.2110 YX= -1.4794 ZX= 0.0046

XY= -1.5891 YY= 25.4670 ZY= 0.0026

XZ= 0.0077 YZ= 0.0046 ZZ= 19.8286

Eigenvalues: 19.8286 24.2603 27.4177

21 H Isotropic = 22.8442 Anisotropy = 7.9668

XX= 28.0526 YX= 1.0093 ZX= 0.0097

XY= 0.4498 YY= 22.9786 ZY= 0.0051

XZ= 0.0118 YZ= 0.0036 ZZ= 17.5014

Eigenvalues: 17.5013 22.8758 28.1554

22 C Isotropic = 150.3001 Anisotropy = 37.0466

XX= 149.1667 YX= -1.2624 ZX= -12.3195

XY= -3.1006 YY= 137.0746 ZY= 9.0930

XZ= -17.2310 YZ= 5.2910 ZZ= 164.6591

Eigenvalues: 135.0362 140.8663 174.9979

23 H Isotropic = 26.5596 Anisotropy = 5.2122

XX= 27.4558 YX= 0.6577 ZX= 0.0127

XY= -1.4546 YY= 29.9728 ZY= 0.0219

XZ= 0.0046 YZ= 0.0140 ZZ= 22.2502

Eigenvalues: 22.2501 27.3943 30.0344

24 C Isotropic = 150.3800 Anisotropy = 36.8993

XX= 149.4331 YX= -1.4156 ZX= 12.3566

XY= -3.2161 YY= 137.1916 ZY= -9.3263

XZ= 16.9725 YZ= -5.5532 ZZ= 164.5152

Eigenvalues: 135.0428 141.1176 174.9795

25 H Isotropic = 29.2736 Anisotropy = 6.4225

XX= 28.2706 YX= -1.0742 ZX= -1.5552

XY= -0.4160 YY= 32.2517 ZY= 1.2501

XZ= -3.5560 YZ= 2.9355 ZZ= 27.2984

Eigenvalues: 24.9869 29.2785 33.5552

26 H Isotropic = 29.3751 Anisotropy = 7.5931

XX= 27.6004 YX= -0.9418 ZX= 0.0984

XY= -0.7542 YY= 26.6378 ZY= -1.1522

XZ= -1.9629 YZ= -2.6867 ZZ= 33.8871

Eigenvalues: 25.5972 28.0910 34.4371

27 H Isotropic = 29.5080 Anisotropy = 9.7199

XX= 34.0825 YX= 2.2946 ZX= -2.4305

XY= 1.7425 YY= 26.6809 ZY= -0.3754

XZ= -4.2876 YZ= -0.6381 ZZ= 27.7605

Eigenvalues: 25.9379 26.5981 35.9879

28 H Isotropic = 29.2741 Anisotropy = 6.4390

XX= 28.2973 YX= -1.1315 ZX= 1.5540

XY= -0.4663 YY= 32.2899 ZY= -1.2061

XZ= 3.5248 YZ= -2.8834 ZZ= 27.2351

Eigenvalues: 24.9945 29.2610 33.5668

29 H Isotropic = 29.5016 Anisotropy = 9.7140

XX= 34.0921 YX= 2.3100 ZX= 2.4363

XY= 1.7411 YY= 26.6903 ZY= 0.3590

XZ= 4.2446 YZ= 0.6176 ZZ= 27.7224

Eigenvalues: 25.9222 26.6050 35.9776

30 H Isotropic = 29.3720 Anisotropy = 7.5917

XX= 27.6019 YX= -0.9239 ZX= -0.0941

XY= -0.7271 YY= 26.5923 ZY= 1.0747

XZ= 1.9657 YZ= 2.5956 ZZ= 33.9218

Eigenvalues: 25.6190 28.0639 34.4331

## Norharman monomer\_iso2 (gas-phase) – PBE0/IGLO-III level

30

C 4.29759 1.03877 0.00271

C 2.97776 1.48705 0.00141

C 1.93285 0.52847 -0.00060

C 2.23150 -0.89920 -0.00143

C 3.58922 -1.32355 -0.00022

C 4.59400 -0.35841 0.00202

C 0.50820 0.59286 -0.00163

N 1.11697 -1.69737 -0.00295

H 3.82157 -2.40043 -0.00105

H 5.65056 -0.67711 0.00337

C -0.48037 1.59252 -0.00101

C 0.08816 -0.82037 -0.00288

C -1.28282 -1.10913 -0.00371

H -0.22873 2.66559 0.00055

C -1.82455 1.22527 -0.00151

N -2.20408 -0.10301 -0.00250

H -2.63906 1.96137 -0.00045

H -1.66363 -2.14109 -0.00477

C -3.65815 -0.44995 0.00000

H 5.12631 1.76617 0.00437

H 2.75413 2.56783 0.00196

C -4.34368 0.03311 1.28681

H -3.67742 -1.55918 -0.00408

C -4.35165 0.04214 -1.27866

H -4.38446 1.14268 1.34577

H -3.81283 -0.34480 2.18669

H -5.38896 -0.34405 1.31688

H -4.39811 1.15176 -1.32573

H -5.39519 -0.34006 -1.30831

H -3.82289 -0.32353 -2.18493

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 55.4743 Anisotropy = 170.6705

XX= 4.8589 YX= -49.3479 ZX= -0.2519

XY= -53.7047 YY= -7.6900 ZY= -0.2068

XZ= -0.2629 YZ= -0.2176 ZZ= 169.2542

Eigenvalues: -53.3230 50.4913 169.2547

2 C Isotropic = 50.9387 Anisotropy = 176.7310

XX= 38.6028 YX= 4.3394 ZX= -0.1531

XY= 4.8713 YY= -54.5457 ZY= -0.1714

XZ= -0.1510 YZ= -0.2122 ZZ= 168.7590

Eigenvalues: -54.7730 38.8297 168.7594

3 C Isotropic = 51.3366 Anisotropy = 163.4500

XX= -9.6336 YX= 17.9374 ZX= -0.1494

XY= 8.0006 YY= 3.3404 ZY= -0.1257

XZ= -0.1596 YZ= -0.1389 ZZ= 160.3030

Eigenvalues: -17.6475 11.3540 160.3033

4 C Isotropic = 8.8534 Anisotropy = 169.7150

XX= -43.9150 YX= 3.2790 ZX= -0.1664

XY= -7.0989 YY= -51.5213 ZY= -0.1321

XZ= -0.1358 YZ= -0.1788 ZZ= 121.9964

Eigenvalues: -51.9741 -43.4625 121.9967

5 C Isotropic = 51.8182 Anisotropy = 160.8980

XX= 28.6081 YX= 30.3108 ZX= -0.1350

XY= 29.6981 YY= -32.2368 ZY= -0.1547

XZ= -0.1361 YZ= -0.0665 ZZ= 159.0833

Eigenvalues: -44.5436 40.9147 159.0835

6 C Isotropic = 43.3475 Anisotropy = 186.0093

XX= -52.9049 YX= 39.2055 ZX= -0.2922

XY= 40.8032 YY= 15.5941 ZY= -0.0655

XZ= -0.2607 YZ= -0.0661 ZZ= 167.3532

Eigenvalues: -71.3185 34.0072 167.3536

7 C Isotropic = 39.1382 Anisotropy = 185.0583

XX= -23.8608 YX= -6.5890 ZX= -0.1026

XY= -13.4417 YY= -21.2348 ZY= -0.1677

XZ= -0.2065 YZ= -0.2285 ZZ= 162.5101

Eigenvalues: -32.6492 -12.4467 162.5104

8 N Isotropic = -17.4307 Anisotropy = 354.3488

XX= -228.0941 YX= 6.8461 ZX= -0.3356

XY= 18.3427 YY= -42.9994 ZY= -0.1772

XZ= -0.3698 YZ= -0.1491 ZZ= 218.8015

Eigenvalues: -228.9474 -42.1465 218.8019

9 H Isotropic = 22.9386 Anisotropy = 6.8001

XX= 27.0978 YX= 1.0621 ZX= 0.0093

XY= 1.3322 YY= 23.6412 ZY= 0.0059

XZ= 0.0108 YZ= 0.0080 ZZ= 18.0767

Eigenvalues: 18.0767 23.2670 27.4719

10 H Isotropic = 23.3171 Anisotropy = 5.7058

XX= 24.2148 YX= 1.1459 ZX= 0.0044

XY= 1.4287 YY= 26.5507 ZY= 0.0085

XZ= 0.0095 YZ= 0.0064 ZZ= 19.1858

Eigenvalues: 19.1857 23.6446 27.1210

11 C Isotropic = 59.4577 Anisotropy = 167.0328

XX= 43.7328 YX= -18.6031 ZX= -0.0572

XY= -15.9603 YY= -36.1721 ZY= -0.2450

XZ= -0.0064 YZ= -0.3369 ZZ= 170.8125

Eigenvalues: -39.7500 47.3102 170.8129

12 C Isotropic = 25.7862 Anisotropy = 155.8582

XX= -14.3777 YX= -17.6349 ZX= -0.1046

XY= -5.1300 YY= -37.9553 ZY= -0.1156

XZ= -0.0803 YZ= -0.0808 ZZ= 129.6915

Eigenvalues: -42.5537 -9.7794 129.6917

13 C Isotropic = 44.9660 Anisotropy = 106.7331

XX= 42.8208 YX= -10.2464 ZX= -0.0118

XY= -7.4234 YY= -24.0441 ZY= -0.1518

XZ= 0.0850 YZ= -0.0864 ZZ= 116.1212

Eigenvalues: -25.1919 43.9685 116.1213

14 H Isotropic = 22.7420 Anisotropy = 7.7472

XX= 27.9032 YX= -0.9072 ZX= 0.0038

XY= 0.6615 YY= 23.6596 ZY= 0.0042

XZ= 0.0008 YZ= 0.0055 ZZ= 16.6632

Eigenvalues: 16.6632 23.6560 27.9068

15 C Isotropic = 61.0212 Anisotropy = 137.9449

XX= 32.1006 YX= 36.8711 ZX= 0.0612

XY= 39.3116 YY= -2.0212 ZY= -0.1525

XZ= 0.1158 YZ= -0.2315 ZZ= 152.9842

Eigenvalues: -26.6982 56.7773 152.9844

16 N Isotropic = 38.9572 Anisotropy = 236.6806

XX= -78.1201 YX= -25.7393 ZX= 0.1932

XY= -16.4821 YY= -1.7524 ZY= -0.1635

XZ= 0.1022 YZ= -0.1826 ZZ= 196.7439

Eigenvalues: -83.5673 3.6946 196.7442

17 H Isotropic = 23.6239 Anisotropy = 10.0621

XX= 26.6485 YX= 4.1568 ZX= 0.0121

XY= 3.0098 YY= 26.8461 ZY= 0.0054

XZ= 0.0019 YZ= 0.0059 ZZ= 17.3772

Eigenvalues: 17.3772 23.1626 30.3319

18 H Isotropic = 22.6172 Anisotropy = 9.6823

XX= 27.5728 YX= -2.5936 ZX= -0.0027

XY= -3.0111 YY= 23.8342 ZY= 0.0113

XZ= -0.0090 YZ= 0.0143 ZZ= 16.4447

Eigenvalues: 16.4447 22.3349 29.0721

19 C Isotropic = 113.4885 Anisotropy = 62.8427

XX= 148.2299 YX= 23.2893 ZX= -0.0101

XY= 15.6117 YY= 102.4968 ZY= -0.0573

XZ= -0.1636 YZ= -0.1094 ZZ= 89.7386

Eigenvalues: 89.7380 95.3438 155.3836

20 H Isotropic = 23.7511 Anisotropy = 5.5324

XX= 26.3794 YX= -1.3549 ZX= 0.0055

XY= -1.5370 YY= 25.4670 ZY= 0.0030

XZ= 0.0083 YZ= 0.0050 ZZ= 19.4070

Eigenvalues: 19.4070 24.4070 27.4394

21 H Isotropic = 22.6921 Anisotropy = 8.2203

XX= 28.0902 YX= 0.9069 ZX= 0.0101

XY= 0.4056 YY= 22.9276 ZY= 0.0054

XZ= 0.0123 YZ= 0.0037 ZZ= 17.0586

Eigenvalues: 17.0586 22.8455 28.1724

22 C Isotropic = 155.7724 Anisotropy = 35.5944

XX= 155.1201 YX= -0.9809 ZX= -11.6773

XY= -2.9522 YY= 142.6633 ZY= 8.8764

XZ= -16.5921 YZ= 4.9765 ZZ= 169.5339

Eigenvalues: 140.7234 147.0918 179.5020

23 H Isotropic = 26.5881 Anisotropy = 5.8239

XX= 27.3876 YX= 0.7584 ZX= 0.0131

XY= -1.4028 YY= 30.4370 ZY= 0.0242

XZ= 0.0048 YZ= 0.0160 ZZ= 21.9398

Eigenvalues: 21.9398 27.3539 30.4707

24 C Isotropic = 155.8488 Anisotropy = 35.4515

XX= 155.3761 YX= -1.1274 ZX= 11.7117

XY= -3.0671 YY= 142.7733 ZY= -9.1044

XZ= 16.3382 YZ= -5.2333 ZZ= 169.3971

Eigenvalues: 140.7258 147.3376 179.4831

25 H Isotropic = 29.2577 Anisotropy = 6.9452

XX= 28.0548 YX= -1.1194 ZX= -1.5739

XY= -0.5054 YY= 32.6139 ZY= 1.3507

XZ= -3.6372 YZ= 3.0316 ZZ= 27.1045

Eigenvalues: 24.7415 29.1438 33.8879

26 H Isotropic = 29.3602 Anisotropy = 7.9610

XX= 27.5396 YX= -1.0339 ZX= 0.3211

XY= -0.8354 YY= 26.4463 ZY= -1.3141

XZ= -1.8955 YZ= -2.8598 ZZ= 34.0947

Eigenvalues: 25.3525 28.0605 34.6675

27 H Isotropic = 29.4981 Anisotropy = 10.2738

XX= 34.4264 YX= 2.4543 ZX= -2.5215

XY= 1.9261 YY= 26.5158 ZY= -0.4019

XZ= -4.3337 YZ= -0.6472 ZZ= 27.5521

Eigenvalues: 25.7248 26.4222 36.3473

28 H Isotropic = 29.2580 Anisotropy = 6.9614

XX= 28.0822 YX= -1.1802 ZX= 1.5734

XY= -0.5591 YY= 32.6530 ZY= -1.3003

XZ= 3.6045 YZ= -2.9730 ZZ= 27.0387

Eigenvalues: 24.7495 29.1256 33.8989

29 H Isotropic = 29.4913 Anisotropy = 10.2689

XX= 34.4341 YX= 2.4716 ZX= 2.5264

XY= 1.9267 YY= 26.5267 ZY= 0.3856

XZ= 4.2913 YZ= 0.6265 ZZ= 27.5129

Eigenvalues: 25.7086 26.4280 36.3372

30 H Isotropic = 29.3565 Anisotropy = 7.9585

XX= 27.5400 YX= -1.0127 ZX= -0.3170

XY= -0.8057 YY= 26.3962 ZY= 1.2318

XZ= 1.8982 YZ= 2.7627 ZZ= 34.1331

Eigenvalues: 25.3742 28.0331 34.6621

## Norharman monomer\_iso2 (IEFPCM solvent = tetrahydrofuran) - BP86/IGLO-III level

30

C 4.29759 1.03877 0.00271

C 2.97776 1.48705 0.00141

C 1.93285 0.52847 -0.00060

C 2.23150 -0.89920 -0.00143

C 3.58922 -1.32355 -0.00022

C 4.59400 -0.35841 0.00202

C 0.50820 0.59286 -0.00163

N 1.11697 -1.69737 -0.00295

H 3.82157 -2.40043 -0.00105

H 5.65056 -0.67711 0.00337

C -0.48037 1.59252 -0.00101

C 0.08816 -0.82037 -0.00288

C -1.28282 -1.10913 -0.00371

H -0.22873 2.66559 0.00055

C -1.82455 1.22527 -0.00151

N -2.20408 -0.10301 -0.00250

H -2.63906 1.96137 -0.00045

H -1.66363 -2.14109 -0.00477

C -3.65815 -0.44995 0.00000

H 5.12631 1.76617 0.00437

H 2.75413 2.56783 0.00196

C -4.34368 0.03311 1.28681

H -3.67742 -1.55918 -0.00408

C -4.35165 0.04214 -1.27866

H -4.38446 1.14268 1.34577

H -3.81283 -0.34480 2.18669

H -5.38896 -0.34405 1.31688

H -4.39811 1.15176 -1.32573

H -5.39519 -0.34006 -1.30831

H -3.82289 -0.32353 -2.18493

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 53.0199 Anisotropy = 165.9785

XX= 1.5645 YX= -47.4193 ZX= -0.2473

XY= -51.1807 YY= -6.1765 ZY= -0.1981

XZ= -0.2571 YZ= -0.2099 ZZ= 163.6717

Eigenvalues: -51.7582 47.1456 163.6722

2 C Isotropic = 48.8315 Anisotropy = 171.9745

XX= 34.3411 YX= 5.9936 ZX= -0.1504

XY= 5.8220 YY= -51.3275 ZY= -0.1631

XZ= -0.1511 YZ= -0.2032 ZZ= 163.4808

Eigenvalues: -51.7331 34.7464 163.4811

3 C Isotropic = 47.1894 Anisotropy = 159.2850

XX= -12.0614 YX= 17.4102 ZX= -0.1461

XY= 8.4858 YY= 0.2504 ZY= -0.1216

XZ= -0.1548 YZ= -0.1369 ZZ= 153.3791

Eigenvalues: -20.2424 8.4311 153.3794

4 C Isotropic = 8.9281 Anisotropy = 158.1998

XX= -38.7992 YX= 1.0315 ZX= -0.1551

XY= -8.0819 YY= -48.8109 ZY= -0.1254

XZ= -0.1251 YZ= -0.1716 ZZ= 114.3944

Eigenvalues: -49.9278 -37.6826 114.3947

5 C Isotropic = 51.0023 Anisotropy = 152.0243

XX= 31.3828 YX= 26.0158 ZX= -0.1273

XY= 26.2591 YY= -30.7275 ZY= -0.1510

XZ= -0.1271 YZ= -0.0643 ZZ= 152.3516

Eigenvalues: -40.2628 40.9179 152.3518

6 C Isotropic = 42.4804 Anisotropy = 179.2922

XX= -51.2858 YX= 35.1782 ZX= -0.2848

XY= 37.2450 YY= 16.7190 ZY= -0.0654

XZ= -0.2549 YZ= -0.0643 ZZ= 162.0081

Eigenvalues: -66.9570 32.3898 162.0086

7 C Isotropic = 37.4068 Anisotropy = 176.2211

XX= -24.7469 YX= -7.2614 ZX= -0.0987

XY= -11.2110 YY= -17.9199 ZY= -0.1566

XZ= -0.1983 YZ= -0.2218 ZZ= 154.8872

Eigenvalues: -31.1805 -11.4866 154.8875

8 N Isotropic = -4.4510 Anisotropy = 318.9958

XX= -189.5486 YX= 6.3627 ZX= -0.3002

XY= 15.7652 YY= -32.0168 ZY= -0.1654

XZ= -0.3343 YZ= -0.1241 ZZ= 208.2125

Eigenvalues: -190.3221 -31.2437 208.2129

9 H Isotropic = 23.1323 Anisotropy = 6.5297

XX= 27.1971 YX= 0.8291 ZX= 0.0086

XY= 1.2902 YY= 23.5912 ZY= 0.0053

XZ= 0.0103 YZ= 0.0072 ZZ= 18.6086

Eigenvalues: 18.6086 23.3029 27.4854

10 H Isotropic = 23.3725 Anisotropy = 5.4627

XX= 24.2155 YX= 1.1237 ZX= 0.0041

XY= 1.2997 YY= 26.4897 ZY= 0.0081

XZ= 0.0090 YZ= 0.0062 ZZ= 19.4122

Eigenvalues: 19.4122 23.6910 27.0143

11 C Isotropic = 56.1816 Anisotropy = 164.5625

XX= 38.0287 YX= -17.8990 ZX= -0.0585

XY= -13.7915 YY= -35.3735 ZY= -0.2369

XZ= -0.0101 YZ= -0.3209 ZZ= 165.8895

Eigenvalues: -38.6483 41.3031 165.8899

12 C Isotropic = 22.8221 Anisotropy = 148.4199

XX= -16.6925 YX= -11.0644 ZX= -0.0963

XY= -1.5671 YY= -36.6098 ZY= -0.1069

XZ= -0.0747 YZ= -0.0738 ZZ= 121.7686

Eigenvalues: -38.4437 -14.8586 121.7687

13 C Isotropic = 41.8316 Anisotropy = 103.6055

XX= 38.4669 YX= -9.0061 ZX= -0.0113

XY= -7.9859 YY= -23.8739 ZY= -0.1464

XZ= 0.0900 YZ= -0.0780 ZZ= 110.9017

Eigenvalues: -25.0111 39.6039 110.9019

14 H Isotropic = 22.7089 Anisotropy = 7.4371

XX= 27.6515 YX= -0.9741 ZX= 0.0034

XY= 0.4724 YY= 23.5794 ZY= 0.0039

XZ= 0.0011 YZ= 0.0054 ZZ= 16.8958

Eigenvalues: 16.8958 23.5640 27.6669

15 C Isotropic = 54.1934 Anisotropy = 140.7719

XX= 23.0351 YX= 33.1919 ZX= 0.0581

XY= 36.2970 YY= -8.4961 ZY= -0.1509

XZ= 0.1247 YZ= -0.2301 ZZ= 148.0411

Eigenvalues: -30.8848 45.4236 148.0413

16 N Isotropic = 25.3261 Anisotropy = 242.6988

XX= -87.3472 YX= -20.5560 ZX= 0.1937

XY= -14.1929 YY= -23.7996 ZY= -0.1752

XZ= 0.1046 YZ= -0.1914 ZZ= 187.1251

Eigenvalues: -91.7873 -19.3597 187.1253

17 H Isotropic = 23.3137 Anisotropy = 9.8755

XX= 26.2965 YX= 4.2069 ZX= 0.0120

XY= 3.0566 YY= 26.2346 ZY= 0.0051

XZ= 0.0031 YZ= 0.0046 ZZ= 17.4101

Eigenvalues: 17.4101 22.6336 29.8974

18 H Isotropic = 22.5699 Anisotropy = 9.3313

XX= 27.5284 YX= -2.3477 ZX= -0.0025

XY= -2.8222 YY= 23.4975 ZY= 0.0106

XZ= -0.0090 YZ= 0.0144 ZZ= 16.6838

Eigenvalues: 16.6838 22.2352 28.7908

19 C Isotropic = 104.9539 Anisotropy = 65.8096

XX= 141.1661 YX= 24.4126 ZX= -0.0110

XY= 17.3940 YY= 91.7887 ZY= -0.0691

XZ= -0.1560 YZ= -0.1203 ZZ= 81.9068

Eigenvalues: 81.9050 84.1297 148.8269

20 H Isotropic = 23.7546 Anisotropy = 5.2580

XX= 26.1260 YX= -1.3593 ZX= 0.0048

XY= -1.5076 YY= 25.4480 ZY= 0.0028

XZ= 0.0078 YZ= 0.0048 ZZ= 19.6899

Eigenvalues: 19.6899 24.3140 27.2600

21 H Isotropic = 22.6612 Anisotropy = 7.8870

XX= 27.8244 YX= 0.9652 ZX= 0.0097

XY= 0.4161 YY= 22.8866 ZY= 0.0052

XZ= 0.0118 YZ= 0.0036 ZZ= 17.2726

Eigenvalues: 17.2726 22.7918 27.9192

22 C Isotropic = 150.3172 Anisotropy = 37.3115

XX= 149.4341 YX= -1.0601 ZX= -12.4973

XY= -2.6838 YY= 137.3405 ZY= 9.3614

XZ= -17.9979 YZ= 5.7424 ZZ= 164.1769

Eigenvalues: 134.7804 140.9796 175.1915

23 H Isotropic = 26.3263 Anisotropy = 5.3027

XX= 27.2162 YX= 0.6969 ZX= 0.0132

XY= -1.4770 YY= 29.8038 ZY= 0.0221

XZ= 0.0046 YZ= 0.0140 ZZ= 21.9587

Eigenvalues: 21.9587 27.1587 29.8614

24 C Isotropic = 150.4108 Anisotropy = 37.1594

XX= 149.7113 YX= -1.2077 ZX= 12.5279

XY= -2.8071 YY= 137.4805 ZY= -9.5942

XZ= 17.7382 YZ= -6.0007 ZZ= 164.0405

Eigenvalues: 134.8161 141.2326 175.1837

25 H Isotropic = 29.2449 Anisotropy = 6.5520

XX= 28.1122 YX= -1.1068 ZX= -1.4785

XY= -0.4983 YY= 32.2989 ZY= 1.2532

XZ= -3.5319 YZ= 2.9805 ZZ= 27.3235

Eigenvalues: 25.0012 29.1206 33.6129

26 H Isotropic = 29.3910 Anisotropy = 7.6342

XX= 27.5978 YX= -0.9867 ZX= 0.1201

XY= -0.7645 YY= 26.6371 ZY= -1.1359

XZ= -1.9882 YZ= -2.6872 ZZ= 33.9380

Eigenvalues: 25.5799 28.1126 34.4805

27 H Isotropic = 29.3688 Anisotropy = 9.7995

XX= 33.9968 YX= 2.3123 ZX= -2.4231

XY= 1.8239 YY= 26.5278 ZY= -0.3886

XZ= -4.2770 YZ= -0.6594 ZZ= 27.5819

Eigenvalues: 25.7765 26.4282 35.9018

28 H Isotropic = 29.2442 Anisotropy = 6.5687

XX= 28.1376 YX= -1.1635 ZX= 1.4793

XY= -0.5483 YY= 32.3371 ZY= -1.2079

XZ= 3.5017 YZ= -2.9279 ZZ= 27.2579

Eigenvalues: 25.0061 29.1032 33.6234

29 H Isotropic = 29.3629 Anisotropy = 9.7946

XX= 34.0064 YX= 2.3286 ZX= 2.4282

XY= 1.8234 YY= 26.5378 ZY= 0.3721

XZ= 4.2353 YZ= 0.6393 ZZ= 27.5444

Eigenvalues: 25.7611 26.4349 35.8926

30 H Isotropic = 29.3878 Anisotropy = 7.6333

XX= 27.5997 YX= -0.9693 ZX= -0.1153

XY= -0.7383 YY= 26.5912 ZY= 1.0584

XZ= 1.9907 YZ= 2.5962 ZZ= 33.9726

Eigenvalues: 25.6007 28.0860 34.4767

## Norharman monomer\_iso2 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level

30

C 4.29759 1.03877 0.00271

C 2.97776 1.48705 0.00141

C 1.93285 0.52847 -0.00060

C 2.23150 -0.89920 -0.00143

C 3.58922 -1.32355 -0.00022

C 4.59400 -0.35841 0.00202

C 0.50820 0.59286 -0.00163

N 1.11697 -1.69737 -0.00295

H 3.82157 -2.40043 -0.00105

H 5.65056 -0.67711 0.00337

C -0.48037 1.59252 -0.00101

C 0.08816 -0.82037 -0.00288

C -1.28282 -1.10913 -0.00371

H -0.22873 2.66559 0.00055

C -1.82455 1.22527 -0.00151

N -2.20408 -0.10301 -0.00250

H -2.63906 1.96137 -0.00045

H -1.66363 -2.14109 -0.00477

C -3.65815 -0.44995 0.00000

H 5.12631 1.76617 0.00437

H 2.75413 2.56783 0.00196

C -4.34368 0.03311 1.28681

H -3.67742 -1.55918 -0.00408

C -4.35165 0.04214 -1.27866

H -4.38446 1.14268 1.34577

H -3.81283 -0.34480 2.18669

H -5.38896 -0.34405 1.31688

H -4.39811 1.15176 -1.32573

H -5.39519 -0.34006 -1.30831

H -3.82289 -0.32353 -2.18493

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 56.4894 Anisotropy = 170.8063

XX= 5.0574 YX= -48.8518 ZX= -0.2529

XY= -52.9910 YY= -5.9490 ZY= -0.2055

XZ= -0.2635 YZ= -0.2180 ZZ= 170.3598

Eigenvalues: -51.6642 50.7721 170.3603

2 C Isotropic = 50.2595 Anisotropy = 179.6692

XX= 35.7932 YX= 4.4458 ZX= -0.1582

XY= 4.7618 YY= -55.0532 ZY= -0.1724

XZ= -0.1560 YZ= -0.2147 ZZ= 170.0386

Eigenvalues: -55.2860 36.0257 170.0390

3 C Isotropic = 51.7693 Anisotropy = 163.2807

XX= -10.2491 YX= 17.1418 ZX= -0.1513

XY= 8.9940 YY= 4.9342 ZY= -0.1233

XZ= -0.1602 YZ= -0.1413 ZZ= 160.6228

Eigenvalues: -17.7705 12.4553 160.6231

4 C Isotropic = 10.8526 Anisotropy = 167.7572

XX= -40.8994 YX= 1.7959 ZX= -0.1648

XY= -8.2349 YY= -49.2332 ZY= -0.1323

XZ= -0.1356 YZ= -0.1729 ZZ= 122.6905

Eigenvalues: -50.3322 -39.8006 122.6907

5 C Isotropic = 53.9690 Anisotropy = 157.8320

XX= 32.6766 YX= 28.7725 ZX= -0.1317

XY= 28.5649 YY= -29.9596 ZY= -0.1538

XZ= -0.1330 YZ= -0.0662 ZZ= 159.1901

Eigenvalues: -41.1000 43.8167 159.1904

6 C Isotropic = 44.1670 Anisotropy = 186.7738

XX= -52.5938 YX= 37.7082 ZX= -0.2948

XY= 39.9228 YY= 16.4126 ZY= -0.0672

XZ= -0.2640 YZ= -0.0678 ZZ= 168.6824

Eigenvalues: -70.0246 33.8429 168.6829

7 C Isotropic = 39.3289 Anisotropy = 184.1092

XX= -26.2091 YX= -6.8034 ZX= -0.1037

XY= -11.7367 YY= -17.8723 ZY= -0.1631

XZ= -0.2052 YZ= -0.2277 ZZ= 162.0680

Eigenvalues: -32.2051 -11.8766 162.0684

8 N Isotropic = 2.0733 Anisotropy = 323.9984

XX= -183.3900 YX= 7.9681 ZX= -0.3005

XY= 16.4125 YY= -28.4620 ZY= -0.1700

XZ= -0.3321 YZ= -0.1231 ZZ= 218.0718

Eigenvalues: -184.3435 -27.5088 218.0722

9 H Isotropic = 22.9808 Anisotropy = 6.7572

XX= 27.1628 YX= 0.9047 ZX= 0.0092

XY= 1.3088 YY= 23.6904 ZY= 0.0059

XZ= 0.0109 YZ= 0.0078 ZZ= 18.0891

Eigenvalues: 18.0891 23.3676 27.4856

10 H Isotropic = 23.2240 Anisotropy = 5.6194

XX= 24.2454 YX= 1.1185 ZX= 0.0047

XY= 1.3573 YY= 26.4079 ZY= 0.0084

XZ= 0.0097 YZ= 0.0064 ZZ= 19.0187

Eigenvalues: 19.0187 23.6831 26.9703

11 C Isotropic = 58.4793 Anisotropy = 170.3805

XX= 40.5029 YX= -17.9558 ZX= -0.0592

XY= -13.6606 YY= -37.1308 ZY= -0.2468

XZ= -0.0120 YZ= -0.3348 ZZ= 172.0659

Eigenvalues: -40.2267 43.5984 172.0663

12 C Isotropic = 25.6145 Anisotropy = 156.4010

XX= -16.9903 YX= -11.1098 ZX= -0.1016

XY= -1.0162 YY= -36.0480 ZY= -0.1124

XZ= -0.0819 YZ= -0.0790 ZZ= 129.8817

Eigenvalues: -37.8134 -15.2250 129.8818

13 C Isotropic = 42.3769 Anisotropy = 113.9405

XX= 36.5794 YX= -9.2916 ZX= -0.0124

XY= -7.6939 YY= -27.7858 ZY= -0.1596

XZ= 0.0905 YZ= -0.0872 ZZ= 118.3370

Eigenvalues: -28.8876 37.6810 118.3372

14 H Isotropic = 22.5125 Anisotropy = 7.6536

XX= 27.6031 YX= -0.9674 ZX= 0.0036

XY= 0.5293 YY= 23.5629 ZY= 0.0044

XZ= 0.0008 YZ= 0.0060 ZZ= 16.3716

Eigenvalues: 16.3716 23.5511 27.6149

15 C Isotropic = 54.7180 Anisotropy = 148.5403

XX= 22.9100 YX= 35.2140 ZX= 0.0608

XY= 38.0877 YY= -12.5006 ZY= -0.1603

XZ= 0.1242 YZ= -0.2464 ZZ= 153.7446

Eigenvalues: -35.4989 45.9080 153.7448

16 N Isotropic = 26.7227 Anisotropy = 257.3198

XX= -95.1448 YX= -22.8515 ZX= 0.2111

XY= -16.2963 YY= -22.9561 ZY= -0.1805

XZ= 0.1126 YZ= -0.2008 ZZ= 198.2689

Eigenvalues: -100.1107 -17.9905 198.2692

17 H Isotropic = 23.1126 Anisotropy = 10.1208

XX= 26.2289 YX= 4.1842 ZX= 0.0120

XY= 3.0761 YY= 26.2305 ZY= 0.0055

XZ= 0.0026 YZ= 0.0057 ZZ= 16.8786

Eigenvalues: 16.8786 22.5995 29.8598

18 H Isotropic = 22.3230 Anisotropy = 9.7236

XX= 27.4627 YX= -2.4618 ZX= -0.0026

XY= -2.9032 YY= 23.4462 ZY= 0.0112

XZ= -0.0088 YZ= 0.0149 ZZ= 16.0600

Eigenvalues: 16.0600 22.1036 28.8054

19 C Isotropic = 112.6764 Anisotropy = 64.6461

XX= 148.2452 YX= 24.1301 ZX= -0.0119

XY= 16.9828 YY= 99.6439 ZY= -0.0674

XZ= -0.1569 YZ= -0.1205 ZZ= 90.1401

Eigenvalues: 90.1381 92.1173 155.7738

20 H Isotropic = 23.6556 Anisotropy = 5.4067

XX= 26.2748 YX= -1.2314 ZX= 0.0057

XY= -1.4436 YY= 25.4442 ZY= 0.0032

XZ= 0.0084 YZ= 0.0053 ZZ= 19.2476

Eigenvalues: 19.2476 24.4591 27.2600

21 H Isotropic = 22.4805 Anisotropy = 8.1309

XX= 27.8244 YX= 0.8721 ZX= 0.0101

XY= 0.3764 YY= 22.8184 ZY= 0.0055

XZ= 0.0124 YZ= 0.0038 ZZ= 16.7987

Eigenvalues: 16.7987 22.7417 27.9010

22 C Isotropic = 155.9023 Anisotropy = 35.8089

XX= 155.4536 YX= -0.7967 ZX= -11.7886

XY= -2.5859 YY= 142.9566 ZY= 9.1215

XZ= -17.1789 YZ= 5.3567 ZZ= 169.2968

Eigenvalues: 140.6164 147.3156 179.7749

23 H Isotropic = 26.3400 Anisotropy = 5.9118

XX= 27.1199 YX= 0.7966 ZX= 0.0136

XY= -1.4280 YY= 30.2496 ZY= 0.0244

XZ= 0.0048 YZ= 0.0160 ZZ= 21.6504

Eigenvalues: 21.6504 27.0884 30.2812

24 C Isotropic = 155.9905 Anisotropy = 35.6618

XX= 155.7177 YX= -0.9379 ZX= 11.8172

XY= -2.7068 YY= 143.0870 ZY= -9.3498

XZ= 16.9254 YZ= -5.6110 ZZ= 169.1666

Eigenvalues: 140.6419 147.5645 179.7650

25 H Isotropic = 29.2150 Anisotropy = 7.0768

XX= 27.8836 YX= -1.1507 ZX= -1.4987

XY= -0.5842 YY= 32.6528 ZY= 1.3482

XZ= -3.6133 YZ= 3.0719 ZZ= 27.1086

Eigenvalues: 24.7371 28.9750 33.9329

26 H Isotropic = 29.3841 Anisotropy = 8.0067

XX= 27.5396 YX= -1.0785 ZX= 0.3488

XY= -0.8454 YY= 26.4560 ZY= -1.2992

XZ= -1.9079 YZ= -2.8646 ZZ= 34.1568

Eigenvalues: 25.3458 28.0846 34.7219

27 H Isotropic = 29.3508 Anisotropy = 10.3543

XX= 34.3363 YX= 2.4735 ZX= -2.5104

XY= 2.0054 YY= 26.3507 ZY= -0.4151

XZ= -4.3163 YZ= -0.6645 ZZ= 27.3653

Eigenvalues: 25.5541 26.2446 36.2536

28 H Isotropic = 29.2141 Anisotropy = 7.0932

XX= 27.9097 YX= -1.2110 ZX= 1.5001

XY= -0.6376 YY= 32.6918 ZY= -1.2965

XZ= 3.5814 YZ= -3.0127 ZZ= 27.0408

Eigenvalues: 24.7426 28.9568 33.9429

29 H Isotropic = 29.3442 Anisotropy = 10.3504

XX= 34.3439 YX= 2.4917 ZX= 2.5148

XY= 2.0069 YY= 26.3622 ZY= 0.3986

XZ= 4.2750 YZ= 0.6440 ZZ= 27.3266

Eigenvalues: 25.5382 26.2500 36.2445

30 H Isotropic = 29.3803 Anisotropy = 8.0048

XX= 27.5403 YX= -1.0576 ZX= -0.3444

XY= -0.8164 YY= 26.4055 ZY= 1.2169

XZ= 1.9104 YZ= 2.7675 ZZ= 34.1952

Eigenvalues: 25.3665 28.0576 34.7168

## Norharman dimer\_iso 1 (gas-phase) - BP86/IGLO-III level

60

C -6.44428 0.64154 -0.01374

C -5.80323 -0.59639 0.01376

C -4.38756 -0.63230 -0.00074

C -3.60730 0.59430 -0.04314

C -4.29094 1.84082 -0.07154

C -5.68541 1.84767 -0.05634

C -3.41409 -1.67675 0.01756

N -2.24905 0.37524 -0.05074

H -3.72306 2.78308 -0.10594

H -6.22025 2.81273 -0.07834

C -3.43051 -3.08191 0.05656

C -2.12466 -0.97929 -0.01534

C -0.94263 -1.73840 -0.00834

H -4.36960 -3.65757 0.08286

C -2.22138 -3.76906 0.06186

N -1.01727 -3.09863 0.02956

H -2.15792 -4.86573 0.09146

H 0.07118 -1.29281 -0.03244

C 0.25233 -3.89768 0.03416

H -7.54543 0.69461 -0.00304

H -6.38998 -1.53022 0.04606

C 1.03361 -3.67623 -1.26864

H -0.08704 -4.95398 0.06976

C 1.07304 -3.60178 1.29736

H 1.42010 -2.63609 -1.33134

H 0.39597 -3.88357 -2.15534

H 1.90391 -4.36737 -1.30064

H 1.46058 -2.55991 1.28776

H 1.94457 -4.29059 1.34266

H 0.46282 -3.75716 2.21356

C 6.44422 -0.64182 -0.01534

C 5.80316 0.59621 0.01406

C 4.38750 0.63213 0.00026

C 3.60713 -0.59437 -0.04274

C 4.29067 -1.84090 -0.07254

C 5.68524 -1.84775 -0.05854

C 3.41411 1.67667 0.01916

N 2.24897 -0.37521 -0.04994

H 3.72279 -2.78316 -0.10744

H 6.22008 -2.81291 -0.08214

C 3.43054 3.08184 0.05826

C 2.12469 0.97932 -0.01404

C 0.94266 1.73843 -0.00744

H 4.36973 3.65750 0.08496

C 2.22140 3.76909 0.06316

N 1.01739 3.09866 0.03026

H 2.15815 4.86567 0.09256

H -0.07116 1.29284 -0.03204

C -0.25221 3.89781 0.03346

H 7.54536 -0.69488 -0.00574

H 6.38991 1.52994 0.04706

C -1.03237 3.67599 -1.26994

H 0.08727 4.95412 0.06886

C -1.07394 3.60258 1.29616

H -1.41897 2.63585 -1.33244

H -0.39401 3.88276 -2.15614

H -1.90258 4.36724 -1.30294

H -1.46148 2.56071 1.28676

H -1.94547 4.29139 1.34026

H -0.46443 3.75844 2.21276

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 52.8837 Anisotropy = 164.8508

XX= -51.0008 YX= -2.7412 ZX= 2.4672

XY= -7.0779 YY= 46.9902 ZY= 3.3669

XZ= 2.5112 YZ= 3.3290 ZZ= 162.6616

Eigenvalues: -51.2791 47.1459 162.7842

2 C Isotropic = 48.8550 Anisotropy = 170.3132

XX= 0.7722 YX= -42.9293 ZX= 2.9892

XY= -42.4156 YY= -16.4182 ZY= 5.4625

XZ= 2.9220 YZ= 5.5051 ZZ= 162.2111

Eigenvalues: -51.5274 35.6954 162.3972

3 C Isotropic = 46.3308 Anisotropy = 159.1736

XX= 5.3850 YX= 10.7069 ZX= 1.3533

XY= 4.3921 YY= -18.6934 ZY= 4.7104

XZ= 1.2519 YZ= 4.7331 ZZ= 152.3007

Eigenvalues: -20.9655 7.5113 152.4465

4 C Isotropic = 9.5134 Anisotropy = 155.3295

XX= -46.1674 YX= 1.7922 ZX= 1.6261

XY= -7.8495 YY= -38.2182 ZY= 4.4465

XZ= 2.1104 YZ= 4.0973 ZZ= 112.9258

Eigenvalues: -47.2517 -37.2745 113.0664

5 C Isotropic = 51.7444 Anisotropy = 149.3224

XX= 31.0462 YX= -29.3972 ZX= 2.3478

XY= -25.6096 YY= -26.9136 ZY= 5.5645

XZ= 2.1898 YZ= 5.6053 ZZ= 151.1005

Eigenvalues: -38.0791 42.0197 151.2926

6 C Isotropic = 42.2358 Anisotropy = 176.4138

XX= 18.7779 YX= 36.1925 ZX= 0.5694

XY= 37.3476 YY= -51.7464 ZY= 5.6931

XZ= 0.4612 YZ= 5.6635 ZZ= 159.6759

Eigenvalues: -67.5409 34.4032 159.8450

7 C Isotropic = 37.0792 Anisotropy = 176.8961

XX= -33.2772 YX= 4.6030 ZX= 1.8951

XY= 0.4387 YY= -10.3484 ZY= 4.6218

XZ= 1.9788 YZ= 4.4857 ZZ= 154.8631

Eigenvalues: -33.5620 -10.2104 155.0099

8 N Isotropic = -7.7262 Anisotropy = 314.7592

XX= -104.0287 YX= 81.4265 ZX= 0.8406

XY= 87.1583 YY= -121.0163 ZY= 8.1164

XZ= 0.9828 YZ= 8.4968 ZZ= 201.8664

Eigenvalues: -197.3189 -27.9729 202.1133

9 H Isotropic = 22.9198 Anisotropy = 9.7125

XX= 29.3459 YX= -0.6016 ZX= 0.0825

XY= -0.5111 YY= 22.9624 ZY= -0.1066

XZ= 0.0955 YZ= -0.1391 ZZ= 16.4511

Eigenvalues: 16.4483 22.9163 29.3948

10 H Isotropic = 23.4092 Anisotropy = 6.7812

XX= 27.4914 YX= 1.3080 ZX= -0.0833

XY= 1.3700 YY= 23.8273 ZY= -0.1249

XZ= -0.0813 YZ= -0.1233 ZZ= 18.9090

Eigenvalues: 18.9056 23.3921 27.9301

11 C Isotropic = 57.4675 Anisotropy = 157.1997

XX= -12.3590 YX= -37.8609 ZX= 3.0078

XY= -36.2226 YY= 22.6448 ZY= 4.3133

XZ= 2.9357 YZ= 4.2136 ZZ= 162.1166

Eigenvalues: -35.9414 46.0766 162.2673

12 C Isotropic = 21.6837 Anisotropy = 147.6141

XX= -32.7035 YX= -14.4955 ZX= 2.1484

XY= -5.5869 YY= -22.1964 ZY= 4.0850

XZ= 1.6215 YZ= 4.3700 ZZ= 119.9510

Eigenvalues: -38.8736 -16.1684 120.0931

13 C Isotropic = 40.7408 Anisotropy = 146.9231

XX= -10.1552 YX= -16.7304 ZX= 2.3520

XY= -21.8080 YY= -6.1638 ZY= 4.3368

XZ= 2.4322 YZ= 4.1884 ZZ= 138.5413

Eigenvalues: -27.6609 11.1937 138.6895

14 H Isotropic = 22.9379 Anisotropy = 7.0980

XX= 25.7469 YX= -2.4302 ZX= -0.0242

XY= -0.8855 YY= 26.2380 ZY= -0.2200

XZ= -0.0907 YZ= -0.2161 ZZ= 16.8288

Eigenvalues: 16.8227 24.3212 27.6699

15 C Isotropic = 52.9381 Anisotropy = 97.7324

XX= 63.9303 YX= -18.9425 ZX= 1.1642

XY= -17.4277 YY= -23.0834 ZY= 4.1449

XZ= 1.1372 YZ= 4.0230 ZZ= 117.9674

Eigenvalues: -26.8546 67.5758 118.0930

16 N Isotropic = 24.9008 Anisotropy = 234.6857

XX= -73.6790 YX= 25.7037 ZX= 2.4997

XY= 32.4311 YY= -32.8011 ZY= 5.4694

XZ= 1.7974 YZ= 5.5632 ZZ= 181.1824

Eigenvalues: -88.7755 -17.8801 181.3579

17 H Isotropic = 23.5559 Anisotropy = 8.3008

XX= 28.9617 YX= 0.8601 ZX= -0.1470

XY= 0.7035 YY= 24.1786 ZY= -0.1560

XZ= -0.2001 YZ= -0.2173 ZZ= 17.5274

Eigenvalues: 17.5201 24.0578 29.0897

18 H Isotropic = 19.0052 Anisotropy = 12.5719

XX= 22.8848 YX= -1.4688 ZX= 0.0224

XY= -0.7371 YY= 27.1141 ZY= -0.1699

XZ= -0.1621 YZ= -0.2809 ZZ= 7.0166

Eigenvalues: 7.0137 22.6154 27.3864

19 C Isotropic = 102.2816 Anisotropy = 65.1099

XX= 121.4740 YX= -34.0697 ZX= 0.5488

XY= -25.4423 YY= 109.1146 ZY= -0.3645

XZ= 0.0130 YZ= -0.3849 ZZ= 76.2561

Eigenvalues: 76.2516 84.9049 145.6882

20 H Isotropic = 23.7396 Anisotropy = 5.1579

XX= 24.7381 YX= -0.1114 ZX= -0.0390

XY= -0.2534 YY= 27.1597 ZY= -0.1967

XZ= -0.0566 YZ= -0.2012 ZZ= 19.3211

Eigenvalues: 19.3155 24.7252 27.1782

21 H Isotropic = 22.6984 Anisotropy = 7.9579

XX= 26.5169 YX= -1.9840 ZX= -0.0326

XY= -2.4773 YY= 24.6559 ZY= -0.1629

XZ= -0.0327 YZ= -0.1713 ZZ= 16.9224

Eigenvalues: 16.9181 23.1734 28.0037

22 C Isotropic = 149.3677 Anisotropy = 31.1509

XX= 151.2796 YX= -4.5581 ZX= -11.9830

XY= -3.1787 YY= 138.7310 ZY= -5.2493

XZ= -18.0645 YZ= 2.0509 ZZ= 158.0924

Eigenvalues: 134.9553 143.0128 170.1350

23 H Isotropic = 26.3972 Anisotropy = 6.3023

XX= 28.2270 YX= 0.3764 ZX= -0.0643

XY= 2.3291 YY= 29.8170 ZY= -0.2209

XZ= -0.1858 YZ= -0.2560 ZZ= 21.1475

Eigenvalues: 21.1399 27.4530 30.5987

24 C Isotropic = 149.6587 Anisotropy = 31.1413

XX= 152.2526 YX= -3.7894 ZX= 12.6194

XY= -1.9148 YY= 139.2690 ZY= 6.8492

XZ= 18.0606 YZ= -0.8121 ZZ= 157.4547

Eigenvalues: 135.1521 143.4045 170.4196

25 H Isotropic = 27.1659 Anisotropy = 9.0163

XX= 27.3611 YX= 3.4768 ZX= -0.8129

XY= 2.5369 YY= 31.6066 ZY= 0.4260

XZ= -1.6714 YZ= 1.6623 ZZ= 22.5301

Eigenvalues: 21.8799 26.4411 33.1768

26 H Isotropic = 29.3290 Anisotropy = 7.1050

XX= 28.3633 YX= 0.8486 ZX= 0.8785

XY= 0.3173 YY= 26.9324 ZY= 1.5273

XZ= -0.1089 YZ= 4.5708 ZZ= 32.6912

Eigenvalues: 25.5648 28.3564 34.0656

27 H Isotropic = 29.1896 Anisotropy = 9.5561

XX= 32.1630 YX= -3.3324 ZX= -1.7271

XY= -3.2195 YY= 29.3146 ZY= 1.6007

XZ= -3.0925 YZ= 3.5406 ZZ= 26.0913

Eigenvalues: 24.6131 27.3954 35.5604

28 H Isotropic = 27.1772 Anisotropy = 9.7392

XX= 27.3639 YX= 3.6608 ZX= 0.6173

XY= 2.9176 YY= 31.8440 ZY= -0.7031

XZ= 1.1132 YZ= -2.4257 ZZ= 22.3237

Eigenvalues: 21.6763 26.1853 33.6700

29 H Isotropic = 29.2275 Anisotropy = 9.4579

XX= 32.3226 YX= -3.2737 ZX= 1.8259

XY= -3.0253 YY= 29.1717 ZY= -1.4942

XZ= 2.9852 YZ= -3.7196 ZZ= 26.1882

Eigenvalues: 24.6276 27.5221 35.5327

30 H Isotropic = 29.3905 Anisotropy = 7.0746

XX= 28.3466 YX= 0.7362 ZX= -0.7279

XY= 0.3713 YY= 26.7626 ZY= -1.0839

XZ= 0.0836 YZ= -4.3255 ZZ= 33.0624

Eigenvalues: 25.6974 28.3673 34.1069

31 C Isotropic = 52.8790 Anisotropy = 164.8575

XX= -51.0193 YX= -2.7368 ZX= -2.2777

XY= -7.0799 YY= 46.9980 ZY= -3.4872

XZ= -2.3401 YZ= -3.4452 ZZ= 162.6583

Eigenvalues: -51.2932 47.1462 162.7840

32 C Isotropic = 48.8409 Anisotropy = 170.3378

XX= 0.7490 YX= -42.9374 ZX= -2.9483

XY= -42.4168 YY= -16.4330 ZY= -5.6363

XZ= -2.8141 YZ= -5.6176 ZZ= 162.2068

Eigenvalues: -51.5538 35.6772 162.3994

33 C Isotropic = 46.3274 Anisotropy = 159.1602

XX= 5.4034 YX= 10.7061 ZX= -1.3028

XY= 4.3855 YY= -18.7061 ZY= -4.8177

XZ= -1.1210 YZ= -4.8137 ZZ= 152.2849

Eigenvalues: -20.9796 7.5275 152.4342

34 C Isotropic = 9.5296 Anisotropy = 155.3320

XX= -46.1546 YX= 1.7798 ZX= -1.5706

XY= -7.8629 YY= -38.1942 ZY= -4.5644

XZ= -2.0780 YZ= -4.2257 ZZ= 112.9377

Eigenvalues: -47.2456 -37.2498 113.0843

35 C Isotropic = 51.7451 Anisotropy = 149.3138

XX= 31.0411 YX= -29.4036 ZX= -2.2812

XY= -25.6070 YY= -26.8923 ZY= -5.7035

XZ= -2.1626 YZ= -5.8061 ZZ= 151.0864

Eigenvalues: -38.0719 42.0194 151.2876

36 C Isotropic = 42.2254 Anisotropy = 176.4125

XX= 18.7644 YX= 36.1883 ZX= -0.4017

XY= 37.3428 YY= -51.7408 ZY= -5.9534

XZ= -0.3146 YZ= -5.9252 ZZ= 159.6527

Eigenvalues: -67.5487 34.3912 159.8338

37 C Isotropic = 37.0821 Anisotropy = 176.9033

XX= -33.2787 YX= 4.6099 ZX= -1.8976

XY= 0.4426 YY= -10.3451 ZY= -4.6555

XZ= -1.9598 YZ= -4.4857 ZZ= 154.8700

Eigenvalues: -33.5645 -10.2069 155.0176

38 N Isotropic = -7.7034 Anisotropy = 314.7433

XX= -103.9982 YX= 81.4225 ZX= -0.7860

XY= 87.1465 YY= -120.9773 ZY= -8.2753

XZ= -1.0198 YZ= -8.8055 ZZ= 201.8652

Eigenvalues: -197.2810 -27.9547 202.1254

39 H Isotropic = 22.9192 Anisotropy = 9.7142

XX= 29.3465 YX= -0.6014 ZX= -0.0843

XY= -0.5102 YY= 22.9612 ZY= 0.1119

XZ= -0.1006 YZ= 0.1451 ZZ= 16.4498

Eigenvalues: 16.4467 22.9155 29.3953

40 H Isotropic = 23.4076 Anisotropy = 6.7808

XX= 27.4901 YX= 1.3068 ZX= 0.0811

XY= 1.3689 YY= 23.8267 ZY= 0.1263

XZ= 0.0748 YZ= 0.1305 ZZ= 18.9060

Eigenvalues: 18.9024 23.3923 27.9281

41 C Isotropic = 57.4546 Anisotropy = 157.2023

XX= -12.3748 YX= -37.8558 ZX= -3.0639

XY= -36.2119 YY= 22.6335 ZY= -4.3375

XZ= -2.9669 YZ= -4.1643 ZZ= 162.1050

Eigenvalues: -35.9503 46.0579 162.2561

42 C Isotropic = 21.6795 Anisotropy = 147.6157

XX= -32.7053 YX= -14.4957 ZX= -2.1879

XY= -5.5822 YY= -22.1994 ZY= -4.1214

XZ= -1.6712 YZ= -4.4602 ZZ= 119.9432

Eigenvalues: -38.8771 -16.1743 120.0900

43 C Isotropic = 40.7440 Anisotropy = 146.9148

XX= -10.1475 YX= -16.7422 ZX= -2.4237

XY= -21.8169 YY= -6.1574 ZY= -4.3260

XZ= -2.5222 YZ= -4.2008 ZZ= 138.5369

Eigenvalues: -27.6674 11.2122 138.6873

44 H Isotropic = 22.9368 Anisotropy = 7.0971

XX= 25.7460 YX= -2.4292 ZX= 0.0236

XY= -0.8850 YY= 26.2369 ZY= 0.2233

XZ= 0.0937 YZ= 0.2166 ZZ= 16.8275

Eigenvalues: 16.8212 24.3209 27.6682

45 C Isotropic = 52.9487 Anisotropy = 97.7482

XX= 63.9408 YX= -18.9511 ZX= -1.1792

XY= -17.4431 YY= -23.0832 ZY= -4.1519

XZ= -1.1434 YZ= -4.0095 ZZ= 117.9884

Eigenvalues: -26.8585 67.5904 118.1141

46 N Isotropic = 24.9031 Anisotropy = 234.6977

XX= -73.6689 YX= 25.6801 ZX= -2.6784

XY= 32.4112 YY= -32.8141 ZY= -5.3993

XZ= -1.9340 YZ= -5.5113 ZZ= 181.1924

Eigenvalues: -88.7519 -17.9070 181.3683

47 H Isotropic = 23.5566 Anisotropy = 8.3011

XX= 28.9630 YX= 0.8585 ZX= 0.1495

XY= 0.7021 YY= 24.1779 ZY= 0.1592

XZ= 0.2042 YZ= 0.2147 ZZ= 17.5289

Eigenvalues: 17.5215 24.0577 29.0907

48 H Isotropic = 19.0051 Anisotropy = 12.5720

XX= 22.8843 YX= -1.4686 ZX= -0.0205

XY= -0.7378 YY= 27.1140 ZY= 0.1725

XZ= 0.1737 YZ= 0.2817 ZZ= 7.0170

Eigenvalues: 7.0139 22.6149 27.3864

49 C Isotropic = 102.2718 Anisotropy = 65.1223

XX= 121.4681 YX= -34.0750 ZX= -0.5069

XY= -25.4473 YY= 109.1084 ZY= 0.3447

XZ= 0.0211 YZ= 0.3504 ZZ= 76.2388

Eigenvalues: 76.2348 84.8938 145.6866

50 H Isotropic = 23.7392 Anisotropy = 5.1583

XX= 24.7369 YX= -0.1115 ZX= 0.0382

XY= -0.2539 YY= 27.1592 ZY= 0.2026

XZ= 0.0494 YZ= 0.2075 ZZ= 19.3216

Eigenvalues: 19.3158 24.7238 27.1781

51 H Isotropic = 22.6986 Anisotropy = 7.9594

XX= 26.5168 YX= -1.9858 ZX= 0.0285

XY= -2.4787 YY= 24.6547 ZY= 0.1678

XZ= 0.0275 YZ= 0.1793 ZZ= 16.9242

Eigenvalues: 16.9197 23.1712 28.0048

52 C Isotropic = 149.3818 Anisotropy = 31.1602

XX= 151.2637 YX= -4.5564 ZX= 11.9820

XY= -3.1853 YY= 138.7437 ZY= 5.2631

XZ= 18.0637 YZ= -2.0497 ZZ= 158.1381

Eigenvalues: 134.9588 143.0314 170.1553

53 H Isotropic = 26.3966 Anisotropy = 6.3017

XX= 28.2266 YX= 0.3766 ZX= 0.0661

XY= 2.3289 YY= 29.8159 ZY= 0.2223

XZ= 0.1909 YZ= 0.2511 ZZ= 21.1474

Eigenvalues: 21.1397 27.4524 30.5978

54 C Isotropic = 149.6536 Anisotropy = 31.1339

XX= 152.2764 YX= -3.7933 ZX= -12.6210

XY= -1.9139 YY= 139.2625 ZY= -6.8293

XZ= -18.0580 YZ= 0.8200 ZZ= 157.4218

Eigenvalues: 135.1567 143.3945 170.4095

55 H Isotropic = 27.1678 Anisotropy = 9.0150

XX= 27.3568 YX= 3.4758 ZX= 0.8109

XY= 2.5378 YY= 31.6091 ZY= -0.4244

XZ= 1.6733 YZ= -1.6613 ZZ= 22.5374

Eigenvalues: 21.8864 26.4391 33.1778

56 H Isotropic = 29.3328 Anisotropy = 7.1045

XX= 28.3670 YX= 0.8488 ZX= -0.8835

XY= 0.3155 YY= 26.9339 ZY= -1.5226

XZ= 0.1051 YZ= -4.5680 ZZ= 32.6976

Eigenvalues: 25.5704 28.3589 34.0692

57 H Isotropic = 29.1906 Anisotropy = 9.5568

XX= 32.1571 YX= -3.3333 ZX= 1.7310

XY= -3.2191 YY= 29.3147 ZY= -1.6029

XZ= 3.0967 YZ= -3.5460 ZZ= 26.1000

Eigenvalues: 24.6165 27.3935 35.5618

58 H Isotropic = 27.1762 Anisotropy = 9.7391

XX= 27.3691 YX= 3.6620 ZX= -0.6200

XY= 2.9160 YY= 31.8416 ZY= 0.7041

XZ= -1.1130 YZ= 2.4261 ZZ= 22.3179

Eigenvalues: 21.6706 26.1891 33.6690

59 H Isotropic = 29.2277 Anisotropy = 9.4581

XX= 32.3287 YX= -3.2743 ZX= -1.8214

XY= -3.0272 YY= 29.1738 ZY= 1.4921

XZ= -2.9801 YZ= 3.7135 ZZ= 26.1806

Eigenvalues: 24.6262 27.5238 35.5331

60 H Isotropic = 29.3883 Anisotropy = 7.0748

XX= 28.3449 YX= 0.7360 ZX= 0.7233

XY= 0.3729 YY= 26.7623 ZY= 1.0892

XZ= -0.0868 YZ= 4.3288 ZZ= 33.0575

Eigenvalues: 25.6933 28.3667 34.1048

## Norharman dimer\_iso 1 (gas-phase) – PBE0/IGLO-III level

60

C -6.44428 0.64154 -0.01374

C -5.80323 -0.59639 0.01376

C -4.38756 -0.63230 -0.00074

C -3.60730 0.59430 -0.04314

C -4.29094 1.84082 -0.07154

C -5.68541 1.84767 -0.05634

C -3.41409 -1.67675 0.01756

N -2.24905 0.37524 -0.05074

H -3.72306 2.78308 -0.10594

H -6.22025 2.81273 -0.07834

C -3.43051 -3.08191 0.05656

C -2.12466 -0.97929 -0.01534

C -0.94263 -1.73840 -0.00834

H -4.36960 -3.65757 0.08286

C -2.22138 -3.76906 0.06186

N -1.01727 -3.09863 0.02956

H -2.15792 -4.86573 0.09146

H 0.07118 -1.29281 -0.03244

C 0.25233 -3.89768 0.03416

H -7.54543 0.69461 -0.00304

H -6.38998 -1.53022 0.04606

C 1.03361 -3.67623 -1.26864

H -0.08704 -4.95398 0.06976

C 1.07304 -3.60178 1.29736

H 1.42010 -2.63609 -1.33134

H 0.39597 -3.88357 -2.15534

H 1.90391 -4.36737 -1.30064

H 1.46058 -2.55991 1.28776

H 1.94457 -4.29059 1.34266

H 0.46282 -3.75716 2.21356

C 6.44422 -0.64182 -0.01534

C 5.80316 0.59621 0.01406

C 4.38750 0.63213 0.00026

C 3.60713 -0.59437 -0.04274

C 4.29067 -1.84090 -0.07254

C 5.68524 -1.84775 -0.05854

C 3.41411 1.67667 0.01916

N 2.24897 -0.37521 -0.04994

H 3.72279 -2.78316 -0.10744

H 6.22008 -2.81291 -0.08214

C 3.43054 3.08184 0.05826

C 2.12469 0.97932 -0.01404

C 0.94266 1.73843 -0.00744

H 4.36973 3.65750 0.08496

C 2.22140 3.76909 0.06316

N 1.01739 3.09866 0.03026

H 2.15815 4.86567 0.09256

H -0.07116 1.29284 -0.03204

C -0.25221 3.89781 0.03346

H 7.54536 -0.69488 -0.00574

H 6.38991 1.52994 0.04706

C -1.03237 3.67599 -1.26994

H 0.08727 4.95412 0.06886

C -1.07394 3.60258 1.29616

H -1.41897 2.63585 -1.33244

H -0.39401 3.88276 -2.15614

H -1.90258 4.36724 -1.30294

H -1.46148 2.56071 1.28676

H -1.94547 4.29139 1.34026

H -0.46443 3.75844 2.21276

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 56.3587 Anisotropy = 169.5554

XX= -50.7344 YX= -4.1451 ZX= 2.5792

XY= -8.9075 YY= 50.5414 ZY= 3.4718

XZ= 2.6383 YZ= 3.4262 ZZ= 169.2689

Eigenvalues: -51.1894 50.8698 169.3956

2 C Isotropic = 50.2789 Anisotropy = 177.8222

XX= -1.3668 YX= -45.9618 ZX= 3.1685

XY= -44.8693 YY= -16.4297 ZY= 5.6713

XZ= 3.0808 YZ= 5.7167 ZZ= 168.6333

Eigenvalues: -55.1150 37.1248 168.8271

3 C Isotropic = 50.7853 Anisotropy = 163.1745

XX= 8.7364 YX= 11.8542 ZX= 1.3620

XY= 6.2523 YY= -15.8000 ZY= 4.8069

XZ= 1.2658 YZ= 4.8380 ZZ= 159.4195

Eigenvalues: -18.8764 11.6640 159.5683

4 C Isotropic = 11.3286 Anisotropy = 165.3392

XX= -47.3830 YX= 3.3307 ZX= 1.6845

XY= -7.4397 YY= -40.0349 ZY= 4.7326

XZ= 2.2265 YZ= 4.4260 ZZ= 121.4036

Eigenvalues: -47.9738 -39.5951 121.5547

5 C Isotropic = 54.8545 Anisotropy = 155.1182

XX= 34.9076 YX= -29.5237 ZX= 2.3858

XY= -25.9551 YY= -28.4107 ZY= 5.8147

XZ= 2.2156 YZ= 5.8660 ZZ= 158.0667

Eigenvalues: -39.0439 45.3408 158.2667

6 C Isotropic = 43.9362 Anisotropy = 183.9025

XX= 20.5996 YX= 36.9822 ZX= 0.6013

XY= 38.1713 YY= -55.1515 ZY= 5.9732

XZ= 0.4815 YZ= 5.9424 ZZ= 166.3605

Eigenvalues: -70.7478 36.0185 166.5379

7 C Isotropic = 38.8891 Anisotropy = 184.6872

XX= -34.0335 YX= 5.9795 ZX= 1.9408

XY= 0.6100 YY= -11.1598 ZY= 4.8352

XZ= 2.0532 YZ= 4.6922 ZZ= 161.8607

Eigenvalues: -34.5075 -10.8391 162.0139

8 N Isotropic = -0.8079 Anisotropy = 320.1839

XX= -98.1254 YX= 80.5574 ZX= 0.9175

XY= 85.2624 YY= -116.6939 ZY= 8.3020

XZ= 1.1377 YZ= 8.6462 ZZ= 212.3955

Eigenvalues: -190.9165 -24.1554 212.6480

9 H Isotropic = 22.8180 Anisotropy = 10.1304

XX= 29.5336 YX= -0.5121 ZX= 0.0750

XY= -0.4818 YY= 22.9628 ZY= -0.1206

XZ= 0.0916 YZ= -0.1564 ZZ= 15.9575

Eigenvalues: 15.9544 22.9279 29.5716

10 H Isotropic = 23.2607 Anisotropy = 7.0026

XX= 27.5246 YX= 1.2299 ZX= -0.0855

XY= 1.3596 YY= 23.7673 ZY= -0.1347

XZ= -0.0827 YZ= -0.1358 ZZ= 18.4901

Eigenvalues: 18.4864 23.3666 27.9291

11 C Isotropic = 59.7944 Anisotropy = 163.2284

XX= -12.0772 YX= -39.8752 ZX= 3.1323

XY= -38.4691 YY= 23.0044 ZY= 4.5024

XZ= 3.0634 YZ= 4.4014 ZZ= 168.4560

Eigenvalues: -37.5790 48.3488 168.6133

12 C Isotropic = 24.3717 Anisotropy = 155.8433

XX= -32.7076 YX= -14.4599 ZX= 2.2339

XY= -4.6845 YY= -22.2960 ZY= 4.2955

XZ= 1.7171 YZ= 4.5780 ZZ= 128.1186

Eigenvalues: -38.4926 -16.6596 128.2672

13 C Isotropic = 40.9900 Anisotropy = 154.9715

XX= -12.9694 YX= -18.2614 ZX= 2.4818

XY= -23.0624 YY= -8.2097 ZY= 4.5637

XZ= 2.5580 YZ= 4.3952 ZZ= 144.1490

Eigenvalues: -31.5227 10.1883 144.3043

14 H Isotropic = 22.7512 Anisotropy = 7.3067

XX= 25.7630 YX= -2.4324 ZX= -0.0277

XY= -0.8430 YY= 26.1772 ZY= -0.2317

XZ= -0.0991 YZ= -0.2311 ZZ= 16.3134

Eigenvalues: 16.3068 24.3244 27.6224

15 C Isotropic = 54.1743 Anisotropy = 106.8596

XX= 63.7533 YX= -20.7523 ZX= 1.3019

XY= -19.2185 YY= -26.5082 ZY= 4.4638

XZ= 1.2728 YZ= 4.3456 ZZ= 125.2778

Eigenvalues: -30.8695 67.9783 125.4140

16 N Isotropic = 26.6889 Anisotropy = 249.3889

XX= -79.5769 YX= 29.5466 ZX= 2.6098

XY= 36.8879 YY= -33.1195 ZY= 5.7368

XZ= 1.8983 YZ= 5.8693 ZZ= 192.7632

Eigenvalues: -96.8832 -15.9982 192.9482

17 H Isotropic = 23.3852 Anisotropy = 8.5603

XX= 28.9507 YX= 0.8910 ZX= -0.1522

XY= 0.7497 YY= 24.2024 ZY= -0.1700

XZ= -0.2035 YZ= -0.2278 ZZ= 17.0023

Eigenvalues: 16.9948 24.0686 29.0920

18 H Isotropic = 18.8979 Anisotropy = 13.0141

XX= 22.8725 YX= -1.5254 ZX= 0.0197

XY= -0.8001 YY= 27.2841 ZY= -0.1815

XZ= -0.1690 YZ= -0.2955 ZZ= 6.5371

Eigenvalues: 6.5339 22.5858 27.5740

19 C Isotropic = 110.1425 Anisotropy = 64.1827

XX= 129.0254 YX= -33.7034 ZX= 0.5408

XY= -25.0864 YY= 116.7793 ZY= -0.3515

XZ= 0.0241 YZ= -0.3597 ZZ= 84.6230

Eigenvalues: 84.6190 92.8776 152.9310

20 H Isotropic = 23.6581 Anisotropy = 5.2796

XX= 24.9324 YX= -0.1470 ZX= -0.0441

XY= -0.3678 YY= 27.1434 ZY= -0.2059

XZ= -0.0565 YZ= -0.2113 ZZ= 18.8986

Eigenvalues: 18.8928 24.9037 27.1779

21 H Isotropic = 22.5357 Anisotropy = 8.1990

XX= 26.4476 YX= -2.0447 ZX= -0.0346

XY= -2.4962 YY= 24.6834 ZY= -0.1757

XZ= -0.0383 YZ= -0.1830 ZZ= 16.4762

Eigenvalues: 16.4715 23.1340 28.0017

22 C Isotropic = 155.1043 Anisotropy = 29.8746

XX= 157.1244 YX= -4.8308 ZX= -11.4409

XY= -3.3274 YY= 144.5674 ZY= -5.1024

XZ= -16.9894 YZ= 2.2004 ZZ= 163.6211

Eigenvalues: 141.0061 149.2861 175.0207

23 H Isotropic = 26.4406 Anisotropy = 6.8990

XX= 28.1705 YX= 0.4567 ZX= -0.0698

XY= 2.4546 YY= 30.2908 ZY= -0.2419

XZ= -0.1932 YZ= -0.2816 ZZ= 20.8604

Eigenvalues: 20.8520 27.4298 31.0399

24 C Isotropic = 155.4020 Anisotropy = 29.8558

XX= 158.0716 YX= -4.0930 ZX= 12.0802

XY= -2.1193 YY= 145.0960 ZY= 6.6789

XZ= 16.9984 YZ= -0.9792 ZZ= 163.0383

Eigenvalues: 141.2234 149.6767 175.3059

25 H Isotropic = 27.1807 Anisotropy = 9.5626

XX= 27.3315 YX= 3.6340 ZX= -0.8580

XY= 2.7596 YY= 31.9022 ZY= 0.3503

XZ= -1.7595 YZ= 1.7121 ZZ= 22.3085

Eigenvalues: 21.6392 26.3472 33.5558

26 H Isotropic = 29.3164 Anisotropy = 7.5917

XX= 28.3295 YX= 0.9077 ZX= 1.1533

XY= 0.3584 YY= 26.7187 ZY= 1.6271

XZ= 0.0558 YZ= 4.8045 ZZ= 32.9009

Eigenvalues: 25.3087 28.2629 34.3775

27 H Isotropic = 29.1694 Anisotropy = 10.1629

XX= 32.3521 YX= -3.6324 ZX= -1.8143

XY= -3.5051 YY= 29.3457 ZY= 1.6740

XZ= -3.0994 YZ= 3.6073 ZZ= 25.8105

Eigenvalues: 24.3541 27.2095 35.9447

28 H Isotropic = 27.1905 Anisotropy = 10.3139

XX= 27.3418 YX= 3.8293 ZX= 0.6502

XY= 3.1513 YY= 32.1508 ZY= -0.6579

XZ= 1.1770 YZ= -2.5124 ZZ= 22.0788

Eigenvalues: 21.4182 26.0868 34.0664

29 H Isotropic = 29.2090 Anisotropy = 10.0631

XX= 32.5172 YX= -3.5687 ZX= 1.9168

XY= -3.3099 YY= 29.1968 ZY= -1.5693

XZ= 2.9914 YZ= -3.8005 ZZ= 25.9131

Eigenvalues: 24.3686 27.3407 35.9177

30 H Isotropic = 29.3808 Anisotropy = 7.5596

XX= 28.3028 YX= 0.7772 ZX= -1.0006

XY= 0.4035 YY= 26.5380 ZY= -1.1563

XZ= -0.0735 YZ= -4.5323 ZZ= 33.3016

Eigenvalues: 25.4517 28.2701 34.4205

31 C Isotropic = 56.3536 Anisotropy = 169.5629

XX= -50.7543 YX= -4.1395 ZX= -2.3852

XY= -8.9084 YY= 50.5493 ZY= -3.5937

XZ= -2.4605 YZ= -3.5428 ZZ= 169.2658

Eigenvalues: -51.2045 50.8698 169.3955

32 C Isotropic = 50.2629 Anisotropy = 177.8492

XX= -1.3917 YX= -45.9702 ZX= -3.1258

XY= -44.8705 YY= -16.4481 ZY= -5.8512

XZ= -2.9700 YZ= -5.8304 ZZ= 168.6285

Eigenvalues: -55.1445 37.1041 168.8290

33 C Isotropic = 50.7823 Anisotropy = 163.1609

XX= 8.7577 YX= 11.8527 ZX= -1.3095

XY= 6.2457 YY= -15.8145 ZY= -4.9173

XZ= -1.1343 YZ= -4.9203 ZZ= 159.4038

Eigenvalues: -18.8908 11.6815 159.5562

34 C Isotropic = 11.3449 Anisotropy = 165.3398

XX= -47.3704 YX= 3.3162 ZX= -1.6251

XY= -7.4550 YY= -40.0087 ZY= -4.8584

XZ= -2.1936 YZ= -4.5664 ZZ= 121.4138

Eigenvalues: -47.9674 -39.5693 121.5715

35 C Isotropic = 54.8559 Anisotropy = 155.1095

XX= 34.9016 YX= -29.5318 ZX= -2.3173

XY= -25.9531 YY= -28.3866 ZY= -5.9614

XZ= -2.1871 YZ= -6.0773 ZZ= 158.0526

Eigenvalues: -39.0352 45.3407 158.2622

36 C Isotropic = 43.9256 Anisotropy = 183.9027

XX= 20.5843 YX= 36.9791 ZX= -0.4279

XY= 38.1672 YY= -55.1449 ZY= -6.2454

XZ= -0.3292 YZ= -6.2166 ZZ= 166.3375

Eigenvalues: -70.7564 36.0059 166.5274

37 C Isotropic = 38.8917 Anisotropy = 184.6944

XX= -34.0361 YX= 5.9876 ZX= -1.9424

XY= 0.6143 YY= -11.1560 ZY= -4.8706

XZ= -2.0318 YZ= -4.6950 ZZ= 161.8672

Eigenvalues: -34.5114 -10.8348 162.0213

38 N Isotropic = -0.7811 Anisotropy = 320.1619

XX= -98.0923 YX= 80.5521 ZX= -0.8629

XY= 85.2493 YY= -116.6449 ZY= -8.4646

XZ= -1.1817 YZ= -8.9648 ZZ= 212.3938

Eigenvalues: -190.8706 -24.1329 212.6601

39 H Isotropic = 22.8174 Anisotropy = 10.1321

XX= 29.5341 YX= -0.5119 ZX= -0.0773

XY= -0.4808 YY= 22.9617 ZY= 0.1263

XZ= -0.0972 YZ= 0.1626 ZZ= 15.9562

Eigenvalues: 15.9528 22.9272 29.5721

40 H Isotropic = 23.2591 Anisotropy = 7.0021

XX= 27.5233 YX= 1.2287 ZX= 0.0829

XY= 1.3585 YY= 23.7667 ZY= 0.1364

XZ= 0.0758 YZ= 0.1435 ZZ= 18.4872

Eigenvalues: 18.4833 23.3668 27.9271

41 C Isotropic = 59.7813 Anisotropy = 163.2321

XX= -12.0945 YX= -39.8701 ZX= -3.1911

XY= -38.4583 YY= 22.9935 ZY= -4.5268

XZ= -3.0922 YZ= -4.3527 ZZ= 168.4451

Eigenvalues: -37.5886 48.3298 168.6027

42 C Isotropic = 24.3666 Anisotropy = 155.8463

XX= -32.7104 YX= -14.4602 ZX= -2.2755

XY= -4.6798 YY= -22.3005 ZY= -4.3334

XZ= -1.7687 YZ= -4.6708 ZZ= 128.1108

Eigenvalues: -38.4974 -16.6668 128.2642

43 C Isotropic = 40.9940 Anisotropy = 154.9619

XX= -12.9602 YX= -18.2736 ZX= -2.5577

XY= -23.0720 YY= -8.2023 ZY= -4.5524

XZ= -2.6518 YZ= -4.4105 ZZ= 144.1444

Eigenvalues: -31.5287 10.2087 144.3019

44 H Isotropic = 22.7500 Anisotropy = 7.3058

XX= 25.7620 YX= -2.4314 ZX= 0.0271

XY= -0.8425 YY= 26.1760 ZY= 0.2351

XZ= 0.1026 YZ= 0.2317 ZZ= 16.3120

Eigenvalues: 16.3053 24.3241 27.6205

45 C Isotropic = 54.1841 Anisotropy = 106.8748

XX= 63.7632 YX= -20.7605 ZX= -1.3212

XY= -19.2339 YY= -26.5087 ZY= -4.4699

XZ= -1.2817 YZ= -4.3310 ZZ= 125.2976

Eigenvalues: -30.8742 67.9924 125.4339

46 N Isotropic = 26.6904 Anisotropy = 249.4031

XX= -79.5672 YX= 29.5218 ZX= -2.8025

XY= 36.8667 YY= -33.1354 ZY= -5.6597

XZ= -2.0440 YZ= -5.8108 ZZ= 192.7738

Eigenvalues: -96.8594 -16.0285 192.9592

47 H Isotropic = 23.3859 Anisotropy = 8.5606

XX= 28.9521 YX= 0.8893 ZX= 0.1551

XY= 0.7482 YY= 24.2017 ZY= 0.1732

XZ= 0.2079 YZ= 0.2253 ZZ= 17.0039

Eigenvalues: 16.9963 24.0685 29.0929

48 H Isotropic = 18.8978 Anisotropy = 13.0142

XX= 22.8720 YX= -1.5252 ZX= -0.0176

XY= -0.8008 YY= 27.2840 ZY= 0.1840

XZ= 0.1805 YZ= 0.2967 ZZ= 6.5374

Eigenvalues: 6.5341 22.5854 27.5740

49 C Isotropic = 110.1329 Anisotropy = 64.1949

XX= 129.0194 YX= -33.7087 ZX= -0.4993

XY= -25.0914 YY= 116.7730 ZY= 0.3324

XZ= 0.0106 YZ= 0.3262 ZZ= 84.6062

Eigenvalues: 84.6026 92.8665 152.9295

50 H Isotropic = 23.6577 Anisotropy = 5.2801

XX= 24.9311 YX= -0.1470 ZX= 0.0427

XY= -0.3682 YY= 27.1429 ZY= 0.2124

XZ= 0.0488 YZ= 0.2180 ZZ= 18.8990

Eigenvalues: 18.8929 24.9023 27.1778

51 H Isotropic = 22.5358 Anisotropy = 8.2006

XX= 26.4474 YX= -2.0467 ZX= 0.0303

XY= -2.4977 YY= 24.6820 ZY= 0.1810

XZ= 0.0330 YZ= 0.1918 ZZ= 16.4779

Eigenvalues: 16.4729 23.1315 28.0029

52 C Isotropic = 155.1179 Anisotropy = 29.8832

XX= 157.1096 YX= -4.8285 ZX= 11.4399

XY= -3.3337 YY= 144.5795 ZY= 5.1157

XZ= 16.9888 YZ= -2.1987 ZZ= 163.6648

Eigenvalues: 141.0097 149.3041 175.0401

53 H Isotropic = 26.4400 Anisotropy = 6.8983

XX= 28.1701 YX= 0.4568 ZX= 0.0717

XY= 2.4544 YY= 30.2897 ZY= 0.2432

XZ= 0.1985 YZ= 0.2764 ZZ= 20.8602

Eigenvalues: 20.8518 27.4293 31.0389

54 C Isotropic = 155.3969 Anisotropy = 29.8486

XX= 158.0944 YX= -4.0974 ZX= -12.0816

XY= -2.1185 YY= 145.0898 ZY= -6.6598

XZ= -16.9957 YZ= 0.9870 ZZ= 163.0067

Eigenvalues: 141.2275 149.6672 175.2960

55 H Isotropic = 27.1825 Anisotropy = 9.5614

XX= 27.3270 YX= 3.6331 ZX= 0.8561

XY= 2.7605 YY= 31.9046 ZY= -0.3486

XZ= 1.7613 YZ= -1.7108 ZZ= 22.3159

Eigenvalues: 21.6457 26.3450 33.5568

56 H Isotropic = 29.3203 Anisotropy = 7.5910

XX= 28.3338 YX= 0.9079 ZX= -1.1588

XY= 0.3566 YY= 26.7201 ZY= -1.6220

XZ= -0.0597 YZ= -4.8013 ZZ= 32.9071

Eigenvalues: 25.3143 28.2656 34.3810

57 H Isotropic = 29.1703 Anisotropy = 10.1634

XX= 32.3459 YX= -3.6332 ZX= 1.8185

XY= -3.5047 YY= 29.3457 ZY= -1.6765

XZ= 3.1039 YZ= -3.6132 ZZ= 25.8194

Eigenvalues: 24.3575 27.2076 35.9459

58 H Isotropic = 27.1896 Anisotropy = 10.3137

XX= 27.3472 YX= 3.8303 ZX= -0.6527

XY= 3.1496 YY= 32.1484 ZY= 0.6589

XZ= -1.1768 YZ= 2.5130 ZZ= 22.0731

Eigenvalues: 21.4126 26.0908 34.0654

59 H Isotropic = 29.2092 Anisotropy = 10.0635

XX= 32.5234 YX= -3.5696 ZX= -1.9119

XY= -3.3120 YY= 29.1990 ZY= 1.5669

XZ= -2.9859 YZ= 3.7940 ZZ= 25.9052

Eigenvalues: 24.3672 27.3423 35.9182

60 H Isotropic = 29.3785 Anisotropy = 7.5601

XX= 28.3007 YX= 0.7771 ZX= 0.9955

XY= 0.4051 YY= 26.5378 ZY= 1.1619

XZ= 0.0702 YZ= 4.5360 ZZ= 33.2969

Eigenvalues: 25.4476 28.2693 34.4185

## Norharman dimer\_iso 1 (IEFPCM solvent = tetrahydrofuran) - BP86/IGLO-III level

60

C -6.44428 0.64154 -0.01374

C -5.80323 -0.59639 0.01376

C -4.38756 -0.63230 -0.00074

C -3.60730 0.59430 -0.04314

C -4.29094 1.84082 -0.07154

C -5.68541 1.84767 -0.05634

C -3.41409 -1.67675 0.01756

N -2.24905 0.37524 -0.05074

H -3.72306 2.78308 -0.10594

H -6.22025 2.81273 -0.07834

C -3.43051 -3.08191 0.05656

C -2.12466 -0.97929 -0.01534

C -0.94263 -1.73840 -0.00834

H -4.36960 -3.65757 0.08286

C -2.22138 -3.76906 0.06186

N -1.01727 -3.09863 0.02956

H -2.15792 -4.86573 0.09146

H 0.07118 -1.29281 -0.03244

C 0.25233 -3.89768 0.03416

H -7.54543 0.69461 -0.00304

H -6.38998 -1.53022 0.04606

C 1.03361 -3.67623 -1.26864

H -0.08704 -4.95398 0.06976

C 1.07304 -3.60178 1.29736

H 1.42010 -2.63609 -1.33134

H 0.39597 -3.88357 -2.15534

H 1.90391 -4.36737 -1.30064

H 1.46058 -2.55991 1.28776

H 1.94457 -4.29059 1.34266

H 0.46282 -3.75716 2.21356

C 6.44422 -0.64182 -0.01534

C 5.80316 0.59621 0.01406

C 4.38750 0.63213 0.00026

C 3.60713 -0.59437 -0.04274

C 4.29067 -1.84090 -0.07254

C 5.68524 -1.84775 -0.05854

C 3.41411 1.67667 0.01916

N 2.24897 -0.37521 -0.04994

H 3.72279 -2.78316 -0.10744

H 6.22008 -2.81291 -0.08214

C 3.43054 3.08184 0.05826

C 2.12469 0.97932 -0.01404

C 0.94266 1.73843 -0.00744

H 4.36973 3.65750 0.08496

C 2.22140 3.76909 0.06316

N 1.01739 3.09866 0.03026

H 2.15815 4.86567 0.09256

H -0.07116 1.29284 -0.03204

C -0.25221 3.89781 0.03346

H 7.54536 -0.69488 -0.00574

H 6.38991 1.52994 0.04706

C -1.03237 3.67599 -1.26994

H 0.08727 4.95412 0.06886

C -1.07394 3.60258 1.29616

H -1.41897 2.63585 -1.33244

H -0.39401 3.88276 -2.15614

H -1.90258 4.36724 -1.30294

H -1.46148 2.56071 1.28676

H -1.94547 4.29139 1.34026

H -0.46443 3.75844 2.21276

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 53.6600 Anisotropy = 165.1575

XX= -50.1726 YX= -2.4611 ZX= 2.4601

XY= -6.8192 YY= 47.5105 ZY= 3.3755

XZ= 2.5054 YZ= 3.3405 ZZ= 163.6422

Eigenvalues: -50.4251 47.6402 163.7650

2 C Isotropic = 48.7903 Anisotropy = 171.8719

XX= -0.0199 YX= -42.1416 ZX= 2.9848

XY= -41.7452 YY= -16.7939 ZY= 5.4912

XZ= 2.9259 YZ= 5.5334 ZZ= 163.1848

Eigenvalues: -51.3562 34.3555 163.3716

3 C Isotropic = 46.7749 Anisotropy = 158.8998

XX= 5.8885 YX= 10.8689 ZX= 1.3468

XY= 5.1827 YY= -18.1267 ZY= 4.6912

XZ= 1.2271 YZ= 4.7226 ZZ= 152.5629

Eigenvalues: -20.6605 8.2771 152.7081

4 C Isotropic = 10.2679 Anisotropy = 154.6282

XX= -45.1110 YX= 1.6191 ZX= 1.6361

XY= -8.0956 YY= -37.2962 ZY= 4.4347

XZ= 2.1054 YZ= 4.1592 ZZ= 113.2108

Eigenvalues: -46.3438 -36.2060 113.3533

5 C Isotropic = 51.8747 Anisotropy = 151.0112

XX= 29.9249 YX= -29.0627 ZX= 2.3852

XY= -24.9530 YY= -26.6572 ZY= 5.5989

XZ= 2.1473 YZ= 5.6131 ZZ= 152.3565

Eigenvalues: -37.6713 40.7466 152.5489

6 C Isotropic = 42.8380 Anisotropy = 177.1873

XX= 18.7418 YX= 36.0161 ZX= 0.5898

XY= 37.0940 YY= -51.0206 ZY= 5.7115

XZ= 0.4834 YZ= 5.6807 ZZ= 160.7929

Eigenvalues: -66.7773 34.3285 160.9629

7 C Isotropic = 37.1686 Anisotropy = 176.1674

XX= -32.8019 YX= 5.3620 ZX= 1.8687

XY= 2.6279 YY= -10.1603 ZY= 4.5884

XZ= 1.9071 YZ= 4.4601 ZZ= 154.4680

Eigenvalues: -33.4925 -9.6152 154.6136

8 N Isotropic = -3.4924 Anisotropy = 309.4627

XX= -98.2281 YX= 81.1038 ZX= 0.9306

XY= 84.6505 YY= -114.8184 ZY= 8.1309

XZ= 0.9828 YZ= 8.2941 ZZ= 202.5694

Eigenvalues: -189.8901 -23.4030 202.8161

9 H Isotropic = 22.7598 Anisotropy = 9.6930

XX= 29.1801 YX= -0.5656 ZX= 0.0803

XY= -0.4546 YY= 22.8720 ZY= -0.1102

XZ= 0.0945 YZ= -0.1423 ZZ= 16.2274

Eigenvalues: 16.2245 22.8332 29.2218

10 H Isotropic = 23.3067 Anisotropy = 6.7101

XX= 27.3578 YX= 1.2636 ZX= -0.0835

XY= 1.3260 YY= 23.7948 ZY= -0.1269

XZ= -0.0807 YZ= -0.1248 ZZ= 18.7675

Eigenvalues: 18.7640 23.3759 27.7801

11 C Isotropic = 56.5417 Anisotropy = 160.5220

XX= -13.7297 YX= -37.3067 ZX= 3.0207

XY= -34.5266 YY= 19.9517 ZY= 4.4025

XZ= 2.9086 YZ= 4.3186 ZZ= 163.4031

Eigenvalues: -36.6750 42.7437 163.5564

12 C Isotropic = 21.6461 Anisotropy = 147.6430

XX= -31.4631 YX= -13.4780 ZX= 2.1057

XY= -4.5326 YY= -23.5296 ZY= 4.1279

XZ= 1.6707 YZ= 4.3903 ZZ= 119.9310

Eigenvalues: -37.4339 -17.7026 120.0747

13 C Isotropic = 40.4229 Anisotropy = 147.2270

XX= -11.5670 YX= -16.4788 ZX= 2.3585

XY= -22.2362 YY= -5.5907 ZY= 4.3311

XZ= 2.4463 YZ= 4.1632 ZZ= 138.4264

Eigenvalues: -28.2920 10.9864 138.5742

14 H Isotropic = 22.7250 Anisotropy = 7.0505

XX= 25.4981 YX= -2.3381 ZX= -0.0270

XY= -0.8336 YY= 26.1176 ZY= -0.2251

XZ= -0.0932 YZ= -0.2211 ZZ= 16.5593

Eigenvalues: 16.5530 24.1966 27.4253

15 C Isotropic = 49.4113 Anisotropy = 105.6619

XX= 55.6816 YX= -19.3805 ZX= 1.2894

XY= -18.3095 YY= -27.1685 ZY= 4.3165

XZ= 1.2848 YZ= 4.1828 ZZ= 119.7208

Eigenvalues: -31.3832 59.7645 119.8526

16 N Isotropic = 19.0424 Anisotropy = 245.2018

XX= -82.3894 YX= 24.7815 ZX= 2.6362

XY= 31.0231 YY= -42.8078 ZY= 5.7963

XZ= 1.9686 YZ= 5.8679 ZZ= 182.3243

Eigenvalues: -96.8084 -28.5748 182.5102

17 H Isotropic = 23.2043 Anisotropy = 8.3288

XX= 28.6371 YX= 0.8055 ZX= -0.1470

XY= 0.6971 YY= 23.8980 ZY= -0.1613

XZ= -0.2008 YZ= -0.2211 ZZ= 17.0777

Eigenvalues: 17.0703 23.7857 28.7568

18 H Isotropic = 19.0064 Anisotropy = 12.5884

XX= 22.8379 YX= -1.5998 ZX= 0.0264

XY= -0.8104 YY= 27.0782 ZY= -0.1690

XZ= -0.1592 YZ= -0.2797 ZZ= 7.1032

Eigenvalues: 7.1002 22.5203 27.3987

19 C Isotropic = 102.5341 Anisotropy = 66.0972

XX= 121.9744 YX= -34.7980 ZX= 0.5609

XY= -26.5367 YY= 108.3992 ZY= -0.3102

XZ= 0.0277 YZ= -0.3269 ZZ= 77.2289

Eigenvalues: 77.2256 83.7779 146.5989

20 H Isotropic = 23.6626 Anisotropy = 5.0838

XX= 24.7330 YX= -0.1003 ZX= -0.0408

XY= -0.2409 YY= 27.0343 ZY= -0.1963

XZ= -0.0586 YZ= -0.2013 ZZ= 19.2204

Eigenvalues: 19.2148 24.7212 27.0517

21 H Isotropic = 22.5453 Anisotropy = 7.8900

XX= 26.3492 YX= -1.9203 ZX= -0.0350

XY= -2.4236 YY= 24.5642 ZY= -0.1668

XZ= -0.0343 YZ= -0.1759 ZZ= 16.7224

Eigenvalues: 16.7179 23.1126 27.8053

22 C Isotropic = 149.4135 Anisotropy = 31.5351

XX= 150.8202 YX= -4.3667 ZX= -12.3515

XY= -3.0906 YY= 139.2077 ZY= -5.2313

XZ= -18.5523 YZ= 1.9022 ZZ= 158.2125

Eigenvalues: 134.9361 142.8674 170.4369

23 H Isotropic = 26.1436 Anisotropy = 6.4993

XX= 27.8966 YX= 0.4216 ZX= -0.0650

XY= 2.4197 YY= 29.6838 ZY= -0.2277

XZ= -0.1872 YZ= -0.2624 ZZ= 20.8503

Eigenvalues: 20.8424 27.1119 30.4764

24 C Isotropic = 149.7356 Anisotropy = 31.5408

XX= 151.8511 YX= -3.5847 ZX= 12.9826

XY= -1.8064 YY= 139.7616 ZY= 6.8000

XZ= 18.5538 YZ= -0.6859 ZZ= 157.5942

Eigenvalues: 135.1603 143.2838 170.7628

25 H Isotropic = 27.4178 Anisotropy = 8.8744

XX= 27.6069 YX= 3.4268 ZX= -0.8062

XY= 2.5008 YY= 31.7847 ZY= 0.4450

XZ= -1.6861 YZ= 1.6429 ZZ= 22.8617

Eigenvalues: 22.1999 26.7194 33.3341

26 H Isotropic = 29.2509 Anisotropy = 7.1992

XX= 28.2504 YX= 0.8869 ZX= 0.9230

XY= 0.3664 YY= 26.8537 ZY= 1.5457

XZ= -0.0796 YZ= 4.6162 ZZ= 32.6485

Eigenvalues: 25.4611 28.2412 34.0504

27 H Isotropic = 29.0474 Anisotropy = 9.6394

XX= 31.9999 YX= -3.3762 ZX= -1.7325

XY= -3.2927 YY= 29.2622 ZY= 1.6066

XZ= -3.0791 YZ= 3.5459 ZZ= 25.8803

Eigenvalues: 24.4316 27.2371 35.4737

28 H Isotropic = 27.4282 Anisotropy = 9.5961

XX= 27.6100 YX= 3.6098 ZX= 0.6166

XY= 2.8814 YY= 32.0212 ZY= -0.7151

XZ= 1.1324 YZ= -2.3991 ZZ= 22.6534

Eigenvalues: 21.9952 26.4638 33.8256

29 H Isotropic = 29.0928 Anisotropy = 9.5368

XX= 32.1642 YX= -3.3161 ZX= 1.8311

XY= -3.0981 YY= 29.1262 ZY= -1.5054

XZ= 2.9727 YZ= -3.7313 ZZ= 25.9879

Eigenvalues: 24.4542 27.3735 35.4506

30 H Isotropic = 29.3135 Anisotropy = 7.1706

XX= 28.2345 YX= 0.7713 ZX= -0.7736

XY= 0.4186 YY= 26.6797 ZY= -1.1022

XZ= 0.0510 YZ= -4.3697 ZZ= 33.0263

Eigenvalues: 25.5916 28.2550 34.0939

31 C Isotropic = 53.6561 Anisotropy = 165.1630

XX= -50.1899 YX= -2.4567 ZX= -2.2704

XY= -6.8211 YY= 47.5194 ZY= -3.4965

XZ= -2.3329 YZ= -3.4570 ZZ= 163.6389

Eigenvalues: -50.4380 47.6416 163.7648

32 C Isotropic = 48.7761 Anisotropy = 171.8962

XX= -0.0429 YX= -42.1495 ZX= -2.9421

XY= -41.7461 YY= -16.8087 ZY= -5.6671

XZ= -2.8166 YZ= -5.6474 ZZ= 163.1801

Eigenvalues: -51.3822 34.3371 163.3736

33 C Isotropic = 46.7712 Anisotropy = 158.8868

XX= 5.9065 YX= 10.8679 ZX= -1.2962

XY= 5.1761 YY= -18.1400 ZY= -4.7991

XZ= -1.0965 YZ= -4.8019 ZZ= 152.5470

Eigenvalues: -20.6747 8.2925 152.6957

34 C Isotropic = 10.2838 Anisotropy = 154.6310

XX= -45.0978 YX= 1.6067 ZX= -1.5809

XY= -8.1091 YY= -37.2732 ZY= -4.5520

XZ= -2.0747 YZ= -4.2885 ZZ= 113.2225

Eigenvalues: -46.3379 -36.1818 113.3712

35 C Isotropic = 51.8758 Anisotropy = 151.0019

XX= 29.9203 YX= -29.0693 ZX= -2.3166

XY= -24.9506 YY= -26.6351 ZY= -5.7392

XZ= -2.1182 YZ= -5.8156 ZZ= 152.3422

Eigenvalues: -37.6634 40.7471 152.5438

36 C Isotropic = 42.8286 Anisotropy = 177.1845

XX= 18.7300 YX= 36.0125 ZX= -0.4213

XY= 37.0897 YY= -51.0138 ZY= -5.9719

XZ= -0.3355 YZ= -5.9429 ZZ= 160.7697

Eigenvalues: -66.7843 34.3185 160.9516

37 C Isotropic = 37.1716 Anisotropy = 176.1744

XX= -32.8031 YX= 5.3695 ZX= -1.8710

XY= 2.6326 YY= -10.1571 ZY= -4.6221

XZ= -1.8862 YZ= -4.4580 ZZ= 154.4750

Eigenvalues: -33.4955 -9.6109 154.6212

38 N Isotropic = -3.4700 Anisotropy = 309.4468

XX= -98.1979 YX= 81.1003 ZX= -0.8762

XY= 84.6385 YY= -114.7798 ZY= -8.2875

XZ= -1.0228 YZ= -8.6041 ZZ= 202.5677

Eigenvalues: -189.8527 -23.3853 202.8279

39 H Isotropic = 22.7592 Anisotropy = 9.6948

XX= 29.1808 YX= -0.5653 ZX= -0.0821

XY= -0.4537 YY= 22.8708 ZY= 0.1157

XZ= -0.0995 YZ= 0.1485 ZZ= 16.2261

Eigenvalues: 16.2229 22.8323 29.2224

40 H Isotropic = 23.3051 Anisotropy = 6.7097

XX= 27.3566 YX= 1.2624 ZX= 0.0812

XY= 1.3250 YY= 23.7942 ZY= 0.1286

XZ= 0.0741 YZ= 0.1322 ZZ= 18.7646

Eigenvalues: 18.7610 23.3761 27.7782

41 C Isotropic = 56.5285 Anisotropy = 160.5257

XX= -13.7459 YX= -37.3011 ZX= -3.0771

XY= -34.5154 YY= 19.9393 ZY= -4.4265

XZ= -2.9394 YZ= -4.2711 ZZ= 163.3920

Eigenvalues: -36.6840 42.7238 163.5456

42 C Isotropic = 21.6419 Anisotropy = 147.6448

XX= -31.4644 YX= -13.4784 ZX= -2.1446

XY= -4.5279 YY= -23.5334 ZY= -4.1646

XZ= -1.7211 YZ= -4.4807 ZZ= 119.9233

Eigenvalues: -37.4375 -17.7086 120.0717

43 C Isotropic = 40.4264 Anisotropy = 147.2183

XX= -11.5590 YX= -16.4910 ZX= -2.4305

XY= -22.2452 YY= -5.5838 ZY= -4.3205

XZ= -2.5392 YZ= -4.1770 ZZ= 138.4218

Eigenvalues: -28.2984 11.0056 138.5719

44 H Isotropic = 22.7238 Anisotropy = 7.0496

XX= 25.4971 YX= -2.3371 ZX= 0.0264

XY= -0.8332 YY= 26.1164 ZY= 0.2285

XZ= 0.0963 YZ= 0.2217 ZZ= 16.5580

Eigenvalues: 16.5516 24.1964 27.4235

45 C Isotropic = 49.4208 Anisotropy = 105.6787

XX= 55.6905 YX= -19.3889 ZX= -1.3096

XY= -18.3246 YY= -27.1695 ZY= -4.3232

XZ= -1.2970 YZ= -4.1677 ZZ= 119.7414

Eigenvalues: -31.3885 59.7777 119.8733

46 N Isotropic = 19.0443 Anisotropy = 245.2150

XX= -82.3795 YX= 24.7576 ZX= -2.8219

XY= 31.0028 YY= -42.8223 ZY= -5.7243

XZ= -2.1118 YZ= -5.8135 ZZ= 182.3346

Eigenvalues: -96.7850 -28.6032 182.5209

47 H Isotropic = 23.2050 Anisotropy = 8.3291

XX= 28.6384 YX= 0.8038 ZX= 0.1496

XY= 0.6957 YY= 23.8973 ZY= 0.1644

XZ= 0.2050 YZ= 0.2186 ZZ= 17.0793

Eigenvalues: 17.0718 23.7855 28.7577

48 H Isotropic = 19.0064 Anisotropy = 12.5886

XX= 22.8375 YX= -1.5997 ZX= -0.0245

XY= -0.8111 YY= 27.0781 ZY= 0.1715

XZ= 0.1706 YZ= 0.2804 ZZ= 7.1036

Eigenvalues: 7.1005 22.5199 27.3988

49 C Isotropic = 102.5243 Anisotropy = 66.1098

XX= 121.9683 YX= -34.8037 ZX= -0.5183

XY= -26.5419 YY= 108.3928 ZY= 0.2900

XZ= 0.0063 YZ= 0.2926 ZZ= 77.2119

Eigenvalues: 77.2091 83.7663 146.5975

50 H Isotropic = 23.6622 Anisotropy = 5.0841

XX= 24.7319 YX= -0.1003 ZX= 0.0399

XY= -0.2413 YY= 27.0338 ZY= 0.2022

XZ= 0.0513 YZ= 0.2076 ZZ= 19.2208

Eigenvalues: 19.2150 24.7199 27.0516

51 H Isotropic = 22.5454 Anisotropy = 7.8915

XX= 26.3491 YX= -1.9222 ZX= 0.0309

XY= -2.4250 YY= 24.5630 ZY= 0.1717

XZ= 0.0290 YZ= 0.1840 ZZ= 16.7242

Eigenvalues: 16.7195 23.1104 27.8064

52 C Isotropic = 149.4270 Anisotropy = 31.5444

XX= 150.8033 YX= -4.3647 ZX= 12.3497

XY= -3.0965 YY= 139.2195 ZY= 5.2449

XZ= 18.5512 YZ= -1.9009 ZZ= 158.2581

Eigenvalues: 134.9392 142.8851 170.4566

53 H Isotropic = 26.1430 Anisotropy = 6.4987

XX= 27.8962 YX= 0.4217 ZX= 0.0668

XY= 2.4195 YY= 29.6827 ZY= 0.2292

XZ= 0.1923 YZ= 0.2574 ZZ= 20.8501

Eigenvalues: 20.8422 27.1113 30.4754

54 C Isotropic = 149.7310 Anisotropy = 31.5327

XX= 151.8758 YX= -3.5886 ZX= -12.9849

XY= -1.8058 YY= 139.7559 ZY= -6.7801

XZ= -18.5512 YZ= 0.6941 ZZ= 157.5613

Eigenvalues: 135.1658 143.2743 170.7528

55 H Isotropic = 27.4197 Anisotropy = 8.8730

XX= 27.6028 YX= 3.4258 ZX= 0.8041

XY= 2.5017 YY= 31.7872 ZY= -0.4433

XZ= 1.6880 YZ= -1.6419 ZZ= 22.8692

Eigenvalues: 22.2065 26.7176 33.3350

56 H Isotropic = 29.2547 Anisotropy = 7.1987

XX= 28.2543 YX= 0.8872 ZX= -0.9281

XY= 0.3646 YY= 26.8552 ZY= -1.5409

XZ= 0.0757 YZ= -4.6133 ZZ= 32.6548

Eigenvalues: 25.4667 28.2436 34.0539

57 H Isotropic = 29.0484 Anisotropy = 9.6400

XX= 31.9940 YX= -3.3771 ZX= 1.7364

XY= -3.2922 YY= 29.2623 ZY= -1.6089

XZ= 3.0834 YZ= -3.5515 ZZ= 25.8890

Eigenvalues: 24.4350 27.2352 35.4751

58 H Isotropic = 27.4272 Anisotropy = 9.5960

XX= 27.6152 YX= 3.6110 ZX= -0.6193

XY= 2.8797 YY= 32.0189 ZY= 0.7161

XZ= -1.1323 YZ= 2.3996 ZZ= 22.6476

Eigenvalues: 21.9895 26.4676 33.8246

59 H Isotropic = 29.0929 Anisotropy = 9.5371

XX= 32.1702 YX= -3.3168 ZX= -1.8266

XY= -3.1001 YY= 29.1283 ZY= 1.5031

XZ= -2.9675 YZ= 3.7251 ZZ= 25.9802

Eigenvalues: 24.4527 27.3751 35.4509

60 H Isotropic = 29.3112 Anisotropy = 7.1710

XX= 28.2327 YX= 0.7711 ZX= 0.7689

XY= 0.4203 YY= 26.6795 ZY= 1.1076

XZ= -0.0543 YZ= 4.3731 ZZ= 33.0214

Eigenvalues: 25.5874 28.2543 34.0919

## Norharman dimer\_iso 1 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level

60

C -6.44428 0.64154 -0.01374

C -5.80323 -0.59639 0.01376

C -4.38756 -0.63230 -0.00074

C -3.60730 0.59430 -0.04314

C -4.29094 1.84082 -0.07154

C -5.68541 1.84767 -0.05634

C -3.41409 -1.67675 0.01756

N -2.24905 0.37524 -0.05074

H -3.72306 2.78308 -0.10594

H -6.22025 2.81273 -0.07834

C -3.43051 -3.08191 0.05656

C -2.12466 -0.97929 -0.01534

C -0.94263 -1.73840 -0.00834

H -4.36960 -3.65757 0.08286

C -2.22138 -3.76906 0.06186

N -1.01727 -3.09863 0.02956

H -2.15792 -4.86573 0.09146

H 0.07118 -1.29281 -0.03244

C 0.25233 -3.89768 0.03416

H -7.54543 0.69461 -0.00304

H -6.38998 -1.53022 0.04606

C 1.03361 -3.67623 -1.26864

H -0.08704 -4.95398 0.06976

C 1.07304 -3.60178 1.29736

H 1.42010 -2.63609 -1.33134

H 0.39597 -3.88357 -2.15534

H 1.90391 -4.36737 -1.30064

H 1.46058 -2.55991 1.28776

H 1.94457 -4.29059 1.34266

H 0.46282 -3.75716 2.21356

C 6.44422 -0.64182 -0.01534

C 5.80316 0.59621 0.01406

C 4.38750 0.63213 0.00026

C 3.60713 -0.59437 -0.04274

C 4.29067 -1.84090 -0.07254

C 5.68524 -1.84775 -0.05854

C 3.41411 1.67667 0.01916

N 2.24897 -0.37521 -0.04994

H 3.72279 -2.78316 -0.10744

H 6.22008 -2.81291 -0.08214

C 3.43054 3.08184 0.05826

C 2.12469 0.97932 -0.01404

C 0.94266 1.73843 -0.00744

H 4.36973 3.65750 0.08496

C 2.22140 3.76909 0.06316

N 1.01739 3.09866 0.03026

H 2.15815 4.86567 0.09256

H -0.07116 1.29284 -0.03204

C -0.25221 3.89781 0.03346

H 7.54536 -0.69488 -0.00574

H 6.38991 1.52994 0.04706

C -1.03237 3.67599 -1.26994

H 0.08727 4.95412 0.06886

C -1.07394 3.60258 1.29616

H -1.41897 2.63585 -1.33244

H -0.39401 3.88276 -2.15614

H -1.90258 4.36724 -1.30294

H -1.46148 2.56071 1.28676

H -1.94547 4.29139 1.34026

H -0.46443 3.75844 2.21276

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 57.0928 Anisotropy = 169.9585

XX= -49.8780 YX= -3.8389 ZX= 2.5712

XY= -8.5716 YY= 50.8850 ZY= 3.4855

XZ= 2.6305 YZ= 3.4426 ZZ= 170.2714

Eigenvalues: -50.2945 51.1744 170.3985

2 C Isotropic = 50.1201 Anisotropy = 179.5947

XX= -2.3465 YX= -44.9735 ZX= 3.1613

XY= -44.0529 YY= -16.9484 ZY= 5.7036

XZ= 3.0819 YZ= 5.7485 ZZ= 169.6553

Eigenvalues: -54.9370 35.4475 169.8499

3 C Isotropic = 51.2847 Anisotropy = 162.7560

XX= 9.3551 YX= 12.0663 ZX= 1.3526

XY= 7.1241 YY= -15.1415 ZY= 4.7838

XZ= 1.2339 YZ= 4.8236 ZZ= 159.6406

Eigenvalues: -18.5478 12.6133 159.7887

4 C Isotropic = 12.1606 Anisotropy = 164.4825

XX= -46.2525 YX= 3.1296 ZX= 1.6940

XY= -7.6796 YY= -38.9288 ZY= 4.7166

XZ= 2.2204 YZ= 4.4723 ZZ= 121.6629

Eigenvalues: -46.9608 -38.3731 121.8155

5 C Isotropic = 54.9838 Anisotropy = 156.7577

XX= 33.6831 YX= -29.1474 ZX= 2.4226

XY= -25.1872 YY= -28.0204 ZY= 5.8444

XZ= 2.1723 YZ= 5.8675 ZZ= 159.2888

Eigenvalues: -38.4770 43.9396 159.4889

6 C Isotropic = 44.4436 Anisotropy = 184.8795

XX= 20.2684 YX= 36.7145 ZX= 0.6276

XY= 37.8048 YY= -54.4557 ZY= 5.9957

XZ= 0.5125 YZ= 5.9621 ZZ= 167.5182

Eigenvalues: -69.9779 35.6121 167.6966

7 C Isotropic = 38.9921 Anisotropy = 183.8960

XX= -33.5779 YX= 6.9637 ZX= 1.9091

XY= 3.1041 YY= -10.8835 ZY= 4.7953

XZ= 1.9763 YZ= 4.6554 ZZ= 161.4378

Eigenvalues: -34.6487 -9.9643 161.5894

8 N Isotropic = 3.7083 Anisotropy = 314.2304

XX= -91.6930 YX= 80.3434 ZX= 0.9961

XY= 82.7776 YY= -110.1256 ZY= 8.3021

XZ= 1.1171 YZ= 8.4250 ZZ= 212.9436

Eigenvalues: -183.0662 -19.0040 213.1952

9 H Isotropic = 22.6483 Anisotropy = 10.0997

XX= 29.3502 YX= -0.4739 ZX= 0.0727

XY= -0.4198 YY= 22.8718 ZY= -0.1246

XZ= 0.0904 YZ= -0.1597 ZZ= 15.7231

Eigenvalues: 15.7199 22.8437 29.3815

10 H Isotropic = 23.1392 Anisotropy = 6.9290

XX= 27.3716 YX= 1.1823 ZX= -0.0857

XY= 1.3119 YY= 23.7223 ZY= -0.1371

XZ= -0.0824 YZ= -0.1376 ZZ= 18.3238

Eigenvalues: 18.3200 23.3391 27.7586

11 C Isotropic = 58.9381 Anisotropy = 166.4378

XX= -13.2715 YX= -39.2685 ZX= 3.1415

XY= -36.5304 YY= 20.3490 ZY= 4.5878

XZ= 3.0309 YZ= 4.5056 ZZ= 169.7369

Eigenvalues: -38.0451 44.9628 169.8967

12 C Isotropic = 24.3844 Anisotropy = 155.7341

XX= -31.1039 YX= -13.2984 ZX= 2.1847

XY= -3.5544 YY= -23.8000 ZY= 4.3405

XZ= 1.7515 YZ= 4.6002 ZZ= 128.0570

Eigenvalues: -36.7378 -18.3162 128.2071

13 C Isotropic = 40.7080 Anisotropy = 155.2674

XX= -14.4170 YX= -17.8909 ZX= 2.4865

XY= -23.5121 YY= -7.5238 ZY= 4.5559

XZ= 2.5765 YZ= 4.3673 ZZ= 144.0647

Eigenvalues: -32.0885 9.9929 144.2196

14 H Isotropic = 22.5234 Anisotropy = 7.2451

XX= 25.5008 YX= -2.3264 ZX= -0.0310

XY= -0.7783 YY= 26.0498 ZY= -0.2375

XZ= -0.1018 YZ= -0.2366 ZZ= 16.0196

Eigenvalues: 16.0128 24.2039 27.3535

15 C Isotropic = 50.4772 Anisotropy = 114.9052

XX= 55.1316 YX= -21.1488 ZX= 1.4290

XY= -20.0817 YY= -30.6385 ZY= 4.6339

XZ= 1.4218 YZ= 4.5036 ZZ= 126.9384

Eigenvalues: -35.4764 59.8272 127.0806

16 N Isotropic = 20.5317 Anisotropy = 260.3619

XX= -88.7557 YX= 28.9000 ZX= 2.7434

XY= 35.5225 YY= -43.5597 ZY= 6.0754

XZ= 2.0728 YZ= 6.1805 ZZ= 193.9107

Eigenvalues: -105.5070 -27.0042 194.1063

17 H Isotropic = 23.0056 Anisotropy = 8.5940

XX= 28.6016 YX= 0.8400 ZX= -0.1524

XY= 0.7444 YY= 23.8935 ZY= -0.1754

XZ= -0.2045 YZ= -0.2321 ZZ= 16.5216

Eigenvalues: 16.5139 23.7679 28.7349

18 H Isotropic = 18.9019 Anisotropy = 13.0244

XX= 22.8318 YX= -1.6550 ZX= 0.0236

XY= -0.8712 YY= 27.2469 ZY= -0.1805

XZ= -0.1659 YZ= -0.2940 ZZ= 6.6270

Eigenvalues: 6.6238 22.4970 27.5848

19 C Isotropic = 110.3701 Anisotropy = 65.2696

XX= 129.5768 YX= -34.4695 ZX= 0.5510

XY= -26.1680 YY= 116.0585 ZY= -0.3015

XZ= 0.0360 YZ= -0.3048 ZZ= 85.4752

Eigenvalues: 85.4722 91.7550 153.8832

20 H Isotropic = 23.5664 Anisotropy = 5.2001

XX= 24.9214 YX= -0.1355 ZX= -0.0461

XY= -0.3521 YY= 27.0001 ZY= -0.2058

XZ= -0.0588 YZ= -0.2116 ZZ= 18.7779

Eigenvalues: 18.7720 24.8941 27.0332

21 H Isotropic = 22.3612 Anisotropy = 8.1234

XX= 26.2612 YX= -1.9723 ZX= -0.0374

XY= -2.4340 YY= 24.5730 ZY= -0.1799

XZ= -0.0401 YZ= -0.1877 ZZ= 16.2495

Eigenvalues: 16.2446 23.0622 27.7768

22 C Isotropic = 155.1991 Anisotropy = 30.1770

XX= 156.7256 YX= -4.6433 ZX= -11.7449

XY= -3.2290 YY= 145.0570 ZY= -5.0856

XZ= -17.3951 YZ= 2.0587 ZZ= 163.8148

Eigenvalues: 141.1114 149.1689 175.3171

23 H Isotropic = 26.1592 Anisotropy = 7.1173

XX= 27.8023 YX= 0.5108 ZX= -0.0706

XY= 2.5535 YY= 30.1364 ZY= -0.2489

XZ= -0.1946 YZ= -0.2881 ZZ= 20.5388

Eigenvalues: 20.5301 27.0434 30.9040

24 C Isotropic = 155.5261 Anisotropy = 30.1749

XX= 157.7228 YX= -3.8966 ZX= 12.3797

XY= -2.0058 YY= 145.6001 ZY= 6.6336

XZ= 17.4104 YZ= -0.8573 ZZ= 163.2556

Eigenvalues: 141.3504 149.5853 175.6428

25 H Isotropic = 27.4439 Anisotropy = 9.4159

XX= 27.5872 YX= 3.5830 ZX= -0.8499

XY= 2.7230 YY= 32.0884 ZY= 0.3724

XZ= -1.7717 YZ= 1.6938 ZZ= 22.6560

Eigenvalues: 21.9746 26.6360 33.7211

26 H Isotropic = 29.2363 Anisotropy = 7.6933

XX= 28.2144 YX= 0.9485 ZX= 1.2038

XY= 0.4107 YY= 26.6397 ZY= 1.6478

XZ= 0.0927 YZ= 4.8519 ZZ= 32.8548

Eigenvalues: 25.2040 28.1398 34.3652

27 H Isotropic = 29.0175 Anisotropy = 10.2509

XX= 32.1786 YX= -3.6813 ZX= -1.8189

XY= -3.5817 YY= 29.2838 ZY= 1.6785

XZ= -3.0831 YZ= 3.6093 ZZ= 25.5901

Eigenvalues: 24.1638 27.0372 35.8514

28 H Isotropic = 27.4531 Anisotropy = 10.1654

XX= 27.5977 YX= 3.7768 ZX= 0.6480

XY= 3.1139 YY= 32.3364 ZY= -0.6729

XZ= 1.1939 YZ= -2.4866 ZZ= 22.4253

Eigenvalues: 21.7533 26.3760 34.2301

29 H Isotropic = 29.0650 Anisotropy = 10.1465

XX= 32.3484 YX= -3.6159 ZX= 1.9217

XY= -3.3862 YY= 29.1430 ZY= -1.5791

XZ= 2.9761 YZ= -3.8086 ZZ= 25.7035

Eigenvalues: 24.1869 27.1788 35.8293

30 H Isotropic = 29.3018 Anisotropy = 7.6635

XX= 28.1880 YX= 0.8142 ZX= -1.0521

XY= 0.4535 YY= 26.4546 ZY= -1.1771

XZ= -0.1139 YZ= -4.5789 ZZ= 33.2628

Eigenvalues: 25.3449 28.1497 34.4108

31 C Isotropic = 57.0886 Anisotropy = 169.9646

XX= -49.8965 YX= -3.8332 ZX= -2.3770

XY= -8.5723 YY= 50.8941 ZY= -3.6085

XZ= -2.4511 YZ= -3.5599 ZZ= 170.2682

Eigenvalues: -50.3082 51.1756 170.3983

32 C Isotropic = 50.1039 Anisotropy = 179.6215

XX= -2.3713 YX= -44.9816 ZX= -3.1163

XY= -44.0537 YY= -16.9670 ZY= -5.8859

XZ= -2.9693 YZ= -5.8640 ZZ= 169.6502

Eigenvalues: -54.9661 35.4263 169.8516

33 C Isotropic = 51.2814 Anisotropy = 162.7427

XX= 9.3760 YX= 12.0645 ZX= -1.2999

XY= 7.1175 YY= -15.1567 ZY= -4.8948

XZ= -1.1027 YZ= -4.9047 ZZ= 159.6248

Eigenvalues: -18.5623 12.6299 159.7765

34 C Isotropic = 12.1766 Anisotropy = 164.4835

XX= -46.2394 YX= 3.1151 ZX= -1.6349

XY= -7.6950 YY= -38.9038 ZY= -4.8415

XZ= -2.1893 YZ= -4.6136 ZZ= 121.6730

Eigenvalues: -46.9547 -38.3478 121.8323

35 C Isotropic = 54.9857 Anisotropy = 156.7481

XX= 33.6778 YX= -29.1556 ZX= -2.3520

XY= -25.1855 YY= -27.9953 ZY= -5.9923

XZ= -2.1420 YZ= -6.0805 ZZ= 159.2746

Eigenvalues: -38.4676 43.9403 159.4844

36 C Isotropic = 44.4340 Anisotropy = 184.8782

XX= 20.2546 YX= 36.7121 ZX= -0.4532

XY= 37.8012 YY= -54.4477 ZY= -6.2678

XZ= -0.3589 YZ= -6.2370 ZZ= 167.4951

Eigenvalues: -69.9855 35.6014 167.6861

37 C Isotropic = 38.9948 Anisotropy = 183.9029

XX= -33.5801 YX= 6.9725 ZX= -1.9106

XY= 3.1092 YY= -10.8798 ZY= -4.8306

XZ= -1.9532 YZ= -4.6560 ZZ= 161.4443

Eigenvalues: -34.6534 -9.9590 161.5968

38 N Isotropic = 3.7348 Anisotropy = 314.2083

XX= -91.6598 YX= 80.3385 ZX= -0.9416

XY= 82.7642 YY= -110.0773 ZY= -8.4623

XZ= -1.1642 YZ= -8.7445 ZZ= 212.9415

Eigenvalues: -183.0207 -18.9819 213.2070

39 H Isotropic = 22.6478 Anisotropy = 10.1014

XX= 29.3507 YX= -0.4737 ZX= -0.0749

XY= -0.4188 YY= 22.8707 ZY= 0.1305

XZ= -0.0959 YZ= 0.1661 ZZ= 15.7218

Eigenvalues: 15.7183 22.8430 29.3820

40 H Isotropic = 23.1376 Anisotropy = 6.9285

XX= 27.3702 YX= 1.1812 ZX= 0.0830

XY= 1.3108 YY= 23.7217 ZY= 0.1390

XZ= 0.0754 YZ= 0.1456 ZZ= 18.3209

Eigenvalues: 18.3169 23.3393 27.7566

41 C Isotropic = 58.9247 Anisotropy = 166.4428

XX= -13.2892 YX= -39.2629 ZX= -3.2004

XY= -36.5190 YY= 20.3368 ZY= -4.6120

XZ= -3.0592 YZ= -4.4587 ZZ= 169.7265

Eigenvalues: -38.0548 44.9423 169.8866

42 C Isotropic = 24.3793 Anisotropy = 155.7373

XX= -31.1060 YX= -13.2988 ZX= -2.2256

XY= -3.5498 YY= -23.8054 ZY= -4.3786

XZ= -1.8037 YZ= -4.6932 ZZ= 128.0492

Eigenvalues: -36.7428 -18.3235 128.2041

43 C Isotropic = 40.7123 Anisotropy = 155.2573

XX= -14.4072 YX= -17.9035 ZX= -2.5628

XY= -23.5220 YY= -7.5157 ZY= -4.5449

XZ= -2.6735 YZ= -4.3841 ZZ= 144.0599

Eigenvalues: -32.0943 10.0141 144.2172

44 H Isotropic = 22.5221 Anisotropy = 7.2442

XX= 25.4997 YX= -2.3255 ZX= 0.0305

XY= -0.7779 YY= 26.0485 ZY= 0.2409

XZ= 0.1053 YZ= 0.2373 ZZ= 16.0182

Eigenvalues: 16.0113 24.2035 27.3516

45 C Isotropic = 50.4858 Anisotropy = 114.9215

XX= 55.1400 YX= -21.1568 ZX= -1.4537

XY= -20.0967 YY= -30.6403 ZY= -4.6397

XZ= -1.4367 YZ= -4.4875 ZZ= 126.9578

Eigenvalues: -35.4825 59.8398 127.1002

46 N Isotropic = 20.5328 Anisotropy = 260.3773

XX= -88.7460 YX= 28.8747 ZX= -2.9434

XY= 35.5010 YY= -43.5773 ZY= -5.9963

XZ= -2.2256 YZ= -6.1194 ZZ= 193.9216

Eigenvalues: -105.4831 -27.0362 194.1176

47 H Isotropic = 23.0063 Anisotropy = 8.5943

XX= 28.6030 YX= 0.8382 ZX= 0.1553

XY= 0.7430 YY= 23.8927 ZY= 0.1785

XZ= 0.2090 YZ= 0.2298 ZZ= 16.5232

Eigenvalues: 16.5154 23.7677 28.7358

48 H Isotropic = 18.9019 Anisotropy = 13.0245

XX= 22.8314 YX= -1.6548 ZX= -0.0215

XY= -0.8720 YY= 27.2468 ZY= 0.1830

XZ= 0.1774 YZ= 0.2951 ZZ= 6.6274

Eigenvalues: 6.6241 22.4966 27.5849

49 C Isotropic = 110.3604 Anisotropy = 65.2821

XX= 129.5707 YX= -34.4752 ZX= -0.5088

XY= -26.1734 YY= 116.0520 ZY= 0.2819

XZ= -0.0014 YZ= 0.2714 ZZ= 85.4586

Eigenvalues: 85.4561 91.7434 153.8818

50 H Isotropic = 23.5660 Anisotropy = 5.2006

XX= 24.9202 YX= -0.1354 ZX= 0.0446

XY= -0.3525 YY= 26.9996 ZY= 0.2122

XZ= 0.0510 YZ= 0.2183 ZZ= 18.7783

Eigenvalues: 18.7722 24.8928 27.0331

51 H Isotropic = 22.3613 Anisotropy = 8.1251

XX= 26.2610 YX= -1.9742 ZX= 0.0330

XY= -2.4355 YY= 24.5717 ZY= 0.1853

XZ= 0.0348 YZ= 0.1967 ZZ= 16.2512

Eigenvalues: 16.2461 23.0598 27.7780

52 C Isotropic = 155.2122 Anisotropy = 30.1857

XX= 156.7099 YX= -4.6408 ZX= 11.7431

XY= -3.2347 YY= 145.0683 ZY= 5.0988

XZ= 17.3942 YZ= -2.0569 ZZ= 163.8582

Eigenvalues: 141.1144 149.1861 175.3360

53 H Isotropic = 26.1586 Anisotropy = 7.1166

XX= 27.8019 YX= 0.5109 ZX= 0.0724

XY= 2.5533 YY= 30.1353 ZY= 0.2502

XZ= 0.1999 YZ= 0.2827 ZZ= 20.5386

Eigenvalues: 20.5300 27.0428 30.9030

54 C Isotropic = 155.5216 Anisotropy = 30.1671

XX= 157.7464 YX= -3.9009 ZX= -12.3817

XY= -2.0053 YY= 145.5946 ZY= -6.6145

XZ= -17.4078 YZ= 0.8653 ZZ= 163.2238

Eigenvalues: 141.3554 149.5764 175.6330

55 H Isotropic = 27.4457 Anisotropy = 9.4145

XX= 27.5829 YX= 3.5821 ZX= 0.8479

XY= 2.7238 YY= 32.0909 ZY= -0.3706

XZ= 1.7736 YZ= -1.6925 ZZ= 22.6635

Eigenvalues: 21.9812 26.6340 33.7221

56 H Isotropic = 29.2402 Anisotropy = 7.6925

XX= 28.2187 YX= 0.9487 ZX= -1.2093

XY= 0.4089 YY= 26.6411 ZY= -1.6427

XZ= -0.0966 YZ= -4.8486 ZZ= 32.8610

Eigenvalues: 25.2096 28.1425 34.3686

57 H Isotropic = 29.0184 Anisotropy = 10.2514

XX= 32.1725 YX= -3.6821 ZX= 1.8232

XY= -3.5812 YY= 29.2838 ZY= -1.6812

XZ= 3.0877 YZ= -3.6152 ZZ= 25.5989

Eigenvalues: 24.1672 27.0353 35.8527

58 H Isotropic = 27.4522 Anisotropy = 10.1652

XX= 27.6032 YX= 3.7779 ZX= -0.6507

XY= 3.1122 YY= 32.3340 ZY= 0.6740

XZ= -1.1937 YZ= 2.4873 ZZ= 22.4196

Eigenvalues: 21.7477 26.3800 34.2290

59 H Isotropic = 29.0651 Anisotropy = 10.1470

XX= 32.3547 YX= -3.6169 ZX= -1.9168

XY= -3.3884 YY= 29.1452 ZY= 1.5764

XZ= -2.9705 YZ= 3.8019 ZZ= 25.6955

Eigenvalues: 24.1854 27.1802 35.8297

60 H Isotropic = 29.2994 Anisotropy = 7.6641

XX= 28.1858 YX= 0.8141 ZX= 1.0470

XY= 0.4551 YY= 26.4544 ZY= 1.1828

XZ= 0.1105 YZ= 4.5827 ZZ= 33.2582

Eigenvalues: 25.3407 28.1488 34.4088

## Norharman dimer\_iso 2 (gas-phase) - BP86/IGLO-III level

60

C -6.41695 0.64808 -0.01475

C -5.75782 -0.58069 0.02255

C -4.34174 -0.59788 -0.00495

C -3.58261 0.64233 -0.07045

C -4.28373 1.87868 -0.10865

C -5.67781 1.86585 -0.08045

C -3.34947 -1.62577 0.01725

N -2.22412 0.44700 -0.08825

H -3.72719 2.82850 -0.16225

H -6.22802 2.82203 -0.11035

C -3.33217 -3.03216 0.07445

C -2.07552 -0.90420 -0.03725

C -0.87869 -1.63850 -0.03285

H -4.25845 -3.62745 0.11725

C -2.10896 -3.69577 0.07765

N -0.92061 -2.99785 0.02465

H -2.02752 -4.78979 0.12145

H 0.13415 -1.19079 -0.07285

C 0.38140 -3.74034 0.03175

H -7.51858 0.68441 0.00575

H -6.33188 -1.52170 0.07235

C 0.56983 -4.50871 1.34705

H 1.14827 -2.93914 -0.01865

C 0.51907 -4.62416 -1.21555

H -0.15569 -5.34505 1.45475

H 0.45979 -3.83214 2.22145

H 1.59235 -4.94368 1.37775

H -0.20706 -5.46693 -1.21785

H 1.54086 -5.06067 -1.24805

H 0.37115 -4.02961 -2.14245

C 6.41678 -0.64827 -0.01525

C 5.75775 0.58050 0.02275

C 4.34167 0.59780 -0.00445

C 3.58253 -0.64241 -0.07005

C 4.28355 -1.87867 -0.10885

C 5.67764 -1.86604 -0.08115

C 3.34950 1.62569 0.01805

N 2.22394 -0.44700 -0.08745

H 3.72692 -2.82859 -0.16265

H 6.22785 -2.82212 -0.11165

C 3.33220 3.03217 0.07515

C 2.07554 0.90422 -0.03625

C 0.87871 1.63862 -0.03175

H 4.25848 3.62737 0.11775

C 2.10909 3.69569 0.07825

N 0.92073 2.99788 0.02555

H 2.02764 4.78981 0.12175

H -0.13423 1.19091 -0.07175

C -0.38128 3.74046 0.03205

H 7.51851 -0.68460 0.00485

H 6.33181 1.52151 0.07295

C -0.56959 4.51054 1.34645

H -1.14826 2.93925 -0.01735

C -0.51898 4.62277 -1.21635

H 0.15592 5.34698 1.45295

H -0.45941 3.83508 2.22165

H -1.59210 4.94541 1.37655

H 0.20746 5.46527 -1.21985

H -1.54058 5.05959 -1.24925

H -0.37131 4.02702 -2.14255

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 52.7766 Anisotropy = 164.5801

XX= -50.9342 YX= -4.5230 ZX= 4.5007

XY= -7.9532 YY= 47.0623 ZY= 4.9853

XZ= 4.4765 YZ= 4.8947 ZZ= 162.2017

Eigenvalues: -51.4373 47.2704 162.4967

2 C Isotropic = 48.8599 Anisotropy = 170.1690

XX= 1.8895 YX= -42.6041 ZX= 4.9775

XY= -42.2605 YY= -17.1815 ZY= 8.2226

XZ= 4.8928 YZ= 8.1761 ZZ= 161.8715

Eigenvalues: -51.5581 35.8318 162.3058

3 C Isotropic = 46.5651 Anisotropy = 158.6358

XX= 6.4332 YX= 11.7260 ZX= 2.4936

XY= 3.3390 YY= -18.7279 ZY= 6.9331

XZ= 2.4654 YZ= 6.8845 ZZ= 151.9901

Eigenvalues: -21.0192 8.3922 152.3224

4 C Isotropic = 10.0898 Anisotropy = 155.9796

XX= -45.7512 YX= 1.3035 ZX= 3.0954

XY= -8.2140 YY= -37.7164 ZY= 6.6270

XZ= 3.9003 YZ= 6.1476 ZZ= 113.7371

Eigenvalues: -47.2232 -36.5835 114.0762

5 C Isotropic = 52.2662 Anisotropy = 146.1631

XX= 33.2850 YX= -29.2196 ZX= 3.7221

XY= -28.6900 YY= -25.7561 ZY= 8.2822

XZ= 3.4552 YZ= 8.3599 ZZ= 149.2697

Eigenvalues: -38.0241 45.1144 149.7083

6 C Isotropic = 42.3756 Anisotropy = 176.3177

XX= 18.1365 YX= 37.0191 ZX= 1.3148

XY= 38.7711 YY= -50.5599 ZY= 8.1943

XZ= 1.0877 YZ= 8.1565 ZZ= 159.5503

Eigenvalues: -67.5720 34.7782 159.9208

7 C Isotropic = 38.2726 Anisotropy = 175.0148

XX= -29.7145 YX= 7.0914 ZX= 3.3456

XY= -0.3324 YY= -10.0797 ZY= 6.8097

XZ= 3.7876 YZ= 6.3654 ZZ= 154.6120

Eigenvalues: -30.3122 -9.8191 154.9492

8 N Isotropic = -7.7788 Anisotropy = 315.3302

XX= -103.7130 YX= 76.5093 ZX= 2.8889

XY= 89.6440 YY= -121.5276 ZY= 11.1718

XZ= 2.7795 YZ= 12.1087 ZZ= 201.9042

Eigenvalues: -196.2882 -29.4895 202.4413

9 H Isotropic = 23.2003 Anisotropy = 8.6535

XX= 28.8636 YX= -0.9309 ZX= 0.1106

XY= -0.5582 YY= 23.6626 ZY= -0.1101

XZ= 0.1004 YZ= -0.1579 ZZ= 17.0749

Eigenvalues: 17.0714 23.5603 28.9693

10 H Isotropic = 23.4279 Anisotropy = 6.5601

XX= 27.2969 YX= 1.3392 ZX= -0.1569

XY= 1.4188 YY= 23.9867 ZY= -0.1932

XZ= -0.1542 YZ= -0.1978 ZZ= 19.0001

Eigenvalues: 18.9911 23.4913 27.8013

11 C Isotropic = 56.7367 Anisotropy = 160.4926

XX= -11.6732 YX= -40.0329 ZX= 5.1592

XY= -36.9060 YY= 18.5362 ZY= 6.7728

XZ= 5.0714 YZ= 6.8196 ZZ= 163.3472

Eigenvalues: -38.2191 44.6975 163.7318

12 C Isotropic = 22.5945 Anisotropy = 146.2795

XX= -31.5824 YX= -13.7915 ZX= 3.8041

XY= -4.4786 YY= -20.4222 ZY= 5.9173

XZ= 2.9586 YZ= 6.3361 ZZ= 119.7882

Eigenvalues: -36.9333 -15.3973 120.1142

13 C Isotropic = 38.1097 Anisotropy = 125.3378

XX= -4.0106 YX= -22.9614 ZX= 3.7925

XY= -23.1055 YY= -3.0135 ZY= 5.8238

XZ= 3.6577 YZ= 5.4746 ZZ= 121.3530

Eigenvalues: -26.8461 19.5069 121.6682

14 H Isotropic = 22.8500 Anisotropy = 7.4573

XX= 25.8186 YX= -2.6161 ZX= -0.0495

XY= -1.1498 YY= 26.0472 ZY= -0.3148

XZ= -0.1530 YZ= -0.3095 ZZ= 16.6842

Eigenvalues: 16.6707 24.0577 27.8215

15 C Isotropic = 57.6963 Anisotropy = 134.1484

XX= 50.6885 YX= -15.5583 ZX= 2.6397

XY= -11.6888 YY= -24.3631 ZY= 7.4429

XZ= 2.3624 YZ= 7.5370 ZZ= 146.7633

Eigenvalues: -27.1104 53.0706 147.1285

16 N Isotropic = 26.2020 Anisotropy = 233.1189

XX= -73.7723 YX= 26.1915 ZX= 4.0937

XY= 36.2653 YY= -28.8276 ZY= 8.2350

XZ= 3.2562 YZ= 8.0158 ZZ= 181.2059

Eigenvalues: -89.7742 -13.2344 181.6146

17 H Isotropic = 23.5077 Anisotropy = 10.1382

XX= 30.2395 YX= 0.9747 ZX= -0.2674

XY= -0.2182 YY= 23.0979 ZY= -0.1755

XZ= -0.3146 YZ= -0.3085 ZZ= 17.1857

Eigenvalues: 17.1700 23.0866 30.2665

18 H Isotropic = 18.3058 Anisotropy = 11.7413

XX= 23.8812 YX= 0.2528 ZX= -0.0444

XY= 0.3263 YY= 26.0900 ZY= -0.2401

XZ= -0.3443 YZ= -0.4291 ZZ= 4.9461

Eigenvalues: 4.9390 23.8451 26.1333

19 C Isotropic = 109.6770 Anisotropy = 61.6870

XX= 140.1163 YX= -19.7377 ZX= -0.1165

XY= -27.5574 YY= 98.4672 ZY= 0.3034

XZ= 0.1401 YZ= -0.0341 ZZ= 90.4474

Eigenvalues: 87.7758 90.4535 150.8016

20 H Isotropic = 23.7522 Anisotropy = 5.2250

XX= 24.7022 YX= -0.1980 ZX= -0.0722

XY= -0.2906 YY= 27.2015 ZY= -0.2927

XZ= -0.1015 YZ= -0.2989 ZZ= 19.3529

Eigenvalues: 19.3401 24.6810 27.2356

21 H Isotropic = 22.7270 Anisotropy = 8.0338

XX= 26.5912 YX= -2.0100 ZX= -0.0825

XY= -2.5374 YY= 24.6161 ZY= -0.2330

XZ= -0.0829 YZ= -0.2543 ZZ= 16.9739

Eigenvalues: 16.9634 23.1348 28.0829

22 C Isotropic = 150.3622 Anisotropy = 35.8982

XX= 142.0613 YX= -4.9514 ZX= 3.3501

XY= -6.3073 YY= 144.4145 ZY= -14.1859

XZ= 8.8002 YZ= -15.1077 ZZ= 164.6108

Eigenvalues: 135.7097 141.0825 174.2943

23 H Isotropic = 24.1619 Anisotropy = 11.0764

XX= 27.3883 YX= 4.0965 ZX= -0.2597

XY= 1.7760 YY= 29.4426 ZY= -0.2276

XZ= -0.4631 YZ= -0.6423 ZZ= 15.6548

Eigenvalues: 15.6346 25.3049 31.5461

24 C Isotropic = 150.3690 Anisotropy = 35.9433

XX= 141.5518 YX= -4.4824 ZX= -2.0984

XY= -6.4654 YY= 147.1468 ZY= 16.2628

XZ= -7.2768 YZ= 16.5580 ZZ= 162.4083

Eigenvalues: 135.7169 141.0588 174.3312

25 H Isotropic = 29.2592 Anisotropy = 7.4577

XX= 29.4850 YX= 1.8328 ZX= 0.0274

XY= 2.5178 YY= 31.3285 ZY= -2.2510

XZ= 0.0655 YZ= -5.2336 ZZ= 26.9641

Eigenvalues: 24.5372 29.0094 34.2310

26 H Isotropic = 29.2028 Anisotropy = 5.9225

XX= 26.3146 YX= -0.1142 ZX= 0.5124

XY= 0.1007 YY= 28.4335 ZY= 0.8794

XZ= 2.2555 YZ= -0.4259 ZZ= 32.8602

Eigenvalues: 26.0329 28.4243 33.1511

27 H Isotropic = 29.2317 Anisotropy = 9.4645

XX= 32.6807 YX= -2.7592 ZX= 1.9440

XY= -3.2543 YY= 28.5198 ZY= -1.6245

XZ= 3.0228 YZ= -3.4717 ZZ= 26.4948

Eigenvalues: 24.7396 27.4142 35.5414

28 H Isotropic = 29.2124 Anisotropy = 7.4138

XX= 29.4367 YX= 2.0054 ZX= -0.2651

XY= 2.5447 YY= 31.8734 ZY= 1.8492

XZ= -0.4802 YZ= 4.5887 ZZ= 26.3271

Eigenvalues: 24.4866 28.9957 34.1549

29 H Isotropic = 29.1666 Anisotropy = 9.5579

XX= 32.4439 YX= -2.8711 ZX= -1.8532

XY= -3.5144 YY= 28.8234 ZY= 1.7867

XZ= -3.0228 YZ= 3.2360 ZZ= 26.2325

Eigenvalues: 24.6666 27.2946 35.5385

30 H Isotropic = 29.1240 Anisotropy = 6.1435

XX= 26.1751 YX= -0.1970 ZX= -0.1677

XY= -0.2525 YY= 28.1739 ZY= -0.3022

XZ= -2.1066 YZ= 0.7431 ZZ= 33.0230

Eigenvalues: 25.9753 28.1770 33.2196

31 C Isotropic = 52.7691 Anisotropy = 164.5786

XX= -50.9405 YX= -4.5181 ZX= -4.4283

XY= -7.9452 YY= 47.0558 ZY= -5.0285

XZ= -4.4174 YZ= -4.9354 ZZ= 162.1922

Eigenvalues: -51.4400 47.2592 162.4882

32 C Isotropic = 48.8615 Anisotropy = 170.1596

XX= 1.8988 YX= -42.6008 ZX= -4.9689

XY= -42.2604 YY= -17.1771 ZY= -8.2974

XZ= -4.8631 YZ= -8.2223 ZZ= 161.8627

Eigenvalues: -51.5533 35.8366 162.3013

33 C Isotropic = 46.5652 Anisotropy = 158.6537

XX= 6.4314 YX= 11.7288 ZX= -2.4671

XY= 3.3350 YY= -18.7361 ZY= -6.9672

XZ= -2.3945 YZ= -6.9386 ZZ= 152.0003

Eigenvalues: -21.0305 8.3918 152.3343

34 C Isotropic = 10.0895 Anisotropy = 155.9685

XX= -45.7432 YX= 1.2971 ZX= -3.0454

XY= -8.2042 YY= -37.7158 ZY= -6.6695

XZ= -3.8658 YZ= -6.1924 ZZ= 113.7275

Eigenvalues: -47.2134 -36.5866 114.0685

35 C Isotropic = 52.2691 Anisotropy = 146.1517

XX= 33.2861 YX= -29.2065 ZX= -3.6937

XY= -28.6889 YY= -25.7395 ZY= -8.3362

XZ= -3.4315 YZ= -8.4243 ZZ= 149.2607

Eigenvalues: -38.0092 45.1129 149.7036

36 C Isotropic = 42.3833 Anisotropy = 176.3121

XX= 18.1386 YX= 37.0223 ZX= -1.2483

XY= 38.7749 YY= -50.5373 ZY= -8.2883

XZ= -1.0278 YZ= -8.2508 ZZ= 159.5486

Eigenvalues: -67.5624 34.7876 159.9247

37 C Isotropic = 38.2820 Anisotropy = 175.0010

XX= -29.6972 YX= 7.0974 ZX= -3.3143

XY= -0.3318 YY= -10.0710 ZY= -6.8040

XZ= -3.7133 YZ= -6.3702 ZZ= 154.6143

Eigenvalues: -30.2948 -9.8085 154.9494

38 N Isotropic = -7.7988 Anisotropy = 315.3203

XX= -103.7150 YX= 76.4980 ZX= -2.8136

XY= 89.6349 YY= -121.5544 ZY= -11.2498

XZ= -2.7385 YZ= -12.1984 ZZ= 201.8731

Eigenvalues: -196.2973 -29.5138 202.4148

39 H Isotropic = 23.1986 Anisotropy = 8.6542

XX= 28.8630 YX= -0.9278 ZX= -0.1140

XY= -0.5560 YY= 23.6624 ZY= 0.1111

XZ= -0.1040 YZ= 0.1602 ZZ= 17.0704

Eigenvalues: 17.0669 23.5608 28.9681

40 H Isotropic = 23.4286 Anisotropy = 6.5603

XX= 27.2970 YX= 1.3405 ZX= 0.1554

XY= 1.4201 YY= 23.9871 ZY= 0.1935

XZ= 0.1514 YZ= 0.2004 ZZ= 19.0017

Eigenvalues: 18.9927 23.4910 27.8022

41 C Isotropic = 56.7484 Anisotropy = 160.4941

XX= -11.6683 YX= -40.0325 ZX= -5.1385

XY= -36.8970 YY= 18.5494 ZY= -6.7481

XZ= -5.0408 YZ= -6.7654 ZZ= 163.3641

Eigenvalues: -38.2037 44.7045 163.7445

42 C Isotropic = 22.5883 Anisotropy = 146.2866

XX= -31.6022 YX= -13.7866 ZX= -3.7828

XY= -4.4706 YY= -20.4182 ZY= -5.9269

XZ= -2.9603 YZ= -6.3666 ZZ= 119.7854

Eigenvalues: -36.9419 -15.4058 120.1127

43 C Isotropic = 38.1068 Anisotropy = 125.3360

XX= -4.0138 YX= -22.9672 ZX= -3.7877

XY= -23.1079 YY= -3.0156 ZY= -5.8079

XZ= -3.6913 YZ= -5.4562 ZZ= 121.3497

Eigenvalues: -26.8527 19.5089 121.6641

44 H Isotropic = 22.8511 Anisotropy = 7.4569

XX= 25.8187 YX= -2.6159 ZX= 0.0485

XY= -1.1492 YY= 26.0493 ZY= 0.3157

XZ= 0.1521 YZ= 0.3082 ZZ= 16.6852

Eigenvalues: 16.6718 24.0591 27.8223

45 C Isotropic = 57.7176 Anisotropy = 134.1169

XX= 50.7124 YX= -15.5738 ZX= -2.6311

XY= -11.6977 YY= -24.3284 ZY= -7.3946

XZ= -2.3850 YZ= -7.4547 ZZ= 146.7688

Eigenvalues: -27.0746 53.0985 147.1289

46 N Isotropic = 26.2304 Anisotropy = 233.0866

XX= -73.7476 YX= 26.1812 ZX= -4.0964

XY= 36.2491 YY= -28.7783 ZY= -8.1803

XZ= -3.2441 YZ= -7.9682 ZZ= 181.2171

Eigenvalues: -89.7337 -13.1966 181.6214

47 H Isotropic = 23.5074 Anisotropy = 10.1366

XX= 30.2383 YX= 0.9743 ZX= 0.2650

XY= -0.2185 YY= 23.1008 ZY= 0.1778

XZ= 0.3130 YZ= 0.3100 ZZ= 17.1832

Eigenvalues: 17.1674 23.0896 30.2652

48 H Isotropic = 18.3055 Anisotropy = 11.7420

XX= 23.8806 YX= 0.2535 ZX= 0.0465

XY= 0.3267 YY= 26.0899 ZY= 0.2416

XZ= 0.3536 YZ= 0.4344 ZZ= 4.9460

Eigenvalues: 4.9386 23.8444 26.1335

49 C Isotropic = 109.6547 Anisotropy = 61.6999

XX= 140.0968 YX= -19.7425 ZX= 0.1297

XY= -27.5651 YY= 98.4545 ZY= -0.2846

XZ= -0.0960 YZ= 0.0380 ZZ= 90.4128

Eigenvalues: 87.7592 90.4169 150.7880

50 H Isotropic = 23.7512 Anisotropy = 5.2242

XX= 24.7028 YX= -0.1981 ZX= 0.0713

XY= -0.2899 YY= 27.1998 ZY= 0.2947

XZ= 0.0997 YZ= 0.3009 ZZ= 19.3509

Eigenvalues: 19.3380 24.6816 27.2340

51 H Isotropic = 22.7267 Anisotropy = 8.0341

XX= 26.5919 YX= -2.0090 ZX= 0.0797

XY= -2.5374 YY= 24.6153 ZY= 0.2341

XZ= 0.0826 YZ= 0.2575 ZZ= 16.9729

Eigenvalues: 16.9623 23.1350 28.0828

52 C Isotropic = 150.3766 Anisotropy = 35.8872

XX= 142.0723 YX= -4.9552 ZX= -3.3465

XY= -6.3119 YY= 144.4589 ZY= 14.2105

XZ= -8.7645 YZ= 15.1155 ZZ= 164.5986

Eigenvalues: 135.7239 141.1046 174.3014

53 H Isotropic = 24.1619 Anisotropy = 11.0745

XX= 27.3876 YX= 4.0960 ZX= 0.2546

XY= 1.7755 YY= 29.4420 ZY= 0.2268

XZ= 0.4620 YZ= 0.6446 ZZ= 15.6562

Eigenvalues: 15.6361 25.3047 31.5449

54 C Isotropic = 150.3611 Anisotropy = 35.9557

XX= 141.5406 YX= -4.4843 ZX= 2.1041

XY= -6.4688 YY= 147.1084 ZY= -16.2402

XZ= 7.3096 YZ= -16.5518 ZZ= 162.4343

Eigenvalues: 135.7095 141.0422 174.3316

55 H Isotropic = 29.2590 Anisotropy = 7.4587

XX= 29.4863 YX= 1.8336 ZX= -0.0297

XY= 2.5193 YY= 31.3359 ZY= 2.2487

XZ= -0.0666 YZ= 5.2266 ZZ= 26.9550

Eigenvalues: 24.5363 29.0093 34.2315

56 H Isotropic = 29.2034 Anisotropy = 5.9296

XX= 26.3148 YX= -0.1143 ZX= -0.5114

XY= 0.1000 YY= 28.4283 ZY= -0.8731

XZ= -2.2520 YZ= 0.4312 ZZ= 32.8672

Eigenvalues: 26.0343 28.4195 33.1565

57 H Isotropic = 29.2327 Anisotropy = 9.4641

XX= 32.6819 YX= -2.7618 ZX= -1.9412

XY= -3.2579 YY= 28.5240 ZY= 1.6259

XZ= -3.0154 YZ= 3.4696 ZZ= 26.4923

Eigenvalues: 24.7401 27.4160 35.5421

58 H Isotropic = 29.2132 Anisotropy = 7.4120

XX= 29.4381 YX= 2.0053 ZX= 0.2616

XY= 2.5438 YY= 31.8663 ZY= -1.8533

XZ= 0.4774 YZ= -4.5961 ZZ= 26.3353

Eigenvalues: 24.4882 28.9969 34.1546

59 H Isotropic = 29.1678 Anisotropy = 9.5582

XX= 32.4425 YX= -2.8708 ZX= 1.8554

XY= -3.5134 YY= 28.8222 ZY= -1.7856

XZ= 3.0285 YZ= -3.2380 ZZ= 26.2387

Eigenvalues: 24.6701 27.2934 35.5400

60 H Isotropic = 29.1235 Anisotropy = 6.1375

XX= 26.1740 YX= -0.1967 ZX= 0.1692

XY= -0.2523 YY= 28.1781 ZY= 0.3101

XZ= 2.1099 YZ= -0.7362 ZZ= 33.0184

Eigenvalues: 25.9733 28.1820 33.2151

## Norharman dimer\_iso 2 (gas-phase) – PBE0/IGLO-III level

60

gaussjob.log Energy: -816885.7719053

C -6.41695 0.64808 -0.01475

C -5.75782 -0.58069 0.02255

C -4.34174 -0.59788 -0.00495

C -3.58261 0.64233 -0.07045

C -4.28373 1.87868 -0.10865

C -5.67781 1.86585 -0.08045

C -3.34947 -1.62577 0.01725

N -2.22412 0.44700 -0.08825

H -3.72719 2.82850 -0.16225

H -6.22802 2.82203 -0.11035

C -3.33217 -3.03216 0.07445

C -2.07552 -0.90420 -0.03725

C -0.87869 -1.63850 -0.03285

H -4.25845 -3.62745 0.11725

C -2.10896 -3.69577 0.07765

N -0.92061 -2.99785 0.02465

H -2.02752 -4.78979 0.12145

H 0.13415 -1.19079 -0.07285

C 0.38140 -3.74034 0.03175

H -7.51858 0.68441 0.00575

H -6.33188 -1.52170 0.07235

C 0.56983 -4.50871 1.34705

H 1.14827 -2.93914 -0.01865

C 0.51907 -4.62416 -1.21555

H -0.15569 -5.34505 1.45475

H 0.45979 -3.83214 2.22145

H 1.59235 -4.94368 1.37775

H -0.20706 -5.46693 -1.21785

H 1.54086 -5.06067 -1.24805

H 0.37115 -4.02961 -2.14245

C 6.41678 -0.64827 -0.01525

C 5.75775 0.58050 0.02275

C 4.34167 0.59780 -0.00445

C 3.58253 -0.64241 -0.07005

C 4.28355 -1.87867 -0.10885

C 5.67764 -1.86604 -0.08115

C 3.34950 1.62569 0.01805

N 2.22394 -0.44700 -0.08745

H 3.72692 -2.82859 -0.16265

H 6.22785 -2.82212 -0.11165

C 3.33220 3.03217 0.07515

C 2.07554 0.90422 -0.03625

C 0.87871 1.63862 -0.03175

H 4.25848 3.62737 0.11775

C 2.10909 3.69569 0.07825

N 0.92073 2.99788 0.02555

H 2.02764 4.78981 0.12175

H -0.13423 1.19091 -0.07175

C -0.38128 3.74046 0.03205

H 7.51851 -0.68460 0.00485

H 6.33181 1.52151 0.07295

C -0.56959 4.51054 1.34645

H -1.14826 2.93925 -0.01735

C -0.51898 4.62277 -1.21635

H 0.15592 5.34698 1.45295

H -0.45941 3.83508 2.22165

H -1.59210 4.94541 1.37655

H 0.20746 5.46527 -1.21985

H -1.54058 5.05959 -1.24925

H -0.37131 4.02702 -2.14255

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 56.2626 Anisotropy = 169.3115

XX= -50.5886 YX= -5.9918 ZX= 4.6893

XY= -9.8528 YY= 50.5453 ZY= 5.1519

XZ= 4.7038 YZ= 5.0464 ZZ= 168.8312

Eigenvalues: -51.3227 50.9736 169.1370

2 C Isotropic = 50.2799 Anisotropy = 177.6937

XX= -0.1969 YX= -45.6194 ZX= 5.2722

XY= -44.7312 YY= -17.2519 ZY= 8.5405

XZ= 5.1561 YZ= 8.5232 ZZ= 168.2885

Eigenvalues: -55.1359 37.2332 168.7424

3 C Isotropic = 50.9944 Anisotropy = 162.6727

XX= 9.6402 YX= 12.8165 ZX= 2.5288

XY= 5.2129 YY= -15.7611 ZY= 7.0671

XZ= 2.4850 YZ= 7.0347 ZZ= 159.1040

Eigenvalues: -18.8353 12.3755 159.4429

4 C Isotropic = 11.8564 Anisotropy = 165.8051

XX= -46.8922 YX= 2.7201 ZX= 3.2274

XY= -7.8195 YY= -39.5708 ZY= 7.0362

XZ= 4.0656 YZ= 6.5958 ZZ= 122.0323

Eigenvalues: -47.8755 -38.9484 122.3932

5 C Isotropic = 55.3125 Anisotropy = 152.0040

XX= 37.0171 YX= -29.2266 ZX= 3.7874

XY= -29.1509 YY= -27.2720 ZY= 8.6480

XZ= 3.5230 YZ= 8.7416 ZZ= 156.1925

Eigenvalues: -39.0023 48.2914 156.6486

6 C Isotropic = 44.0613 Anisotropy = 183.8020

XX= 19.9158 YX= 37.7806 ZX= 1.3786

XY= 39.6503 YY= -53.9392 ZY= 8.6027

XZ= 1.1360 YZ= 8.5670 ZZ= 166.2071

Eigenvalues: -70.7454 36.3332 166.5959

7 C Isotropic = 40.1858 Anisotropy = 182.8721

XX= -30.3328 YX= 8.4155 ZX= 3.4453

XY= -0.1082 YY= -10.8575 ZY= 7.1296

XZ= 3.9197 YZ= 6.6851 ZZ= 161.7477

Eigenvalues: -31.2077 -10.3355 162.1006

8 N Isotropic = -1.1580 Anisotropy = 321.0255

XX= -97.8524 YX= 75.5713 ZX= 3.0077

XY= 88.2928 YY= -117.9296 ZY= 11.4897

XZ= 3.0042 YZ= 12.3305 ZZ= 212.3080

Eigenvalues: -190.5550 -25.7780 212.8590

9 H Isotropic = 23.0663 Anisotropy = 9.0430

XX= 29.0101 YX= -0.8241 ZX= 0.0967

XY= -0.5279 YY= 23.6425 ZY= -0.1317

XZ= 0.0962 YZ= -0.1836 ZZ= 16.5464

Eigenvalues: 16.5424 23.5616 29.0950

10 H Isotropic = 23.2797 Anisotropy = 6.7729

XX= 27.3279 YX= 1.2640 ZX= -0.1606

XY= 1.4079 YY= 23.9251 ZY= -0.2074

XZ= -0.1586 YZ= -0.2127 ZZ= 18.5860

Eigenvalues: 18.5764 23.4677 27.7949

11 C Isotropic = 58.9666 Anisotropy = 166.4547

XX= -11.2600 YX= -42.2293 ZX= 5.3677

XY= -39.2480 YY= 18.6242 ZY= 7.0708

XZ= 5.2812 YZ= 7.1090 ZZ= 169.5357

Eigenvalues: -40.0492 47.0126 169.9364

12 C Isotropic = 25.3152 Anisotropy = 154.4617

XX= -31.5980 YX= -13.6056 ZX= 3.9610

XY= -3.3988 YY= -20.4052 ZY= 6.2157

XZ= 3.1123 YZ= 6.6423 ZZ= 127.9487

Eigenvalues: -36.4126 -15.9316 128.2897

13 C Isotropic = 38.4084 Anisotropy = 133.6483

XX= -6.7856 YX= -24.3955 ZX= 4.0399

XY= -24.1182 YY= -5.1613 ZY= 6.1929

XZ= 3.8329 YZ= 5.8468 ZZ= 127.1722

Eigenvalues: -30.5560 18.2740 127.5073

14 H Isotropic = 22.6622 Anisotropy = 7.6811

XX= 25.8258 YX= -2.6309 ZX= -0.0580

XY= -1.1174 YY= 25.9839 ZY= -0.3324

XZ= -0.1655 YZ= -0.3306 ZZ= 16.1769

Eigenvalues: 16.1625 24.0412 27.7829

15 C Isotropic = 58.4454 Anisotropy = 141.4943

XX= 51.0284 YX= -17.4973 ZX= 2.8245

XY= -13.7190 YY= -28.0795 ZY= 7.8733

XZ= 2.5676 YZ= 7.9762 ZZ= 152.3874

Eigenvalues: -31.4215 53.9828 152.7750

16 N Isotropic = 28.2351 Anisotropy = 247.9097

XX= -79.3146 YX= 29.7988 ZX= 4.2941

XY= 40.7453 YY= -29.0571 ZY= 8.6563

XZ= 3.4362 YZ= 8.4659 ZZ= 193.0769

Eigenvalues: -97.4945 -11.3085 193.5082

17 H Isotropic = 23.3275 Anisotropy = 10.4131

XX= 30.2376 YX= 0.9825 ZX= -0.2799

XY= -0.1435 YY= 23.1138 ZY= -0.1970

XZ= -0.3215 YZ= -0.3213 ZZ= 16.6310

Eigenvalues: 16.6147 23.0982 30.2695

18 H Isotropic = 18.2017 Anisotropy = 12.1561

XX= 23.7777 YX= 0.2454 ZX= -0.0443

XY= 0.2924 YY= 26.2708 ZY= -0.2564

XZ= -0.3480 YZ= -0.4501 ZZ= 4.5567

Eigenvalues: 4.5491 23.7503 26.3058

19 C Isotropic = 116.7759 Anisotropy = 61.3964

XX= 147.2301 YX= -19.3160 ZX= -0.1409

XY= -27.1388 YY= 106.2106 ZY= 0.2601

XZ= 0.1211 YZ= -0.1085 ZZ= 96.8870

Eigenvalues: 95.7302 96.8907 157.7068

20 H Isotropic = 23.6718 Anisotropy = 5.3461

XX= 24.8971 YX= -0.2292 ZX= -0.0821

XY= -0.4030 YY= 27.1825 ZY= -0.3060

XZ= -0.1015 YZ= -0.3128 ZZ= 18.9359

Eigenvalues: 18.9225 24.8571 27.2359

21 H Isotropic = 22.5615 Anisotropy = 8.2751

XX= 26.5186 YX= -2.0741 ZX= -0.0868

XY= -2.5557 YY= 24.6411 ZY= -0.2517

XZ= -0.0926 YZ= -0.2663 ZZ= 16.5248

Eigenvalues: 16.5137 23.0926 28.0783

22 C Isotropic = 155.8344 Anisotropy = 34.4369

XX= 147.9900 YX= -5.0320 ZX= 3.0075

XY= -6.5540 YY= 150.0569 ZY= -13.5788

XZ= 8.5190 YZ= -14.4722 ZZ= 169.4563

Eigenvalues: 141.4534 147.2575 178.7924

23 H Isotropic = 24.2419 Anisotropy = 11.6592

XX= 27.6745 YX= 4.3744 ZX= -0.2785

XY= 2.0038 YY= 29.6392 ZY= -0.2434

XZ= -0.4789 YZ= -0.6630 ZZ= 15.4119

Eigenvalues: 15.3909 25.3200 32.0147

24 C Isotropic = 155.8496 Anisotropy = 34.4940

XX= 147.5304 YX= -4.6092 ZX= -1.7557

XY= -6.7209 YY= 152.6585 ZY= 15.6028

XZ= -7.0318 YZ= 15.8829 ZZ= 167.3599

Eigenvalues: 141.4256 147.2776 178.8456

25 H Isotropic = 29.2311 Anisotropy = 8.0311

XX= 29.4631 YX= 2.1399 ZX= -0.0379

XY= 2.7884 YY= 31.4839 ZY= -2.3541

XZ= 0.0323 YZ= -5.3938 ZZ= 26.7463

Eigenvalues: 24.2668 28.8413 34.5852

26 H Isotropic = 29.1808 Anisotropy = 6.2086

XX= 26.1066 YX= -0.1861 ZX= 0.4683

XY= 0.0609 YY= 28.4178 ZY= 1.1583

XZ= 2.3056 YZ= -0.3047 ZZ= 33.0181

Eigenvalues: 25.8307 28.3918 33.3199

27 H Isotropic = 29.2070 Anisotropy = 10.0308

XX= 32.9537 YX= -3.0033 ZX= 2.0207

XY= -3.4738 YY= 28.4339 ZY= -1.6740

XZ= 3.0408 YZ= -3.5464 ZZ= 26.2333

Eigenvalues: 24.4827 27.2441 35.8942

28 H Isotropic = 29.1836 Anisotropy = 7.9838

XX= 29.4159 YX= 2.3145 ZX= -0.2331

XY= 2.8185 YY= 32.0466 ZY= 1.9116

XZ= -0.4822 YZ= 4.7039 ZZ= 26.0881

Eigenvalues: 24.2145 28.8301 34.5061

29 H Isotropic = 29.1441 Anisotropy = 10.1259

XX= 32.7213 YX= -3.1169 ZX= -1.9256

XY= -3.7343 YY= 28.7444 ZY= 1.8356

XZ= -3.0470 YZ= 3.2949 ZZ= 25.9667

Eigenvalues: 24.4107 27.1269 35.8948

30 H Isotropic = 29.0978 Anisotropy = 6.4253

XX= 25.9642 YX= -0.2788 ZX= -0.0962

XY= -0.3106 YY= 28.1181 ZY= -0.5551

XZ= -2.1418 YZ= 0.6340 ZZ= 33.2112

Eigenvalues: 25.7608 28.1514 33.3814

31 C Isotropic = 56.2549 Anisotropy = 169.3118

XX= -50.5962 YX= -5.9857 ZX= -4.6153

XY= -9.8436 YY= 50.5381 ZY= -5.1959

XZ= -4.6426 YZ= -5.0875 ZZ= 168.8227

Eigenvalues: -51.3262 50.9613 169.1294

32 C Isotropic = 50.2826 Anisotropy = 177.6832

XX= -0.1855 YX= -45.6152 ZX= -5.2633

XY= -44.7306 YY= -17.2466 ZY= -8.6179

XZ= -5.1250 YZ= -8.5703 ZZ= 168.2799

Eigenvalues: -55.1289 37.2386 168.7381

33 C Isotropic = 50.9930 Anisotropy = 162.6923

XX= 9.6373 YX= 12.8196 ZX= -2.5014

XY= 5.2099 YY= -15.7720 ZY= -7.1024

XZ= -2.4129 YZ= -7.0896 ZZ= 159.1139

Eigenvalues: -18.8494 12.3739 159.4546

34 C Isotropic = 11.8570 Anisotropy = 165.7947

XX= -46.8838 YX= 2.7129 ZX= -3.1746

XY= -7.8093 YY= -39.5691 ZY= -7.0816

XZ= -4.0294 YZ= -6.6434 ZZ= 122.0239

Eigenvalues: -47.8650 -38.9508 122.3868

35 C Isotropic = 55.3158 Anisotropy = 151.9939

XX= 37.0179 YX= -29.2134 ZX= -3.7579

XY= -29.1508 YY= -27.2550 ZY= -8.7052

XZ= -3.4986 YZ= -8.8093 ZZ= 156.1844

Eigenvalues: -38.9877 48.2900 156.6450

36 C Isotropic = 44.0692 Anisotropy = 183.7959

XX= 19.9175 YX= 37.7845 ZX= -1.3099

XY= 39.6545 YY= -53.9150 ZY= -8.7010

XZ= -1.0743 YZ= -8.6654 ZZ= 166.2051

Eigenvalues: -70.7349 36.3428 166.5998

37 C Isotropic = 40.1969 Anisotropy = 182.8563

XX= -30.3123 YX= 8.4225 ZX= -3.4122

XY= -0.1070 YY= -10.8475 ZY= -7.1239

XZ= -3.8433 YZ= -6.6912 ZZ= 161.7504

Eigenvalues: -31.1879 -10.3226 162.1011

38 N Isotropic = -1.1808 Anisotropy = 321.0216

XX= -97.8593 YX= 75.5606 ZX= -2.9318

XY= 88.2842 YY= -117.9609 ZY= -11.5687

XZ= -2.9653 YZ= -12.4242 ZZ= 212.2779

Eigenvalues: -190.5696 -25.8063 212.8336

39 H Isotropic = 23.0646 Anisotropy = 9.0439

XX= 29.0095 YX= -0.8209 ZX= -0.1003

XY= -0.5257 YY= 23.6422 ZY= 0.1329

XZ= -0.1000 YZ= 0.1860 ZZ= 16.5421

Eigenvalues: 16.5379 23.5621 29.0938

40 H Isotropic = 23.2804 Anisotropy = 6.7733

XX= 27.3281 YX= 1.2652 ZX= 0.1589

XY= 1.4092 YY= 23.9256 ZY= 0.2079

XZ= 0.1556 YZ= 0.2155 ZZ= 18.5874

Eigenvalues: 18.5778 23.4675 27.7959

41 C Isotropic = 58.9778 Anisotropy = 166.4552

XX= -11.2553 YX= -42.2290 ZX= -5.3462

XY= -39.2384 YY= 18.6371 ZY= -7.0448

XZ= -5.2473 YZ= -7.0532 ZZ= 169.5517

Eigenvalues: -40.0334 47.0189 169.9479

42 C Isotropic = 25.3091 Anisotropy = 154.4687

XX= -31.6184 YX= -13.5993 ZX= -3.9383

XY= -3.3895 YY= -20.4002 ZY= -6.2258

XZ= -3.1120 YZ= -6.6736 ZZ= 127.9460

Eigenvalues: -36.4205 -15.9404 128.2882

43 C Isotropic = 38.4044 Anisotropy = 133.6490

XX= -6.7917 YX= -24.4015 ZX= -4.0346

XY= -24.1209 YY= -5.1647 ZY= -6.1758

XZ= -3.8692 YZ= -5.8261 ZZ= 127.1695

Eigenvalues: -30.5649 18.2743 127.5037

44 H Isotropic = 22.6634 Anisotropy = 7.6805

XX= 25.8259 YX= -2.6307 ZX= 0.0570

XY= -1.1168 YY= 25.9861 ZY= 0.3332

XZ= 0.1647 YZ= 0.3291 ZZ= 16.1782

Eigenvalues: 16.1638 24.0427 27.7837

45 C Isotropic = 58.4703 Anisotropy = 141.4574

XX= 51.0568 YX= -17.5141 ZX= -2.8155

XY= -13.7283 YY= -28.0392 ZY= -7.8217

XZ= -2.5879 YZ= -7.8894 ZZ= 152.3931

Eigenvalues: -31.3804 54.0160 152.7752

46 N Isotropic = 28.2664 Anisotropy = 247.8726

XX= -79.2873 YX= 29.7851 ZX= -4.2994

XY= 40.7255 YY= -29.0015 ZY= -8.5975

XZ= -3.4294 YZ= -8.4121 ZZ= 193.0881

Eigenvalues: -97.4476 -11.2679 193.5148

47 H Isotropic = 23.3275 Anisotropy = 10.4109

XX= 30.2363 YX= 0.9820 ZX= 0.2774

XY= -0.1439 YY= 23.1170 ZY= 0.1992

XZ= 0.3199 YZ= 0.3228 ZZ= 16.6291

Eigenvalues: 16.6128 23.1016 30.2681

48 H Isotropic = 18.2013 Anisotropy = 12.1567

XX= 23.7769 YX= 0.2460 ZX= 0.0463

XY= 0.2929 YY= 26.2705 ZY= 0.2577

XZ= 0.3573 YZ= 0.4553 ZZ= 4.5565

Eigenvalues: 4.5486 23.7495 26.3058

49 C Isotropic = 116.7548 Anisotropy = 61.4097

XX= 147.2123 YX= -19.3209 ZX= 0.1536

XY= -27.1463 YY= 106.1983 ZY= -0.2416

XZ= -0.0775 YZ= 0.1107 ZZ= 96.8540

Eigenvalues: 95.7143 96.8556 157.6946

50 H Isotropic = 23.6707 Anisotropy = 5.3453

XX= 24.8976 YX= -0.2293 ZX= 0.0809

XY= -0.4022 YY= 27.1808 ZY= 0.3083

XZ= 0.0995 YZ= 0.3149 ZZ= 18.9338

Eigenvalues: 18.9203 24.8576 27.2343

51 H Isotropic = 22.5613 Anisotropy = 8.2753

XX= 26.5194 YX= -2.0729 ZX= 0.0839

XY= -2.5557 YY= 24.6404 ZY= 0.2530

XZ= 0.0923 YZ= 0.2699 ZZ= 16.5239

Eigenvalues: 16.5127 23.0930 28.0781

52 C Isotropic = 155.8481 Anisotropy = 34.4264

XX= 148.0006 YX= -5.0362 ZX= -3.0034

XY= -6.5587 YY= 150.0992 ZY= 13.6025

XZ= -8.4844 YZ= 14.4801 ZZ= 169.4444

Eigenvalues: 141.4660 147.2792 178.7990

53 H Isotropic = 24.2419 Anisotropy = 11.6574

XX= 27.6738 YX= 4.3740 ZX= 0.2730

XY= 2.0033 YY= 29.6384 ZY= 0.2423

XZ= 0.4775 YZ= 0.6652 ZZ= 15.4134

Eigenvalues: 15.3925 25.3197 32.0135

54 C Isotropic = 155.8419 Anisotropy = 34.5059

XX= 147.5192 YX= -4.6110 ZX= 1.7615

XY= -6.7240 YY= 152.6220 ZY= -15.5810

XZ= 7.0637 YZ= -15.8766 ZZ= 167.3846

Eigenvalues: 141.4184 147.2614 178.8459

55 H Isotropic = 29.2310 Anisotropy = 8.0322

XX= 29.4643 YX= 2.1407 ZX= 0.0351

XY= 2.7898 YY= 31.4915 ZY= 2.3515

XZ= -0.0337 YZ= 5.3865 ZZ= 26.7370

Eigenvalues: 24.2659 28.8412 34.5857

56 H Isotropic = 29.1814 Anisotropy = 6.2155

XX= 26.1068 YX= -0.1863 ZX= -0.4671

XY= 0.0601 YY= 28.4119 ZY= -1.1518

XZ= -2.3020 YZ= 0.3104 ZZ= 33.0255

Eigenvalues: 25.8322 28.3870 33.3251

57 H Isotropic = 29.2080 Anisotropy = 10.0305

XX= 32.9551 YX= -3.0059 ZX= -2.0176

XY= -3.4774 YY= 28.4381 ZY= 1.6753

XZ= -3.0333 YZ= 3.5442 ZZ= 26.2307

Eigenvalues: 24.4830 27.2459 35.8950

58 H Isotropic = 29.1845 Anisotropy = 7.9820

XX= 29.4176 YX= 2.3144 ZX= 0.2292

XY= 2.8177 YY= 32.0392 ZY= -1.9162

XZ= 0.4791 YZ= -4.7121 ZZ= 26.0966

Eigenvalues: 24.2162 28.8314 34.5058

59 H Isotropic = 29.1454 Anisotropy = 10.1262

XX= 32.7198 YX= -3.1166 ZX= 1.9280

XY= -3.7334 YY= 28.7434 ZY= -1.8346

XZ= 3.0529 YZ= -3.2970 ZZ= 25.9729

Eigenvalues: 24.4143 27.1256 35.8962

60 H Isotropic = 29.0973 Anisotropy = 6.4192

XX= 25.9632 YX= -0.2786 ZX= 0.0979

XY= -0.3104 YY= 28.1228 ZY= 0.5633

XZ= 2.1453 YZ= -0.6269 ZZ= 33.2060

Eigenvalues: 25.7588 28.1565 33.3768

## Norharman dimer\_iso 2 (IEFPCM solvent = tetrahydrofuran) - BP86/IGLO-III level

60

C -6.41695 0.64808 -0.01475

C -5.75782 -0.58069 0.02255

C -4.34174 -0.59788 -0.00495

C -3.58261 0.64233 -0.07045

C -4.28373 1.87868 -0.10865

C -5.67781 1.86585 -0.08045

C -3.34947 -1.62577 0.01725

N -2.22412 0.44700 -0.08825

H -3.72719 2.82850 -0.16225

H -6.22802 2.82203 -0.11035

C -3.33217 -3.03216 0.07445

C -2.07552 -0.90420 -0.03725

C -0.87869 -1.63850 -0.03285

H -4.25845 -3.62745 0.11725

C -2.10896 -3.69577 0.07765

N -0.92061 -2.99785 0.02465

H -2.02752 -4.78979 0.12145

H 0.13415 -1.19079 -0.07285

C 0.38140 -3.74034 0.03175

H -7.51858 0.68441 0.00575

H -6.33188 -1.52170 0.07235

C 0.56983 -4.50871 1.34705

H 1.14827 -2.93914 -0.01865

C 0.51907 -4.62416 -1.21555

H -0.15569 -5.34505 1.45475

H 0.45979 -3.83214 2.22145

H 1.59235 -4.94368 1.37775

H -0.20706 -5.46693 -1.21785

H 1.54086 -5.06067 -1.24805

H 0.37115 -4.02961 -2.14245

C 6.41678 -0.64827 -0.01525

C 5.75775 0.58050 0.02275

C 4.34167 0.59780 -0.00445

C 3.58253 -0.64241 -0.07005

C 4.28355 -1.87867 -0.10885

C 5.67764 -1.86604 -0.08115

C 3.34950 1.62569 0.01805

N 2.22394 -0.44700 -0.08745

H 3.72692 -2.82859 -0.16265

H 6.22785 -2.82212 -0.11165

C 3.33220 3.03217 0.07515

C 2.07554 0.90422 -0.03625

C 0.87871 1.63862 -0.03175

H 4.25848 3.62737 0.11775

C 2.10909 3.69569 0.07825

N 0.92073 2.99788 0.02555

H 2.02764 4.78981 0.12175

H -0.13423 1.19091 -0.07175

C -0.38128 3.74046 0.03205

H 7.51851 -0.68460 0.00485

H 6.33181 1.52151 0.07295

C -0.56959 4.51054 1.34645

H -1.14826 2.93925 -0.01735

C -0.51898 4.62277 -1.21635

H 0.15592 5.34698 1.45295

H -0.45941 3.83508 2.22165

H -1.59210 4.94541 1.37655

H 0.20746 5.46527 -1.21985

H -1.54058 5.05959 -1.24925

H -0.37131 4.02702 -2.14255

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 53.4332 Anisotropy = 165.1841

XX= -50.2743 YX= -4.2102 ZX= 4.4936

XY= -7.6797 YY= 47.3143 ZY= 5.0117

XZ= 4.4721 YZ= 4.9266 ZZ= 163.2598

Eigenvalues: -50.7418 47.4856 163.5560

2 C Isotropic = 48.7766 Anisotropy = 171.8052

XX= 0.9778 YX= -41.7870 ZX= 4.9795

XY= -41.5731 YY= -17.5255 ZY= 8.2619

XZ= 4.9000 YZ= 8.2162 ZZ= 162.8774

Eigenvalues: -51.3912 34.4076 163.3134

3 C Isotropic = 47.0088 Anisotropy = 158.3934

XX= 6.8182 YX= 11.8826 ZX= 2.4861

XY= 4.1521 YY= -18.0659 ZY= 6.8955

XZ= 2.4343 YZ= 6.8578 ZZ= 152.2740

Eigenvalues: -20.6276 9.0495 152.6044

4 C Isotropic = 10.8721 Anisotropy = 155.1719

XX= -44.8764 YX= 1.1165 ZX= 3.1125

XY= -8.3636 YY= -36.4838 ZY= 6.5911

XZ= 3.8953 YZ= 6.2392 ZZ= 113.9766

Eigenvalues: -46.4169 -35.2868 114.3201

5 C Isotropic = 52.5217 Anisotropy = 148.3069

XX= 31.9356 YX= -28.8182 ZX= 3.7969

XY= -27.7581 YY= -25.3231 ZY= 8.3380

XZ= 3.4087 YZ= 8.3898 ZZ= 150.9524

Eigenvalues: -37.3814 43.5535 151.3929

6 C Isotropic = 42.8121 Anisotropy = 177.4696

XX= 17.7464 YX= 36.8371 ZX= 1.3596

XY= 38.4877 YY= -50.0615 ZY= 8.2377

XZ= 1.1374 YZ= 8.2027 ZZ= 160.7513

Eigenvalues: -67.0477 34.3588 161.1252

7 C Isotropic = 38.2552 Anisotropy = 174.5256

XX= -29.4282 YX= 7.8942 ZX= 3.3042

XY= 1.8085 YY= -10.0774 ZY= 6.7607

XZ= 3.6808 YZ= 6.3414 ZZ= 154.2711

Eigenvalues: -30.5959 -9.2441 154.6056

8 N Isotropic = -1.6812 Anisotropy = 307.6036

XX= -95.0843 YX= 74.8459 ZX= 2.9706

XY= 85.9071 YY= -112.8140 ZY= 11.1098

XZ= 2.7840 YZ= 11.7445 ZZ= 202.8546

Eigenvalues: -184.9252 -23.5063 203.3878

9 H Isotropic = 23.0189 Anisotropy = 8.6069

XX= 28.6601 YX= -0.9035 ZX= 0.1072

XY= -0.5008 YY= 23.5934 ZY= -0.1167

XZ= 0.0977 YZ= -0.1639 ZZ= 16.8031

Eigenvalues: 16.7996 23.5003 28.7568

10 H Isotropic = 23.3153 Anisotropy = 6.4892

XX= 27.1533 YX= 1.2961 ZX= -0.1577

XY= 1.3752 YY= 23.9420 ZY= -0.1964

XZ= -0.1540 YZ= -0.1999 ZZ= 18.8505

Eigenvalues: 18.8415 23.4630 27.6414

11 C Isotropic = 55.7935 Anisotropy = 163.7760

XX= -12.8766 YX= -39.2595 ZX= 5.1738

XY= -35.2190 YY= 15.6696 ZY= 6.9046

XZ= 5.0428 YZ= 6.9704 ZZ= 164.5874

Eigenvalues: -38.8103 41.2132 164.9775

12 C Isotropic = 22.4954 Anisotropy = 146.3489

XX= -30.2775 YX= -12.5422 ZX= 3.7237

XY= -3.4102 YY= -21.9682 ZY= 5.9818

XZ= 3.0188 YZ= 6.3672 ZZ= 119.7319

Eigenvalues: -35.3560 -17.2191 120.0614

13 C Isotropic = 38.0269 Anisotropy = 125.3529

XX= -5.2175 YX= -22.9314 ZX= 3.8166

XY= -23.8260 YY= -1.9835 ZY= 5.8090

XZ= 3.6769 YZ= 5.4169 ZZ= 121.2816

Eigenvalues: -27.3255 19.8106 121.5955

14 H Isotropic = 22.6344 Anisotropy = 7.3993

XX= 25.5685 YX= -2.5187 ZX= -0.0543

XY= -1.1000 YY= 25.9248 ZY= -0.3225

XZ= -0.1559 YZ= -0.3178 ZZ= 16.4098

Eigenvalues: 16.3959 23.9400 27.5672

15 C Isotropic = 53.7257 Anisotropy = 141.1032

XX= 42.8487 YX= -16.2643 ZX= 2.8355

XY= -12.1037 YY= -29.0870 ZY= 7.6799

XZ= 2.5555 YZ= 7.7776 ZZ= 147.4153

Eigenvalues: -32.1478 45.5303 147.7945

16 N Isotropic = 19.5387 Anisotropy = 244.2484

XX= -82.7206 YX= 26.0471 ZX= 4.2888

XY= 34.1578 YY= -40.5964 ZY= 8.8173

XZ= 3.5524 YZ= 8.5591 ZZ= 181.9331

Eigenvalues: -98.3987 -25.3562 182.3710

17 H Isotropic = 23.1428 Anisotropy = 10.1533

XX= 29.8881 YX= 0.9195 ZX= -0.2664

XY= -0.2294 YY= 22.7624 ZY= -0.1790

XZ= -0.3145 YZ= -0.3092 ZZ= 16.7780

Eigenvalues: 16.7622 22.7546 29.9117

18 H Isotropic = 18.3277 Anisotropy = 11.5785

XX= 23.8901 YX= 0.1848 ZX= -0.0391

XY= 0.2329 YY= 26.0207 ZY= -0.2365

XZ= -0.3409 YZ= -0.4270 ZZ= 5.0725

Eigenvalues: 5.0654 23.8711 26.0467

19 C Isotropic = 108.0991 Anisotropy = 62.6795

XX= 139.3338 YX= -20.0814 ZX= -0.1267

XY= -27.6342 YY= 95.9409 ZY= 0.3748

XZ= 0.1074 YZ= 0.0419 ZZ= 89.0226

Eigenvalues: 85.3798 89.0320 149.8854

20 H Isotropic = 23.6669 Anisotropy = 5.1532

XX= 24.6861 YX= -0.1865 ZX= -0.0754

XY= -0.2765 YY= 27.0697 ZY= -0.2922

XZ= -0.1046 YZ= -0.2992 ZZ= 19.2450

Eigenvalues: 19.2320 24.6663 27.1024

21 H Isotropic = 22.5708 Anisotropy = 7.9663

XX= 26.4211 YX= -1.9491 ZX= -0.0866

XY= -2.4798 YY= 24.5229 ZY= -0.2391

XZ= -0.0848 YZ= -0.2614 ZZ= 16.7683

Eigenvalues: 16.7575 23.0732 27.8816

22 C Isotropic = 150.5688 Anisotropy = 36.1369

XX= 142.5895 YX= -5.1676 ZX= 3.1918

XY= -6.3922 YY= 144.5928 ZY= -14.3611

XZ= 8.9721 YZ= -15.7406 ZZ= 164.5242

Eigenvalues: 135.5736 141.4727 174.6601

23 H Isotropic = 24.2646 Anisotropy = 10.9042

XX= 27.4416 YX= 4.0399 ZX= -0.2540

XY= 1.6607 YY= 29.5195 ZY= -0.2257

XZ= -0.4537 YZ= -0.6401 ZZ= 15.8327

Eigenvalues: 15.8127 25.4470 31.5341

24 C Isotropic = 150.5728 Anisotropy = 36.1698

XX= 142.0827 YX= -4.6385 ZX= -1.9590

XY= -6.5565 YY= 147.3781 ZY= 16.3998

XZ= -7.4718 YZ= 17.1653 ZZ= 162.2576

Eigenvalues: 135.5928 141.4396 174.6860

25 H Isotropic = 29.1319 Anisotropy = 7.6080

XX= 29.3045 YX= 1.9540 ZX= -0.0119

XY= 2.6043 YY= 31.2516 ZY= -2.2255

XZ= 0.0371 YZ= -5.2516 ZZ= 26.8395

Eigenvalues: 24.4126 28.7792 34.2039

26 H Isotropic = 29.2264 Anisotropy = 5.9441

XX= 26.3156 YX= -0.1398 ZX= 0.4880

XY= 0.1032 YY= 28.4573 ZY= 0.8564

XZ= 2.2599 YZ= -0.4557 ZZ= 32.9063

Eigenvalues: 26.0393 28.4508 33.1891

27 H Isotropic = 29.1276 Anisotropy = 9.5265

XX= 32.6060 YX= -2.8183 ZX= 1.9324

XY= -3.2781 YY= 28.4073 ZY= -1.6056

XZ= 3.0297 YZ= -3.4689 ZZ= 26.3696

Eigenvalues: 24.6309 27.2734 35.4786

28 H Isotropic = 29.0879 Anisotropy = 7.5626

XX= 29.2611 YX= 2.1303 ZX= -0.2341

XY= 2.6307 YY= 31.7975 ZY= 1.8158

XZ= -0.4571 YZ= 4.5977 ZZ= 26.2049

Eigenvalues: 24.3654 28.7686 34.1296

29 H Isotropic = 29.0554 Anisotropy = 9.6249

XX= 32.3672 YX= -2.9300 ZX= -1.8392

XY= -3.5402 YY= 28.6990 ZY= 1.7680

XZ= -3.0306 YZ= 3.2353 ZZ= 26.1000

Eigenvalues: 24.5479 27.1463 35.4720

30 H Isotropic = 29.1463 Anisotropy = 6.1655

XX= 26.1735 YX= -0.2176 ZX= -0.1414

XY= -0.2498 YY= 28.2038 ZY= -0.2791

XZ= -2.1103 YZ= 0.7744 ZZ= 33.0616

Eigenvalues: 25.9776 28.2047 33.2566

31 C Isotropic = 53.4257 Anisotropy = 165.1826

XX= -50.2811 YX= -4.2053 ZX= -4.4210

XY= -7.6715 YY= 47.3079 ZY= -5.0554

XZ= -4.4129 YZ= -4.9675 ZZ= 163.2503

Eigenvalues: -50.7450 47.4747 163.5475

32 C Isotropic = 48.7785 Anisotropy = 171.7955

XX= 0.9876 YX= -41.7839 ZX= -4.9700

XY= -41.5732 YY= -17.5207 ZY= -8.3374

XZ= -4.8692 YZ= -8.2636 ZZ= 162.8686

Eigenvalues: -51.3861 34.4128 163.3088

33 C Isotropic = 47.0085 Anisotropy = 158.4116

XX= 6.8161 YX= 11.8851 ZX= -2.4596

XY= 4.1477 YY= -18.0747 ZY= -6.9300

XZ= -2.3636 YZ= -6.9117 ZZ= 152.2841

Eigenvalues: -20.6391 9.0484 152.6163

34 C Isotropic = 10.8722 Anisotropy = 155.1607

XX= -44.8682 YX= 1.1098 ZX= -3.0623

XY= -8.3540 YY= -36.4826 ZY= -6.6331

XZ= -3.8614 YZ= -6.2828 ZZ= 113.9674

Eigenvalues: -46.4069 -35.2891 114.3127

35 C Isotropic = 52.5247 Anisotropy = 148.2955

XX= 31.9373 YX= -28.8053 ZX= -3.7673

XY= -27.7577 YY= -25.3068 ZY= -8.3929

XZ= -3.3844 YZ= -8.4549 ZZ= 150.9436

Eigenvalues: -37.3670 43.5527 151.3883

36 C Isotropic = 42.8200 Anisotropy = 177.4642

XX= 17.7486 YX= 36.8403 ZX= -1.2926

XY= 38.4915 YY= -50.0387 ZY= -8.3319

XZ= -1.0771 YZ= -8.2970 ZZ= 160.7500

Eigenvalues: -67.0378 34.3683 161.1294

37 C Isotropic = 38.2646 Anisotropy = 174.5122

XX= -29.4107 YX= 7.8999 ZX= -3.2731

XY= 1.8089 YY= -10.0693 ZY= -6.7555

XZ= -3.6064 YZ= -6.3461 ZZ= 154.2737

Eigenvalues: -30.5792 -9.2331 154.6060

38 N Isotropic = -1.7012 Anisotropy = 307.5935

XX= -95.0866 YX= 74.8350 ZX= -2.8953

XY= 85.8987 YY= -112.8405 ZY= -11.1837

XZ= -2.7448 YZ= -11.8350 ZZ= 202.8234

Eigenvalues: -184.9348 -23.5299 203.3611

39 H Isotropic = 23.0171 Anisotropy = 8.6077

XX= 28.6595 YX= -0.9004 ZX= -0.1107

XY= -0.4986 YY= 23.5931 ZY= 0.1178

XZ= -0.1013 YZ= 0.1662 ZZ= 16.7987

Eigenvalues: 16.7951 23.5007 28.7556

40 H Isotropic = 23.3160 Anisotropy = 6.4896

XX= 27.1534 YX= 1.2973 ZX= 0.1562

XY= 1.3765 YY= 23.9425 ZY= 0.1968

XZ= 0.1511 YZ= 0.2026 ZZ= 18.8519

Eigenvalues: 18.8428 23.4627 27.6423

41 C Isotropic = 55.8049 Anisotropy = 163.7766

XX= -12.8712 YX= -39.2593 ZX= -5.1529

XY= -35.2101 YY= 15.6823 ZY= -6.8796

XZ= -5.0104 YZ= -6.9159 ZZ= 164.6036

Eigenvalues: -38.7947 41.2201 164.9893

42 C Isotropic = 22.4891 Anisotropy = 146.3562

XX= -30.2970 YX= -12.5370 ZX= -3.7024

XY= -3.4022 YY= -21.9648 ZY= -5.9916

XZ= -3.0203 YZ= -6.3985 ZZ= 119.7291

Eigenvalues: -35.3635 -17.2291 120.0599

43 C Isotropic = 38.0235 Anisotropy = 125.3509

XX= -5.2218 YX= -22.9370 ZX= -3.8119

XY= -23.8280 YY= -1.9853 ZY= -5.7931

XZ= -3.7118 YZ= -5.3995 ZZ= 121.2776

Eigenvalues: -27.3324 19.8121 121.5908

44 H Isotropic = 22.6355 Anisotropy = 7.3988

XX= 25.5687 YX= -2.5184 ZX= 0.0533

XY= -1.0994 YY= 25.9269 ZY= 0.3233

XZ= 0.1551 YZ= 0.3165 ZZ= 16.4109

Eigenvalues: 16.3971 23.9414 27.5681

45 C Isotropic = 53.7479 Anisotropy = 141.0709

XX= 42.8740 YX= -16.2799 ZX= -2.8266

XY= -12.1132 YY= -29.0517 ZY= -7.6297

XZ= -2.5782 YZ= -7.6936 ZZ= 147.4212

Eigenvalues: -32.1117 45.5601 147.7951

46 N Isotropic = 19.5676 Anisotropy = 244.2165

XX= -82.6969 YX= 26.0349 ZX= -4.2918

XY= 34.1411 YY= -40.5456 ZY= -8.7592

XZ= -3.5418 YZ= -8.5068 ZZ= 181.9453

Eigenvalues: -98.3573 -25.3185 182.3786

47 H Isotropic = 23.1426 Anisotropy = 10.1513

XX= 29.8867 YX= 0.9192 ZX= 0.2639

XY= -0.2298 YY= 22.7653 ZY= 0.1813

XZ= 0.3128 YZ= 0.3106 ZZ= 16.7759

Eigenvalues: 16.7601 22.7576 29.9102

48 H Isotropic = 18.3275 Anisotropy = 11.5791

XX= 23.8895 YX= 0.1855 ZX= 0.0412

XY= 0.2333 YY= 26.0206 ZY= 0.2379

XZ= 0.3502 YZ= 0.4321 ZZ= 5.0724

Eigenvalues: 5.0650 23.8705 26.0469

49 C Isotropic = 108.0763 Anisotropy = 62.6934

XX= 139.3145 YX= -20.0866 ZX= 0.1395

XY= -27.6420 YY= 95.9272 ZY= -0.3537

XZ= -0.0637 YZ= -0.0366 ZZ= 88.9872

Eigenvalues: 85.3626 88.9944 149.8719

50 H Isotropic = 23.6659 Anisotropy = 5.1524

XX= 24.6866 YX= -0.1866 ZX= 0.0745

XY= -0.2758 YY= 27.0680 ZY= 0.2943

XZ= 0.1027 YZ= 0.3012 ZZ= 19.2429

Eigenvalues: 19.2299 24.6669 27.1008

51 H Isotropic = 22.5704 Anisotropy = 7.9665

XX= 26.4218 YX= -1.9480 ZX= 0.0839

XY= -2.4798 YY= 24.5222 ZY= 0.2402

XZ= 0.0846 YZ= 0.2647 ZZ= 16.7673

Eigenvalues: 16.7564 23.0735 27.8815

52 C Isotropic = 150.5836 Anisotropy = 36.1257

XX= 142.6011 YX= -5.1703 ZX= -3.1878

XY= -6.3965 YY= 144.6378 ZY= 14.3857

XZ= -8.9360 YZ= 15.7482 ZZ= 164.5120

Eigenvalues: 135.5885 141.4950 174.6674

53 H Isotropic = 24.2646 Anisotropy = 10.9023

XX= 27.4410 YX= 4.0394 ZX= 0.2490

XY= 1.6602 YY= 29.5188 ZY= 0.2249

XZ= 0.4526 YZ= 0.6425 ZZ= 15.8341

Eigenvalues: 15.8143 25.4468 31.5329

54 C Isotropic = 150.5639 Anisotropy = 36.1829

XX= 142.0696 YX= -4.6409 ZX= 1.9651

XY= -6.5595 YY= 147.3384 ZY= -16.3775

XZ= 7.5047 YZ= -17.1594 ZZ= 162.2836

Eigenvalues: 135.5849 141.4210 174.6858

55 H Isotropic = 29.1317 Anisotropy = 7.6092

XX= 29.3058 YX= 1.9548 ZX= 0.0095

XY= 2.6058 YY= 31.2590 ZY= 2.2233

XZ= -0.0382 YZ= 5.2449 ZZ= 26.8304

Eigenvalues: 24.4115 28.7792 34.2045

56 H Isotropic = 29.2268 Anisotropy = 5.9511

XX= 26.3154 YX= -0.1399 ZX= -0.4869

XY= 0.1024 YY= 28.4519 ZY= -0.8502

XZ= -2.2564 YZ= 0.4612 ZZ= 32.9130

Eigenvalues: 26.0403 28.4458 33.1942

57 H Isotropic = 29.1286 Anisotropy = 9.5261

XX= 32.6072 YX= -2.8209 ZX= -1.9295

XY= -3.2816 YY= 28.4114 ZY= 1.6071

XZ= -3.0223 YZ= 3.4669 ZZ= 26.3672

Eigenvalues: 24.6313 27.2752 35.4794

58 H Isotropic = 29.0888 Anisotropy = 7.5608

XX= 29.2626 YX= 2.1300 ZX= 0.2304

XY= 2.6297 YY= 31.7905 ZY= -1.8199

XZ= 0.4541 YZ= -4.6053 ZZ= 26.2132

Eigenvalues: 24.3672 28.7698 34.1293

59 H Isotropic = 29.0566 Anisotropy = 9.6251

XX= 32.3657 YX= -2.9297 ZX= 1.8415

XY= -3.5393 YY= 28.6980 ZY= -1.7668

XZ= 3.0363 YZ= -3.2373 ZZ= 26.1061

Eigenvalues: 24.5514 27.1450 35.4733

60 H Isotropic = 29.1460 Anisotropy = 6.1594

XX= 26.1727 YX= -0.2174 ZX= 0.1429

XY= -0.2495 YY= 28.2081 ZY= 0.2870

XZ= 2.1135 YZ= -0.7677 ZZ= 33.0571

Eigenvalues: 25.9758 28.2099 33.2522

## Norharman dimer\_iso 2 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level

60

C -6.41695 0.64808 -0.01475

C -5.75782 -0.58069 0.02255

C -4.34174 -0.59788 -0.00495

C -3.58261 0.64233 -0.07045

C -4.28373 1.87868 -0.10865

C -5.67781 1.86585 -0.08045

C -3.34947 -1.62577 0.01725

N -2.22412 0.44700 -0.08825

H -3.72719 2.82850 -0.16225

H -6.22802 2.82203 -0.11035

C -3.33217 -3.03216 0.07445

C -2.07552 -0.90420 -0.03725

C -0.87869 -1.63850 -0.03285

H -4.25845 -3.62745 0.11725

C -2.10896 -3.69577 0.07765

N -0.92061 -2.99785 0.02465

H -2.02752 -4.78979 0.12145

H 0.13415 -1.19079 -0.07285

C 0.38140 -3.74034 0.03175

H -7.51858 0.68441 0.00575

H -6.33188 -1.52170 0.07235

C 0.56983 -4.50871 1.34705

H 1.14827 -2.93914 -0.01865

C 0.51907 -4.62416 -1.21555

H -0.15569 -5.34505 1.45475

H 0.45979 -3.83214 2.22145

H 1.59235 -4.94368 1.37775

H -0.20706 -5.46693 -1.21785

H 1.54086 -5.06067 -1.24805

H 0.37115 -4.02961 -2.14245

C 6.41678 -0.64827 -0.01525

C 5.75775 0.58050 0.02275

C 4.34167 0.59780 -0.00445

C 3.58253 -0.64241 -0.07005

C 4.28355 -1.87867 -0.10885

C 5.67764 -1.86604 -0.08115

C 3.34950 1.62569 0.01805

N 2.22394 -0.44700 -0.08745

H 3.72692 -2.82859 -0.16265

H 6.22785 -2.82212 -0.11165

C 3.33220 3.03217 0.07515

C 2.07554 0.90422 -0.03625

C 0.87871 1.63862 -0.03175

H 4.25848 3.62737 0.11775

C 2.10909 3.69569 0.07825

N 0.92073 2.99788 0.02555

H 2.02764 4.78981 0.12175

H -0.13423 1.19091 -0.07175

C -0.38128 3.74046 0.03205

H 7.51851 -0.68460 0.00485

H 6.33181 1.52151 0.07295

C -0.56959 4.51054 1.34645

H -1.14826 2.93925 -0.01735

C -0.51898 4.62277 -1.21635

H 0.15592 5.34698 1.45295

H -0.45941 3.83508 2.22165

H -1.59210 4.94541 1.37655

H 0.20746 5.46527 -1.21985

H -1.54058 5.05959 -1.24925

H -0.37131 4.02702 -2.14255

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 56.8658 Anisotropy = 170.0187

XX= -49.9199 YX= -5.6408 ZX= 4.6807

XY= -9.4805 YY= 50.6129 ZY= 5.1851

XZ= 4.6954 YZ= 5.0854 ZZ= 169.9045

Eigenvalues: -50.6014 50.9873 170.2117

2 C Isotropic = 50.1041 Anisotropy = 179.5444

XX= -1.2973 YX= -44.5893 ZX= 5.2703

XY= -43.9018 YY= -17.7352 ZY= 8.5847

XZ= 5.1627 YZ= 8.5664 ZZ= 169.3447

Eigenvalues: -54.9582 35.4701 169.8004

3 C Isotropic = 51.4866 Anisotropy = 162.2765

XX= 10.1438 YX= 13.0388 ZX= 2.5151

XY= 6.1135 YY= -15.0183 ZY= 7.0236

XZ= 2.4405 YZ= 7.0037 ZZ= 159.3344

Eigenvalues: -18.4416 13.2306 159.6710

4 C Isotropic = 12.7193 Anisotropy = 164.8620

XX= -46.0035 YX= 2.5086 ZX= 3.2436

XY= -7.9446 YY= -38.1018 ZY= 6.9917

XZ= 4.0591 YZ= 6.6615 ZZ= 122.2632

Eigenvalues: -47.0309 -37.4385 122.6273

5 C Isotropic = 55.5691 Anisotropy = 154.0549

XX= 35.5713 YX= -28.7900 ZX= 3.8615

XY= -28.1115 YY= -26.6787 ZY= 8.6944

XZ= 3.4804 YZ= 8.7597 ZZ= 157.8148

Eigenvalues: -38.1796 46.6146 158.2724

6 C Isotropic = 44.3921 Anisotropy = 185.1664

XX= 19.2118 YX= 37.5167 ZX= 1.4328

XY= 39.2563 YY= -53.4790 ZY= 8.6523

XZ= 1.2011 YZ= 8.6187 ZZ= 167.4437

Eigenvalues: -70.2281 35.5681 167.8364

7 C Isotropic = 40.1383 Anisotropy = 182.3351

XX= -30.1420 YX= 9.4248 ZX= 3.3975

XY= 2.3607 YY= -10.7888 ZY= 7.0689

XZ= 3.8050 YZ= 6.6440 ZZ= 161.3457

Eigenvalues: -31.8088 -9.4714 161.6950

8 N Isotropic = 5.2731 Anisotropy = 312.4789

XX= -88.5203 YX= 74.0082 ZX= 3.0657

XY= 84.6006 YY= -108.7078 ZY= 11.3970

XZ= 2.9719 YZ= 11.9360 ZZ= 213.0473

Eigenvalues: -178.6750 -19.0981 213.5923

9 H Isotropic = 22.8718 Anisotropy = 8.9832

XX= 28.7852 YX= -0.7918 ZX= 0.0932

XY= -0.4625 YY= 23.5702 ZY= -0.1391

XZ= 0.0933 YZ= -0.1900 ZZ= 16.2599

Eigenvalues: 16.2557 23.4991 28.8606

10 H Isotropic = 23.1473 Anisotropy = 6.6997

XX= 27.1639 YX= 1.2189 ZX= -0.1615

XY= 1.3604 YY= 23.8672 ZY= -0.2112

XZ= -0.1587 YZ= -0.2151 ZZ= 18.4108

Eigenvalues: 18.4011 23.4270 27.6137

11 C Isotropic = 58.1087 Anisotropy = 169.6214

XX= -12.2876 YX= -41.4004 ZX= 5.3766

XY= -37.2968 YY= 15.8300 ZY= 7.1950

XZ= 5.2420 YZ= 7.2568 ZZ= 170.7838

Eigenvalues: -40.3561 43.4926 171.1896

12 C Isotropic = 25.2651 Anisotropy = 154.3934

XX= -29.8956 YX= -12.1954 ZX= 3.8673

XY= -2.2480 YY= -22.1591 ZY= 6.2840

XZ= 3.1492 YZ= 6.6762 ZZ= 127.8499

Eigenvalues: -34.4686 -17.9301 128.1940

13 C Isotropic = 38.3436 Anisotropy = 133.7030

XX= -8.0901 YX= -24.1932 ZX= 4.0604

XY= -24.8524 YY= -4.0244 ZY= 6.1753

XZ= 3.8603 YZ= 5.7829 ZZ= 127.1453

Eigenvalues: -30.9709 18.5228 127.4790

14 H Isotropic = 22.4319 Anisotropy = 7.6081

XX= 25.5630 YX= -2.5186 ZX= -0.0636

XY= -1.0543 YY= 25.8550 ZY= -0.3411

XZ= -0.1691 YZ= -0.3398 ZZ= 15.8776

Eigenvalues: 15.8626 23.9291 27.5040

15 C Isotropic = 54.3642 Anisotropy = 148.5646

XX= 42.8979 YX= -18.1534 ZX= 3.0236

XY= -14.1586 YY= -32.8109 ZY= 8.1104

XZ= 2.7645 YZ= 8.2144 ZZ= 153.0057

Eigenvalues: -36.5026 46.1880 153.4073

16 N Isotropic = 21.2577 Anisotropy = 259.5127

XX= -88.8293 YX= 29.8710 ZX= 4.4898

XY= 38.7438 YY= -41.2026 ZY= 9.2528

XZ= 3.7381 YZ= 9.0196 ZZ= 193.8051

Eigenvalues: -106.7792 -23.7138 194.2662

17 H Isotropic = 22.9386 Anisotropy = 10.4275

XX= 29.8619 YX= 0.9286 ZX= -0.2789

XY= -0.1506 YY= 22.7555 ZY= -0.2008

XZ= -0.3218 YZ= -0.3224 ZZ= 16.1986

Eigenvalues: 16.1822 22.7434 29.8903

18 H Isotropic = 18.2278 Anisotropy = 11.9978

XX= 23.7907 YX= 0.1706 ZX= -0.0389

XY= 0.2027 YY= 26.2059 ZY= -0.2530

XZ= -0.3442 YZ= -0.4476 ZZ= 4.6868

Eigenvalues: 4.6792 23.7778 26.2263

19 C Isotropic = 115.2475 Anisotropy = 62.4624

XX= 146.5212 YX= -19.6968 ZX= -0.1497

XY= -27.2730 YY= 103.6910 ZY= 0.3343

XZ= 0.0908 YZ= -0.0283 ZZ= 95.5301

Eigenvalues: 93.3159 95.5374 156.8890

20 H Isotropic = 23.5706 Anisotropy = 5.2697

XX= 24.8734 YX= -0.2169 ZX= -0.0856

XY= -0.3847 YY= 27.0322 ZY= -0.3059

XZ= -0.1052 YZ= -0.3131 ZZ= 18.8063

Eigenvalues: 18.7928 24.8354 27.0837

21 H Isotropic = 22.3832 Anisotropy = 8.1998

XX= 26.3297 YX= -2.0036 ZX= -0.0915

XY= -2.4889 YY= 24.5291 ZY= -0.2582

XZ= -0.0953 YZ= -0.2738 ZZ= 16.2909

Eigenvalues: 16.2794 23.0204 27.8498

22 C Isotropic = 156.1154 Anisotropy = 34.6584

XX= 148.5350 YX= -5.2476 ZX= 2.8365

XY= -6.6577 YY= 150.2817 ZY= -13.7176

XZ= 8.6414 YZ= -15.0043 ZZ= 169.5296

Eigenvalues: 141.4127 147.7126 179.2210

23 H Isotropic = 24.3458 Anisotropy = 11.4807

XX= 27.7298 YX= 4.3179 ZX= -0.2731

XY= 1.8839 YY= 29.7158 ZY= -0.2414

XZ= -0.4696 YZ= -0.6607 ZZ= 15.5917

Eigenvalues: 15.5709 25.4669 31.9995

24 C Isotropic = 156.1274 Anisotropy = 34.7037

XX= 148.0805 YX= -4.7679 ZX= -1.5976

XY= -6.8265 YY= 152.9250 ZY= 15.7147

XZ= -7.1722 YZ= 16.4001 ZZ= 167.3765

Eigenvalues: 141.3970 147.7219 179.2632

25 H Isotropic = 29.0882 Anisotropy = 8.1899

XX= 29.2700 YX= 2.2650 ZX= -0.0767

XY= 2.8793 YY= 31.3939 ZY= -2.3272

XZ= 0.0037 YZ= -5.4104 ZZ= 26.6007

Eigenvalues: 24.1232 28.5933 34.5481

26 H Isotropic = 29.2128 Anisotropy = 6.2340

XX= 26.1137 YX= -0.2102 ZX= 0.4412

XY= 0.0647 YY= 28.4470 ZY= 1.1366

XZ= 2.3061 YZ= -0.3272 ZZ= 33.0777

Eigenvalues: 25.8442 28.4254 33.3688

27 H Isotropic = 29.0980 Anisotropy = 10.0951

XX= 32.8730 YX= -3.0659 ZX= 2.0083

XY= -3.5026 YY= 28.3169 ZY= -1.6541

XZ= 3.0437 YZ= -3.5401 ZZ= 26.1042

Eigenvalues: 24.3716 27.0944 35.8281

28 H Isotropic = 29.0436 Anisotropy = 8.1411

XX= 29.2277 YX= 2.4432 ZX= -0.2032

XY= 2.9088 YY= 31.9576 ZY= 1.8759

XZ= -0.4598 YZ= 4.7107 ZZ= 25.9454

Eigenvalues: 24.0746 28.5852 34.4710

29 H Isotropic = 29.0274 Anisotropy = 10.1958

XX= 32.6384 YX= -3.1792 ZX= -1.9105

XY= -3.7647 YY= 28.6144 ZY= 1.8161

XZ= -3.0507 YZ= 3.2914 ZZ= 25.8295

Eigenvalues: 24.2886 26.9691 35.8246

30 H Isotropic = 29.1279 Anisotropy = 6.4517

XX= 25.9682 YX= -0.2978 ZX= -0.0670

XY= -0.3061 YY= 28.1522 ZY= -0.5329

XZ= -2.1415 YZ= 0.6586 ZZ= 33.2634

Eigenvalues: 25.7695 28.1852 33.4290

31 C Isotropic = 56.8578 Anisotropy = 170.0194

XX= -49.9281 YX= -5.6347 ZX= -4.6065

XY= -9.4712 YY= 50.6056 ZY= -5.2298

XZ= -4.6341 YZ= -5.1270 ZZ= 169.8960

Eigenvalues: -50.6055 50.9749 170.2041

32 C Isotropic = 50.1071 Anisotropy = 179.5337

XX= -1.2855 YX= -44.5853 ZX= -5.2603

XY= -43.9014 YY= -17.7294 ZY= -8.6630

XZ= -5.1303 YZ= -8.6148 ZZ= 169.3363

Eigenvalues: -54.9510 35.4761 169.7963

33 C Isotropic = 51.4849 Anisotropy = 162.2967

XX= 10.1404 YX= 13.0413 ZX= -2.4877

XY= 6.1100 YY= -15.0300 ZY= -7.0592

XZ= -2.3686 YZ= -7.0584 ZZ= 159.3444

Eigenvalues: -18.4561 13.2281 159.6828

34 C Isotropic = 12.7202 Anisotropy = 164.8509

XX= -45.9947 YX= 2.5012 ZX= -3.1907

XY= -7.9343 YY= -38.0993 ZY= -7.0367

XZ= -4.0234 YZ= -6.7080 ZZ= 122.2547

Eigenvalues: -47.0201 -37.4401 122.6208

35 C Isotropic = 55.5725 Anisotropy = 154.0450

XX= 35.5725 YX= -28.7771 ZX= -3.8308

XY= -28.1121 YY= -26.6621 ZY= -8.7523

XZ= -3.4552 YZ= -8.8281 ZZ= 157.8070

Eigenvalues: -38.1656 46.6138 158.2692

36 C Isotropic = 44.4002 Anisotropy = 185.1604

XX= 19.2136 YX= 37.5206 ZX= -1.3635

XY= 39.2605 YY= -53.4547 ZY= -8.7508

XZ= -1.1388 YZ= -8.7172 ZZ= 167.4418

Eigenvalues: -70.2176 35.5778 167.8405

37 C Isotropic = 40.1494 Anisotropy = 182.3198

XX= -30.1211 YX= 9.4316 ZX= -3.3645

XY= 2.3617 YY= -10.7794 ZY= -7.0638

XZ= -3.7285 YZ= -6.6501 ZZ= 161.3487

Eigenvalues: -31.7898 -9.4579 161.6959

38 N Isotropic = 5.2505 Anisotropy = 312.4744

XX= -88.5273 YX= 73.9975 ZX= -2.9899

XY= 84.5926 YY= -108.7384 ZY= -11.4719

XZ= -2.9352 YZ= -12.0302 ZZ= 213.0170

Eigenvalues: -178.6896 -19.1257 213.5667

39 H Isotropic = 22.8700 Anisotropy = 8.9840

XX= 28.7846 YX= -0.7887 ZX= -0.0969

XY= -0.4603 YY= 23.5699 ZY= 0.1404

XZ= -0.0971 YZ= 0.1925 ZZ= 16.2556

Eigenvalues: 16.2513 23.4994 28.8594

40 H Isotropic = 23.1480 Anisotropy = 6.7000

XX= 27.1641 YX= 1.2201 ZX= 0.1598

XY= 1.3617 YY= 23.8677 ZY= 0.2117

XZ= 0.1556 YZ= 0.2180 ZZ= 18.4122

Eigenvalues: 18.4024 23.4269 27.6147

41 C Isotropic = 58.1199 Anisotropy = 169.6211

XX= -12.2819 YX= -41.4005 ZX= -5.3549

XY= -37.2875 YY= 15.8424 ZY= -7.1687

XZ= -5.2063 YZ= -7.2008 ZZ= 170.7993

Eigenvalues: -40.3400 43.4991 171.2006

42 C Isotropic = 25.2589 Anisotropy = 154.4005

XX= -29.9157 YX= -12.1884 ZX= -3.8447

XY= -2.2385 YY= -22.1548 ZY= -6.2942

XZ= -3.1488 YZ= -6.7082 ZZ= 127.8472

Eigenvalues: -34.4749 -17.9410 128.1926

43 C Isotropic = 38.3390 Anisotropy = 133.7037

XX= -8.0975 YX= -24.1988 ZX= -4.0552

XY= -24.8545 YY= -4.0275 ZY= -6.1582

XZ= -3.8977 YZ= -5.7634 ZZ= 127.1419

Eigenvalues: -30.9801 18.5223 127.4748

44 H Isotropic = 22.4331 Anisotropy = 7.6076

XX= 25.5633 YX= -2.5183 ZX= 0.0626

XY= -1.0536 YY= 25.8572 ZY= 0.3419

XZ= 0.1684 YZ= 0.3384 ZZ= 15.8788

Eigenvalues: 15.8639 23.9305 27.5048

45 C Isotropic = 54.3903 Anisotropy = 148.5271

XX= 42.9281 YX= -18.1705 ZX= -3.0141

XY= -14.1686 YY= -32.7697 ZY= -8.0568

XZ= -2.7850 YZ= -8.1259 ZZ= 153.0125

Eigenvalues: -36.4610 46.2235 153.4084

46 N Isotropic = 21.2895 Anisotropy = 259.4765

XX= -88.8036 YX= 29.8553 ZX= -4.4955

XY= 38.7233 YY= -41.1455 ZY= -9.1905

XZ= -3.7332 YZ= -8.9611 ZZ= 193.8177

Eigenvalues: -106.7318 -23.6734 194.2739

47 H Isotropic = 22.9387 Anisotropy = 10.4253

XX= 29.8606 YX= 0.9281 ZX= 0.2764

XY= -0.1511 YY= 22.7588 ZY= 0.2030

XZ= 0.3203 YZ= 0.3239 ZZ= 16.1968

Eigenvalues: 16.1804 22.7469 29.8889

48 H Isotropic = 18.2274 Anisotropy = 11.9985

XX= 23.7899 YX= 0.1712 ZX= 0.0409

XY= 0.2031 YY= 26.2057 ZY= 0.2543

XZ= 0.3535 YZ= 0.4527 ZZ= 4.6865

Eigenvalues: 4.6788 23.7770 26.2264

49 C Isotropic = 115.2261 Anisotropy = 62.4765

XX= 146.5037 YX= -19.7019 ZX= 0.1622

XY= -27.2807 YY= 103.6779 ZY= -0.3135

XZ= -0.0476 YZ= 0.0320 ZZ= 95.4966

Eigenvalues: 93.2996 95.5015 156.8770

50 H Isotropic = 23.5695 Anisotropy = 5.2689

XX= 24.8739 YX= -0.2170 ZX= 0.0844

XY= -0.3839 YY= 27.0304 ZY= 0.3081

XZ= 0.1032 YZ= 0.3152 ZZ= 18.8042

Eigenvalues: 18.7906 24.8359 27.0821

51 H Isotropic = 22.3830 Anisotropy = 8.2000

XX= 26.3305 YX= -2.0025 ZX= 0.0886

XY= -2.4889 YY= 24.5284 ZY= 0.2595

XZ= 0.0951 YZ= 0.2775 ZZ= 16.2900

Eigenvalues: 16.2784 23.0208 27.8496

52 C Isotropic = 156.1294 Anisotropy = 34.6476

XX= 148.5461 YX= -5.2508 ZX= -2.8322

XY= -6.6621 YY= 150.3246 ZY= 13.7414

XZ= -8.6065 YZ= 15.0120 ZZ= 169.5176

Eigenvalues: 141.4260 147.7344 179.2278

53 H Isotropic = 24.3458 Anisotropy = 11.4788

XX= 27.7292 YX= 4.3176 ZX= 0.2676

XY= 1.8835 YY= 29.7150 ZY= 0.2404

XZ= 0.4683 YZ= 0.6630 ZZ= 15.5932

Eigenvalues: 15.5725 25.4666 31.9984

54 C Isotropic = 156.1188 Anisotropy = 34.7162

XX= 148.0677 YX= -4.7702 ZX= 1.6038

XY= -6.8294 YY= 152.8874 ZY= -15.6932

XZ= 7.2040 YZ= -16.3939 ZZ= 167.4014

Eigenvalues: 141.3894 147.7041 179.2630

55 H Isotropic = 29.0881 Anisotropy = 8.1910

XX= 29.2713 YX= 2.2658 ZX= 0.0737

XY= 2.8808 YY= 31.4015 ZY= 2.3245

XZ= -0.0052 YZ= 5.4031 ZZ= 26.5914

Eigenvalues: 24.1222 28.5932 34.5487

56 H Isotropic = 29.2131 Anisotropy = 6.2410

XX= 26.1136 YX= -0.2104 ZX= -0.4400

XY= 0.0639 YY= 28.4410 ZY= -1.1302

XZ= -2.3025 YZ= 0.3329 ZZ= 33.0848

Eigenvalues: 25.8452 28.4203 33.3738

57 H Isotropic = 29.0990 Anisotropy = 10.0949

XX= 32.8744 YX= -3.0685 ZX= -2.0050

XY= -3.5061 YY= 28.3210 ZY= 1.6554

XZ= -3.0362 YZ= 3.5379 ZZ= 26.1016

Eigenvalues: 24.3719 27.0963 35.8289

58 H Isotropic = 29.0446 Anisotropy = 8.1392

XX= 29.2295 YX= 2.4430 ZX= 0.1991

XY= 2.9079 YY= 31.9502 ZY= -1.8804

XZ= 0.4566 YZ= -4.7189 ZZ= 25.9541

Eigenvalues: 24.0765 28.5866 34.4708

59 H Isotropic = 29.0286 Anisotropy = 10.1959

XX= 32.6368 YX= -3.1790 ZX= 1.9131

XY= -3.7638 YY= 28.6134 ZY= -1.8150

XZ= 3.0565 YZ= -3.2934 ZZ= 25.8356

Eigenvalues: 24.2922 26.9678 35.8259

60 H Isotropic = 29.1276 Anisotropy = 6.4455

XX= 25.9674 YX= -0.2976 ZX= 0.0688

XY= -0.3058 YY= 28.1570 ZY= 0.5410

XZ= 2.1450 YZ= -0.6515 ZZ= 33.2584

Eigenvalues: 25.7678 28.1904 33.4246

# NMR chemical shift calculations – BETAINE motif (compounds 2 and[2]2)

## BETAINE monomer\_iso1 (gas-phase) - BP86/IGLO-III level

32

c 0.0915 -0.0647 -4.0409

c -1.3554 -0.3808 -4.4431

c 1.0937 -1.1457 -4.4667

h 2.1246 -0.8830 -4.1461

h 1.0879 -1.2404 -5.5740

h 0.8373 -2.1396 -4.0404

c 0.5686 1.4653 -2.1614

h 0.7870 2.2030 -2.9436

c 0.6505 1.7212 -0.7780

h 0.9375 2.7348 -0.4529

c 0.3752 0.7363 0.1587

h 0.4344 0.9643 1.2340

c -0.0264 -0.6062 -0.2554

c -0.0930 -0.7705 -1.6926

h -0.4003 -1.7455 -2.0958

c -0.2017 -1.6815 1.8651

c -1.2598 -2.1762 2.6790

h -2.2046 -2.4509 2.1820

c -1.1095 -2.3122 4.0651

h -1.9531 -2.6920 4.6672

c 0.1057 -1.9777 4.6931

h 0.2243 -2.0932 5.7831

c 1.1707 -1.5070 3.9040

h 2.1375 -1.2578 4.3756

c 1.0238 -1.3563 2.5167

h 1.8796 -1.0142 1.9100

n 0.1914 0.2136 -2.5682

n -0.3782 -1.6366 0.4901

h -1.4240 -0.4570 -5.5499

h -2.0476 0.4207 -4.1068

h -1.7025 -1.3455 -4.0144

h 0.3861 0.8912 -4.5207

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 106.0416 Anisotropy = 62.7669

XX= 141.9771 YX= -12.3013 ZX= 6.4083

XY= -21.0333 YY= 90.4916 ZY= -2.7881

XZ= 8.5107 YZ= -1.9635 ZZ= 85.6560

Eigenvalues: 84.6426 85.5959 147.8862

2 C Isotropic = 151.4787 Anisotropy = 36.9810

XX= 143.3629 YX= -6.4874 ZX= -2.7785

XY= -8.8921 YY= 152.1965 ZY= 19.7725

XZ= -4.6134 YZ= 17.1028 ZZ= 158.8768

Eigenvalues: 134.9769 143.3266 176.1328

3 C Isotropic = 151.1940 Anisotropy = 36.7806

XX= 142.5358 YX= -3.4473 ZX= 3.5419

XY= -4.0635 YY= 137.0384 ZY= -7.2071

XZ= 6.1021 YZ= -4.1068 ZZ= 174.0078

Eigenvalues: 134.8934 142.9741 175.7144

4 H Isotropic = 29.4487 Anisotropy = 8.1838

XX= 26.3399 YX= -0.7801 ZX= 0.3219

XY= -0.3294 YY= 28.8483 ZY= 2.6398

XZ= 0.5414 YZ= 3.8613 ZZ= 33.1578

Eigenvalues: 25.9293 27.5121 34.9045

5 H Isotropic = 29.7643 Anisotropy = 8.9224

XX= 33.0067 YX= -2.0112 ZX= 3.0054

XY= -2.2280 YY= 26.6919 ZY= -0.6705

XZ= 3.8792 YZ= -1.0922 ZZ= 29.5944

Eigenvalues: 26.0330 27.5473 35.7126

6 H Isotropic = 29.4468 Anisotropy = 5.5057

XX= 28.9873 YX= 1.8641 ZX= 0.0092

XY= 2.1801 YY= 29.6416 ZY= -2.0252

XZ= -0.5803 YZ= -3.4973 ZZ= 29.7114

Eigenvalues: 26.2512 28.9718 33.1172

7 C Isotropic = 61.0909 Anisotropy = 73.8557

XX= 30.7130 YX= -42.4388 ZX= 8.0057

XY= -41.1141 YY= 49.9274 ZY= 16.5510

XZ= 14.6721 YZ= 25.9417 ZZ= 102.6324

Eigenvalues: -7.0431 79.9879 110.3281

8 H Isotropic = 25.2366 Anisotropy = 5.3169

XX= 24.7414 YX= -1.7240 ZX= 0.6692

XY= -1.2793 YY= 27.8574 ZY= -1.5313

XZ= 0.6952 YZ= -0.8117 ZZ= 23.1110

Eigenvalues: 22.7673 24.1612 28.7812

9 C Isotropic = 44.2761 Anisotropy = 162.9084

XX= 40.0599 YX= 13.4889 ZX= -9.9892

XY= 18.5274 YY= -39.7613 ZY= 60.5880

XZ= -17.2116 YZ= 62.6420 ZZ= 132.5297

Eigenvalues: -63.1834 43.1300 152.8817

10 H Isotropic = 24.7983 Anisotropy = 3.8216

XX= 27.2553 YX= 0.6414 ZX= 0.0221

XY= 0.1835 YY= 23.9360 ZY= -0.2090

XZ= -0.7446 YZ= -0.5829 ZZ= 23.2036

Eigenvalues: 23.0236 24.0253 27.3461

11 C Isotropic = 45.9469 Anisotropy = 180.6878

XX= -30.1304 YX= 18.9755 ZX= -11.6500

XY= 17.0420 YY= 10.8478 ZY= 43.2050

XZ= -54.1598 YZ= 11.0209 ZZ= 157.1232

Eigenvalues: -45.0948 16.5301 166.4054

12 H Isotropic = 23.8050 Anisotropy = 9.5471

XX= 24.9724 YX= 4.4739 ZX= -2.4211

XY= 4.0696 YY= 25.9757 ZY= -0.6635

XZ= -4.1964 YZ= 1.5466 ZZ= 20.4670

Eigenvalues: 17.8628 23.3825 30.1698

13 C Isotropic = 20.3727 Anisotropy = 137.3143

XX= -35.5340 YX= 26.5467 ZX= -12.2993

XY= 1.7078 YY= -4.6059 ZY= 38.3019

XZ= -9.4819 YZ= 31.1582 ZZ= 101.2578

Eigenvalues: -45.0261 -5.7715 111.9156

14 C Isotropic = 36.9939 Anisotropy = 125.5710

XX= 21.9927 YX= 3.1139 ZX= -4.7423

XY= -0.4043 YY= -11.3250 ZY= 38.3320

XZ= 3.7785 YZ= 65.4499 ZZ= 100.3139

Eigenvalues: -31.7573 22.0311 120.7079

15 H Isotropic = 24.5819 Anisotropy = 9.9039

XX= 30.7951 YX= 2.3405 ZX= -0.1827

XY= 1.4321 YY= 20.8395 ZY= 0.8038

XZ= 1.0394 YZ= 1.4943 ZZ= 22.1110

Eigenvalues: 19.9679 22.5932 31.1845

16 C Isotropic = 15.9263 Anisotropy = 168.7014

XX= -68.0615 YX= 11.5179 ZX= -4.0793

XY= 21.6978 YY= 41.3378 ZY= -66.1501

XZ= -17.5243 YZ= -67.1538 ZZ= 74.5025

Eigenvalues: -70.5348 -10.0803 128.3939

17 C Isotropic = 45.7545 Anisotropy = 152.0202

XX= 28.5240 YX= 25.8211 ZX= 3.2068

XY= 20.8006 YY= 28.3793 ZY= -89.3343

XZ= 19.7286 YZ= -88.2780 ZZ= 80.3601

Eigenvalues: -46.8263 36.9884 147.1013

18 H Isotropic = 24.3416 Anisotropy = 6.1070

XX= 27.7282 YX= 1.2713 ZX= 1.4817

XY= 1.2213 YY= 23.2757 ZY= 0.8474

XZ= 1.3010 YZ= 0.4842 ZZ= 22.0210

Eigenvalues: 21.6018 23.0101 28.4130

19 C Isotropic = 40.8984 Anisotropy = 179.3717

XX= -4.1703 YX= -31.7438 ZX= -44.4780

XY= -30.6471 YY= 48.3820 ZY= -91.4667

XZ= -41.0467 YZ= -98.2607 ZZ= 78.4834

Eigenvalues: -72.0530 34.2687 160.4795

20 H Isotropic = 23.8814 Anisotropy = 4.6505

XX= 25.8237 YX= -1.5694 ZX= -0.8214

XY= -1.4467 YY= 23.6606 ZY= 1.6061

XZ= -0.7817 YZ= 1.1196 ZZ= 22.1600

Eigenvalues: 21.3529 23.3097 26.9818

21 C Isotropic = 51.8630 Anisotropy = 167.0104

XX= -46.5659 YX= 23.5198 ZX= -5.0691

XY= 26.5085 YY= 87.8751 ZY= -57.1966

XZ= -3.0634 YZ= -60.7233 ZZ= 114.2797

Eigenvalues: -51.3624 43.7481 163.2033

22 H Isotropic = 24.3745 Anisotropy = 3.6957

XX= 24.5708 YX= 0.2802 ZX= 0.4369

XY= 0.3383 YY= 24.8981 ZY= 2.4803

XZ= 0.6582 YZ= 2.1836 ZZ= 23.6545

Eigenvalues: 21.8402 24.4450 26.8383

23 C Isotropic = 42.9256 Anisotropy = 176.1499

XX= 24.9785 YX= 35.4127 ZX= 12.9456

XY= 33.1724 YY= 27.7740 ZY= -103.0027

XZ= 9.8284 YZ= -106.0416 ZZ= 76.0244

Eigenvalues: -67.8602 36.2782 160.3588

24 H Isotropic = 24.0591 Anisotropy = 4.8218

XX= 27.0773 YX= 0.6437 ZX= 0.9700

XY= 0.4805 YY= 22.6640 ZY= 1.1172

XZ= 0.2757 YZ= 1.1781 ZZ= 22.4360

Eigenvalues: 21.3954 23.5083 27.2736

25 C Isotropic = 58.2705 Anisotropy = 154.6222

XX= 12.2660 YX= -17.3477 ZX= -27.9990

XY= -23.6964 YY= 61.3132 ZY= -74.7494

XZ= -50.5773 YZ= -75.1778 ZZ= 101.2323

Eigenvalues: -33.2777 46.7373 161.3520

26 H Isotropic = 24.1664 Anisotropy = 7.9327

XX= 28.0054 YX= -2.4168 ZX= -2.6836

XY= -1.6936 YY= 22.5617 ZY= 0.7014

XZ= -1.7302 YZ= 1.1803 ZZ= 21.9321

Eigenvalues: 21.1274 21.9169 29.4549

27 N Isotropic = 2.9997 Anisotropy = 257.1641

XX= -105.4975 YX= 42.1049 ZX= -25.8040

XY= 22.5322 YY= -36.5512 ZY= 62.8145

XZ= -25.6372 YZ= 75.1707 ZZ= 151.0476

Eigenvalues: -127.9832 -37.4603 174.4424

28 N Isotropic = -11.6868 Anisotropy = 282.1001

XX= -191.7891 YX= -31.0168 ZX= 16.9169

XY= -32.2014 YY= -15.5539 ZY= 24.5412

XZ= -89.6969 YZ= -11.3250 ZZ= 172.2826

Eigenvalues: -200.5277 -10.9127 176.3799

29 H Isotropic = 29.7873 Anisotropy = 8.9665

XX= 33.4746 YX= -3.3216 ZX= -1.0492

XY= -3.9304 YY= 28.1566 ZY= 1.1618

XZ= -1.7672 YZ= 1.6981 ZZ= 27.7306

Eigenvalues: 26.0120 27.5848 35.7649

30 H Isotropic = 29.5409 Anisotropy = 8.1117

XX= 26.5349 YX= -0.9106 ZX= -0.6147

XY= -0.6901 YY= 27.2687 ZY= 1.0615

XZ= -1.1364 YZ= -0.1444 ZZ= 34.8190

Eigenvalues: 25.9929 27.6810 34.9487

31 H Isotropic = 29.4720 Anisotropy = 5.8322

XX= 29.0494 YX= 1.2901 ZX= -0.7855

XY= 2.1070 YY= 32.3796 ZY= 0.8633

XZ= -0.5065 YZ= 2.4412 ZZ= 26.9870

Eigenvalues: 26.0794 28.9764 33.3601

32 H Isotropic = 27.4735 Anisotropy = 3.9483

XX= 28.1258 YX= 2.0284 ZX= -0.3555

XY= 0.3026 YY= 29.1014 ZY= -1.1989

XZ= -0.0016 YZ= -1.0876 ZZ= 25.1934

Eigenvalues: 24.8776 27.4373 30.1058

## BETAINE monomer\_iso1 (gas-phase) – PBE0/IGLO-III level

32

c 0.0915 -0.0647 -4.0409

c -1.3554 -0.3808 -4.4431

c 1.0937 -1.1457 -4.4667

h 2.1246 -0.8830 -4.1461

h 1.0879 -1.2404 -5.5740

h 0.8373 -2.1396 -4.0404

c 0.5686 1.4653 -2.1614

h 0.7870 2.2030 -2.9436

c 0.6505 1.7212 -0.7780

h 0.9375 2.7348 -0.4529

c 0.3752 0.7363 0.1587

h 0.4344 0.9643 1.2340

c -0.0264 -0.6062 -0.2554

c -0.0930 -0.7705 -1.6926

h -0.4003 -1.7455 -2.0958

c -0.2017 -1.6815 1.8651

c -1.2598 -2.1762 2.6790

h -2.2046 -2.4509 2.1820

c -1.1095 -2.3122 4.0651

h -1.9531 -2.6920 4.6672

c 0.1057 -1.9777 4.6931

h 0.2243 -2.0932 5.7831

c 1.1707 -1.5070 3.9040

h 2.1375 -1.2578 4.3756

c 1.0238 -1.3563 2.5167

h 1.8796 -1.0142 1.9100

n 0.1914 0.2136 -2.5682

n -0.3782 -1.6366 0.4901

h -1.4240 -0.4570 -5.5499

h -2.0476 0.4207 -4.1068

h -1.7025 -1.3455 -4.0144

h 0.3861 0.8912 -4.5207

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 113.4450 Anisotropy = 62.0343

XX= 148.9788 YX= -12.1734 ZX= 6.2995

XY= -20.7519 YY= 98.0348 ZY= -2.7202

XZ= 8.4148 YZ= -1.8616 ZZ= 93.3216

Eigenvalues: 92.3404 93.1935 154.8012

2 C Isotropic = 156.8015 Anisotropy = 35.5143

XX= 149.3424 YX= -6.4205 ZX= -2.4136

XY= -9.0736 YY= 157.3553 ZY= 18.9072

XZ= -4.8579 YZ= 16.5103 ZZ= 163.7068

Eigenvalues: 140.6941 149.2326 180.4777

3 C Isotropic = 156.5927 Anisotropy = 35.2402

XX= 148.5864 YX= -3.6215 ZX= 3.2844

XY= -4.1884 YY= 142.8499 ZY= -6.8415

XZ= 6.4489 YZ= -4.0315 ZZ= 178.3416

Eigenvalues: 140.6600 149.0319 180.0861

4 H Isotropic = 29.4280 Anisotropy = 8.5949

XX= 26.1540 YX= -0.9062 ZX= 0.2518

XY= -0.3602 YY= 28.9020 ZY= 2.9620

XZ= 0.7504 YZ= 3.9828 ZZ= 33.2280

Eigenvalues: 25.6665 27.4595 35.1579

5 H Isotropic = 29.7273 Anisotropy = 9.5320

XX= 33.3083 YX= -2.1928 ZX= 3.1697

XY= -2.3696 YY= 26.5165 ZY= -0.7249

XZ= 4.0625 YZ= -1.1904 ZZ= 29.3570

Eigenvalues: 25.8111 27.2888 36.0819

6 H Isotropic = 29.3817 Anisotropy = 6.0668

XX= 28.9186 YX= 2.1355 ZX= -0.1144

XY= 2.4549 YY= 29.7183 ZY= -2.1768

XZ= -0.5499 YZ= -3.7737 ZZ= 29.5081

Eigenvalues: 25.8988 28.8200 33.4262

7 C Isotropic = 63.8017 Anisotropy = 83.4404

XX= 29.5062 YX= -44.3452 ZX= 8.1623

XY= -42.4447 YY= 50.5029 ZY= 18.9285

XZ= 14.3477 YZ= 27.5908 ZZ= 111.3959

Eigenvalues: -9.1689 81.1454 119.4286

8 H Isotropic = 25.0232 Anisotropy = 5.6804

XX= 24.7507 YX= -1.6943 ZX= 0.6728

XY= -1.1380 YY= 27.8785 ZY= -1.7408

XZ= 0.6713 YZ= -1.1003 ZZ= 22.4405

Eigenvalues: 22.0490 24.2105 28.8101

9 C Isotropic = 46.5273 Anisotropy = 171.6092

XX= 41.5268 YX= 14.1705 ZX= -10.3575

XY= 19.6990 YY= -41.5771 ZY= 63.7475

XZ= -17.0474 YZ= 65.8044 ZZ= 139.6321

Eigenvalues: -66.1900 44.8384 160.9334

10 H Isotropic = 24.5223 Anisotropy = 4.0731

XX= 27.1421 YX= 0.7443 ZX= -0.0018

XY= 0.1621 YY= 23.8602 ZY= -0.3647

XZ= -0.6449 YZ= -0.7669 ZZ= 22.5647

Eigenvalues: 22.3479 23.9813 27.2378

11 C Isotropic = 48.8765 Anisotropy = 185.2064

XX= -28.3398 YX= 19.6773 ZX= -12.2109

XY= 19.1707 YY= 12.5211 ZY= 45.2701

XZ= -52.1044 YZ= 15.7151 ZZ= 162.4482

Eigenvalues: -44.4612 18.7433 172.3474

12 H Isotropic = 23.6202 Anisotropy = 10.1479

XX= 25.0769 YX= 4.5252 ZX= -2.3998

XY= 4.2922 YY= 25.9086 ZY= -0.8284

XZ= -4.1812 YZ= 1.0375 ZZ= 19.8751

Eigenvalues: 17.6606 22.8146 30.3855

13 C Isotropic = 20.6680 Anisotropy = 151.0820

XX= -41.5201 YX= 29.7218 ZX= -13.7435

XY= 3.1433 YY= -5.7733 ZY= 41.2182

XZ= -11.9047 YZ= 35.9586 ZZ= 109.2974

Eigenvalues: -52.6229 -6.7625 121.3894

14 C Isotropic = 38.8917 Anisotropy = 132.7896

XX= 22.4944 YX= 3.0432 ZX= -4.8990

XY= -0.6226 YY= -13.2854 ZY= 40.9007

XZ= 2.7295 YZ= 65.0574 ZZ= 107.4661

Eigenvalues: -33.2752 22.5323 127.4181

15 H Isotropic = 24.2140 Anisotropy = 10.4229

XX= 30.7406 YX= 2.5057 ZX= -0.2139

XY= 1.5635 YY= 20.7000 ZY= 0.5886

XZ= 0.8797 YZ= 1.2426 ZZ= 21.2016

Eigenvalues: 19.7985 21.6810 31.1627

16 C Isotropic = 17.5395 Anisotropy = 178.7474

XX= -72.7561 YX= 13.1741 ZX= -4.8818

XY= 23.4856 YY= 45.0318 ZY= -69.6290

XZ= -17.5969 YZ= -70.1372 ZZ= 80.3429

Eigenvalues: -75.5459 -8.5400 136.7044

17 C Isotropic = 48.1063 Anisotropy = 158.4319

XX= 29.6693 YX= 27.6230 ZX= 4.4811

XY= 22.7733 YY= 31.0659 ZY= -91.9845

XZ= 19.4710 YZ= -92.9812 ZZ= 83.5838

Eigenvalues: -48.3968 38.9882 153.7276

18 H Isotropic = 24.1583 Anisotropy = 6.4056

XX= 27.7080 YX= 1.2690 ZX= 1.5377

XY= 1.1174 YY= 23.0884 ZY= 1.0751

XZ= 1.4992 YZ= 0.8104 ZZ= 21.6785

Eigenvalues: 21.0807 22.9655 28.4287

19 C Isotropic = 42.8630 Anisotropy = 186.7196

XX= -4.4886 YX= -32.9644 ZX= -46.3669

XY= -31.5944 YY= 50.1999 ZY= -95.5689

XZ= -42.4272 YZ= -101.2014 ZZ= 82.8776

Eigenvalues: -74.3304 35.5766 167.3427

20 H Isotropic = 23.7321 Anisotropy = 4.8145

XX= 25.7949 YX= -1.5848 ZX= -0.7932

XY= -1.4348 YY= 23.4922 ZY= 1.7775

XZ= -0.7226 YZ= 1.3743 ZZ= 21.9091

Eigenvalues: 20.9317 23.3227 26.9417

21 C Isotropic = 54.7594 Anisotropy = 172.9617

XX= -47.4330 YX= 24.3758 ZX= -5.3117

XY= 26.8407 YY= 91.7978 ZY= -59.5323

XZ= -3.4804 YZ= -62.1942 ZZ= 119.9134

Eigenvalues: -52.2666 46.4776 170.0672

22 H Isotropic = 24.2529 Anisotropy = 3.8416

XX= 24.6659 YX= 0.2370 ZX= 0.4646

XY= 0.2869 YY= 24.7259 ZY= 2.6740

XZ= 0.6216 YZ= 2.4110 ZZ= 23.3670

Eigenvalues: 21.3919 24.5529 26.8140

23 C Isotropic = 44.7846 Anisotropy = 183.6889

XX= 25.7127 YX= 37.0423 ZX= 13.7264

XY= 34.6686 YY= 29.7962 ZY= -107.0796

XZ= 10.5323 YZ= -110.8568 ZZ= 78.8449

Eigenvalues: -70.6100 37.7199 167.2439

24 H Isotropic = 23.8926 Anisotropy = 5.0113

XX= 27.0347 YX= 0.6257 ZX= 0.9968

XY= 0.4527 YY= 22.5172 ZY= 1.3152

XZ= 0.3087 YZ= 1.3556 ZZ= 22.1260

Eigenvalues: 20.9685 23.4759 27.2335

25 C Isotropic = 59.2598 Anisotropy = 161.9744

XX= 11.3641 YX= -18.5589 ZX= -29.7295

XY= -23.3006 YY= 64.5371 ZY= -77.9113

XZ= -53.8395 YZ= -80.4248 ZZ= 101.8780

Eigenvalues: -36.8674 47.4040 167.2427

26 H Isotropic = 24.0100 Anisotropy = 8.3704

XX= 28.0022 YX= -2.5287 ZX= -2.7107

XY= -1.7478 YY= 22.3684 ZY= 0.9336

XZ= -2.0382 YZ= 1.3961 ZZ= 21.6595

Eigenvalues: 20.6805 21.7593 29.5903

27 N Isotropic = 1.8057 Anisotropy = 278.6993

XX= -117.0760 YX= 46.2703 ZX= -28.0775

XY= 26.3745 YY= -40.7613 ZY= 68.0178

XZ= -25.8041 YZ= 78.7164 ZZ= 163.2544

Eigenvalues: -141.5123 -40.6758 187.6052

28 N Isotropic = 1.8776 Anisotropy = 281.1960

XX= -179.0917 YX= -25.1796 ZX= 15.9529

XY= -22.4933 YY= -0.8613 ZY= 24.1598

XZ= -85.3584 YZ= -9.4753 ZZ= 185.5857

Eigenvalues: -185.2478 1.5389 189.3416

29 H Isotropic = 29.7462 Anisotropy = 9.5740

XX= 33.7860 YX= -3.5506 ZX= -1.0524

XY= -4.1285 YY= 28.0255 ZY= 1.1420

XZ= -1.8052 YZ= 1.7062 ZZ= 27.4272

Eigenvalues: 25.7883 27.3215 36.1289

30 H Isotropic = 29.5088 Anisotropy = 8.5147

XX= 26.3369 YX= -0.9702 ZX= -0.5292

XY= -0.7943 YY= 27.1291 ZY= 0.8714

XZ= -1.3406 YZ= -0.1450 ZZ= 35.0603

Eigenvalues: 25.7275 27.6135 35.1853

31 H Isotropic = 29.4091 Anisotropy = 6.3824

XX= 28.9771 YX= 1.5841 ZX= -0.8098

XY= 2.3378 YY= 32.5790 ZY= 0.8120

XZ= -0.6618 YZ= 2.5010 ZZ= 26.6710

Eigenvalues: 25.7264 28.8368 33.6640

32 H Isotropic = 27.4268 Anisotropy = 4.6148

XX= 28.2854 YX= 2.3035 ZX= -0.4141

XY= 0.5425 YY= 29.2331 ZY= -1.3435

XZ= -0.0240 YZ= -1.2344 ZZ= 24.7621

Eigenvalues: 24.4101 27.3671 30.5033

## BETAINE monomer\_iso1 (IEFPCM solvent = tetrahydrofuran) – BP86/IGLO-III level

32

c 0.0915 -0.0647 -4.0409

c -1.3554 -0.3808 -4.4431

c 1.0937 -1.1457 -4.4667

h 2.1246 -0.8830 -4.1461

h 1.0879 -1.2404 -5.5740

h 0.8373 -2.1396 -4.0404

c 0.5686 1.4653 -2.1614

h 0.7870 2.2030 -2.9436

c 0.6505 1.7212 -0.7780

h 0.9375 2.7348 -0.4529

c 0.3752 0.7363 0.1587

h 0.4344 0.9643 1.2340

c -0.0264 -0.6062 -0.2554

c -0.0930 -0.7705 -1.6926

h -0.4003 -1.7455 -2.0958

c -0.2017 -1.6815 1.8651

c -1.2598 -2.1762 2.6790

h -2.2046 -2.4509 2.1820

c -1.1095 -2.3122 4.0651

h -1.9531 -2.6920 4.6672

c 0.1057 -1.9777 4.6931

h 0.2243 -2.0932 5.7831

c 1.1707 -1.5070 3.9040

h 2.1375 -1.2578 4.3756

c 1.0238 -1.3563 2.5167

h 1.8796 -1.0142 1.9100

n 0.1914 0.2136 -2.5682

n -0.3782 -1.6366 0.4901

h -1.4240 -0.4570 -5.5499

h -2.0476 0.4207 -4.1068

h -1.7025 -1.3455 -4.0144

h 0.3861 0.8912 -4.5207

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 105.1836 Anisotropy = 64.9389

XX= 142.1224 YX= -13.7495 ZX= 6.7809

XY= -21.8875 YY= 88.0951 ZY= -2.2010

XZ= 8.8155 YZ= -1.2953 ZZ= 85.3334

Eigenvalues: 82.5677 84.5070 148.4762

2 C Isotropic = 151.3765 Anisotropy = 37.2034

XX= 143.8874 YX= -6.4749 ZX= -2.8732

XY= -8.9768 YY= 152.4707 ZY= 19.7080

XZ= -5.6578 YZ= 17.7508 ZZ= 157.7716

Eigenvalues: 134.9257 143.0251 176.1788

3 C Isotropic = 151.1395 Anisotropy = 37.0128

XX= 143.0396 YX= -3.3010 ZX= 3.6496

XY= -3.5769 YY= 136.6725 ZY= -7.5614

XZ= 7.0441 YZ= -5.1638 ZZ= 173.7064

Eigenvalues: 134.7607 142.8430 175.8147

4 H Isotropic = 29.4499 Anisotropy = 8.1436

XX= 26.3298 YX= -0.7645 ZX= 0.3378

XY= -0.2184 YY= 28.8138 ZY= 2.6540

XZ= 0.8665 YZ= 3.6898 ZZ= 33.2062

Eigenvalues: 25.9086 27.5622 34.8790

5 H Isotropic = 29.5847 Anisotropy = 9.1366

XX= 32.9629 YX= -2.0485 ZX= 3.0374

XY= -2.1865 YY= 26.4870 ZY= -0.6862

XZ= 4.0051 YZ= -1.1849 ZZ= 29.3043

Eigenvalues: 25.8493 27.2291 35.6758

6 H Isotropic = 29.4447 Anisotropy = 5.6337

XX= 28.9866 YX= 1.9026 ZX= -0.0266

XY= 2.2295 YY= 29.6550 ZY= -2.0104

XZ= -0.4777 YZ= -3.6908 ZZ= 29.6924

Eigenvalues: 26.1399 28.9937 33.2005

7 C Isotropic = 55.3697 Anisotropy = 88.4891

XX= 22.0998 YX= -41.8816 ZX= 7.3648

XY= -39.9060 YY= 38.2702 ZY= 21.1895

XZ= 12.3017 YZ= 29.4373 ZZ= 105.7393

Eigenvalues: -16.1724 67.9191 114.3625

8 H Isotropic = 24.6549 Anisotropy = 5.5759

XX= 24.4622 YX= -1.7611 ZX= 0.6875

XY= -1.3430 YY= 27.3042 ZY= -1.6562

XZ= 0.7129 YZ= -1.0945 ZZ= 22.1983

Eigenvalues: 21.8102 23.7824 28.3722

9 C Isotropic = 43.5539 Anisotropy = 169.2264

XX= 36.2519 YX= 12.3098 ZX= -9.7992

XY= 16.2390 YY= -41.4817 ZY= 61.9776

XZ= -15.6279 YZ= 63.5731 ZZ= 135.8915

Eigenvalues: -64.4842 38.7744 156.3715

10 H Isotropic = 24.4245 Anisotropy = 4.0062

XX= 26.9905 YX= 0.6933 ZX= 0.0096

XY= 0.2732 YY= 23.7583 ZY= -0.3510

XZ= -0.6412 YZ= -0.7385 ZZ= 22.5245

Eigenvalues: 22.3150 23.8631 27.0953

11 C Isotropic = 49.3125 Anisotropy = 176.4004

XX= -26.7780 YX= 19.4931 ZX= -11.7284

XY= 16.0457 YY= 16.0339 ZY= 41.5663

XZ= -42.9649 YZ= 14.5304 ZZ= 158.6814

Eigenvalues: -39.6094 20.6341 166.9127

12 H Isotropic = 23.7860 Anisotropy = 9.4196

XX= 25.0671 YX= 4.2605 ZX= -2.2999

XY= 3.9357 YY= 25.9782 ZY= -0.7908

XZ= -3.6388 YZ= 0.8372 ZZ= 20.3128

Eigenvalues: 18.3460 22.9464 30.0657

13 C Isotropic = 19.4362 Anisotropy = 145.0190

XX= -39.6707 YX= 17.6714 ZX= -9.4815

XY= -3.1273 YY= -6.6893 ZY= 39.8459

XZ= -10.1844 YZ= 33.8964 ZZ= 104.6687

Eigenvalues: -43.7104 -14.0965 116.1156

14 C Isotropic = 36.5903 Anisotropy = 128.8548

XX= 20.7623 YX= -0.3203 ZX= -3.7340

XY= -1.1036 YY= -14.8222 ZY= 39.8454

XZ= 3.6322 YZ= 61.3981 ZZ= 103.8306

Eigenvalues: -33.4919 20.7693 122.4934

15 H Isotropic = 24.1856 Anisotropy = 10.1553

XX= 30.6683 YX= 2.0654 ZX= -0.0820

XY= 1.2491 YY= 20.5215 ZY= 0.6699

XZ= 0.7352 YZ= 1.2679 ZZ= 21.3671

Eigenvalues: 19.7456 21.8554 30.9558

16 C Isotropic = 14.9084 Anisotropy = 170.3886

XX= -68.1150 YX= 10.3230 ZX= -5.2480

XY= 21.2028 YY= 39.4775 ZY= -68.3128

XZ= -16.9446 YZ= -68.2400 ZZ= 73.3628

Eigenvalues: -70.3932 -13.3824 128.5008

17 C Isotropic = 46.6898 Anisotropy = 148.4909

XX= 30.4300 YX= 27.4663 ZX= 5.4504

XY= 20.2326 YY= 31.6461 ZY= -85.3257

XZ= 22.2421 YZ= -90.1540 ZZ= 77.9933

Eigenvalues: -45.7519 40.1375 145.6837

18 H Isotropic = 24.3358 Anisotropy = 6.0977

XX= 27.6796 YX= 1.3444 ZX= 1.5372

XY= 1.0477 YY= 23.2860 ZY= 0.7482

XZ= 1.5167 YZ= 0.4465 ZZ= 22.0418

Eigenvalues: 21.5977 23.0088 28.4009

19 C Isotropic = 40.9807 Anisotropy = 180.4371

XX= -4.4967 YX= -31.1377 ZX= -44.4525

XY= -30.5037 YY= 49.1677 ZY= -91.4840

XZ= -41.0192 YZ= -99.4180 ZZ= 78.2712

Eigenvalues: -72.0568 33.7268 161.2722

20 H Isotropic = 23.7872 Anisotropy = 4.6012

XX= 25.7675 YX= -1.5302 ZX= -0.7764

XY= -1.3753 YY= 23.5917 ZY= 1.6237

XZ= -0.7652 YZ= 1.0869 ZZ= 22.0023

Eigenvalues: 21.2251 23.2818 26.8546

21 C Isotropic = 53.4200 Anisotropy = 166.0270

XX= -44.4971 YX= 23.1587 ZX= -5.2613

XY= 25.6872 YY= 89.1001 ZY= -57.1666

XZ= -3.3475 YZ= -59.9584 ZZ= 115.6572

Eigenvalues: -49.0753 45.2307 164.1047

22 H Isotropic = 24.3184 Anisotropy = 3.5798

XX= 24.5976 YX= 0.2222 ZX= 0.4119

XY= 0.2644 YY= 24.8240 ZY= 2.4696

XZ= 0.6279 YZ= 2.1593 ZZ= 23.5335

Eigenvalues: 21.7505 24.4997 26.7049

23 C Isotropic = 42.3049 Anisotropy = 178.3275

XX= 23.7618 YX= 34.8427 ZX= 12.3851

XY= 33.2639 YY= 27.8987 ZY= -103.9099

XZ= 8.9026 YZ= -107.5340 ZZ= 75.2542

Eigenvalues: -68.7936 34.5183 161.1899

24 H Isotropic = 23.9131 Anisotropy = 4.8116

XX= 26.9324 YX= 0.6104 ZX= 0.9614

XY= 0.4889 YY= 22.5629 ZY= 1.1152

XZ= 0.2656 YZ= 1.1385 ZZ= 22.2440

Eigenvalues: 21.2634 23.3550 27.1208

25 C Isotropic = 55.8382 Anisotropy = 158.3580

XX= 8.9332 YX= -17.2971 ZX= -28.7787

XY= -20.9103 YY= 61.2667 ZY= -75.5020

XZ= -53.3254 YZ= -78.7979 ZZ= 97.3146

Eigenvalues: -37.1743 43.2786 161.4102

26 H Isotropic = 23.9643 Anisotropy = 8.2458

XX= 27.7816 YX= -2.5283 ZX= -2.7945

XY= -1.7007 YY= 22.4370 ZY= 0.7482

XZ= -2.2973 YZ= 1.1233 ZZ= 21.6743

Eigenvalues: 20.7277 21.7037 29.4615

27 N Isotropic = -3.1812 Anisotropy = 272.3135

XX= -115.2001 YX= 37.2810 ZX= -24.7067

XY= 19.0850 YY= -48.8152 ZY= 67.3271

XZ= -23.5426 YZ= 77.5543 ZZ= 154.4716

Eigenvalues: -134.5513 -53.3535 178.3611

28 N Isotropic = 10.9365 Anisotropy = 245.1003

XX= -142.3438 YX= -26.0172 ZX= 14.8291

XY= -21.5665 YY= 4.8920 ZY= 17.9475

XZ= -86.1560 YZ= -17.0096 ZZ= 170.2613

Eigenvalues: -149.9553 8.4281 174.3367

29 H Isotropic = 29.5993 Anisotropy = 9.1795

XX= 33.4314 YX= -3.3658 ZX= -1.0460

XY= -3.9527 YY= 27.9705 ZY= 1.1088

XZ= -1.8729 YZ= 1.7074 ZZ= 27.3959

Eigenvalues: 25.8243 27.2546 35.7190

30 H Isotropic = 29.5310 Anisotropy = 8.0919

XX= 26.5321 YX= -0.8980 ZX= -0.6342

XY= -0.7563 YY= 27.3189 ZY= 1.0315

XZ= -1.4722 YZ= 0.0065 ZZ= 34.7419

Eigenvalues: 25.9639 27.7034 34.9256

31 H Isotropic = 29.4717 Anisotropy = 5.9463

XX= 29.0443 YX= 1.3423 ZX= -0.7770

XY= 2.0993 YY= 32.4574 ZY= 0.7906

XZ= -0.6225 YZ= 2.5506 ZZ= 26.9133

Eigenvalues: 25.9806 28.9985 33.4358

32 H Isotropic = 27.0809 Anisotropy = 4.2448

XX= 27.8563 YX= 2.1757 ZX= -0.3931

XY= 0.3286 YY= 28.8100 ZY= -1.2884

XZ= 0.0309 YZ= -1.1706 ZZ= 24.5764

Eigenvalues: 24.2383 27.0936 29.9107

## BETAINE monomer\_iso1 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level

32

c 0.0915 -0.0647 -4.0409

c -1.3554 -0.3808 -4.4431

c 1.0937 -1.1457 -4.4667

h 2.1246 -0.8830 -4.1461

h 1.0879 -1.2404 -5.5740

h 0.8373 -2.1396 -4.0404

c 0.5686 1.4653 -2.1614

h 0.7870 2.2030 -2.9436

c 0.6505 1.7212 -0.7780

h 0.9375 2.7348 -0.4529

c 0.3752 0.7363 0.1587

h 0.4344 0.9643 1.2340

c -0.0264 -0.6062 -0.2554

c -0.0930 -0.7705 -1.6926

h -0.4003 -1.7455 -2.0958

c -0.2017 -1.6815 1.8651

c -1.2598 -2.1762 2.6790

h -2.2046 -2.4509 2.1820

c -1.1095 -2.3122 4.0651

h -1.9531 -2.6920 4.6672

c 0.1057 -1.9777 4.6931

h 0.2243 -2.0932 5.7831

c 1.1707 -1.5070 3.9040

h 2.1375 -1.2578 4.3756

c 1.0238 -1.3563 2.5167

h 1.8796 -1.0142 1.9100

n 0.1914 0.2136 -2.5682

n -0.3782 -1.6366 0.4901

h -1.4240 -0.4570 -5.5499

h -2.0476 0.4207 -4.1068

h -1.7025 -1.3455 -4.0144

h 0.3861 0.8912 -4.5207

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 112.6173 Anisotropy = 64.2669

XX= 149.1788 YX= -13.6027 ZX= 6.6826

XY= -21.6716 YY= 95.7022 ZY= -2.1623

XZ= 8.7183 YZ= -1.2475 ZZ= 92.9709

Eigenvalues: 90.2206 92.1693 155.4619

2 C Isotropic = 156.8209 Anisotropy = 35.6868

XX= 149.8888 YX= -6.4305 ZX= -2.4627

XY= -9.1528 YY= 157.6637 ZY= 18.8402

XZ= -5.6818 YZ= 17.0379 ZZ= 162.9100

Eigenvalues: 140.7408 149.1098 180.6120

3 C Isotropic = 156.6460 Anisotropy = 35.4216

XX= 149.1130 YX= -3.5283 ZX= 3.3624

XY= -3.8081 YY= 142.6457 ZY= -7.1182

XZ= 7.2120 YZ= -4.9046 ZZ= 178.1792

Eigenvalues: 140.6513 149.0262 180.2603

4 H Isotropic = 29.4374 Anisotropy = 8.5698

XX= 26.1480 YX= -0.8855 ZX= 0.2631

XY= -0.2564 YY= 28.8839 ZY= 2.9807

XZ= 1.0389 YZ= 3.8427 ZZ= 33.2803

Eigenvalues: 25.6556 27.5060 35.1506

5 H Isotropic = 29.5451 Anisotropy = 9.7373

XX= 33.2607 YX= -2.2295 ZX= 3.2006

XY= -2.3412 YY= 26.3056 ZY= -0.7390

XZ= 4.1700 YZ= -1.2650 ZZ= 29.0690

Eigenvalues: 25.6164 26.9823 36.0367

6 H Isotropic = 29.3823 Anisotropy = 6.1830

XX= 28.9147 YX= 2.1747 ZX= -0.1417

XY= 2.5021 YY= 29.7369 ZY= -2.1609

XZ= -0.4592 YZ= -3.9442 ZZ= 29.4953

Eigenvalues: 25.8007 28.8419 33.5043

7 C Isotropic = 57.5309 Anisotropy = 98.2672

XX= 20.4842 YX= -43.6525 ZX= 7.4551

XY= -41.2068 YY= 38.2052 ZY= 23.6377

XZ= 12.2157 YZ= 31.4657 ZZ= 113.9035

Eigenvalues: -18.8046 68.3550 123.0424

8 H Isotropic = 24.4157 Anisotropy = 5.9231

XX= 24.4206 YX= -1.7371 ZX= 0.6962

XY= -1.2224 YY= 27.2951 ZY= -1.8543

XZ= 0.6912 YZ= -1.3400 ZZ= 21.5313

Eigenvalues: 21.0876 23.7951 28.3644

9 C Isotropic = 45.7600 Anisotropy = 177.5392

XX= 37.6010 YX= 12.7337 ZX= -10.1144

XY= 16.9269 YY= -43.0034 ZY= 64.9592

XZ= -15.6431 YZ= 66.6461 ZZ= 142.6823

Eigenvalues: -67.0741 40.2346 164.1194

10 H Isotropic = 24.1499 Anisotropy = 4.2438

XX= 26.8645 YX= 0.7824 ZX= -0.0046

XY= 0.2536 YY= 23.6798 ZY= -0.5033

XZ= -0.5815 YZ= -0.9119 ZZ= 21.9053

Eigenvalues: 21.6554 23.8151 26.9790

11 C Isotropic = 51.6718 Anisotropy = 182.0729

XX= -26.3059 YX= 20.0239 ZX= -12.3132

XY= 17.2481 YY= 17.3782 ZY= 43.6666

XZ= -43.7024 YZ= 18.0232 ZZ= 163.9430

Eigenvalues: -40.0620 22.0236 173.0537

12 H Isotropic = 23.6005 Anisotropy = 9.9769

XX= 25.1132 YX= 4.3193 ZX= -2.2775

XY= 4.1127 YY= 25.9511 ZY= -0.9580

XZ= -3.7345 YZ= 0.4619 ZZ= 19.7370

Eigenvalues: 18.0247 22.5250 30.2517

13 C Isotropic = 19.6252 Anisotropy = 158.3924

XX= -45.5658 YX= 18.9919 ZX= -10.4988

XY= -2.5607 YY= -8.1024 ZY= 42.6968

XZ= -11.8850 YZ= 38.0674 ZZ= 112.5439

Eigenvalues: -50.1147 -16.2298 125.2201

14 C Isotropic = 38.4254 Anisotropy = 136.0382

XX= 21.5138 YX= -0.4784 ZX= -3.8588

XY= -1.6398 YY= -16.6453 ZY= 42.3067

XZ= 2.6034 YZ= 62.1124 ZZ= 110.4076

Eigenvalues: -35.3577 21.5163 129.1175

15 H Isotropic = 23.8495 Anisotropy = 10.6650

XX= 30.6357 YX= 2.2008 ZX= -0.1014

XY= 1.4016 YY= 20.3839 ZY= 0.4752

XZ= 0.6837 YZ= 1.0422 ZZ= 20.5289

Eigenvalues: 19.5629 21.0261 30.9595

16 C Isotropic = 16.3249 Anisotropy = 180.8051

XX= -73.0426 YX= 11.9410 ZX= -6.0272

XY= 22.8403 YY= 43.0061 ZY= -71.8768

XZ= -17.2109 YZ= -71.6186 ZZ= 79.0112

Eigenvalues: -75.6033 -12.2836 136.8616

17 C Isotropic = 49.2293 Anisotropy = 154.7575

XX= 31.7856 YX= 29.0914 ZX= 6.5736

XY= 22.3906 YY= 34.2279 ZY= -88.1492

XZ= 21.5275 YZ= -94.3133 ZZ= 81.6745

Eigenvalues: -46.9757 42.2627 152.4010

18 H Isotropic = 24.1508 Anisotropy = 6.3960

XX= 27.6585 YX= 1.3337 ZX= 1.5911

XY= 0.9574 YY= 23.0883 ZY= 0.9916

XZ= 1.6826 YZ= 0.7938 ZZ= 21.7055

Eigenvalues: 21.0922 22.9453 28.4148

19 C Isotropic = 42.8067 Anisotropy = 188.1092

XX= -5.1008 YX= -32.1784 ZX= -46.2257

XY= -31.3181 YY= 50.8682 ZY= -95.7347

XZ= -42.3125 YZ= -102.4874 ZZ= 82.6527

Eigenvalues: -74.3903 34.5976 168.2128

20 H Isotropic = 23.6164 Anisotropy = 4.7667

XX= 25.7238 YX= -1.5407 ZX= -0.7418

XY= -1.3625 YY= 23.3958 ZY= 1.8014

XZ= -0.7095 YZ= 1.3452 ZZ= 21.7298

Eigenvalues: 20.7787 23.2763 26.7943

21 C Isotropic = 56.1974 Anisotropy = 172.2731

XX= -45.3667 YX= 23.9573 ZX= -5.5533

XY= 26.0315 YY= 92.8789 ZY= -59.6583

XZ= -3.6534 YZ= -61.8199 ZZ= 121.0799

Eigenvalues: -49.9892 47.5351 171.0461

22 H Isotropic = 24.1793 Anisotropy = 3.7205

XX= 24.6897 YX= 0.1751 ZX= 0.4404

XY= 0.2122 YY= 24.6256 ZY= 2.6684

XZ= 0.6032 YZ= 2.3855 ZZ= 23.2227

Eigenvalues: 21.2753 24.6030 26.6597

23 C Isotropic = 44.0664 Anisotropy = 186.1711

XX= 24.1689 YX= 36.3954 ZX= 13.0622

XY= 34.6217 YY= 29.8028 ZY= -108.1319

XZ= 9.4483 YZ= -112.3221 ZZ= 78.2276

Eigenvalues: -71.5394 35.5582 168.1805

24 H Isotropic = 23.7244 Anisotropy = 4.9963

XX= 26.8669 YX= 0.5862 ZX= 0.9858

XY= 0.4528 YY= 22.3871 ZY= 1.3213

XZ= 0.2957 YZ= 1.3325 ZZ= 21.9193

Eigenvalues: 20.8016 23.3164 27.0553

25 C Isotropic = 57.2384 Anisotropy = 165.4285

XX= 8.2832 YX= -18.3097 ZX= -30.3756

XY= -20.8009 YY= 64.5062 ZY= -78.6642

XZ= -55.9850 YZ= -83.2555 ZZ= 98.9257

Eigenvalues: -40.0101 44.2011 167.5240

26 H Isotropic = 23.7980 Anisotropy = 8.6537

XX= 27.7737 YX= -2.6345 ZX= -2.8126

XY= -1.7522 YY= 22.2314 ZY= 0.9896

XZ= -2.5213 YZ= 1.3416 ZZ= 21.3888

Eigenvalues: 20.3200 21.5068 29.5671

27 N Isotropic = -4.2680 Anisotropy = 293.1477

XX= -126.8356 YX= 41.1742 ZX= -26.9122

XY= 22.7100 YY= -52.1553 ZY= 72.1689

XZ= -24.1505 YZ= 81.3523 ZZ= 166.1867

Eigenvalues: -147.8594 -56.1085 191.1638

28 N Isotropic = 26.1645 Anisotropy = 241.9557

XX= -126.1394 YX= -21.2614 ZX= 13.8342

XY= -14.0396 YY= 21.0573 ZY= 17.1755

XZ= -83.4267 YZ= -16.4981 ZZ= 183.5756

Eigenvalues: -132.0029 23.0281 187.4683

29 H Isotropic = 29.5578 Anisotropy = 9.7774

XX= 33.7398 YX= -3.5936 ZX= -1.0457

XY= -4.1531 YY= 27.8275 ZY= 1.0958

XZ= -1.8887 YZ= 1.7084 ZZ= 27.1060

Eigenvalues: 25.5899 27.0074 36.0761

30 H Isotropic = 29.5108 Anisotropy = 8.5064

XX= 26.3422 YX= -0.9532 ZX= -0.5475

XY= -0.8496 YY= 27.1788 ZY= 0.8430

XZ= -1.6423 YZ= -0.0182 ZZ= 35.0114

Eigenvalues: 25.7114 27.6393 35.1817

31 H Isotropic = 29.4106 Anisotropy = 6.4884

XX= 28.9719 YX= 1.6308 ZX= -0.8067

XY= 2.3337 YY= 32.6534 ZY= 0.7424

XZ= -0.7660 YZ= 2.5994 ZZ= 26.6063

Eigenvalues: 25.6375 28.8580 33.7361

32 H Isotropic = 27.0321 Anisotropy = 4.9011

XX= 27.9973 YX= 2.4609 ZX= -0.4535

XY= 0.5728 YY= 28.9249 ZY= -1.4214

XZ= -0.0003 YZ= -1.3059 ZZ= 24.1740

Eigenvalues: 23.8026 26.9941 30.2995

## BETAINE dimer\_iso1 (gas-phase) - BP86/IGLO-III level

64

c 0.9103 2.7214 -2.5483

c -0.4089 2.5606 -3.3137

c 1.8662 1.5359 -2.7204

h 2.7949 1.6818 -2.1268

h 2.1466 1.4511 -3.7921

h 1.3863 0.5793 -2.4209

c 0.8154 4.2780 -0.6398

h 1.1930 5.0150 -1.3595

c 0.4844 4.5691 0.6933

h 0.5919 5.6079 1.0460

c 0.0295 3.5771 1.5524

h -0.2424 3.8278 2.5891

c -0.1004 2.2004 1.1035

c 0.1916 2.0025 -0.3000

h 0.0105 1.0163 -0.7685

c -0.7621 1.2508 3.1813

c -2.0262 0.8321 3.6826

h -2.7910 0.5172 2.9536

c -2.2990 0.8253 5.0584

h -3.2930 0.5017 5.4128

c -1.3201 1.2276 5.9862

h -1.5349 1.2187 7.0675

c -0.0616 1.6407 5.5112

h 0.7203 1.9537 6.2252

c 0.2155 1.6563 4.1353

h 1.2117 1.9689 3.7791

n 0.6382 2.9986 -1.0927

n -0.5050 1.1525 1.8150

h -0.1986 2.4665 -4.4006

h -1.0676 3.4425 -3.1598

h -0.9501 1.6429 -2.9993

h 1.4213 3.6401 -2.9052

c 0.9112 -2.7208 2.5483

c -0.4075 -2.5598 3.3145

c 1.8671 -1.5353 2.7196

h 2.7956 -1.6812 2.1256

h 2.1481 -1.4501 3.7911

h 1.3871 -0.5788 2.4200

c 0.8167 -4.2776 0.6401

h 1.1954 -5.0141 1.3596

c 0.4854 -4.5692 -0.6928

h 0.5934 -5.6079 -1.0454

c 0.0294 -3.5778 -1.5518

h -0.2429 -3.8288 -2.5884

c -0.1012 -2.2011 -1.1032

c 0.1907 -2.0027 0.3003

h 0.0091 -1.0166 0.7688

c -0.7619 -1.2516 -3.1815

c -2.0249 -0.8315 -3.6843

h -2.7903 -0.5161 -2.9562

c -2.2960 -0.8242 -5.0605

h -3.2892 -0.4994 -5.4160

c -1.3165 -1.2275 -5.9871

h -1.5300 -1.2183 -7.0687

c -0.0591 -1.6422 -5.5107

h 0.7233 -1.9561 -6.2237

c 0.2164 -1.6582 -4.1345

h 1.2119 -1.9719 -3.7772

n 0.6385 -2.9984 1.0929

n -0.5062 -1.1533 -1.8149

h -0.1965 -2.4675 4.4014

h -1.0672 -3.4407 3.1597

h -0.9478 -1.6410 3.0019

h 1.4224 -3.6394 2.9051

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 102.8504 Anisotropy = 64.6279

XX= 140.7762 YX= -11.0240 ZX= 19.9831

XY= -5.1938 YY= 86.1522 ZY= -0.2929

XZ= 12.0010 YZ= -2.1132 ZZ= 81.6229

Eigenvalues: 77.4881 85.1274 145.9357

2 C Isotropic = 150.8353 Anisotropy = 35.6625

XX= 151.9184 YX= -1.1794 ZX= -12.4307

XY= 0.4879 YY= 136.7715 ZY= 0.6115

XZ= -18.6138 YZ= 4.0813 ZZ= 163.8161

Eigenvalues: 136.4259 141.4697 174.6104

3 C Isotropic = 152.8254 Anisotropy = 31.2167

XX= 149.4017 YX= 3.2380 ZX= 5.6568

XY= 4.5858 YY= 153.5764 ZY= 18.7065

XZ= 6.5905 YZ= 15.2245 ZZ= 155.4981

Eigenvalues: 137.3684 147.4712 173.6366

4 H Isotropic = 29.8637 Anisotropy = 7.4301

XX= 27.6920 YX= 0.2713 ZX= -1.8814

XY= 0.3030 YY= 27.6185 ZY= 1.2207

XZ= -1.6206 YZ= 0.6685 ZZ= 34.2805

Eigenvalues: 26.8664 27.9075 34.8171

5 H Isotropic = 30.2036 Anisotropy = 7.4947

XX= 33.3487 YX= 0.2135 ZX= 2.8533

XY= 1.4316 YY= 27.7908 ZY= -1.3909

XZ= 3.6286 YZ= -0.2400 ZZ= 29.4712

Eigenvalues: 26.5889 28.8217 35.2001

6 H Isotropic = 28.5941 Anisotropy = 8.9521

XX= 25.8319 YX= 0.2155 ZX= 0.1500

XY= 2.1129 YY= 33.2313 ZY= -4.2426

XZ= 0.5418 YZ= -1.9172 ZZ= 26.7190

Eigenvalues: 24.8534 26.3666 34.5621

7 C Isotropic = 59.0096 Anisotropy = 80.9578

XX= 67.2543 YX= 24.6565 ZX= -17.1514

XY= 26.1819 YY= 9.1528 ZY= 35.4387

XZ= -14.1615 YZ= 32.0805 ZZ= 100.6217

Eigenvalues: -12.5731 76.6204 112.9815

8 H Isotropic = 25.0827 Anisotropy = 6.2082

XX= 26.7730 YX= 2.8426 ZX= 0.0035

XY= 2.5400 YY= 26.0909 ZY= -0.8520

XZ= -0.1128 YZ= -1.1993 ZZ= 22.3842

Eigenvalues: 21.9992 24.0275 29.2215

9 C Isotropic = 44.9122 Anisotropy = 164.5149

XX= 11.7812 YX= -53.9567 ZX= -21.2830

XY= -61.1645 YY= -17.4676 ZY= 31.4298

XZ= -24.2697 YZ= 29.4036 ZZ= 140.4230

Eigenvalues: -62.7565 42.9044 154.5888

10 H Isotropic = 24.7219 Anisotropy = 3.8196

XX= 25.9568 YX= -1.4414 ZX= 1.1160

XY= -1.0328 YY= 25.4965 ZY= -1.0325

XZ= 0.5191 YZ= -0.5537 ZZ= 22.7123

Eigenvalues: 22.4256 24.4717 27.2683

11 C Isotropic = 49.6718 Anisotropy = 170.5004

XX= -31.3948 YX= -10.3540 ZX= -43.8059

XY= -11.2388 YY= 37.7749 ZY= 29.9640

XZ= -33.0634 YZ= 46.7498 ZZ= 142.6351

Eigenvalues: -39.6063 25.2829 163.3387

12 H Isotropic = 24.0331 Anisotropy = 10.1588

XX= 21.7140 YX= -2.0980 ZX= -0.5351

XY= -3.0354 YY= 29.2524 ZY= -2.6123

XZ= -0.9291 YZ= -3.4460 ZZ= 21.1328

Eigenvalues: 19.0930 22.2006 30.8056

13 C Isotropic = 17.2759 Anisotropy = 144.5085

XX= -39.2723 YX= -15.5743 ZX= -26.7214

XY= 3.0126 YY= -7.2061 ZY= 25.1879

XZ= -39.2835 YZ= 34.9274 ZZ= 98.3060

Eigenvalues: -46.7881 -14.9991 113.6149

14 C Isotropic = 35.0584 Anisotropy = 140.7987

XX= 4.0268 YX= -18.1620 ZX= -14.3466

XY= -18.7020 YY= -19.7172 ZY= 43.0201

XZ= -14.0229 YZ= 14.1400 ZZ= 120.8655

Eigenvalues: -32.1911 8.4421 128.9242

15 H Isotropic = 21.9875 Anisotropy = 7.6452

XX= 25.2756 YX= -3.1292 ZX= 1.6070

XY= -1.2298 YY= 23.0524 ZY= -1.7928

XZ= -0.0041 YZ= -3.4263 ZZ= 17.6344

Eigenvalues: 16.5813 22.2968 27.0843

16 C Isotropic = 13.5823 Anisotropy = 172.4384

XX= -64.1168 YX= 38.5652 ZX= -5.1224

XY= 28.8889 YY= 106.2754 ZY= 44.8324

XZ= -8.4146 YZ= 49.6751 ZZ= -1.4116

Eigenvalues: -74.4187 -13.3756 128.5413

17 C Isotropic = 45.1700 Anisotropy = 154.6718

XX= 0.6625 YX= 6.4862 ZX= 45.5904

XY= 19.0012 YY= 128.6275 ZY= 45.7264

XZ= 54.6103 YZ= 41.9721 ZZ= 6.2200

Eigenvalues: -49.4260 36.6514 148.2845

18 H Isotropic = 24.2395 Anisotropy = 6.0700

XX= 25.1796 YX= -1.0516 ZX= 2.8680

XY= -1.0826 YY= 22.6372 ZY= -0.9040

XZ= 3.0353 YZ= -0.5687 ZZ= 24.9016

Eigenvalues: 21.9782 22.4541 28.2861

19 C Isotropic = 39.9943 Anisotropy = 181.8547

XX= 31.0455 YX= 27.8235 ZX= -18.9361

XY= 30.1822 YY= 132.7010 ZY= 66.2428

XZ= -11.7306 YZ= 74.5154 ZZ= -43.7635

Eigenvalues: -74.0166 32.7688 161.2308

20 H Isotropic = 23.7694 Anisotropy = 4.7905

XX= 26.9440 YX= -0.1834 ZX= -0.4578

XY= -0.2535 YY= 21.4274 ZY= -0.6821

XZ= 0.0218 YZ= 0.0104 ZZ= 22.9368

Eigenvalues: 21.3440 23.0011 26.9631

21 C Isotropic = 51.6107 Anisotropy = 168.1238

XX= -40.8713 YX= 38.5864 ZX= -12.5500

XY= 35.7296 YY= 143.8307 ZY= 39.3413

XZ= -9.9334 YZ= 41.1153 ZZ= 51.8727

Eigenvalues: -51.6779 42.8168 163.6932

22 H Isotropic = 24.2860 Anisotropy = 2.9810

XX= 24.9225 YX= 0.1216 ZX= -0.4148

XY= 0.1376 YY= 22.1813 ZY= -1.4788

XZ= -0.1561 YZ= -1.2029 ZZ= 25.7542

Eigenvalues: 21.7338 24.8508 26.2734

23 C Isotropic = 41.9621 Anisotropy = 178.4468

XX= -11.3141 YX= 8.1315 ZX= 59.0658

XY= 7.9022 YY= 143.0687 ZY= 46.4358

XZ= 55.4607 YZ= 49.8901 ZZ= -5.8684

Eigenvalues: -69.7018 34.6614 160.9266

24 H Isotropic = 23.8866 Anisotropy = 4.6485

XX= 26.0400 YX= -0.8276 ZX= 1.6782

XY= -0.8776 YY= 22.0487 ZY= -1.4205

XZ= 1.0356 YZ= -1.0786 ZZ= 23.5709

Eigenvalues: 21.3451 23.3290 26.9856

25 C Isotropic = 51.4558 Anisotropy = 159.9290

XX= 34.8743 YX= 24.1778 ZX= -9.5745

XY= 20.4340 YY= 131.8868 ZY= 55.2595

XZ= -26.1812 YZ= 73.1715 ZZ= -12.3936

Eigenvalues: -44.5792 40.8715 158.0752

26 H Isotropic = 24.1356 Anisotropy = 7.4895

XX= 28.5431 YX= -0.4810 ZX= -1.9491

XY= -1.1683 YY= 23.1121 ZY= 0.3943

XZ= -1.9885 YZ= -0.0985 ZZ= 20.7517

Eigenvalues: 20.2816 22.9967 29.1286

27 N Isotropic = -2.6820 Anisotropy = 266.8617

XX= -121.3246 YX= -26.7031 ZX= -51.9127

XY= -7.4328 YY= -31.8382 ZY= 60.2271

XZ= -54.6173 YZ= 63.7688 ZZ= 145.1169

Eigenvalues: -131.8747 -51.3970 175.2259

28 N Isotropic = 2.9377 Anisotropy = 239.9516

XX= -109.0689 YX= 68.1700 ZX= -53.8902

XY= 35.6296 YY= 8.7999 ZY= 58.7708

XZ= -91.0283 YZ= 109.9886 ZZ= 109.0820

Eigenvalues: -165.3346 11.2423 162.9054

29 H Isotropic = 30.5557 Anisotropy = 7.0074

XX= 34.6953 YX= -1.0006 ZX= -0.9798

XY= -0.9001 YY= 30.0363 ZY= -0.0677

XZ= -2.5795 YZ= -0.5738 ZZ= 26.9355

Eigenvalues: 26.4702 29.9695 35.2273

30 H Isotropic = 30.0228 Anisotropy = 7.4812

XX= 27.8749 YX= 0.7387 ZX= -1.3531

XY= 1.1087 YY= 31.5380 ZY= 3.4801

XZ= -1.7285 YZ= 4.2631 ZZ= 30.6556

Eigenvalues: 25.7360 29.3223 35.0103

31 H Isotropic = 29.2826 Anisotropy = 10.4562

XX= 26.8680 YX= 1.6940 ZX= -1.8728

XY= 3.2616 YY= 33.0089 ZY= -2.4839

XZ= -3.2232 YZ= -5.0393 ZZ= 27.9709

Eigenvalues: 24.7699 26.8245 36.2535

32 H Isotropic = 27.6002 Anisotropy = 5.5232

XX= 27.1371 YX= -0.3039 ZX= 0.8929

XY= 1.7965 YY= 30.1173 ZY= -2.4087

XZ= 0.1987 YZ= -2.6202 ZZ= 25.5462

Eigenvalues: 24.2121 27.3061 31.2823

33 C Isotropic = 102.8522 Anisotropy = 64.6466

XX= 140.7677 YX= -11.0326 ZX= -20.0155

XY= -5.1760 YY= 86.1390 ZY= 0.3092

XZ= -12.0558 YZ= 2.1467 ZZ= 81.6499

Eigenvalues: 77.4961 85.1106 145.9499

34 C Isotropic = 150.8665 Anisotropy = 35.6577

XX= 151.9559 YX= -1.1783 ZX= 12.4497

XY= 0.5035 YY= 136.8020 ZY= -0.6125

XZ= 18.5914 YZ= -4.0978 ZZ= 163.8415

Eigenvalues: 136.4514 141.5098 174.6383

35 C Isotropic = 152.8316 Anisotropy = 31.2278

XX= 149.3763 YX= 3.2340 ZX= -5.6568

XY= 4.5847 YY= 153.5960 ZY= -18.7027

XZ= -6.5905 YZ= -15.2199 ZZ= 155.5225

Eigenvalues: 137.3933 147.4514 173.6501

36 H Isotropic = 29.8625 Anisotropy = 7.4295

XX= 27.6934 YX= 0.2704 ZX= 1.8852

XY= 0.3026 YY= 27.6171 ZY= -1.2187

XZ= 1.6258 YZ= -0.6665 ZZ= 34.2770

Eigenvalues: 26.8659 27.9061 34.8155

37 H Isotropic = 30.2021 Anisotropy = 7.4974

XX= 33.3421 YX= 0.2137 ZX= -2.8564

XY= 1.4331 YY= 27.7875 ZY= 1.3898

XZ= -3.6346 YZ= 0.2378 ZZ= 29.4766

Eigenvalues: 26.5873 28.8186 35.2004

38 H Isotropic = 28.5919 Anisotropy = 8.9561

XX= 25.8241 YX= 0.2120 ZX= -0.1499

XY= 2.1096 YY= 33.2313 ZY= 4.2455

XZ= -0.5451 YZ= 1.9182 ZZ= 26.7202

Eigenvalues: 24.8499 26.3631 34.5626

39 C Isotropic = 59.0253 Anisotropy = 80.9413

XX= 67.2928 YX= 24.6206 ZX= 17.1934

XY= 26.1444 YY= 9.2190 ZY= -35.5169

XZ= 14.2138 YZ= -32.1264 ZZ= 100.5641

Eigenvalues: -12.5443 76.6340 112.9862

40 H Isotropic = 25.0844 Anisotropy = 6.2079

XX= 26.7745 YX= 2.8424 ZX= -0.0047

XY= 2.5411 YY= 26.0917 ZY= 0.8513

XZ= 0.1115 YZ= 1.2002 ZZ= 22.3871

Eigenvalues: 22.0012 24.0291 29.2230

41 C Isotropic = 44.9367 Anisotropy = 164.5035

XX= 11.8561 YX= -53.9684 ZX= 21.3379

XY= -61.1876 YY= -17.4202 ZY= -31.4724

XZ= 24.3536 YZ= -29.4351 ZZ= 140.3744

Eigenvalues: -62.7149 42.9194 154.6057

42 H Isotropic = 24.7235 Anisotropy = 3.8186

XX= 25.9584 YX= -1.4403 ZX= -1.1180

XY= -1.0323 YY= 25.4974 ZY= 1.0339

XZ= -0.5186 YZ= 0.5531 ZZ= 22.7146

Eigenvalues: 22.4275 24.4737 27.2692

43 C Isotropic = 49.6738 Anisotropy = 170.5175

XX= -31.3466 YX= -10.3800 ZX= 43.9142

XY= -11.2818 YY= 37.8395 ZY= -29.9852

XZ= 33.1865 YZ= -46.9081 ZZ= 142.5286

Eigenvalues: -39.6106 25.2798 163.3522

44 H Isotropic = 24.0287 Anisotropy = 10.1507

XX= 21.7134 YX= -2.1000 ZX= 0.5363

XY= -3.0356 YY= 29.2413 ZY= 2.6073

XZ= 0.9348 YZ= 3.4506 ZZ= 21.1313

Eigenvalues: 19.0872 22.2029 30.7958

45 C Isotropic = 17.2473 Anisotropy = 144.5246

XX= -39.3093 YX= -15.6079 ZX= 26.7333

XY= 3.0364 YY= -7.2199 ZY= -25.1761

XZ= 39.3027 YZ= -34.9782 ZZ= 98.2710

Eigenvalues: -46.8318 -15.0233 113.5970

46 C Isotropic = 35.0429 Anisotropy = 140.8382

XX= 4.0413 YX= -18.1280 ZX= 14.3934

XY= -18.7395 YY= -19.7896 ZY= -43.1255

XZ= 14.0958 YZ= -13.9659 ZZ= 120.8769

Eigenvalues: -32.2345 8.4281 128.9350

47 H Isotropic = 21.9829 Anisotropy = 7.6360

XX= 25.2711 YX= -3.1189 ZX= -1.6075

XY= -1.2238 YY= 23.0468 ZY= 1.7915

XZ= 0.0007 YZ= 3.4332 ZZ= 17.6308

Eigenvalues: 16.5756 22.2996 27.0736

48 C Isotropic = 13.5762 Anisotropy = 172.4252

XX= -64.1196 YX= 38.5736 ZX= 5.0174

XY= 28.9183 YY= 106.1168 ZY= -44.9884

XZ= 8.3227 YZ= -49.8163 ZZ= -1.2687

Eigenvalues: -74.4028 -13.3950 128.5263

49 C Isotropic = 45.1635 Anisotropy = 154.6758

XX= 0.7164 YX= 6.4808 ZX= -45.6177

XY= 18.9455 YY= 128.4886 ZY= -45.8926

XZ= -54.6388 YZ= -42.1442 ZZ= 6.2855

Eigenvalues: -49.4331 36.6429 148.2807

50 H Isotropic = 24.2399 Anisotropy = 6.0671

XX= 25.1821 YX= -1.0544 ZX= -2.8682

XY= -1.0870 YY= 22.6422 ZY= 0.9009

XZ= -3.0330 YZ= 0.5693 ZZ= 24.8955

Eigenvalues: 21.9763 22.4588 28.2846

51 C Isotropic = 40.0059 Anisotropy = 181.8387

XX= 31.0471 YX= 27.9232 ZX= 18.9269

XY= 30.2525 YY= 132.4687 ZY= -66.4778

XZ= 11.7198 YZ= -74.8004 ZZ= -43.4981

Eigenvalues: -73.9951 32.7811 161.2318

52 H Isotropic = 23.7710 Anisotropy = 4.7894

XX= 26.9447 YX= -0.1820 ZX= 0.4596

XY= -0.2524 YY= 21.4321 ZY= 0.6856

XZ= -0.0195 YZ= -0.0103 ZZ= 22.9361

Eigenvalues: 21.3478 23.0012 26.9639

53 C Isotropic = 51.6323 Anisotropy = 168.0847

XX= -40.8250 YX= 38.6443 ZX= 12.4243

XY= 35.8030 YY= 143.6837 ZY= -39.4590

XZ= 9.7857 YZ= -41.2425 ZZ= 52.0381

Eigenvalues: -51.6252 42.8333 163.6887

54 H Isotropic = 24.2872 Anisotropy = 2.9787

XX= 24.9259 YX= 0.1206 ZX= 0.4137

XY= 0.1377 YY= 22.1862 ZY= 1.4858

XZ= 0.1534 YZ= 1.2094 ZZ= 25.7494

Eigenvalues: 21.7336 24.8549 26.2730

55 C Isotropic = 41.9746 Anisotropy = 178.4218

XX= -11.2069 YX= 8.0632 ZX= -59.0855

XY= 7.8380 YY= 142.9025 ZY= -46.6654

XZ= -55.4775 YZ= -50.1430 ZZ= -5.7717

Eigenvalues: -69.6829 34.6843 160.9225

56 H Isotropic = 23.8884 Anisotropy = 4.6489

XX= 26.0438 YX= -0.8317 ZX= -1.6749

XY= -0.8815 YY= 22.0564 ZY= 1.4245

XZ= -1.0321 YZ= 1.0803 ZZ= 23.5649

Eigenvalues: 21.3469 23.3305 26.9876

57 C Isotropic = 51.4748 Anisotropy = 159.9568

XX= 34.8282 YX= 24.2347 ZX= 9.5626

XY= 20.4024 YY= 131.7120 ZY= -55.5001

XZ= 26.2571 YZ= -73.4294 ZZ= -12.1156

Eigenvalues: -44.5674 40.8792 158.1127

58 H Isotropic = 24.1325 Anisotropy = 7.4948

XX= 28.5428 YX= -0.4840 ZX= 1.9544

XY= -1.1697 YY= 23.1123 ZY= -0.3909

XZ= 1.9862 YZ= 0.0987 ZZ= 20.7423

Eigenvalues: 20.2720 22.9965 29.1290

59 N Isotropic = -2.6903 Anisotropy = 266.8797

XX= -121.2736 YX= -26.7752 ZX= 52.0383

XY= -7.5367 YY= -31.7882 ZY= -60.3466

XZ= 54.7391 YZ= -63.8495 ZZ= 144.9908

Eigenvalues: -131.8801 -51.4204 175.2295

60 N Isotropic = 2.9243 Anisotropy = 240.0541

XX= -109.1797 YX= 68.2380 ZX= 53.8020

XY= 35.5208 YY= 8.7477 ZY= -58.8282

XZ= 90.8913 YZ= -109.9279 ZZ= 109.2047

Eigenvalues: -165.3257 11.1381 162.9603

61 H Isotropic = 30.5566 Anisotropy = 7.0087

XX= 34.6968 YX= -1.0144 ZX= 0.9737

XY= -0.9102 YY= 30.0394 ZY= 0.0756

XZ= 2.5687 YZ= 0.5725 ZZ= 26.9337

Eigenvalues: 26.4707 29.9702 35.2291

62 H Isotropic = 30.0266 Anisotropy = 7.4796

XX= 27.8802 YX= 0.7391 ZX= 1.3504

XY= 1.1102 YY= 31.5318 ZY= -3.4810

XZ= 1.7247 YZ= -4.2639 ZZ= 30.6677

Eigenvalues: 25.7422 29.3245 35.0130

63 H Isotropic = 29.2846 Anisotropy = 10.4932

XX= 26.8630 YX= 1.7080 ZX= 1.8808

XY= 3.2832 YY= 33.0309 ZY= 2.4906

XZ= 3.2291 YZ= 5.0406 ZZ= 27.9600

Eigenvalues: 24.7574 26.8164 36.2801

64 H Isotropic = 27.6011 Anisotropy = 5.5238

XX= 27.1403 YX= -0.3044 ZX= -0.8922

XY= 1.7976 YY= 30.1178 ZY= 2.4097

XZ= -0.1974 YZ= 2.6217 ZZ= 25.5451

Eigenvalues: 24.2111 27.3085 31.2836

## BETAINE dimer\_iso1 (gas-phase) – PBE0/IGLO-III level

64

c 0.9103 2.7214 -2.5483

c -0.4089 2.5606 -3.3137

c 1.8662 1.5359 -2.7204

h 2.7949 1.6818 -2.1268

h 2.1466 1.4511 -3.7921

h 1.3863 0.5793 -2.4209

c 0.8154 4.2780 -0.6398

h 1.1930 5.0150 -1.3595

c 0.4844 4.5691 0.6933

h 0.5919 5.6079 1.0460

c 0.0295 3.5771 1.5524

h -0.2424 3.8278 2.5891

c -0.1004 2.2004 1.1035

c 0.1916 2.0025 -0.3000

h 0.0105 1.0163 -0.7685

c -0.7621 1.2508 3.1813

c -2.0262 0.8321 3.6826

h -2.7910 0.5172 2.9536

c -2.2990 0.8253 5.0584

h -3.2930 0.5017 5.4128

c -1.3201 1.2276 5.9862

h -1.5349 1.2187 7.0675

c -0.0616 1.6407 5.5112

h 0.7203 1.9537 6.2252

c 0.2155 1.6563 4.1353

h 1.2117 1.9689 3.7791

n 0.6382 2.9986 -1.0927

n -0.5050 1.1525 1.8150

h -0.1986 2.4665 -4.4006

h -1.0676 3.4425 -3.1598

h -0.9501 1.6429 -2.9993

h 1.4213 3.6401 -2.9052

c 0.9112 -2.7208 2.5483

c -0.4075 -2.5598 3.3145

c 1.8671 -1.5353 2.7196

h 2.7956 -1.6812 2.1256

h 2.1481 -1.4501 3.7911

h 1.3871 -0.5788 2.4200

c 0.8167 -4.2776 0.6401

h 1.1954 -5.0141 1.3596

c 0.4854 -4.5692 -0.6928

h 0.5934 -5.6079 -1.0454

c 0.0294 -3.5778 -1.5518

h -0.2429 -3.8288 -2.5884

c -0.1012 -2.2011 -1.1032

c 0.1907 -2.0027 0.3003

h 0.0091 -1.0166 0.7688

c -0.7619 -1.2516 -3.1815

c -2.0249 -0.8315 -3.6843

h -2.7903 -0.5161 -2.9562

c -2.2960 -0.8242 -5.0605

h -3.2892 -0.4994 -5.4160

c -1.3165 -1.2275 -5.9871

h -1.5300 -1.2183 -7.0687

c -0.0591 -1.6422 -5.5107

h 0.7233 -1.9561 -6.2237

c 0.2164 -1.6582 -4.1345

h 1.2119 -1.9719 -3.7772

n 0.6385 -2.9984 1.0929

n -0.5062 -1.1533 -1.8149

h -0.1965 -2.4675 4.4014

h -1.0672 -3.4407 3.1597

h -0.9478 -1.6410 3.0019

h 1.4224 -3.6394 2.9051

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 110.4587 Anisotropy = 63.9734

XX= 148.0773 YX= -11.0440 ZX= 19.6221

XY= -5.1261 YY= 93.7837 ZY= -0.3491

XZ= 11.6277 YZ= -2.2543 ZZ= 89.5152

Eigenvalues: 85.5397 92.7289 153.1077

2 C Isotropic = 156.5424 Anisotropy = 34.1402

XX= 158.1929 YX= -1.1667 ZX= -11.5131

XY= 0.5893 YY= 142.8804 ZY= 0.7426

XZ= -18.3259 YZ= 4.3026 ZZ= 168.5538

Eigenvalues: 142.4523 147.8723 179.3025

3 C Isotropic = 158.4022 Anisotropy = 29.5761

XX= 155.7232 YX= 2.9661 ZX= 5.3377

XY= 4.5785 YY= 158.6043 ZY= 17.9481

XZ= 6.3875 YZ= 14.5168 ZZ= 160.8791

Eigenvalues: 143.3293 153.7577 178.1196

4 H Isotropic = 29.8548 Anisotropy = 7.8822

XX= 27.6228 YX= 0.2538 ZX= -2.1819

XY= 0.4095 YY= 27.4061 ZY= 1.1684

XZ= -1.6406 YZ= 0.6295 ZZ= 34.5354

Eigenvalues: 26.6756 27.7791 35.1095

5 H Isotropic = 30.2035 Anisotropy = 8.0674

XX= 33.6932 YX= 0.1931 ZX= 3.0472

XY= 1.4205 YY= 27.6363 ZY= -1.5197

XZ= 3.8302 YZ= -0.3222 ZZ= 29.2810

Eigenvalues: 26.3147 28.7141 35.5818

6 H Isotropic = 28.5458 Anisotropy = 9.7054

XX= 25.6040 YX= 0.1670 ZX= 0.1691

XY= 2.2579 YY= 33.5275 ZY= -4.5950

XZ= 0.6379 YZ= -2.2367 ZZ= 26.5060

Eigenvalues: 24.4627 26.1586 35.0161

7 C Isotropic = 61.4313 Anisotropy = 90.3839

XX= 67.9301 YX= 25.4958 ZX= -19.2374

XY= 27.0370 YY= 8.1179 ZY= 38.5932

XZ= -15.2883 YZ= 34.6888 ZZ= 108.2459

Eigenvalues: -15.0161 77.6227 121.6872

8 H Isotropic = 24.8756 Anisotropy = 6.6151

XX= 26.7065 YX= 2.9482 ZX= 0.0986

XY= 2.5518 YY= 26.1618 ZY= -1.0790

XZ= 0.0279 YZ= -1.4588 ZZ= 21.7586

Eigenvalues: 21.2738 24.0674 29.2857

9 C Isotropic = 47.1117 Anisotropy = 172.7978

XX= 12.2231 YX= -56.1462 ZX= -22.4197

XY= -63.5167 YY= -18.4664 ZY= 33.0430

XZ= -25.0133 YZ= 31.0828 ZZ= 147.5784

Eigenvalues: -65.4686 44.4934 162.3102

10 H Isotropic = 24.4695 Anisotropy = 4.0523

XX= 25.8311 YX= -1.4563 ZX= 1.2190

XY= -0.8872 YY= 25.4476 ZY= -1.1781

XZ= 0.6327 YZ= -0.7104 ZZ= 22.1299

Eigenvalues: 21.7807 24.4568 27.1711

11 C Isotropic = 52.2744 Anisotropy = 176.1036

XX= -30.7274 YX= -10.7777 ZX= -45.6014

XY= -13.0671 YY= 39.3533 ZY= 30.2767

XZ= -36.0396 YZ= 47.4822 ZZ= 148.1972

Eigenvalues: -39.7629 26.9093 169.6768

12 H Isotropic = 23.8544 Anisotropy = 10.7749

XX= 21.6571 YX= -2.1005 ZX= -0.4042

XY= -3.1445 YY= 29.4513 ZY= -2.8878

XZ= -0.7752 YZ= -3.4412 ZZ= 20.4548

Eigenvalues: 18.7152 21.8103 31.0376

13 C Isotropic = 17.3973 Anisotropy = 158.4247

XX= -45.6824 YX= -16.3157 ZX= -29.8025

XY= 2.9523 YY= -8.3926 ZY= 28.0283

XZ= -43.2209 YZ= 37.1930 ZZ= 106.2670

Eigenvalues: -54.0140 -16.8078 123.0138

14 C Isotropic = 36.3845 Anisotropy = 148.1282

XX= 3.2347 YX= -19.2523 ZX= -15.1788

XY= -19.9263 YY= -20.1753 ZY= 45.0274

XZ= -14.8520 YZ= 17.3732 ZZ= 126.0943

Eigenvalues: -34.0048 8.0217 135.1367

15 H Isotropic = 21.7211 Anisotropy = 8.1543

XX= 25.2192 YX= -3.2472 ZX= 1.7569

XY= -1.2180 YY= 23.0301 ZY= -2.0070

XZ= 0.1022 YZ= -3.6588 ZZ= 16.9139

Eigenvalues: 15.8031 22.2028 27.1573

16 C Isotropic = 15.2578 Anisotropy = 182.7831

XX= -68.5342 YX= 40.5043 ZX= -6.2590

XY= 31.1091 YY= 113.6117 ZY= 47.5694

XZ= -9.2380 YZ= 52.0921 ZZ= 0.6958

Eigenvalues: -79.4638 -11.8760 137.1132

17 C Isotropic = 47.1566 Anisotropy = 161.3343

XX= -0.1279 YX= 7.1706 ZX= 47.8413

XY= 19.2243 YY= 134.8330 ZY= 45.9199

XZ= 56.4344 YZ= 44.0965 ZZ= 6.7648

Eigenvalues: -51.5575 38.3146 154.7128

18 H Isotropic = 24.0402 Anisotropy = 6.4247

XX= 25.1392 YX= -1.1046 ZX= 2.9063

XY= -1.0759 YY= 22.1218 ZY= -1.0282

XZ= 3.1006 YZ= -0.7498 ZZ= 24.8596

Eigenvalues: 21.7562 22.0411 28.3234

19 C Isotropic = 42.0023 Anisotropy = 189.0446

XX= 32.1082 YX= 28.9826 ZX= -19.6270

XY= 30.8553 YY= 138.0159 ZY= 70.2672

XZ= -12.4980 YZ= 77.1791 ZZ= -44.1173

Eigenvalues: -76.1685 34.1433 168.0320

20 H Isotropic = 23.6210 Anisotropy = 4.9427

XX= 26.8935 YX= -0.2257 ZX= -0.4649

XY= -0.3350 YY= 21.0391 ZY= -0.7442

XZ= 0.0385 YZ= -0.1393 ZZ= 22.9306

Eigenvalues: 20.9238 23.0231 26.9162

21 C Isotropic = 54.3771 Anisotropy = 174.3526

XX= -41.3897 YX= 39.9038 ZX= -12.8791

XY= 37.0857 YY= 149.8363 ZY= 41.3285

XZ= -10.7077 YZ= 42.6825 ZZ= 54.6847

Eigenvalues: -52.6726 45.1918 170.6122

22 H Isotropic = 24.1496 Anisotropy = 3.1091

XX= 25.0058 YX= 0.0450 ZX= -0.4018

XY= 0.0112 YY= 21.7882 ZY= -1.6169

XZ= -0.1841 YZ= -1.3386 ZZ= 25.6546

Eigenvalues: 21.2869 24.9395 26.2223

23 C Isotropic = 43.9550 Anisotropy = 185.6910

XX= -11.7343 YX= 8.7824 ZX= 61.2419

XY= 8.5790 YY= 149.3265 ZY= 47.7947

XZ= 57.6570 YZ= 51.6886 ZZ= -5.7272

Eigenvalues: -72.0391 36.1551 167.7490

24 H Isotropic = 23.7319 Anisotropy = 4.7983

XX= 26.0134 YX= -0.8615 ZX= 1.6330

XY= -0.8911 YY= 21.6961 ZY= -1.5414

XZ= 0.9896 YZ= -1.2084 ZZ= 23.4861

Eigenvalues: 20.9456 23.3193 26.9307

25 C Isotropic = 52.9392 Anisotropy = 167.2253

XX= 35.3757 YX= 26.0129 ZX= -10.9909

XY= 21.3545 YY= 137.7729 ZY= 56.6920

XZ= -26.9507 YZ= 75.5644 ZZ= -14.3309

Eigenvalues: -47.3846 41.7796 164.4228

26 H Isotropic = 23.9605 Anisotropy = 7.9034

XX= 28.5752 YX= -0.5193 ZX= -2.0649

XY= -1.3039 YY= 22.7211 ZY= 0.2614

XZ= -2.1852 YZ= -0.1421 ZZ= 20.5852

Eigenvalues: 20.0450 22.6071 29.2295

27 N Isotropic = -3.7566 Anisotropy = 288.0357

XX= -134.3213 YX= -28.0984 ZX= -56.5125

XY= -7.5878 YY= -33.2727 ZY= 64.5677

XZ= -58.7842 YZ= 67.2283 ZZ= 156.3242

Eigenvalues: -145.6106 -53.9263 188.2672

28 N Isotropic = 17.7527 Anisotropy = 238.7469

XX= -98.5949 YX= 65.4850 ZX= -53.5805

XY= 32.7778 YY= 28.1006 ZY= 57.1105

XZ= -88.7937 YZ= 107.8485 ZZ= 123.7525

Eigenvalues: -149.7171 26.0580 176.9173

29 H Isotropic = 30.5851 Anisotropy = 7.5543

XX= 35.1194 YX= -1.0645 ZX= -0.9533

XY= -0.9334 YY= 29.9969 ZY= -0.1127

XZ= -2.5924 YZ= -0.6542 ZZ= 26.6390

Eigenvalues: 26.1951 29.9389 35.6213

30 H Isotropic = 30.0409 Anisotropy = 8.0124

XX= 27.7962 YX= 0.8850 ZX= -1.2363

XY= 1.1795 YY= 31.7186 ZY= 3.7785

XZ= -1.9202 YZ= 4.5672 ZZ= 30.6079

Eigenvalues: 25.4579 29.2823 35.3825

31 H Isotropic = 29.2890 Anisotropy = 11.1333

XX= 26.7114 YX= 1.6729 ZX= -1.8706

XY= 3.3913 YY= 33.3632 ZY= -2.6885

XZ= -3.5097 YZ= -5.3688 ZZ= 27.7925

Eigenvalues: 24.4364 26.7196 36.7112

32 H Isotropic = 27.5866 Anisotropy = 6.2093

XX= 27.0562 YX= -0.3948 ZX= 1.0079

XY= 1.7692 YY= 30.4198 ZY= -2.7283

XZ= 0.3187 YZ= -2.9988 ZZ= 25.2837

Eigenvalues: 23.7657 27.2679 31.7261

33 C Isotropic = 110.4606 Anisotropy = 63.9905

XX= 148.0683 YX= -11.0525 ZX= -19.6543

XY= -5.1082 YY= 93.7713 ZY= 0.3646

XZ= -11.6820 YZ= 2.2865 ZZ= 89.5422

Eigenvalues: 85.5475 92.7133 153.1209

34 C Isotropic = 156.5726 Anisotropy = 34.1356

XX= 158.2270 YX= -1.1666 ZX= 11.5311

XY= 0.6047 YY= 142.9103 ZY= -0.7444

XZ= 18.3029 YZ= -4.3195 ZZ= 168.5804

Eigenvalues: 142.4766 147.9115 179.3296

35 C Isotropic = 158.4079 Anisotropy = 29.5870

XX= 155.6987 YX= 2.9625 ZX= -5.3386

XY= 4.5788 YY= 158.6225 ZY= -17.9435

XZ= -6.3894 YZ= -14.5122 ZZ= 160.9027

Eigenvalues: 143.3536 153.7376 178.1326

36 H Isotropic = 29.8535 Anisotropy = 7.8816

XX= 27.6243 YX= 0.2530 ZX= 2.1859

XY= 0.4094 YY= 27.4046 ZY= -1.1663

XZ= 1.6457 YZ= -0.6277 ZZ= 34.5317

Eigenvalues: 26.6750 27.7777 35.1079

37 H Isotropic = 30.2020 Anisotropy = 8.0702

XX= 33.6863 YX= 0.1935 ZX= -3.0509

XY= 1.4222 YY= 27.6329 ZY= 1.5187

XZ= -3.8368 YZ= 0.3198 ZZ= 29.2867

Eigenvalues: 26.3130 28.7108 35.5821

38 H Isotropic = 28.5434 Anisotropy = 9.7094

XX= 25.5963 YX= 0.1635 ZX= -0.1689

XY= 2.2544 YY= 33.5272 ZY= 4.5980

XZ= -0.6417 YZ= 2.2374 ZZ= 26.5068

Eigenvalues: 24.4591 26.1548 35.0163

39 C Isotropic = 61.4468 Anisotropy = 90.3689

XX= 67.9682 YX= 25.4582 ZX= 19.2841

XY= 26.9968 YY= 8.1887 ZY= -38.6778

XZ= 15.3459 YZ= -34.7408 ZZ= 108.1835

Eigenvalues: -14.9874 77.6350 121.6927

40 H Isotropic = 24.8772 Anisotropy = 6.6153

XX= 26.7078 YX= 2.9483 ZX= -0.0999

XY= 2.5533 YY= 26.1624 ZY= 1.0791

XZ= -0.0299 YZ= 1.4603 ZZ= 21.7614

Eigenvalues: 21.2751 24.0692 29.2874

41 C Isotropic = 47.1376 Anisotropy = 172.7844

XX= 12.3000 YX= -56.1595 ZX= 22.4771

XY= -63.5380 YY= -18.4155 ZY= -33.0883

XZ= 25.0940 YZ= -31.1194 ZZ= 147.5283

Eigenvalues: -65.4243 44.5099 162.3273

42 H Isotropic = 24.4710 Anisotropy = 4.0513

XX= 25.8326 YX= -1.4550 ZX= -1.2213

XY= -0.8862 YY= 25.4484 ZY= 1.1798

XZ= -0.6328 YZ= 0.7098 ZZ= 22.1321

Eigenvalues: 21.7822 24.4589 27.1719

43 C Isotropic = 52.2756 Anisotropy = 176.1206

XX= -30.6797 YX= -10.8038 ZX= 45.7145

XY= -13.1090 YY= 39.4132 ZY= -30.3007

XZ= 36.1531 YZ= -47.6292 ZZ= 148.0932

Eigenvalues: -39.7679 26.9053 169.6893

44 H Isotropic = 23.8497 Anisotropy = 10.7667

XX= 21.6560 YX= -2.1025 ZX= 0.4052

XY= -3.1439 YY= 29.4402 ZY= 2.8828

XZ= 0.7794 YZ= 3.4451 ZZ= 20.4530

Eigenvalues: 18.7105 21.8112 31.0276

45 C Isotropic = 17.3674 Anisotropy = 158.4458

XX= -45.7171 YX= -16.3489 ZX= 29.8163

XY= 2.9692 YY= -8.4136 ZY= -28.0208

XZ= 43.2454 YZ= -37.2389 ZZ= 106.2329

Eigenvalues: -54.0569 -16.8388 122.9979

46 C Isotropic = 36.3692 Anisotropy = 148.1658

XX= 3.2511 YX= -19.2222 ZX= 15.2258

XY= -19.9658 YY= -20.2437 ZY= -45.1351

XZ= 14.9285 YZ= -17.2153 ZZ= 126.1002

Eigenvalues: -34.0474 8.0085 135.1464

47 H Isotropic = 21.7164 Anisotropy = 8.1454

XX= 25.2147 YX= -3.2369 ZX= -1.7578

XY= -1.2119 YY= 23.0241 ZY= 2.0065

XZ= -0.1064 YZ= 3.6653 ZZ= 16.9104

Eigenvalues: 15.7972 22.2053 27.1466

48 C Isotropic = 15.2490 Anisotropy = 182.7754

XX= -68.5402 YX= 40.5144 ZX= 6.1467

XY= 31.1419 YY= 113.4457 ZY= -47.7322

XZ= 9.1339 YZ= -52.2436 ZZ= 0.8414

Eigenvalues: -79.4490 -11.9033 137.0992

49 C Isotropic = 47.1521 Anisotropy = 161.3378

XX= -0.0705 YX= 7.1640 ZX= -47.8705

XY= 19.1667 YY= 134.6925 ZY= -46.0923

XZ= -56.4640 YZ= -44.2771 ZZ= 6.8344

Eigenvalues: -51.5625 38.3082 154.7106

50 H Isotropic = 24.0406 Anisotropy = 6.4221

XX= 25.1417 YX= -1.1077 ZX= -2.9065

XY= -1.0805 YY= 22.1272 ZY= 1.0260

XZ= -3.0984 YZ= 0.7511 ZZ= 24.8530

Eigenvalues: 21.7578 22.0421 28.3220

51 C Isotropic = 42.0138 Anisotropy = 189.0292

XX= 32.1092 YX= 29.0860 ZX= 19.6173

XY= 30.9313 YY= 137.7712 ZY= -70.5151

XZ= 12.4864 YZ= -77.4728 ZZ= -43.8389

Eigenvalues: -76.1478 34.1560 168.0333

52 H Isotropic = 23.6224 Anisotropy = 4.9417

XX= 26.8941 YX= -0.2244 ZX= 0.4668

XY= -0.3342 YY= 21.0437 ZY= 0.7479

XZ= -0.0359 YZ= 0.1402 ZZ= 22.9295

Eigenvalues: 20.9272 23.0232 26.9169

53 C Isotropic = 54.4014 Anisotropy = 174.3115

XX= -41.3394 YX= 39.9639 ZX= 12.7511

XY= 37.1625 YY= 149.6839 ZY= -41.4522

XZ= 10.5596 YZ= -42.8145 ZZ= 54.8598

Eigenvalues: -52.6171 45.2123 170.6091

54 H Isotropic = 24.1507 Anisotropy = 3.1069

XX= 25.0094 YX= 0.0440 ZX= 0.4010

XY= 0.0113 YY= 21.7933 ZY= 1.6244

XZ= 0.1820 YZ= 1.3458 ZZ= 25.6493

Eigenvalues: 21.2864 24.9437 26.2219

55 C Isotropic = 43.9675 Anisotropy = 185.6684

XX= -11.6217 YX= 8.7115 ZX= -61.2637

XY= 8.5127 YY= 149.1563 ZY= -48.0346

XZ= -57.6768 YZ= -51.9532 ZZ= -5.6320

Eigenvalues: -72.0220 36.1782 167.7465

56 H Isotropic = 23.7335 Anisotropy = 4.7991

XX= 26.0172 YX= -0.8657 ZX= -1.6298

XY= -0.8951 YY= 21.7038 ZY= 1.5460

XZ= -0.9860 YZ= 1.2110 ZZ= 23.4795

Eigenvalues: 20.9470 23.3206 26.9329

57 C Isotropic = 52.9554 Anisotropy = 167.2532

XX= 35.3269 YX= 26.0740 ZX= 10.9747

XY= 21.3278 YY= 137.5924 ZY= -56.9376

XZ= 27.0201 YZ= -75.8333 ZZ= -14.0531

Eigenvalues: -47.3746 41.7833 164.4575

58 H Isotropic = 23.9575 Anisotropy = 7.9096

XX= 28.5754 YX= -0.5223 ZX= 2.0703

XY= -1.3059 YY= 22.7215 ZY= -0.2572

XZ= 2.1843 YZ= 0.1432 ZZ= 20.5757

Eigenvalues: 20.0345 22.6074 29.2306

59 N Isotropic = -3.7628 Anisotropy = 288.0539

XX= -134.2620 YX= -28.1775 ZX= 56.6502

XY= -7.7019 YY= -33.2160 ZY= -64.6951

XZ= 58.9221 YZ= -67.3159 ZZ= 156.1898

Eigenvalues: -145.6132 -53.9482 188.2732

60 N Isotropic = 17.7379 Anisotropy = 238.8484

XX= -98.6965 YX= 65.5447 ZX= 53.4884

XY= 32.6641 YY= 28.0491 ZY= -57.1647

XZ= 88.6723 YZ= -107.8067 ZZ= 123.8610

Eigenvalues: -149.7080 25.9515 176.9702

61 H Isotropic = 30.5861 Anisotropy = 7.5554

XX= 35.1205 YX= -1.0792 ZX= 0.9468

XY= -0.9446 YY= 30.0003 ZY= 0.1212

XZ= 2.5808 YZ= 0.6529 ZZ= 26.6374

Eigenvalues: 26.1955 29.9397 35.6230

62 H Isotropic = 30.0447 Anisotropy = 8.0102

XX= 27.8019 YX= 0.8855 ZX= 1.2333

XY= 1.1809 YY= 31.7113 ZY= -3.7794

XZ= 1.9163 YZ= -4.5679 ZZ= 30.6210

Eigenvalues: 25.4644 29.2849 35.3849

63 H Isotropic = 29.2912 Anisotropy = 11.1724

XX= 26.7061 YX= 1.6880 ZX= 1.8795

XY= 3.4142 YY= 33.3865 ZY= 2.6956

XZ= 3.5153 YZ= 5.3698 ZZ= 27.7808

Eigenvalues: 24.4236 26.7105 36.7394

64 H Isotropic = 27.5874 Anisotropy = 6.2098

XX= 27.0596 YX= -0.3952 ZX= -1.0073

XY= 1.7706 YY= 30.4201 ZY= 2.7295

XZ= -0.3176 YZ= 3.0003 ZZ= 25.2826

Eigenvalues: 23.7645 27.2705 31.7273

## BETAINE dimer\_iso1 (IEFPCM solvent = tetrahydrofuran) – BP86/IGLO-III level

64

c 0.9103 2.7214 -2.5483

c -0.4089 2.5606 -3.3137

c 1.8662 1.5359 -2.7204

h 2.7949 1.6818 -2.1268

h 2.1466 1.4511 -3.7921

h 1.3863 0.5793 -2.4209

c 0.8154 4.2780 -0.6398

h 1.1930 5.0150 -1.3595

c 0.4844 4.5691 0.6933

h 0.5919 5.6079 1.0460

c 0.0295 3.5771 1.5524

h -0.2424 3.8278 2.5891

c -0.1004 2.2004 1.1035

c 0.1916 2.0025 -0.3000

h 0.0105 1.0163 -0.7685

c -0.7621 1.2508 3.1813

c -2.0262 0.8321 3.6826

h -2.7910 0.5172 2.9536

c -2.2990 0.8253 5.0584

h -3.2930 0.5017 5.4128

c -1.3201 1.2276 5.9862

h -1.5349 1.2187 7.0675

c -0.0616 1.6407 5.5112

h 0.7203 1.9537 6.2252

c 0.2155 1.6563 4.1353

h 1.2117 1.9689 3.7791

n 0.6382 2.9986 -1.0927

n -0.5050 1.1525 1.8150

h -0.1986 2.4665 -4.4006

h -1.0676 3.4425 -3.1598

h -0.9501 1.6429 -2.9993

h 1.4213 3.6401 -2.9052

c 0.9112 -2.7208 2.5483

c -0.4075 -2.5598 3.3145

c 1.8671 -1.5353 2.7196

h 2.7956 -1.6812 2.1256

h 2.1481 -1.4501 3.7911

h 1.3871 -0.5788 2.4200

c 0.8167 -4.2776 0.6401

h 1.1954 -5.0141 1.3596

c 0.4854 -4.5692 -0.6928

h 0.5934 -5.6079 -1.0454

c 0.0294 -3.5778 -1.5518

h -0.2429 -3.8288 -2.5884

c -0.1012 -2.2011 -1.1032

c 0.1907 -2.0027 0.3003

h 0.0091 -1.0166 0.7688

c -0.7619 -1.2516 -3.1815

c -2.0249 -0.8315 -3.6843

h -2.7903 -0.5161 -2.9562

c -2.2960 -0.8242 -5.0605

h -3.2892 -0.4994 -5.4160

c -1.3165 -1.2275 -5.9871

h -1.5300 -1.2183 -7.0687

c -0.0591 -1.6422 -5.5107

h 0.7233 -1.9561 -6.2237

c 0.2164 -1.6582 -4.1345

h 1.2119 -1.9719 -3.7772

n 0.6385 -2.9984 1.0929

n -0.5062 -1.1533 -1.8149

h -0.1965 -2.4675 4.4014

h -1.0672 -3.4407 3.1597

h -0.9478 -1.6410 3.0019

h 1.4224 -3.6394 2.9051

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 103.2685 Anisotropy = 65.5318

XX= 141.9003 YX= -10.9033 ZX= 19.8313

XY= -5.3274 YY= 85.5951 ZY= 0.2662

XZ= 12.0937 YZ= -1.5170 ZZ= 82.3102

Eigenvalues: 78.0208 84.8284 146.9564

2 C Isotropic = 150.9206 Anisotropy = 36.0149

XX= 151.8676 YX= -1.3913 ZX= -12.5467

XY= 0.0685 YY= 136.9919 ZY= 0.6055

XZ= -19.0546 YZ= 4.0378 ZZ= 163.9024

Eigenvalues: 136.7144 141.1169 174.9306

3 C Isotropic = 152.9993 Anisotropy = 31.7941

XX= 149.1962 YX= 3.1203 ZX= 5.9425

XY= 4.4836 YY= 154.0029 ZY= 18.8761

XZ= 6.9686 YZ= 15.3894 ZZ= 155.7989

Eigenvalues: 137.4657 147.3369 174.1954

4 H Isotropic = 29.7584 Anisotropy = 7.5076

XX= 27.5359 YX= 0.2668 ZX= -1.9157

XY= 0.3232 YY= 27.4942 ZY= 1.2046

XZ= -1.5713 YZ= 0.6225 ZZ= 34.2451

Eigenvalues: 26.7347 27.7771 34.7635

5 H Isotropic = 30.1236 Anisotropy = 7.6034

XX= 33.2990 YX= 0.1662 ZX= 2.9138

XY= 1.3662 YY= 27.7222 ZY= -1.4295

XZ= 3.7202 YZ= -0.2937 ZZ= 29.3496

Eigenvalues: 26.4551 28.7232 35.1925

6 H Isotropic = 28.7694 Anisotropy = 8.8887

XX= 26.0565 YX= 0.1881 ZX= 0.1860

XY= 2.0999 YY= 33.3880 ZY= -4.2249

XZ= 0.6068 YZ= -1.8902 ZZ= 26.8638

Eigenvalues: 25.0070 26.6060 34.6953

7 C Isotropic = 55.5603 Anisotropy = 89.3525

XX= 60.8549 YX= 22.5513 ZX= -18.5080

XY= 23.5377 YY= 3.8707 ZY= 37.0304

XZ= -15.1933 YZ= 34.0546 ZZ= 101.9553

Eigenvalues: -17.1557 68.7080 115.1286

8 H Isotropic = 24.7328 Anisotropy = 6.2978

XX= 26.5155 YX= 2.8096 ZX= 0.0706

XY= 2.5328 YY= 25.8125 ZY= -0.9279

XZ= -0.0353 YZ= -1.2717 ZZ= 21.8705

Eigenvalues: 21.4534 23.8138 28.9313

9 C Isotropic = 44.1157 Anisotropy = 168.5810

XX= 9.7408 YX= -53.3532 ZX= -22.3826

XY= -59.7626 YY= -19.2166 ZY= 32.7291

XZ= -25.3762 YZ= 30.3911 ZZ= 141.8228

Eigenvalues: -63.6679 39.5119 156.5030

10 H Isotropic = 24.4775 Anisotropy = 3.8795

XX= 25.6960 YX= -1.4090 ZX= 1.1318

XY= -1.0086 YY= 25.3684 ZY= -1.0984

XZ= 0.5682 YZ= -0.6328 ZZ= 22.3682

Eigenvalues: 22.0530 24.3157 27.0639

11 C Isotropic = 50.6854 Anisotropy = 169.3146

XX= -29.7417 YX= -10.6893 ZX= -43.4428

XY= -9.5817 YY= 38.7983 ZY= 30.3997

XZ= -33.6435 YZ= 45.5522 ZZ= 142.9995

Eigenvalues: -38.0098 26.5042 163.5618

12 H Isotropic = 24.0113 Anisotropy = 10.0612

XX= 21.7840 YX= -2.0102 ZX= -0.4995

XY= -2.8995 YY= 29.2327 ZY= -2.6152

XZ= -0.8443 YZ= -3.3514 ZZ= 21.0172

Eigenvalues: 19.1644 22.1507 30.7187

13 C Isotropic = 17.0847 Anisotropy = 146.6354

XX= -38.1568 YX= -13.3845 ZX= -27.0883

XY= 3.5897 YY= -9.6154 ZY= 26.0372

XZ= -39.9913 YZ= 36.6831 ZZ= 99.0261

Eigenvalues: -46.0944 -17.4932 114.8416

14 C Isotropic = 36.0300 Anisotropy = 139.6564

XX= 6.0166 YX= -18.1113 ZX= -14.0334

XY= -19.6251 YY= -19.2191 ZY= 42.8660

XZ= -12.6007 YZ= 14.0816 ZZ= 121.2925

Eigenvalues: -31.8362 10.7919 129.1343

15 H Isotropic = 21.9515 Anisotropy = 7.7525

XX= 25.3609 YX= -3.1251 ZX= 1.6504

XY= -1.2474 YY= 22.9922 ZY= -1.8129

XZ= -0.0347 YZ= -3.4014 ZZ= 17.5014

Eigenvalues: 16.4603 22.2744 27.1199

16 C Isotropic = 13.0657 Anisotropy = 173.7945

XX= -64.4709 YX= 38.6444 ZX= -5.1066

XY= 28.5260 YY= 106.4282 ZY= 45.7822

XZ= -7.9553 YZ= 50.1097 ZZ= -2.7602

Eigenvalues: -74.7107 -15.0208 128.9287

17 C Isotropic = 45.2739 Anisotropy = 153.2254

XX= 1.0766 YX= 6.4835 ZX= 46.2255

XY= 19.9197 YY= 128.1849 ZY= 43.6491

XZ= 55.6184 YZ= 41.4524 ZZ= 6.5603

Eigenvalues: -49.5628 37.9604 147.4242

18 H Isotropic = 24.2365 Anisotropy = 6.1038

XX= 25.1788 YX= -1.0195 ZX= 2.9121

XY= -0.9701 YY= 22.6396 ZY= -0.8769

XZ= 3.0995 YZ= -0.5628 ZZ= 24.8912

Eigenvalues: 21.9626 22.4412 28.3057

19 C Isotropic = 40.2661 Anisotropy = 182.5854

XX= 30.8639 YX= 27.8352 ZX= -18.7939

XY= 30.6791 YY= 133.5276 ZY= 65.9531

XZ= -11.4716 YZ= 74.5307 ZZ= -43.5932

Eigenvalues: -73.6586 32.4672 161.9897

20 H Isotropic = 23.6870 Anisotropy = 4.7581

XX= 26.8412 YX= -0.1910 ZX= -0.4408

XY= -0.2800 YY= 21.3480 ZY= -0.7512

XZ= 0.0559 YZ= -0.0194 ZZ= 22.8719

Eigenvalues: 21.2427 22.9593 26.8591

21 C Isotropic = 52.4139 Anisotropy = 168.2147

XX= -39.7136 YX= 38.4850 ZX= -12.4813

XY= 35.9688 YY= 144.5740 ZY= 39.6487

XZ= -9.9314 YZ= 41.1810 ZZ= 52.3814

Eigenvalues: -50.5960 43.2808 164.5570

22 H Isotropic = 24.2154 Anisotropy = 2.9077

XX= 24.9280 YX= 0.0957 ZX= -0.4155

XY= 0.1278 YY= 22.0845 ZY= -1.4806

XZ= -0.1393 YZ= -1.1941 ZZ= 25.6337

Eigenvalues: 21.6369 24.8554 26.1539

23 C Isotropic = 41.8280 Anisotropy = 179.9971

XX= -11.6388 YX= 8.5633 ZX= 58.5984

XY= 8.2538 YY= 143.8252 ZY= 46.6620

XZ= 55.0183 YZ= 50.5467 ZZ= -6.7024

Eigenvalues: -69.8362 33.4942 161.8260

24 H Isotropic = 23.7684 Anisotropy = 4.6198

XX= 25.9235 YX= -0.8198 ZX= 1.6417

XY= -0.8801 YY= 21.9166 ZY= -1.4419

XZ= 1.0096 YZ= -1.0827 ZZ= 23.4650

Eigenvalues: 21.2077 23.2492 26.8482

25 C Isotropic = 50.1517 Anisotropy = 162.8077

XX= 32.2995 YX= 24.8914 ZX= -9.9126

XY= 19.6829 YY= 132.9211 ZY= 54.5819

XZ= -26.3887 YZ= 73.9861 ZZ= -14.7654

Eigenvalues: -46.7203 38.4854 158.6902

26 H Isotropic = 23.9954 Anisotropy = 7.5962

XX= 28.4371 YX= -0.4640 ZX= -1.9979

XY= -1.2251 YY= 22.9917 ZY= 0.3524

XZ= -2.1011 YZ= -0.0369 ZZ= 20.5575

Eigenvalues: 20.0555 22.8712 29.0595

27 N Isotropic = -5.5200 Anisotropy = 273.4315

XX= -124.7053 YX= -25.3963 ZX= -53.0907

XY= -7.2048 YY= -37.7106 ZY= 62.5489

XZ= -55.4956 YZ= 65.9544 ZZ= 145.8560

Eigenvalues: -135.3700 -57.9576 176.7677

28 N Isotropic = 10.8292 Anisotropy = 227.4353

XX= -95.6640 YX= 65.1850 ZX= -49.2380

XY= 29.5537 YY= 20.7593 ZY= 55.5839

XZ= -88.4774 YZ= 109.4027 ZZ= 107.3924

Eigenvalues: -148.2294 18.2643 162.4528

29 H Isotropic = 30.5011 Anisotropy = 7.0723

XX= 34.6733 YX= -1.0635 ZX= -0.9524

XY= -0.9913 YY= 30.0054 ZY= -0.1129

XZ= -2.5623 YZ= -0.5994 ZZ= 26.8248

Eigenvalues: 26.3599 29.9275 35.2160

30 H Isotropic = 29.9317 Anisotropy = 7.5925

XX= 27.7462 YX= 0.7348 ZX= -1.3192

XY= 1.0951 YY= 31.5214 ZY= 3.5117

XZ= -1.8115 YZ= 4.3279 ZZ= 30.5276

Eigenvalues: 25.5937 29.2081 34.9934

31 H Isotropic = 29.5061 Anisotropy = 10.3045

XX= 27.1550 YX= 1.6429 ZX= -1.8646

XY= 3.1898 YY= 33.1754 ZY= -2.4148

XZ= -3.2680 YZ= -5.0005 ZZ= 28.1878

Eigenvalues: 25.0028 27.1397 36.3757

32 H Isotropic = 27.3227 Anisotropy = 5.7607

XX= 26.8045 YX= -0.3647 ZX= 0.9308

XY= 1.7821 YY= 29.9669 ZY= -2.4925

XZ= 0.2342 YZ= -2.7430 ZZ= 25.1967

Eigenvalues: 23.8142 26.9907 31.1632

33 C Isotropic = 103.2698 Anisotropy = 65.5512

XX= 141.8914 YX= -10.9122 ZX= -19.8650

XY= -5.3103 YY= 85.5809 ZY= -0.2511

XZ= -12.1496 YZ= 1.5498 ZZ= 82.3371

Eigenvalues: 78.0310 84.8079 146.9706

34 C Isotropic = 150.9530 Anisotropy = 36.0106

XX= 151.9043 YX= -1.3898 ZX= 12.5662

XY= 0.0847 YY= 137.0250 ZY= -0.6062

XZ= 19.0330 YZ= -4.0540 ZZ= 163.9296

Eigenvalues: 136.7430 141.1558 174.9601

35 C Isotropic = 153.0050 Anisotropy = 31.8052

XX= 149.1707 YX= 3.1165 ZX= -5.9430

XY= 4.4828 YY= 154.0221 ZY= -18.8721

XZ= -6.9704 YZ= -15.3842 ZZ= 155.8221

Eigenvalues: 137.4894 147.3170 174.2084

36 H Isotropic = 29.7573 Anisotropy = 7.5068

XX= 27.5374 YX= 0.2658 ZX= 1.9196

XY= 0.3230 YY= 27.4929 ZY= -1.2025

XZ= 1.5762 YZ= -0.6207 ZZ= 34.2417

Eigenvalues: 26.7343 27.7758 34.7619

37 H Isotropic = 30.1220 Anisotropy = 7.6063

XX= 33.2922 YX= 0.1666 ZX= -2.9170

XY= 1.3679 YY= 27.7187 ZY= 1.4285

XZ= -3.7265 YZ= 0.2914 ZZ= 29.3550

Eigenvalues: 26.4533 28.7198 35.1928

38 H Isotropic = 28.7670 Anisotropy = 8.8929

XX= 26.0484 YX= 0.1847 ZX= -0.1858

XY= 2.0968 YY= 33.3878 ZY= 4.2280

XZ= -0.6103 YZ= 1.8910 ZZ= 26.8649

Eigenvalues: 25.0033 26.6021 34.6956

39 C Isotropic = 55.5720 Anisotropy = 89.3437

XX= 60.8887 YX= 22.5126 ZX= 18.5534

XY= 23.4987 YY= 3.9328 ZY= -37.1140

XZ= 15.2500 YZ= -34.1045 ZZ= 101.8945

Eigenvalues: -17.1336 68.7152 115.1345

40 H Isotropic = 24.7347 Anisotropy = 6.2971

XX= 26.5170 YX= 2.8096 ZX= -0.0717

XY= 2.5341 YY= 25.8128 ZY= 0.9271

XZ= 0.0339 YZ= 1.2724 ZZ= 21.8743

Eigenvalues: 21.4562 23.8151 28.9327

41 C Isotropic = 44.1396 Anisotropy = 168.5738

XX= 9.8141 YX= -53.3656 ZX= 22.4407

XY= -59.7860 YY= -19.1693 ZY= -32.7753

XZ= 25.4608 YZ= -30.4273 ZZ= 141.7740

Eigenvalues: -63.6277 39.5243 156.5222

42 H Isotropic = 24.4792 Anisotropy = 3.8783

XX= 25.6974 YX= -1.4080 ZX= -1.1337

XY= -1.0080 YY= 25.3691 ZY= 1.0999

XZ= -0.5679 YZ= 0.6321 ZZ= 22.3709

Eigenvalues: 22.0552 24.3176 27.0647

43 C Isotropic = 50.6859 Anisotropy = 169.3356

XX= -29.6972 YX= -10.7124 ZX= 43.5510

XY= -9.6229 YY= 38.8585 ZY= -30.4238

XZ= 33.7617 YZ= -45.7074 ZZ= 142.8965

Eigenvalues: -38.0171 26.4986 163.5763

44 H Isotropic = 24.0068 Anisotropy = 10.0530

XX= 21.7831 YX= -2.0123 ZX= 0.5007

XY= -2.8996 YY= 29.2216 ZY= 2.6102

XZ= 0.8496 YZ= 3.3556 ZZ= 21.0158

Eigenvalues: 19.1591 22.1526 30.7088

45 C Isotropic = 17.0558 Anisotropy = 146.6567

XX= -38.1916 YX= -13.4145 ZX= 27.1011

XY= 3.6136 YY= -9.6338 ZY= -26.0283

XZ= 40.0150 YZ= -36.7351 ZZ= 98.9928

Eigenvalues: -46.1379 -17.5217 114.8269

46 C Isotropic = 36.0151 Anisotropy = 139.6957

XX= 6.0325 YX= -18.0782 ZX= 14.0788

XY= -19.6621 YY= -19.2893 ZY= -42.9708

XZ= 12.6728 YZ= -13.9226 ZZ= 121.3020

Eigenvalues: -31.8795 10.7792 129.1455

47 H Isotropic = 21.9467 Anisotropy = 7.7434

XX= 25.3562 YX= -3.1148 ZX= -1.6511

XY= -1.2413 YY= 22.9865 ZY= 1.8119

XZ= 0.0310 YZ= 3.4077 ZZ= 17.4973

Eigenvalues: 16.4542 22.2769 27.1090

48 C Isotropic = 13.0610 Anisotropy = 173.7796

XX= -64.4702 YX= 38.6523 ZX= 5.0025

XY= 28.5553 YY= 106.2677 ZY= -45.9407

XZ= 7.8639 YZ= -50.2529 ZZ= -2.6144

Eigenvalues: -74.6918 -15.0392 128.9141

49 C Isotropic = 45.2685 Anisotropy = 153.2269

XX= 1.1335 YX= 6.4778 ZX= -46.2513

XY= 19.8590 YY= 128.0514 ZY= -43.8089

XZ= -55.6461 YZ= -41.6229 ZZ= 6.6205

Eigenvalues: -49.5673 37.9530 147.4198

50 H Isotropic = 24.2370 Anisotropy = 6.1011

XX= 25.1814 YX= -1.0223 ZX= -2.9125

XY= -0.9741 YY= 22.6445 ZY= 0.8735

XZ= -3.0975 YZ= 0.5635 ZZ= 24.8852

Eigenvalues: 21.9606 22.4461 28.3044

51 C Isotropic = 40.2772 Anisotropy = 182.5700

XX= 30.8647 YX= 27.9351 ZX= 18.7847

XY= 30.7508 YY= 133.2957 ZY= -66.1877

XZ= 11.4592 YZ= -74.8163 ZZ= -43.3289

Eigenvalues: -73.6371 32.4781 161.9905

52 H Isotropic = 23.6886 Anisotropy = 4.7568

XX= 26.8419 YX= -0.1897 ZX= 0.4427

XY= -0.2791 YY= 21.3531 ZY= 0.7547

XZ= -0.0534 YZ= 0.0195 ZZ= 22.8709

Eigenvalues: 21.2467 22.9593 26.8599

53 C Isotropic = 52.4368 Anisotropy = 168.1729

XX= -39.6645 YX= 38.5424 ZX= 12.3569

XY= 36.0437 YY= 144.4256 ZY= -39.7667

XZ= 9.7843 YZ= -41.3078 ZZ= 52.5491

Eigenvalues: -50.5413 43.2996 164.5520

54 H Isotropic = 24.2168 Anisotropy = 2.9053

XX= 24.9316 YX= 0.0946 ZX= 0.4145

XY= 0.1280 YY= 22.0898 ZY= 1.4875

XZ= 0.1368 YZ= 1.2006 ZZ= 25.6290

Eigenvalues: 21.6371 24.8596 26.1536

55 C Isotropic = 41.8412 Anisotropy = 179.9704

XX= -11.5307 YX= 8.4964 ZX= -58.6182

XY= 8.1904 YY= 143.6582 ZY= -46.8911

XZ= -55.0362 YZ= -50.8017 ZZ= -6.6038

Eigenvalues: -69.8166 33.5188 161.8215

56 H Isotropic = 23.7703 Anisotropy = 4.6201

XX= 25.9272 YX= -0.8238 ZX= -1.6384

XY= -0.8840 YY= 21.9246 ZY= 1.4461

XZ= -1.0061 YZ= 1.0844 ZZ= 23.4590

Eigenvalues: 21.2098 23.2507 26.8503

57 C Isotropic = 50.1710 Anisotropy = 162.8335

XX= 32.2533 YX= 24.9494 ZX= 9.8996

XY= 19.6469 YY= 132.7485 ZY= -54.8221

XZ= 26.4639 YZ= -74.2469 ZZ= -14.4887

Eigenvalues: -46.7063 38.4926 158.7267

58 H Isotropic = 23.9926 Anisotropy = 7.6014

XX= 28.4368 YX= -0.4668 ZX= 2.0033

XY= -1.2268 YY= 22.9925 ZY= -0.3488

XZ= 2.0995 YZ= 0.0367 ZZ= 20.5483

Eigenvalues: 20.0459 22.8716 29.0602

59 N Isotropic = -5.5297 Anisotropy = 273.4543

XX= -124.6531 YX= -25.4688 ZX= 53.2200

XY= -7.3102 YY= -37.6628 ZY= -62.6750

XZ= 55.6240 YZ= -66.0404 ZZ= 145.7267

Eigenvalues: -135.3754 -57.9869 176.7731

60 N Isotropic = 10.8307 Anisotropy = 227.5201

XX= -95.7395 YX= 65.2393 ZX= 49.1467

XY= 29.4388 YY= 20.7196 ZY= -55.6424

XZ= 88.3476 YZ= -109.3470 ZZ= 107.5119

Eigenvalues: -148.1870 18.1683 162.5107

61 H Isotropic = 30.5015 Anisotropy = 7.0741

XX= 34.6742 YX= -1.0771 ZX= 0.9463

XY= -1.0014 YY= 30.0080 ZY= 0.1209

XZ= 2.5515 YZ= 0.5983 ZZ= 26.8223

Eigenvalues: 26.3594 29.9275 35.2176

62 H Isotropic = 29.9359 Anisotropy = 7.5908

XX= 27.7520 YX= 0.7352 ZX= 1.3167

XY= 1.0964 YY= 31.5154 ZY= -3.5127

XZ= 1.8081 YZ= -4.3287 ZZ= 30.5402

Eigenvalues: 25.6002 29.2110 34.9964

63 H Isotropic = 29.5083 Anisotropy = 10.3413

XX= 27.1502 YX= 1.6568 ZX= 1.8725

XY= 3.2110 YY= 33.1975 ZY= 2.4217

XZ= 3.2738 YZ= 5.0019 ZZ= 28.1771

Eigenvalues: 24.9906 27.1317 36.4025

64 H Isotropic = 27.3235 Anisotropy = 5.7614

XX= 26.8078 YX= -0.3651 ZX= -0.9302

XY= 1.7833 YY= 29.9673 ZY= 2.4936

XZ= -0.2330 YZ= 2.7446 ZZ= 25.1956

Eigenvalues: 23.8131 26.9931 31.1645

## BETAINE dimer\_iso1 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level

64

c 0.9103 2.7214 -2.5483

c -0.4089 2.5606 -3.3137

c 1.8662 1.5359 -2.7204

h 2.7949 1.6818 -2.1268

h 2.1466 1.4511 -3.7921

h 1.3863 0.5793 -2.4209

c 0.8154 4.2780 -0.6398

h 1.1930 5.0150 -1.3595

c 0.4844 4.5691 0.6933

h 0.5919 5.6079 1.0460

c 0.0295 3.5771 1.5524

h -0.2424 3.8278 2.5891

c -0.1004 2.2004 1.1035

c 0.1916 2.0025 -0.3000

h 0.0105 1.0163 -0.7685

c -0.7621 1.2508 3.1813

c -2.0262 0.8321 3.6826

h -2.7910 0.5172 2.9536

c -2.2990 0.8253 5.0584

h -3.2930 0.5017 5.4128

c -1.3201 1.2276 5.9862

h -1.5349 1.2187 7.0675

c -0.0616 1.6407 5.5112

h 0.7203 1.9537 6.2252

c 0.2155 1.6563 4.1353

h 1.2117 1.9689 3.7791

n 0.6382 2.9986 -1.0927

n -0.5050 1.1525 1.8150

h -0.1986 2.4665 -4.4006

h -1.0676 3.4425 -3.1598

h -0.9501 1.6429 -2.9993

h 1.4213 3.6401 -2.9052

c 0.9112 -2.7208 2.5483

c -0.4075 -2.5598 3.3145

c 1.8671 -1.5353 2.7196

h 2.7956 -1.6812 2.1256

h 2.1481 -1.4501 3.7911

h 1.3871 -0.5788 2.4200

c 0.8167 -4.2776 0.6401

h 1.1954 -5.0141 1.3596

c 0.4854 -4.5692 -0.6928

h 0.5934 -5.6079 -1.0454

c 0.0294 -3.5778 -1.5518

h -0.2429 -3.8288 -2.5884

c -0.1012 -2.2011 -1.1032

c 0.1907 -2.0027 0.3003

h 0.0091 -1.0166 0.7688

c -0.7619 -1.2516 -3.1815

c -2.0249 -0.8315 -3.6843

h -2.7903 -0.5161 -2.9562

c -2.2960 -0.8242 -5.0605

h -3.2892 -0.4994 -5.4160

c -1.3165 -1.2275 -5.9871

h -1.5300 -1.2183 -7.0687

c -0.0591 -1.6422 -5.5107

h 0.7233 -1.9561 -6.2237

c 0.2164 -1.6582 -4.1345

h 1.2119 -1.9719 -3.7772

n 0.6385 -2.9984 1.0929

n -0.5062 -1.1533 -1.8149

h -0.1965 -2.4675 4.4014

h -1.0672 -3.4407 3.1597

h -0.9478 -1.6410 3.0019

h 1.4224 -3.6394 2.9051

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 110.8711 Anisotropy = 64.9359

XX= 149.2382 YX= -10.9179 ZX= 19.4893

XY= -5.2153 YY= 93.2518 ZY= 0.1679

XZ= 11.7311 YZ= -1.6936 ZZ= 90.1233

Eigenvalues: 86.0247 92.4269 154.1617

2 C Isotropic = 156.6791 Anisotropy = 34.4618

XX= 158.1672 YX= -1.3673 ZX= -11.6182

XY= 0.2271 YY= 143.1359 ZY= 0.7774

XZ= -18.6827 YZ= 4.2955 ZZ= 168.7343

Eigenvalues: 142.7622 147.6215 179.6537

3 C Isotropic = 158.6124 Anisotropy = 30.1104

XX= 155.5705 YX= 2.8610 ZX= 5.5839

XY= 4.4817 YY= 159.0335 ZY= 18.1051

XZ= 6.6982 YZ= 14.6835 ZZ= 161.2332

Eigenvalues: 143.4864 153.6648 178.6860

4 H Isotropic = 29.7465 Anisotropy = 7.9696

XX= 27.4630 YX= 0.2478 ZX= -2.2192

XY= 0.4278 YY= 27.2757 ZY= 1.1479

XZ= -1.6021 YZ= 0.5808 ZZ= 34.5008

Eigenvalues: 26.5407 27.6392 35.0595

5 H Isotropic = 30.1206 Anisotropy = 8.1780

XX= 33.6405 YX= 0.1433 ZX= 3.1099

XY= 1.3528 YY= 27.5618 ZY= -1.5601

XZ= 3.9192 YZ= -0.3759 ZZ= 29.1597

Eigenvalues: 26.1757 28.6137 35.5726

6 H Isotropic = 28.7293 Anisotropy = 9.6342

XX= 25.8366 YX= 0.1400 ZX= 0.2048

XY= 2.2458 YY= 33.6863 ZY= -4.5780

XZ= 0.6987 YZ= -2.2056 ZZ= 26.6650

Eigenvalues: 24.6277 26.4081 35.1521

7 C Isotropic = 57.6670 Anisotropy = 99.0170

XX= 61.0912 YX= 23.3057 ZX= -20.6297

XY= 24.2801 YY= 2.4699 ZY= 40.2094

XZ= -16.3653 YZ= 36.5870 ZZ= 109.4399

Eigenvalues: -19.8808 69.2035 123.6783

8 H Isotropic = 24.4976 Anisotropy = 6.7070

XX= 26.4167 YX= 2.9183 ZX= 0.1636

XY= 2.5518 YY= 25.8519 ZY= -1.1524

XZ= 0.1022 YZ= -1.5313 ZZ= 21.2241

Eigenvalues: 20.7060 23.8178 28.9689

9 C Isotropic = 46.3101 Anisotropy = 176.7844

XX= 10.1903 YX= -55.3924 ZX= -23.5615

XY= -61.8524 YY= -20.1508 ZY= 34.3623

XZ= -26.2074 YZ= 32.0851 ZZ= 148.8909

Eigenvalues: -66.1373 40.9013 164.1664

10 H Isotropic = 24.2099 Anisotropy = 4.1168

XX= 25.5540 YX= -1.4161 ZX= 1.2353

XY= -0.8666 YY= 25.3135 ZY= -1.2493

XZ= 0.6757 YZ= -0.7863 ZZ= 21.7623

Eigenvalues: 21.3852 24.2902 26.9545

11 C Isotropic = 53.0256 Anisotropy = 175.3407

XX= -29.4654 YX= -11.1006 ZX= -45.3449

XY= -11.3321 YY= 40.1846 ZY= 30.7673

XZ= -36.9890 YZ= 46.7319 ZZ= 148.3575

Eigenvalues: -38.6305 27.7879 169.9194

12 H Isotropic = 23.8237 Anisotropy = 10.6656

XX= 21.7092 YX= -2.0003 ZX= -0.3758

XY= -3.0049 YY= 29.4206 ZY= -2.8835

XZ= -0.7337 YZ= -3.3546 ZZ= 20.3412

Eigenvalues: 18.7378 21.7992 30.9340

13 C Isotropic = 17.2394 Anisotropy = 160.3699

XX= -43.9875 YX= -13.7105 ZX= -30.1477

XY= 3.7270 YY= -11.1980 ZY= 29.0071

XZ= -43.7179 YZ= 39.0930 ZZ= 106.9037

Eigenvalues: -52.7723 -19.6620 124.1527

14 C Isotropic = 37.5292 Anisotropy = 146.6985

XX= 5.7302 YX= -19.2362 ZX= -14.7606

XY= -20.9005 YY= -19.6529 ZY= 44.8714

XZ= -13.3961 YZ= 17.3103 ZZ= 126.5102

Eigenvalues: -33.5826 10.8420 135.3281

15 H Isotropic = 21.6987 Anisotropy = 8.2440

XX= 25.3200 YX= -3.2279 ZX= 1.7942

XY= -1.2316 YY= 22.9747 ZY= -2.0223

XZ= 0.0876 YZ= -3.6279 ZZ= 16.8016

Eigenvalues: 15.7033 22.1982 27.1947

16 C Isotropic = 14.6775 Anisotropy = 184.2217

XX= -68.9795 YX= 40.6185 ZX= -6.2475

XY= 30.7653 YY= 113.7512 ZY= 48.4836

XZ= -8.7987 YZ= 52.5863 ZZ= -0.7392

Eigenvalues: -79.8601 -13.5994 137.4920

17 C Isotropic = 47.3900 Anisotropy = 159.7563

XX= 0.3790 YX= 7.1798 ZX= 48.4617

XY= 19.7820 YY= 134.4454 ZY= 44.0281

XZ= 57.1975 YZ= 43.5367 ZZ= 7.3457

Eigenvalues: -51.4509 39.7267 153.8943

18 H Isotropic = 24.0360 Anisotropy = 6.4520

XX= 25.1358 YX= -1.0714 ZX= 2.9448

XY= -0.9768 YY= 22.1178 ZY= -1.0054

XZ= 3.1507 YZ= -0.7469 ZZ= 24.8543

Eigenvalues: 21.7925 21.9782 28.3373

19 C Isotropic = 42.2192 Anisotropy = 189.9470

XX= 31.6803 YX= 29.0097 ZX= -19.3771

XY= 31.3591 YY= 138.8724 ZY= 70.0742

XZ= -12.2100 YZ= 77.1934 ZZ= -43.8951

Eigenvalues: -75.7786 33.5857 168.8506

20 H Isotropic = 23.5231 Anisotropy = 4.9093

XX= 26.7739 YX= -0.2380 ZX= -0.4427

XY= -0.3656 YY= 20.9372 ZY= -0.8144

XZ= 0.0742 YZ= -0.1751 ZZ= 22.8581

Eigenvalues: 20.7982 22.9750 26.7960

21 C Isotropic = 55.1183 Anisotropy = 174.6216

XX= -40.2459 YX= 39.7975 ZX= -12.7714

XY= 37.3638 YY= 150.6062 ZY= 41.6964

XZ= -10.6292 YZ= 42.8328 ZZ= 54.9946

Eigenvalues: -51.6025 45.4248 171.5327

22 H Isotropic = 24.0636 Anisotropy = 3.0323

XX= 25.0048 YX= 0.0144 ZX= -0.4011

XY= -0.0013 YY= 21.6690 ZY= -1.6188

XZ= -0.1657 YZ= -1.3315 ZZ= 25.5169

Eigenvalues: 21.1667 24.9389 26.0851

23 C Isotropic = 43.7365 Anisotropy = 187.4613

XX= -12.1778 YX= 9.2783 ZX= 60.6722

XY= 9.0122 YY= 150.0800 ZY= 48.1543

XZ= 57.1060 YZ= 52.4459 ZZ= -6.6927

Eigenvalues: -72.2012 34.7000 168.7107

24 H Isotropic = 23.5939 Anisotropy = 4.7710

XX= 25.8830 YX= -0.8549 ZX= 1.5902

XY= -0.8926 YY= 21.5347 ZY= -1.5624

XZ= 0.9595 YZ= -1.2152 ZZ= 23.3639

Eigenvalues: 20.7803 23.2268 26.7745

25 C Isotropic = 51.7480 Anisotropy = 170.0012

XX= 32.8661 YX= 26.6450 ZX= -11.2465

XY= 20.7092 YY= 138.7714 ZY= 56.1660

XZ= -27.0129 YZ= 76.2909 ZZ= -16.3937

Eigenvalues: -49.2558 39.4176 165.0821

26 H Isotropic = 23.8140 Anisotropy = 8.0004

XX= 28.4594 YX= -0.5016 ZX= -2.1113

XY= -1.3512 YY= 22.5847 ZY= 0.2158

XZ= -2.2873 YZ= -0.0880 ZZ= 20.3979

Eigenvalues: 19.8265 22.4680 29.1476

27 N Isotropic = -6.5439 Anisotropy = 294.3933

XX= -137.5621 YX= -26.2544 ZX= -57.7824

XY= -7.1151 YY= -39.0263 ZY= 66.8774

XZ= -59.7139 YZ= 69.4414 ZZ= 156.9565

Eigenvalues: -148.9798 -60.3703 189.7183

28 N Isotropic = 26.3751 Anisotropy = 225.1395

XX= -83.3636 YX= 62.5205 ZX= -48.6982

XY= 27.1381 YY= 40.2864 ZY= 53.8994

XZ= -85.7367 YZ= 106.9426 ZZ= 122.2024

Eigenvalues: -131.1878 33.8449 176.4681

29 H Isotropic = 30.5329 Anisotropy = 7.6145

XX= 35.0968 YX= -1.1327 ZX= -0.9228

XY= -1.0242 YY= 29.9676 ZY= -0.1576

XZ= -2.5665 YZ= -0.6807 ZZ= 26.5344

Eigenvalues: 26.0912 29.8984 35.6093

30 H Isotropic = 29.9471 Anisotropy = 8.1336

XX= 27.6597 YX= 0.8810 ZX= -1.2007

XY= 1.1699 YY= 31.7050 ZY= 3.8130

XZ= -1.9925 YZ= 4.6357 ZZ= 30.4767

Eigenvalues: 25.3136 29.1583 35.3695

31 H Isotropic = 29.5227 Anisotropy = 10.9776

XX= 27.0092 YX= 1.6194 ZX= -1.8613

XY= 3.3234 YY= 33.5389 ZY= -2.6180

XZ= -3.5500 YZ= -5.3283 ZZ= 28.0201

Eigenvalues: 24.6812 27.0459 36.8411

32 H Isotropic = 27.2897 Anisotropy = 6.4620

XX= 26.6887 YX= -0.4605 ZX= 1.0428

XY= 1.7507 YY= 30.2563 ZY= -2.8139

XZ= 0.3509 YZ= -3.1182 ZZ= 24.9242

Eigenvalues: 23.3586 26.9129 31.5978

33 C Isotropic = 110.8723 Anisotropy = 64.9537

XX= 149.2287 YX= -10.9266 ZX= -19.5228

XY= -5.1980 YY= 93.2382 ZY= -0.1537

XZ= -11.7866 YZ= 1.7251 ZZ= 90.1499

Eigenvalues: 86.0342 92.4078 154.1748

34 C Isotropic = 156.7104 Anisotropy = 34.4577

XX= 158.2004 YX= -1.3667 ZX= 11.6368

XY= 0.2431 YY= 143.1683 ZY= -0.7790

XZ= 18.6604 YZ= -4.3124 ZZ= 168.7626

Eigenvalues: 142.7893 147.6598 179.6823

35 C Isotropic = 158.6177 Anisotropy = 30.1214

XX= 155.5459 YX= 2.8576 ZX= -5.5852

XY= 4.4822 YY= 159.0513 ZY= -18.1003

XZ= -6.7016 YZ= -14.6784 ZZ= 161.2558

Eigenvalues: 143.5097 153.6447 178.6986

36 H Isotropic = 29.7454 Anisotropy = 7.9688

XX= 27.4647 YX= 0.2469 ZX= 2.2233

XY= 0.4279 YY= 27.2744 ZY= -1.1458

XZ= 1.6069 YZ= -0.5791 ZZ= 34.4971

Eigenvalues: 26.5402 27.6380 35.0579

37 H Isotropic = 30.1190 Anisotropy = 8.1811

XX= 33.6335 YX= 0.1438 ZX= -3.1136

XY= 1.3546 YY= 27.5581 ZY= 1.5591

XZ= -3.9260 YZ= 0.3735 ZZ= 29.1653

Eigenvalues: 26.1738 28.6100 35.5730

38 H Isotropic = 28.7266 Anisotropy = 9.6384

XX= 25.8285 YX= 0.1366 ZX= -0.2045

XY= 2.2426 YY= 33.6858 ZY= 4.5813

XZ= -0.7026 YZ= 2.2061 ZZ= 26.6656

Eigenvalues: 24.6238 26.4039 35.1522

39 C Isotropic = 57.6779 Anisotropy = 99.0110

XX= 61.1237 YX= 23.2649 ZX= 20.6801

XY= 24.2382 YY= 2.5356 ZY= -40.2998

XZ= 16.4272 YZ= -36.6436 ZZ= 109.3745

Eigenvalues: -19.8596 69.2081 123.6853

40 H Isotropic = 24.4990 Anisotropy = 6.7072

XX= 26.4180 YX= 2.9186 ZX= -0.1651

XY= 2.5535 YY= 25.8521 ZY= 1.1525

XZ= -0.1045 YZ= 1.5330 ZZ= 21.2269

Eigenvalues: 20.7072 23.8193 28.9705

41 C Isotropic = 46.3355 Anisotropy = 176.7746

XX= 10.2659 YX= -55.4062 ZX= 23.6221

XY= -61.8739 YY= -20.0996 ZY= -34.4111

XZ= 26.2889 YZ= -32.1261 ZZ= 148.8401

Eigenvalues: -66.0939 40.9151 164.1852

42 H Isotropic = 24.2113 Anisotropy = 4.1159

XX= 25.5553 YX= -1.4148 ZX= -1.2376

XY= -0.8655 YY= 25.3142 ZY= 1.2511

XZ= -0.6762 YZ= 0.7858 ZZ= 21.7644

Eigenvalues: 21.3864 24.2922 26.9552

43 C Isotropic = 53.0246 Anisotropy = 175.3630

XX= -29.4219 YX= -11.1247 ZX= 45.4581

XY= -11.3729 YY= 40.2398 ZY= -30.7944

XZ= 37.1000 YZ= -46.8771 ZZ= 148.2558

Eigenvalues: -38.6398 27.7803 169.9332

44 H Isotropic = 23.8188 Anisotropy = 10.6576

XX= 21.7078 YX= -2.0024 ZX= 0.3766

XY= -3.0041 YY= 29.4095 ZY= 2.8787

XZ= 0.7375 YZ= 3.3581 ZZ= 20.3390

Eigenvalues: 18.7332 21.7994 30.9239

45 C Isotropic = 17.2094 Anisotropy = 160.3958

XX= -44.0181 YX= -13.7387 ZX= 30.1623

XY= 3.7446 YY= -11.2246 ZY= -29.0027

XZ= 43.7468 YZ= -39.1413 ZZ= 106.8710

Eigenvalues: -52.8132 -19.6985 124.1400

46 C Isotropic = 37.5147 Anisotropy = 146.7359

XX= 5.7491 YX= -19.2065 ZX= 14.8058

XY= -20.9393 YY= -19.7197 ZY= -44.9787

XZ= 13.4713 YZ= -17.1666 ZZ= 126.5147

Eigenvalues: -33.6256 10.8311 135.3386

47 H Isotropic = 21.6939 Anisotropy = 8.2352

XX= 25.3154 YX= -3.2175 ZX= -1.7953

XY= -1.2254 YY= 22.9686 ZY= 2.0221

XZ= -0.0922 YZ= 3.6339 ZZ= 16.7975

Eigenvalues: 15.6970 22.2006 27.1840

48 C Isotropic = 14.6700 Anisotropy = 184.2123

XX= -68.9821 YX= 40.6282 ZX= 6.1357

XY= 30.7980 YY= 113.5831 ZY= -48.6491

XZ= 8.6950 YZ= -52.7399 ZZ= -0.5910

Eigenvalues: -79.8421 -13.6261 137.4782

49 C Isotropic = 47.3866 Anisotropy = 159.7574

XX= 0.4392 YX= 7.1729 ZX= -48.4895

XY= 19.7196 YY= 134.3102 ZY= -44.1940

XZ= -57.2258 YZ= -43.7156 ZZ= 7.4104

Eigenvalues: -51.4533 39.7215 153.8915

50 H Isotropic = 24.0364 Anisotropy = 6.4495

XX= 25.1385 YX= -1.0746 ZX= -2.9451

XY= -0.9811 YY= 22.1229 ZY= 1.0029

XZ= -3.1487 YZ= 0.7483 ZZ= 24.8478

Eigenvalues: 21.7938 21.9793 28.3361

51 C Isotropic = 42.2301 Anisotropy = 189.9325

XX= 31.6804 YX= 29.1131 ZX= 19.3671

XY= 31.4362 YY= 138.6280 ZY= -70.3219

XZ= 12.1966 YZ= -77.4877 ZZ= -43.6180

Eigenvalues: -75.7583 33.5968 168.8517

52 H Isotropic = 23.5245 Anisotropy = 4.9083

XX= 26.7746 YX= -0.2368 ZX= 0.4446

XY= -0.3649 YY= 20.9421 ZY= 0.8183

XZ= -0.0715 YZ= 0.1761 ZZ= 22.8568

Eigenvalues: 20.8017 22.9751 26.7967

53 C Isotropic = 55.1438 Anisotropy = 174.5780

XX= -40.1930 YX= 39.8570 ZX= 12.6447

XY= 37.4422 YY= 150.4523 ZY= -41.8207

XZ= 10.4815 YZ= -42.9648 ZZ= 55.1720

Eigenvalues: -51.5452 45.4474 171.5291

54 H Isotropic = 24.0649 Anisotropy = 3.0300

XX= 25.0085 YX= 0.0133 ZX= 0.4003

XY= -0.0012 YY= 21.6744 ZY= 1.6262

XZ= 0.1637 YZ= 1.3386 ZZ= 25.5117

Eigenvalues: 21.1666 24.9431 26.0849

55 C Isotropic = 43.7498 Anisotropy = 187.4372

XX= -12.0645 YX= 9.2090 ZX= -60.6942

XY= 8.9468 YY= 149.9086 ZY= -48.3943

XZ= -57.1267 YZ= -52.7127 ZZ= -6.5946

Eigenvalues: -72.1834 34.7249 168.7080

56 H Isotropic = 23.5956 Anisotropy = 4.7718

XX= 25.8867 YX= -0.8589 ZX= -1.5869

XY= -0.8965 YY= 21.5427 ZY= 1.5671

XZ= -0.9560 YZ= 1.2177 ZZ= 23.3573

Eigenvalues: 20.7818 23.2282 26.7768

57 C Isotropic = 51.7646 Anisotropy = 170.0270

XX= 32.8177 YX= 26.7069 ZX= 11.2293

XY= 20.6781 YY= 138.5929 ZY= -56.4110

XZ= 27.0814 YZ= -76.5624 ZZ= -16.1168

Eigenvalues: -49.2434 39.4213 165.1159

58 H Isotropic = 23.8112 Anisotropy = 8.0066

XX= 28.4596 YX= -0.5045 ZX= 2.1168

XY= -1.3535 YY= 22.5855 ZY= -0.2113

XZ= 2.2870 YZ= 0.0887 ZZ= 20.3884

Eigenvalues: 19.8160 22.4686 29.1489

59 N Isotropic = -6.5509 Anisotropy = 294.4155

XX= -137.5004 YX= -26.3327 ZX= 57.9242

XY= -7.2300 YY= -38.9711 ZY= -67.0115

XZ= 59.8585 YZ= -69.5343 ZZ= 156.8188

Eigenvalues: -148.9811 -60.3978 189.7260

60 N Isotropic = 26.3775 Anisotropy = 225.2192

XX= -83.4247 YX= 62.5660 ZX= 48.6028

XY= 27.0186 YY= 40.2494 ZY= -53.9538

XZ= 85.6204 YZ= -106.9040 ZZ= 122.3079

Eigenvalues: -131.1396 33.7485 176.5237

61 H Isotropic = 30.5333 Anisotropy = 7.6161

XX= 35.0972 YX= -1.1474 ZX= 0.9162

XY= -1.0354 YY= 29.9705 ZY= 0.1663

XZ= 2.5549 YZ= 0.6796 ZZ= 26.5321

Eigenvalues: 26.0906 29.8985 35.6107

62 H Isotropic = 29.9514 Anisotropy = 8.1312

XX= 27.6659 YX= 0.8815 ZX= 1.1979

XY= 1.1712 YY= 31.6980 ZY= -3.8139

XZ= 1.9889 YZ= -4.6365 ZZ= 30.4902

Eigenvalues: 25.3205 29.1615 35.3721

63 H Isotropic = 29.5250 Anisotropy = 11.0165

XX= 27.0041 YX= 1.6343 ZX= 1.8702

XY= 3.3460 YY= 33.5623 ZY= 2.6252

XZ= 3.5556 YZ= 5.3293 ZZ= 28.0087

Eigenvalues: 24.6687 27.0370 36.8694

64 H Isotropic = 27.2905 Anisotropy = 6.4626

XX= 26.6921 YX= -0.4607 ZX= -1.0422

XY= 1.7522 YY= 30.2565 ZY= 2.8152

XZ= -0.3497 YZ= 3.1197 ZZ= 24.9231

Eigenvalues: 23.3572 26.9155 31.5989

## BETAINE monomer\_iso2 (gas-phase) - BP86/IGLO-III level

32

C 3.74540 -0.60622 0.35301

C 4.48918 0.31833 1.30253

C 4.53810 -0.92755 -0.90306

H 3.95698 -1.55493 -1.57608

H 5.44696 -1.46037 -0.62807

H 4.82519 -0.02100 -1.43227

C 2.38403 1.14974 -0.66779

H 3.32134 1.62088 -0.90636

C 1.12927 1.66740 -0.99963

H 1.09043 2.60023 -1.54550

C -0.03348 1.01934 -0.65453

H -0.98953 1.43737 -0.93707

C -0.00219 -0.24149 0.06199

C 1.32044 -0.70451 0.35227

H 1.46335 -1.64116 0.87116

C -2.30381 -0.52870 0.24777

C -3.23959 -1.31441 -0.44077

H -2.90640 -2.25463 -0.86019

C -4.56066 -0.89839 -0.58057

H -5.26206 -1.51982 -1.12197

C -4.98440 0.30711 -0.02194

H -6.01215 0.62676 -0.12505

C -4.07076 1.08940 0.68378

H -4.38981 2.01852 1.13841

C -2.74762 0.67698 0.81802

H -2.04599 1.27601 1.38590

N 2.42756 -0.03002 -0.00197

N -1.00463 -1.00790 0.42121

H 5.39630 -0.17528 1.64754

H 3.87388 0.55963 2.16715

H 4.77617 1.24478 0.80911

H 3.51132 -1.53372 0.87210

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 111.1637 Anisotropy = 63.2302

XX= 134.4099 YX= -27.6505 ZX= 16.8932

XY= -20.7749 YY= 105.1584 ZY= -9.9437

XZ= 12.4405 YZ= -9.8877 ZZ= 93.9227

Eigenvalues: 88.1233 92.0505 153.3171

2 C Isotropic = 156.0738 Anisotropy = 37.2623

XX= 151.9014 YX= 5.9321 ZX= 12.3743

XY= 6.7273 YY= 153.6829 ZY= 18.3649

XZ= 10.0167 YZ= 14.7421 ZZ= 162.6372

Eigenvalues: 140.5393 146.7668 180.9154

3 C Isotropic = 156.1942 Anisotropy = 37.0440

XX= 153.2621 YX= -7.9191 ZX= -12.0317

XY= -5.7806 YY= 145.6264 ZY= 8.9744

XZ= -12.3356 YZ= 12.9458 ZZ= 169.6942

Eigenvalues: 140.7923 146.9001 180.8902

4 H Isotropic = 30.2516 Anisotropy = 8.4462

XX= 28.5939 YX= 0.6758 ZX= 0.0600

XY= 1.0176 YY= 30.0799 ZY= 4.0056

XZ= 0.7579 YZ= 5.1845 ZZ= 32.0809

Eigenvalues: 26.3044 28.5679 35.8824

5 H Isotropic = 30.4517 Anisotropy = 9.2915

XX= 33.6101 YX= -4.4873 ZX= -0.1186

XY= -4.4497 YY= 29.6258 ZY= 0.7058

XZ= -1.2614 YZ= 1.1129 ZZ= 28.1190

Eigenvalues: 26.6173 28.0917 36.6460

6 H Isotropic = 30.2552 Anisotropy = 5.9178

XX= 29.5634 YX= 0.8505 ZX= -2.5306

XY= -0.1973 YY= 30.3954 ZY= -1.5629

XZ= -3.2184 YZ= -2.9700 ZZ= 30.8069

Eigenvalues: 26.7880 29.7772 34.2005

7 C Isotropic = 68.9130 Anisotropy = 111.4626

XX= 23.2181 YX= -29.0823 ZX= 12.4777

XY= -29.5458 YY= 68.4200 ZY= 42.1318

XZ= 19.5221 YZ= 49.5371 ZZ= 115.1010

Eigenvalues: -2.6738 66.1914 143.2214

8 H Isotropic = 25.6391 Anisotropy = 7.6629

XX= 25.2015 YX= -3.4688 ZX= 2.1251

XY= -1.8101 YY= 27.6655 ZY= -2.8617

XZ= 1.4103 YZ= -2.1494 ZZ= 24.0503

Eigenvalues: 22.6299 23.5397 30.7477

9 C Isotropic = 48.0345 Anisotropy = 167.4397

XX= 42.6721 YX= 8.6753 ZX= -8.9641

XY= 12.7481 YY= -1.4623 ZY= 94.2000

XZ= -16.7856 YZ= 96.4548 ZZ= 102.8936

Eigenvalues: -60.3770 44.8195 159.6609

10 H Isotropic = 25.1550 Anisotropy = 4.4850

XX= 28.0756 YX= 0.5196 ZX= -0.1019

XY= 0.0394 YY= 23.7641 ZY= -0.2091

XZ= -0.8086 YZ= -0.5941 ZZ= 23.6253

Eigenvalues: 23.2808 24.0391 28.1450

11 C Isotropic = 50.9402 Anisotropy = 175.3394

XX= -22.3921 YX= 17.0229 ZX= -13.6578

XY= 11.0434 YY= 35.7902 ZY= 71.2264

XZ= -46.4047 YZ= 44.5758 ZZ= 139.4224

Eigenvalues: -37.8626 22.8500 167.8331

12 H Isotropic = 24.3360 Anisotropy = 10.9280

XX= 26.5184 YX= 4.1049 ZX= -3.5377

XY= 4.0673 YY= 25.7655 ZY= -1.5876

XZ= -5.5660 YZ= 0.4711 ZZ= 20.7241

Eigenvalues: 17.8922 23.4945 31.6213

13 C Isotropic = 20.9320 Anisotropy = 139.1622

XX= -31.4512 YX= 25.8591 ZX= -16.2506

XY= 5.1558 YY= 13.8256 ZY= 60.2426

XZ= -10.9305 YZ= 54.8120 ZZ= 80.4214

Eigenvalues: -46.5729 -4.3380 113.7067

14 C Isotropic = 38.6042 Anisotropy = 83.5356

XX= 48.0044 YX= 2.0208 ZX= -1.3322

XY= -4.6971 YY= 11.7338 ZY= 46.0162

XZ= 6.5222 YZ= 66.2412 ZZ= 56.0743

Eigenvalues: -26.5329 48.0508 94.2946

15 H Isotropic = 24.8184 Anisotropy = 7.9878

XX= 29.6789 YX= 1.6306 ZX= -0.5336

XY= 2.1416 YY= 22.4606 ZY= 0.6024

XZ= -0.1336 YZ= 1.2057 ZZ= 22.3156

Eigenvalues: 21.1853 23.1262 30.1435

16 C Isotropic = 16.3369 Anisotropy = 171.7186

XX= -57.6284 YX= 28.7233 ZX= -28.6796

XY= 33.7718 YY= 17.4111 ZY= -55.6382

XZ= -44.1725 YZ= -54.5729 ZZ= 89.2279

Eigenvalues: -70.9584 -10.8469 130.8160

17 C Isotropic = 50.0719 Anisotropy = 155.7337

XX= 37.9681 YX= 31.9817 ZX= -17.5597

XY= 29.5025 YY= 2.2715 ZY= -75.1335

XZ= -1.4975 YZ= -77.1480 ZZ= 109.9762

Eigenvalues: -43.7787 40.1001 153.8944

18 H Isotropic = 24.7014 Anisotropy = 6.1928

XX= 28.0346 YX= 1.0539 ZX= 1.8952

XY= 0.9812 YY= 23.5524 ZY= 0.5029

XZ= 1.8154 YZ= 0.3678 ZZ= 22.5174

Eigenvalues: 21.9415 23.3329 28.8300

19 C Isotropic = 43.7471 Anisotropy = 183.3068

XX= 0.9862 YX= -24.0819 ZX= -60.2689

XY= -23.8990 YY= 31.4625 ZY= -81.9006

XZ= -58.1110 YZ= -90.4372 ZZ= 98.7928

Eigenvalues: -70.3488 35.6386 165.9517

20 H Isotropic = 24.1758 Anisotropy = 4.8559

XX= 25.8346 YX= -2.0004 ZX= -0.1035

XY= -1.9332 YY= 24.7520 ZY= 1.1309

XZ= -0.3016 YZ= 0.5050 ZZ= 21.9409

Eigenvalues: 21.6866 23.4278 27.4131

21 C Isotropic = 54.6315 Anisotropy = 170.9208

XX= -33.0457 YX= 40.5486 ZX= -33.4276

XY= 43.3868 YY= 65.8890 ZY= -46.6423

XZ= -32.5440 YZ= -49.5138 ZZ= 131.0513

Eigenvalues: -49.7750 45.0908 168.5787

22 H Isotropic = 24.7089 Anisotropy = 3.8696

XX= 24.7084 YX= 0.3160 ZX= 0.7769

XY= 0.4148 YY= 25.8567 ZY= 2.2238

XZ= 0.8439 YZ= 1.9252 ZZ= 23.5615

Eigenvalues: 22.2276 24.6103 27.2886

23 C Isotropic = 46.0765 Anisotropy = 179.5969

XX= 37.0407 YX= 41.7750 ZX= -12.4226

XY= 39.3885 YY= -7.0018 ZY= -88.5563

XZ= -15.5721 YZ= -92.1090 ZZ= 108.1906

Eigenvalues: -65.0693 37.4911 165.8078

24 H Isotropic = 24.3858 Anisotropy = 4.9673

XX= 27.3969 YX= 0.2692 ZX= 1.4843

XY= 0.0249 YY= 23.0641 ZY= 0.8408

XZ= 0.8501 YZ= 0.9330 ZZ= 22.6965

Eigenvalues: 21.8471 23.6131 27.6974

25 C Isotropic = 58.1143 Anisotropy = 158.6413

XX= 15.8189 YX= -9.4127 ZX= -43.6296

XY= -20.4616 YY= 46.4037 ZY= -64.1746

XZ= -66.3104 YZ= -67.4988 ZZ= 112.1203

Eigenvalues: -34.9111 45.3788 163.8751

26 H Isotropic = 24.5646 Anisotropy = 7.9455

XX= 27.8182 YX= -3.5004 ZX= -1.8579

XY= -2.5635 YY= 23.6561 ZY= 0.6096

XZ= -1.4230 YZ= 1.0938 ZZ= 22.2195

Eigenvalues: 21.7721 22.0601 29.8616

27 N Isotropic = 7.3136 Anisotropy = 260.7754

XX= -102.8288 YX= 37.1039 ZX= -28.5922

XY= 20.3000 YY= 5.3935 ZY= 99.6974

XZ= -23.9267 YZ= 108.2086 ZZ= 119.3760

Eigenvalues: -124.3122 -34.9109 181.1639

28 N Isotropic = -10.1593 Anisotropy = 278.1063

XX= -189.1047 YX= -8.2076 ZX= 9.2081

XY= -36.9625 YY= 5.2931 ZY= 66.3257

XZ= -94.2232 YZ= 35.3116 ZZ= 153.3336

Eigenvalues: -195.6708 -10.0521 175.2449

29 H Isotropic = 30.4169 Anisotropy = 9.1621

XX= 33.3318 YX= -2.0511 ZX= 4.0517

XY= -1.1630 YY= 27.6988 ZY= -0.0395

XZ= 4.4189 YZ= -0.3920 ZZ= 30.2201

Eigenvalues: 26.6229 28.1028 36.5249

30 H Isotropic = 30.1393 Anisotropy = 8.4183

XX= 28.5181 YX= 0.3031 ZX= -0.8844

XY= -0.2214 YY= 27.4787 ZY= 3.6197

XZ= -1.6808 YZ= 2.4362 ZZ= 34.4211

Eigenvalues: 26.2319 28.4345 35.7515

31 H Isotropic = 30.2557 Anisotropy = 5.9180

XX= 29.3174 YX= 2.6029 ZX= 0.6745

XY= 2.5548 YY= 32.8364 ZY= -1.4278

XZ= 1.6834 YZ= -0.0616 ZZ= 28.6134

Eigenvalues: 26.8548 29.7113 34.2010

32 H Isotropic = 27.8927 Anisotropy = 3.9692

XX= 28.3997 YX= 0.0718 ZX= 0.1245

XY= 1.8730 YY= 28.9570 ZY= -1.9863

XZ= -1.1719 YZ= -1.8556 ZZ= 26.3213

Eigenvalues: 25.3096 27.8295 30.5388

## BETAINE monomer\_iso2 (gas-phase) – PBE0/IGLO-III level

32

C 3.74540 -0.60622 0.35301

C 4.48918 0.31833 1.30253

C 4.53810 -0.92755 -0.90306

H 3.95698 -1.55493 -1.57608

H 5.44696 -1.46037 -0.62807

H 4.82519 -0.02100 -1.43227

C 2.38403 1.14974 -0.66779

H 3.32134 1.62088 -0.90636

C 1.12927 1.66740 -0.99963

H 1.09043 2.60023 -1.54550

C -0.03348 1.01934 -0.65453

H -0.98953 1.43737 -0.93707

C -0.00219 -0.24149 0.06199

C 1.32044 -0.70451 0.35227

H 1.46335 -1.64116 0.87116

C -2.30381 -0.52870 0.24777

C -3.23959 -1.31441 -0.44077

H -2.90640 -2.25463 -0.86019

C -4.56066 -0.89839 -0.58057

H -5.26206 -1.51982 -1.12197

C -4.98440 0.30711 -0.02194

H -6.01215 0.62676 -0.12505

C -4.07076 1.08940 0.68378

H -4.38981 2.01852 1.13841

C -2.74762 0.67698 0.81802

H -2.04599 1.27601 1.38590

N 2.42756 -0.03002 -0.00197

N -1.00463 -1.00790 0.42121

H 5.39630 -0.17528 1.64754

H 3.87388 0.55963 2.16715

H 4.77617 1.24478 0.80911

H 3.51132 -1.53372 0.87210

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 118.4769 Anisotropy = 62.2239

XX= 141.3534 YX= -27.3325 ZX= 16.6715

XY= -20.4073 YY= 112.5138 ZY= -9.6563

XZ= 12.2388 YZ= -9.5911 ZZ= 101.5635

Eigenvalues: 95.9427 99.5286 159.9595

2 C Isotropic = 161.1736 Anisotropy = 35.6633

XX= 157.5924 YX= 5.2473 ZX= 12.0149

XY= 6.5407 YY= 158.7217 ZY= 17.7258

XZ= 10.2920 YZ= 13.7626 ZZ= 167.2065

Eigenvalues: 146.0182 152.5534 184.9491

3 C Isotropic = 161.2643 Anisotropy = 35.5181

XX= 158.8594 YX= -7.9429 ZX= -11.2438

XY= -6.0237 YY= 150.9802 ZY= 8.3216

XZ= -12.1815 YZ= 12.5290 ZZ= 173.9533

Eigenvalues: 146.1992 152.6507 184.9430

4 H Isotropic = 30.2226 Anisotropy = 8.8389

XX= 28.5679 YX= 0.8460 ZX= 0.2630

XY= 1.0418 YY= 30.0688 ZY= 4.1949

XZ= 0.6576 YZ= 5.4972 ZZ= 32.0310

Eigenvalues: 26.0268 28.5258 36.1151

5 H Isotropic = 30.4246 Anisotropy = 9.9076

XX= 33.8614 YX= -4.7480 ZX= -0.0665

XY= -4.7447 YY= 29.5619 ZY= 0.6287

XZ= -1.2237 YZ= 1.0348 ZZ= 27.8505

Eigenvalues: 26.4105 27.8336 37.0297

6 H Isotropic = 30.2386 Anisotropy = 6.4644

XX= 29.4111 YX= 0.9783 ZX= -2.6348

XY= -0.0725 YY= 30.5516 ZY= -1.8527

XZ= -3.4862 YZ= -3.1940 ZZ= 30.7530

Eigenvalues: 26.4922 29.6754 34.5482

7 C Isotropic = 71.0662 Anisotropy = 118.7912

XX= 22.0177 YX= -30.9744 ZX= 13.3905

XY= -31.0304 YY= 70.3031 ZY= 44.9225

XZ= 19.9664 YZ= 51.9549 ZZ= 120.8777

Eigenvalues: -4.9398 67.8780 150.2603

8 H Isotropic = 25.4571 Anisotropy = 7.9993

XX= 25.2159 YX= -3.4366 ZX= 2.1111

XY= -1.7059 YY= 27.5824 ZY= -3.1952

XZ= 1.3166 YZ= -2.5786 ZZ= 23.5731

Eigenvalues: 22.0061 23.5752 30.7900

9 C Isotropic = 50.1707 Anisotropy = 175.4859

XX= 44.2329 YX= 9.2767 ZX= -9.3260

XY= 13.6771 YY= -1.4814 ZY= 98.6747

XZ= -16.7858 YZ= 100.9583 ZZ= 107.7607

Eigenvalues: -63.1909 46.5417 167.1613

10 H Isotropic = 24.9049 Anisotropy = 4.7388

XX= 27.9913 YX= 0.6208 ZX= -0.1592

XY= 0.0210 YY= 23.6048 ZY= -0.4676

XZ= -0.7257 YZ= -0.8757 ZZ= 23.1186

Eigenvalues: 22.6413 24.0093 28.0642

11 C Isotropic = 53.7573 Anisotropy = 180.1518

XX= -20.3676 YX= 17.7861 ZX= -14.2341

XY= 12.5964 YY= 38.6353 ZY= 73.8643

XZ= -46.2664 YZ= 49.2580 ZZ= 143.0042

Eigenvalues: -37.3013 24.7147 173.8585

12 H Isotropic = 24.1894 Anisotropy = 11.5679

XX= 26.6752 YX= 4.1686 ZX= -3.5523

XY= 4.2528 YY= 25.5682 ZY= -1.8388

XZ= -5.7013 YZ= -0.0856 ZZ= 20.3248

Eigenvalues: 17.6942 22.9727 31.9013

13 C Isotropic = 21.1930 Anisotropy = 152.5961

XX= -36.9775 YX= 29.2283 ZX= -18.5515

XY= 6.7888 YY= 14.3974 ZY= 64.8717

XZ= -13.4574 YZ= 61.1223 ZZ= 86.1591

Eigenvalues: -54.4212 -4.9236 122.9238

14 C Isotropic = 41.2520 Anisotropy = 92.2383

XX= 48.1417 YX= 2.0183 ZX= -1.4594

XY= -4.6757 YY= 12.1685 ZY= 50.5938

XZ= 5.8342 YZ= 68.6811 ZZ= 63.4458

Eigenvalues: -27.1790 48.1908 102.7442

15 H Isotropic = 24.4944 Anisotropy = 8.5291

XX= 29.6510 YX= 1.8007 ZX= -0.6230

XY= 2.2599 YY= 22.2177 ZY= 0.2566

XZ= -0.2893 YZ= 0.8274 ZZ= 21.6147

Eigenvalues: 21.0120 22.2908 30.1805

16 C Isotropic = 18.4926 Anisotropy = 180.9596

XX= -60.6919 YX= 31.2740 ZX= -31.0416

XY= 36.7377 YY= 20.2725 ZY= -57.8552

XZ= -45.6287 YZ= -56.4885 ZZ= 95.8972

Eigenvalues: -75.1672 -8.4874 139.1324

17 C Isotropic = 52.1975 Anisotropy = 161.8507

XX= 39.5131 YX= 34.2189 ZX= -17.1583

XY= 31.6936 YY= 3.0817 ZY= -77.4019

XZ= -2.9508 YZ= -80.7992 ZZ= 113.9977

Eigenvalues: -45.4389 41.9335 160.0979

18 H Isotropic = 24.5347 Anisotropy = 6.4945

XX= 27.9925 YX= 1.0228 ZX= 2.0125

XY= 0.9057 YY= 23.4699 ZY= 0.6780

XZ= 2.0691 YZ= 0.6120 ZZ= 22.1416

Eigenvalues: 21.4427 23.2969 28.8644

19 C Isotropic = 45.8528 Anisotropy = 190.0700

XX= 0.9406 YX= -25.0549 ZX= -62.7345

XY= -24.5032 YY= 32.7589 ZY= -85.0683

XZ= -60.0600 YZ= -92.2573 ZZ= 103.8589

Eigenvalues: -72.0855 37.0778 172.5661

20 H Isotropic = 24.0463 Anisotropy = 5.0157

XX= 25.8059 YX= -2.0468 ZX= -0.0299

XY= -1.9335 YY= 24.6606 ZY= 1.2784

XZ= -0.1790 YZ= 0.7488 ZZ= 21.6725

Eigenvalues: 21.2940 23.4549 27.3901

21 C Isotropic = 57.4240 Anisotropy = 176.7104

XX= -33.4646 YX= 41.8401 ZX= -34.6882

XY= 44.2437 YY= 68.9836 ZY= -48.4398

XZ= -33.7136 YZ= -50.6050 ZZ= 136.7531

Eigenvalues: -50.5677 47.6089 175.2310

22 H Isotropic = 24.5980 Anisotropy = 4.0174

XX= 24.7937 YX= 0.2326 ZX= 0.8712

XY= 0.3072 YY= 25.7724 ZY= 2.3824

XZ= 0.8925 YZ= 2.1195 ZZ= 23.2280

Eigenvalues: 21.7808 24.7369 27.2763

23 C Isotropic = 48.1074 Anisotropy = 186.4936

XX= 38.4070 YX= 43.6697 ZX= -12.7014

XY= 41.2116 YY= -6.4231 ZY= -91.8554

XZ= -15.8752 YZ= -95.9663 ZZ= 112.3383

Eigenvalues: -67.2358 39.1216 172.4365

24 H Isotropic = 24.2379 Anisotropy = 5.1475

XX= 27.3518 YX= 0.2184 ZX= 1.5553

XY= -0.0284 YY= 22.9945 ZY= 1.0094

XZ= 0.9327 YZ= 1.0835 ZZ= 22.3675

Eigenvalues: 21.4314 23.6128 27.6696

25 C Isotropic = 59.1090 Anisotropy = 165.8289

XX= 15.3161 YX= -10.1427 ZX= -45.8191

XY= -20.2982 YY= 48.2534 ZY= -67.4585

XZ= -69.9895 YZ= -72.0009 ZZ= 113.7576

Eigenvalues: -38.4929 46.1584 169.6616

26 H Isotropic = 24.4003 Anisotropy = 8.3848

XX= 27.7897 YX= -3.6479 ZX= -1.8174

XY= -2.7198 YY= 23.5371 ZY= 0.8173

XZ= -1.6263 YZ= 1.2706 ZZ= 21.8741

Eigenvalues: 21.3529 21.8578 29.9902

27 N Isotropic = 6.1094 Anisotropy = 281.4110

XX= -114.2350 YX= 40.1826 ZX= -30.8684

XY= 23.9556 YY= 4.3726 ZY= 107.3722

XZ= -24.7768 YZ= 114.9461 ZZ= 128.1905

Eigenvalues: -137.2552 -38.1334 193.7167

28 N Isotropic = 3.4314 Anisotropy = 277.1223

XX= -175.5392 YX= -2.6026 ZX= 6.7286

XY= -26.3343 YY= 19.2628 ZY= 65.9449

XZ= -91.8455 YZ= 36.4876 ZZ= 166.5707

Eigenvalues: -181.0975 3.2121 188.1796

29 H Isotropic = 30.3917 Anisotropy = 9.7945

XX= 33.5812 YX= -2.2239 ZX= 4.2636

XY= -1.3368 YY= 27.5557 ZY= -0.1546

XZ= 4.6931 YZ= -0.5110 ZZ= 30.0381

Eigenvalues: 26.3998 27.8540 36.9214

30 H Isotropic = 30.1240 Anisotropy = 8.7999

XX= 28.5182 YX= 0.2095 ZX= -1.1404

XY= -0.1595 YY= 27.2448 ZY= 3.7859

XZ= -1.6376 YZ= 2.4924 ZZ= 34.6089

Eigenvalues: 25.9810 28.4003 35.9905

31 H Isotropic = 30.2347 Anisotropy = 6.4783

XX= 29.1692 YX= 2.7497 ZX= 0.6200

XY= 2.8421 YY= 33.0823 ZY= -1.6010

XZ= 1.7221 YZ= -0.2894 ZZ= 28.4526

Eigenvalues: 26.5579 29.5927 34.5536

32 H Isotropic = 27.8513 Anisotropy = 4.6195

XX= 28.3153 YX= 0.0979 ZX= 0.1094

XY= 1.9882 YY= 29.1776 ZY= -2.3621

XZ= -1.1972 YZ= -2.2487 ZZ= 26.0612

Eigenvalues: 24.8367 27.7863 30.9310

## BETAINE monomer\_iso2 (IEFPCM solvent = tetrahydrofuran) – BP86/IGLO-III level

32

C 3.74540 -0.60622 0.35301

C 4.48918 0.31833 1.30253

C 4.53810 -0.92755 -0.90306

H 3.95698 -1.55493 -1.57608

H 5.44696 -1.46037 -0.62807

H 4.82519 -0.02100 -1.43227

C 2.38403 1.14974 -0.66779

H 3.32134 1.62088 -0.90636

C 1.12927 1.66740 -0.99963

H 1.09043 2.60023 -1.54550

C -0.03348 1.01934 -0.65453

H -0.98953 1.43737 -0.93707

C -0.00219 -0.24149 0.06199

C 1.32044 -0.70451 0.35227

H 1.46335 -1.64116 0.87116

C -2.30381 -0.52870 0.24777

C -3.23959 -1.31441 -0.44077

H -2.90640 -2.25463 -0.86019

C -4.56066 -0.89839 -0.58057

H -5.26206 -1.51982 -1.12197

C -4.98440 0.30711 -0.02194

H -6.01215 0.62676 -0.12505

C -4.07076 1.08940 0.68378

H -4.38981 2.01852 1.13841

C -2.74762 0.67698 0.81802

H -2.04599 1.27601 1.38590

N 2.42756 -0.03002 -0.00197

N -1.00463 -1.00790 0.42121

H 5.39630 -0.17528 1.64754

H 3.87388 0.55963 2.16715

H 4.77617 1.24478 0.80911

H 3.51132 -1.53372 0.87210

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 110.3039 Anisotropy = 64.8081

XX= 133.7162 YX= -28.6018 ZX= 17.3731

XY= -22.2881 YY= 103.6540 ZY= -9.0483

XZ= 13.2961 YZ= -8.9509 ZZ= 93.5413

Eigenvalues: 88.2233 89.1790 153.5092

2 C Isotropic = 156.0192 Anisotropy = 37.2827

XX= 152.1873 YX= 5.8185 ZX= 12.7238

XY= 7.1547 YY= 153.8487 ZY= 17.8636

XZ= 11.6608 YZ= 14.0078 ZZ= 162.0217

Eigenvalues: 140.5828 146.6005 180.8744

3 C Isotropic = 156.1161 Anisotropy = 37.1355

XX= 153.5348 YX= -8.2521 ZX= -12.1216

XY= -6.8309 YY= 145.7273 ZY= 8.2263

XZ= -13.4626 YZ= 12.4158 ZZ= 169.0863

Eigenvalues: 140.7774 146.6978 180.8731

4 H Isotropic = 30.2661 Anisotropy = 8.4041

XX= 28.6280 YX= 0.7081 ZX= 0.0216

XY= 0.8614 YY= 30.1390 ZY= 3.9654

XZ= 0.4387 YZ= 5.2843 ZZ= 32.0314

Eigenvalues: 26.2719 28.6577 35.8689

5 H Isotropic = 30.2798 Anisotropy = 9.5044

XX= 33.5308 YX= -4.5180 ZX= -0.1033

XY= -4.5871 YY= 29.4802 ZY= 0.6258

XZ= -1.3170 YZ= 1.0759 ZZ= 27.8283

Eigenvalues: 26.4392 27.7841 36.6160

6 H Isotropic = 30.2023 Anisotropy = 6.1152

XX= 29.4633 YX= 0.9551 ZX= -2.5027

XY= -0.1512 YY= 30.3833 ZY= -1.6176

XZ= -3.4086 YZ= -3.0211 ZZ= 30.7602

Eigenvalues: 26.6617 29.6661 34.2791

7 C Isotropic = 63.3184 Anisotropy = 123.8624

XX= 14.9040 YX= -29.0759 ZX= 12.2848

XY= -30.0565 YY= 60.2230 ZY= 48.2307

XZ= 18.3745 YZ= 54.8626 ZZ= 114.8284

Eigenvalues: -11.9640 56.0260 145.8934

8 H Isotropic = 25.0422 Anisotropy = 7.8963

XX= 24.8586 YX= -3.5151 ZX= 2.1413

XY= -1.8929 YY= 26.9784 ZY= -2.9730

XZ= 1.4355 YZ= -2.3983 ZZ= 23.2895

Eigenvalues: 21.8050 23.0151 30.3064

9 C Isotropic = 47.1854 Anisotropy = 173.2160

XX= 38.7951 YX= 7.4429 ZX= -8.2934

XY= 10.7994 YY= -2.2005 ZY= 96.2388

XZ= -14.9369 YZ= 98.2949 ZZ= 104.9618

Eigenvalues: -61.5574 40.4510 162.6628

10 H Isotropic = 24.8142 Anisotropy = 4.6515

XX= 27.8368 YX= 0.5585 ZX= -0.1294

XY= 0.1332 YY= 23.5245 ZY= -0.4293

XZ= -0.7585 YZ= -0.8095 ZZ= 23.0813

Eigenvalues: 22.6397 23.8877 27.9152

11 C Isotropic = 54.0827 Anisotropy = 171.6710

XX= -19.0663 YX= 17.8560 ZX= -14.1525

XY= 10.9298 YY= 40.7279 ZY= 68.7532

XZ= -38.3383 YZ= 46.1827 ZZ= 140.5863

Eigenvalues: -32.8210 26.5390 168.5300

12 H Isotropic = 24.3645 Anisotropy = 10.7376

XX= 26.6060 YX= 3.8951 ZX= -3.3629

XY= 3.9898 YY= 25.6897 ZY= -1.7287

XZ= -5.1009 YZ= -0.1855 ZZ= 20.7977

Eigenvalues: 18.4005 23.1701 31.5229

13 C Isotropic = 20.2011 Anisotropy = 146.3895

XX= -35.7628 YX= 18.4049 ZX= -11.7371

XY= 0.8702 YY= 13.7433 ZY= 62.4165

XZ= -10.4551 YZ= 58.2305 ZZ= 82.6227

Eigenvalues: -44.3019 -12.8890 117.7940

14 C Isotropic = 38.3217 Anisotropy = 88.8112

XX= 45.2780 YX= -0.8310 ZX= 0.1950

XY= -5.3460 YY= 9.6320 ZY= 49.0781

XZ= 6.6614 YZ= 65.6478 ZZ= 60.0550

Eigenvalues: -28.0865 45.5224 97.5291

15 H Isotropic = 24.4890 Anisotropy = 8.2450

XX= 29.6214 YX= 1.3929 ZX= -0.3998

XY= 1.9666 YY= 22.1179 ZY= 0.3908

XZ= -0.3106 YZ= 0.9325 ZZ= 21.7276

Eigenvalues: 21.0194 22.4619 29.9856

16 C Isotropic = 15.4013 Anisotropy = 173.7682

XX= -58.1037 YX= 27.8211 ZX= -29.8342

XY= 33.7630 YY= 15.3753 ZY= -57.5473

XZ= -43.4380 YZ= -55.5222 ZZ= 88.9322

Eigenvalues: -71.2666 -13.7763 131.2468

17 C Isotropic = 50.5629 Anisotropy = 152.8832

XX= 39.0698 YX= 34.4831 ZX= -14.9290

XY= 29.3826 YY= 4.7019 ZY= -72.6984

XZ= 0.9928 YZ= -79.9190 ZZ= 107.9169

Eigenvalues: -43.5559 42.7595 152.4850

18 H Isotropic = 24.6811 Anisotropy = 6.2077

XX= 27.9466 YX= 1.1520 ZX= 1.9293

XY= 0.8904 YY= 23.5263 ZY= 0.3984

XZ= 2.0315 YZ= 0.3330 ZZ= 22.5703

Eigenvalues: 21.9190 23.3047 28.8195

19 C Isotropic = 43.7549 Anisotropy = 184.4750

XX= 0.6064 YX= -23.1212 ZX= -60.2898

XY= -23.5327 YY= 31.9728 ZY= -81.9502

XZ= -58.3515 YZ= -91.7191 ZZ= 98.6856

Eigenvalues: -70.3548 34.8813 166.7383

20 H Isotropic = 24.0792 Anisotropy = 4.8199

XX= 25.7902 YX= -1.9627 ZX= -0.0477

XY= -1.8610 YY= 24.6694 ZY= 1.1500

XZ= -0.2917 YZ= 0.4619 ZZ= 21.7781

Eigenvalues: 21.5371 23.4081 27.2925

21 C Isotropic = 55.5829 Anisotropy = 170.8245

XX= -31.8241 YX= 40.0773 ZX= -33.6303

XY= 42.7396 YY= 66.5986 ZY= -47.0335

XZ= -32.7059 YZ= -49.2592 ZZ= 131.9741

Eigenvalues: -48.3089 45.5917 169.4659

22 H Isotropic = 24.6311 Anisotropy = 3.7751

XX= 24.6866 YX= 0.2513 ZX= 0.7759

XY= 0.3488 YY= 25.7742 ZY= 2.2048

XZ= 0.8337 YZ= 1.8958 ZZ= 23.4327

Eigenvalues: 22.1221 24.6234 27.1479

23 C Isotropic = 45.4939 Anisotropy = 181.7578

XX= 35.7442 YX= 41.3455 ZX= -13.1693

XY= 39.5894 YY= -7.0608 ZY= -89.3980

XZ= -16.7869 YZ= -93.3242 ZZ= 107.7984

Eigenvalues: -65.7507 35.5667 166.6658

24 H Isotropic = 24.2420 Anisotropy = 4.9626

XX= 27.2560 YX= 0.2403 ZX= 1.4901

XY= 0.0228 YY= 22.9591 ZY= 0.8394

XZ= 0.8408 YZ= 0.8976 ZZ= 22.5110

Eigenvalues: 21.7024 23.4733 27.5504

25 C Isotropic = 55.5618 Anisotropy = 162.5004

XX= 12.8326 YX= -9.1150 ZX= -44.7026

XY= -18.6655 YY= 45.2749 ZY= -65.3958

XZ= -69.8534 YZ= -70.7193 ZZ= 108.5779

Eigenvalues: -39.5265 42.3164 163.8954

26 H Isotropic = 24.3427 Anisotropy = 8.2936

XX= 27.5912 YX= -3.6301 ZX= -1.9568

XY= -2.6842 YY= 23.5033 ZY= 0.6379

XZ= -1.9441 YZ= 1.0400 ZZ= 21.9336

Eigenvalues: 21.2978 21.8585 29.8718

27 N Isotropic = 0.9332 Anisotropy = 275.6207

XX= -113.0740 YX= 31.4907 ZX= -25.5468

XY= 17.5542 YY= -3.8668 ZY= 106.7533

XZ= -21.4423 YZ= 114.0708 ZZ= 119.7405

Eigenvalues: -130.8131 -51.0676 184.6804

28 N Isotropic = 13.4760 Anisotropy = 240.1935

XX= -136.9400 YX= -6.3261 ZX= 7.4435

XY= -26.9011 YY= 21.9055 ZY= 55.7614

XZ= -93.1862 YZ= 25.5240 ZZ= 155.4625

Eigenvalues: -143.8084 10.6314 173.6050

29 H Isotropic = 30.2495 Anisotropy = 9.3900

XX= 33.2582 YX= -2.0819 ZX= 4.0728

XY= -1.1823 YY= 27.5021 ZY= -0.1061

XZ= 4.5889 YZ= -0.5096 ZZ= 29.9880

Eigenvalues: 26.4420 27.7970 36.5094

30 H Isotropic = 30.1639 Anisotropy = 8.3610

XX= 28.5606 YX= 0.3463 ZX= -0.8940

XY= -0.0389 YY= 27.4389 ZY= 3.6650

XZ= -1.3636 YZ= 2.3365 ZZ= 34.4923

Eigenvalues: 26.2080 28.5459 35.7379

31 H Isotropic = 30.2126 Anisotropy = 6.1134

XX= 29.2285 YX= 2.6246 ZX= 0.5596

XY= 2.7380 YY= 32.8627 ZY= -1.4503

XZ= 1.7509 YZ= -0.0930 ZZ= 28.5467

Eigenvalues: 26.7449 29.6048 34.2882

32 H Isotropic = 27.6048 Anisotropy = 4.1772

XX= 28.2264 YX= 0.0109 ZX= 0.1552

XY= 1.9107 YY= 28.7213 ZY= -2.1638

XZ= -1.1829 YZ= -2.0546 ZZ= 25.8667

Eigenvalues: 24.7472 27.6776 30.3896

## BETAINE monomer\_iso2 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level

32

C 3.74540 -0.60622 0.35301

C 4.48918 0.31833 1.30253

C 4.53810 -0.92755 -0.90306

H 3.95698 -1.55493 -1.57608

H 5.44696 -1.46037 -0.62807

H 4.82519 -0.02100 -1.43227

C 2.38403 1.14974 -0.66779

H 3.32134 1.62088 -0.90636

C 1.12927 1.66740 -0.99963

H 1.09043 2.60023 -1.54550

C -0.03348 1.01934 -0.65453

H -0.98953 1.43737 -0.93707

C -0.00219 -0.24149 0.06199

C 1.32044 -0.70451 0.35227

H 1.46335 -1.64116 0.87116

C -2.30381 -0.52870 0.24777

C -3.23959 -1.31441 -0.44077

H -2.90640 -2.25463 -0.86019

C -4.56066 -0.89839 -0.58057

H -5.26206 -1.51982 -1.12197

C -4.98440 0.30711 -0.02194

H -6.01215 0.62676 -0.12505

C -4.07076 1.08940 0.68378

H -4.38981 2.01852 1.13841

C -2.74762 0.67698 0.81802

H -2.04599 1.27601 1.38590

N 2.42756 -0.03002 -0.00197

N -1.00463 -1.00790 0.42121

H 5.39630 -0.17528 1.64754

H 3.87388 0.55963 2.16715

H 4.77617 1.24478 0.80911

H 3.51132 -1.53372 0.87210

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 117.6238 Anisotropy = 63.9423

XX= 140.7529 YX= -28.3350 ZX= 17.1945

XY= -21.9051 YY= 111.0131 ZY= -8.8276

XZ= 13.0841 YZ= -8.7292 ZZ= 101.1053

Eigenvalues: 95.9084 96.7109 160.2520

2 C Isotropic = 161.2171 Anisotropy = 35.6921

XX= 157.9465 YX= 5.1156 ZX= 12.3174

XY= 6.8625 YY= 158.9600 ZY= 17.3118

XZ= 11.6781 YZ= 13.1653 ZZ= 166.7447

Eigenvalues: 146.0703 152.5691 185.0118

3 C Isotropic = 161.2871 Anisotropy = 35.6061

XX= 159.2074 YX= -8.2477 ZX= -11.2884

XY= -6.9386 YY= 151.1188 ZY= 7.6845

XZ= -13.1131 YZ= 12.0666 ZZ= 173.5352

Eigenvalues: 146.2076 152.6292 185.0246

4 H Isotropic = 30.2488 Anisotropy = 8.8055

XX= 28.6088 YX= 0.8812 ZX= 0.2280

XY= 0.9015 YY= 30.1373 ZY= 4.1609

XZ= 0.3702 YZ= 5.5931 ZZ= 32.0003

Eigenvalues: 26.0067 28.6207 36.1191

5 H Isotropic = 30.2513 Anisotropy = 10.1100

XX= 33.7786 YX= -4.7794 ZX= -0.0449

XY= -4.8727 YY= 29.4082 ZY= 0.5577

XZ= -1.2613 YZ= 1.0011 ZZ= 27.5672

Eigenvalues: 26.2235 27.5392 36.9913

6 H Isotropic = 30.1783 Anisotropy = 6.6601

XX= 29.3019 YX= 1.0854 ZX= -2.6081

XY= -0.0249 YY= 30.5330 ZY= -1.9020

XZ= -3.6661 YZ= -3.2465 ZZ= 30.7001

Eigenvalues: 26.3624 29.5543 34.6184

7 C Isotropic = 65.0385 Anisotropy = 131.4305

XX= 13.3948 YX= -30.8865 ZX= 13.1273

XY= -31.4704 YY= 61.6207 ZY= 51.1521

XZ= 18.9767 YZ= 57.6484 ZZ= 120.1000

Eigenvalues: -14.6383 57.0950 152.6589

8 H Isotropic = 24.8360 Anisotropy = 8.2166

XX= 24.8315 YX= -3.4781 ZX= 2.1290

XY= -1.8044 YY= 26.8787 ZY= -3.2947

XZ= 1.3535 YZ= -2.7881 ZZ= 22.7978

Eigenvalues: 21.1390 23.0553 30.3137

9 C Isotropic = 49.2919 Anisotropy = 181.0114

XX= 40.2004 YX= 7.8449 ZX= -8.5669

XY= 11.3189 YY= -2.0389 ZY= 100.5061

XZ= -14.9408 YZ= 102.6116 ZZ= 109.7141

Eigenvalues: -64.0228 41.9323 169.9662

10 H Isotropic = 24.5605 Anisotropy = 4.8979

XX= 27.7406 YX= 0.6487 ZX= -0.1745

XY= 0.1141 YY= 23.3615 ZY= -0.6861

XZ= -0.7070 YZ= -1.0874 ZZ= 22.5794

Eigenvalues: 21.9967 23.8590 27.8258

11 C Isotropic = 56.4488 Anisotropy = 177.3085

XX= -18.2256 YX= 18.4566 ZX= -14.6773

XY= 11.6033 YY= 43.1768 ZY= 71.5476

XZ= -39.8457 YZ= 50.0192 ZZ= 144.3953

Eigenvalues: -33.1134 27.8053 174.6545

12 H Isotropic = 24.2139 Anisotropy = 11.3463

XX= 26.7110 YX= 3.9727 ZX= -3.3820

XY= 4.1326 YY= 25.5467 ZY= -1.9940

XZ= -5.3040 YZ= -0.6382 ZZ= 20.3841

Eigenvalues: 18.0986 22.7651 31.7781

13 C Isotropic = 20.3919 Anisotropy = 159.4890

XX= -41.2819 YX= 20.1729 ZX= -13.2466

XY= 1.7584 YY= 14.0789 ZY= 66.9993

XZ= -12.1724 YZ= 64.0186 ZZ= 88.3788

Eigenvalues: -50.8585 -14.6836 126.7179

14 C Isotropic = 40.8072 Anisotropy = 97.4100

XX= 45.5189 YX= -0.9088 ZX= 0.1159

XY= -5.5648 YY= 10.1014 ZY= 53.4551

XZ= 5.9528 YZ= 68.5863 ZZ= 66.8012

Eigenvalues: -29.0884 45.7627 105.7472

15 H Isotropic = 24.1821 Anisotropy = 8.7805

XX= 29.6140 YX= 1.5446 ZX= -0.4740

XY= 2.1019 YY= 21.8726 ZY= 0.0691

XZ= -0.3910 YZ= 0.5774 ZZ= 21.0597

Eigenvalues: 20.7953 21.7153 30.0358

16 C Isotropic = 17.4235 Anisotropy = 183.2456

XX= -61.3616 YX= 30.4263 ZX= -32.1294

XY= 36.5529 YY= 18.1578 ZY= -59.7824

XZ= -45.1050 YZ= -57.7401 ZZ= 95.4744

Eigenvalues: -75.6353 -11.6814 139.5872

17 C Isotropic = 52.8768 Anisotropy = 158.8333

XX= 40.8370 YX= 36.4616 ZX= -14.6599

XY= 31.6324 YY= 5.5122 ZY= -75.0249

XZ= -0.8521 YZ= -82.9013 ZZ= 112.2813

Eigenvalues: -44.8315 44.6963 158.7657

18 H Isotropic = 24.5136 Anisotropy = 6.5073

XX= 27.9067 YX= 1.1115 ZX= 2.0493

XY= 0.8228 YY= 23.4443 ZY= 0.5907

XZ= 2.2517 YZ= 0.5979 ZZ= 22.1897

Eigenvalues: 21.4352 23.2538 28.8518

19 C Isotropic = 45.7536 Anisotropy = 191.4880

XX= 0.3636 YX= -23.9063 ZX= -62.7067

XY= -23.9723 YY= 33.0890 ZY= -85.2168

XZ= -60.2698 YZ= -93.5745 ZZ= 103.8082

Eigenvalues: -72.0981 35.9466 173.4122

20 H Isotropic = 23.9312 Anisotropy = 4.9797

XX= 25.7489 YX= -2.0054 ZX= 0.0331

XY= -1.8619 YY= 24.5535 ZY= 1.3028

XZ= -0.1689 YZ= 0.7127 ZZ= 21.4911

Eigenvalues: 21.1242 23.4183 27.2510

21 C Isotropic = 58.2666 Anisotropy = 176.8697

XX= -32.2649 YX= 41.3176 ZX= -34.9354

XY= 43.6101 YY= 69.4928 ZY= -48.9615

XZ= -33.8754 YZ= -50.6556 ZZ= 137.5719

Eigenvalues: -49.1237 47.7438 176.1797

22 H Isotropic = 24.5036 Anisotropy = 3.9200

XX= 24.7662 YX= 0.1622 ZX= 0.8745

XY= 0.2388 YY= 25.6669 ZY= 2.3687

XZ= 0.8910 YZ= 2.0908 ZZ= 23.0776

Eigenvalues: 21.6487 24.7450 27.1169

23 C Isotropic = 47.4153 Anisotropy = 188.9372

XX= 36.8151 YX= 43.1706 ZX= -13.5807

XY= 41.2897 YY= -6.6227 ZY= -92.8088

XZ= -17.2289 YZ= -97.1271 ZZ= 112.0536

Eigenvalues: -67.9642 36.8367 173.3734

24 H Isotropic = 24.0725 Anisotropy = 5.1397

XX= 27.1876 YX= 0.1816 ZX= 1.5603

XY= -0.0397 YY= 22.8668 ZY= 1.0143

XZ= 0.9246 YZ= 1.0627 ZZ= 22.1631

Eigenvalues: 21.2533 23.4653 27.4990

25 C Isotropic = 56.9444 Anisotropy = 169.3651

XX= 12.4748 YX= -9.7153 ZX= -46.8146

XY= -18.6524 YY= 47.2641 ZY= -68.5458

XZ= -72.6916 YZ= -74.5293 ZZ= 111.0944

Eigenvalues: -42.2829 43.2617 169.8545

26 H Isotropic = 24.1754 Anisotropy = 8.7000

XX= 27.5573 YX= -3.7713 ZX= -1.9093

XY= -2.8269 YY= 23.3814 ZY= 0.8548

XZ= -2.0770 YZ= 1.2204 ZZ= 21.5874

Eigenvalues: 20.9814 21.5694 29.9754

27 N Isotropic = -0.1874 Anisotropy = 295.7199

XX= -124.4883 YX= 34.5759 ZX= -27.8371

XY= 20.9613 YY= -4.3956 ZY= 114.0003

XZ= -22.4830 YZ= 120.6858 ZZ= 128.3218

Eigenvalues: -143.6488 -53.8726 196.9592

28 N Isotropic = 28.5323 Anisotropy = 237.0840

XX= -120.5792 YX= -1.8204 ZX= 5.2963

XY= -18.6334 YY= 37.1683 ZY= 54.6752

XZ= -91.4902 YZ= 25.3877 ZZ= 169.0078

Eigenvalues: -126.9762 25.9848 186.5883

29 H Isotropic = 30.2225 Anisotropy = 10.0079

XX= 33.5026 YX= -2.2587 ZX= 4.2834

XY= -1.3674 YY= 27.3566 ZY= -0.2157

XZ= 4.8405 YZ= -0.6147 ZZ= 29.8084

Eigenvalues: 26.2106 27.5625 36.8945

30 H Isotropic = 30.1570 Anisotropy = 8.7540

XX= 28.5625 YX= 0.2534 ZX= -1.1544

XY= 0.0050 YY= 27.2188 ZY= 3.8291

XZ= -1.3558 YZ= 2.4029 ZZ= 34.6896

Eigenvalues: 25.9674 28.5105 35.9930

31 H Isotropic = 30.1810 Anisotropy = 6.6730

XX= 29.0671 YX= 2.7759 ZX= 0.5068

XY= 3.0175 YY= 33.0973 ZY= -1.6295

XZ= 1.7811 YZ= -0.3192 ZZ= 28.3785

Eigenvalues: 26.4390 29.4743 34.6296

32 H Isotropic = 27.5653 Anisotropy = 4.8130

XX= 28.1279 YX= 0.0383 ZX= 0.1418

XY= 2.0255 YY= 28.9423 ZY= -2.5246

XZ= -1.2081 YZ= -2.4279 ZZ= 25.6258

Eigenvalues: 24.3037 27.6182 30.7740

## BETAINE dimer\_iso2 (gas-phase) - BP86/IGLO-III level

64

C -2.67201 -2.22598 -0.31674

C -3.37269 -2.04059 1.01697

C -3.38185 -3.20840 -1.23044

H -2.83168 -3.34418 -2.16024

H -4.36773 -2.80899 -1.46523

H -3.51552 -4.17982 -0.75635

C -0.97964 -3.83369 0.46234

H -1.81100 -4.46883 0.71564

C 0.35849 -4.16103 0.67122

H 0.58981 -5.12769 1.09731

C 1.37413 -3.28576 0.34552

H 2.40373 -3.57519 0.50241

C 1.08224 -2.00100 -0.23976

C -0.30658 -1.75512 -0.44765

H -0.67317 -0.82604 -0.86794

C 3.26610 -1.11818 -0.28467

C 4.23037 -0.70079 -1.22178

H 3.89280 -0.46795 -2.22457

C 5.57573 -0.59136 -0.88129

H 6.29177 -0.27419 -1.62889

C 6.00334 -0.89266 0.41251

H 7.04792 -0.80907 0.67890

C 5.06349 -1.30645 1.35741

H 5.37683 -1.53309 2.36870

C 3.71801 -1.41648 1.01712

H 2.99616 -1.69937 1.77362

N -1.25930 -2.63403 -0.09895

N 1.92787 -1.06525 -0.64816

H -4.34987 -1.58962 0.84288

H -2.80274 -1.36782 1.65547

H -3.51018 -2.99209 1.53106

H -2.60069 -1.25864 -0.80763

C 2.67238 2.22495 -0.31504

C 3.37287 2.04224 1.01905

C 3.38245 3.20518 -1.23084

H 2.83212 3.33938 -2.16073

H 4.36800 2.80489 -1.46515

H 3.51695 4.17757 -0.75873

C 0.97971 3.83536 0.45749

H 1.81082 4.47210 0.70769

C -0.35861 4.16300 0.66560

H -0.59029 5.13126 1.08771

C -1.37391 3.28592 0.34390

H -2.40349 3.57585 0.49951

C -1.08179 1.99937 -0.23731

C 0.30730 1.75238 -0.44293

H 0.67433 0.82169 -0.85914

C -3.26612 1.11746 -0.28280

C -4.22933 0.69906 -1.22050

H -3.89054 0.46409 -2.22240

C -5.57524 0.59114 -0.88169

H -6.29042 0.27325 -1.62969

C -6.00435 0.89536 0.41092

H -7.04939 0.81288 0.67603

C -5.06565 1.31007 1.35631

H -5.38031 1.53903 2.36672

C -3.71972 1.41869 1.01780

H -2.99863 1.70279 1.77470

N 1.25969 2.63329 -0.09842

N -1.92744 1.06292 -0.64421

H 4.35024 1.59127 0.84614

H 2.80295 1.37046 1.65875

H 3.50979 2.99475 1.53146

H 2.60123 1.25662 -0.80415

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 112.9589 Anisotropy = 62.6005

XX= 141.4957 YX= -26.2060 ZX= 11.4712

XY= -23.0306 YY= 101.9709 ZY= -0.5857

XZ= 7.0800 YZ= -2.6831 ZZ= 95.4101

Eigenvalues: 88.9271 95.2570 154.6926

2 C Isotropic = 155.9160 Anisotropy = 34.8107

XX= 150.7055 YX= -4.4822 ZX= -12.7238

XY= -6.2100 YY= 147.3110 ZY= 5.9422

XZ= -13.2060 YZ= 9.8784 ZZ= 169.7314

Eigenvalues: 143.1540 145.4708 179.1231

3 C Isotropic = 158.1128 Anisotropy = 34.6573

XX= 153.5188 YX= 6.4897 ZX= 9.9768

XY= 7.1473 YY= 157.4829 ZY= 17.8932

XZ= 9.2043 YZ= 13.2261 ZZ= 163.3367

Eigenvalues: 144.4171 148.7037 181.2176

4 H Isotropic = 30.5047 Anisotropy = 8.4811

XX= 28.0729 YX= 0.4455 ZX= -0.9876

XY= 0.0352 YY= 28.7479 ZY= 4.2365

XZ= -0.7804 YZ= 2.1831 ZZ= 34.6932

Eigenvalues: 27.0162 28.3391 36.1587

5 H Isotropic = 30.5395 Anisotropy = 7.6983

XX= 33.6795 YX= -1.7126 ZX= 3.4538

XY= -0.7118 YY= 30.0519 ZY= 2.0368

XZ= 4.2537 YZ= 0.1145 ZZ= 27.8872

Eigenvalues: 25.4656 30.4813 35.6717

6 H Isotropic = 30.6705 Anisotropy = 7.7176

XX= 28.7890 YX= 1.9794 ZX= 0.6532

XY= 1.8542 YY= 35.2852 ZY= -0.9836

XZ= 2.0624 YZ= -0.2340 ZZ= 27.9373

Eigenvalues: 26.6189 29.5771 35.8156

7 C Isotropic = 64.7552 Anisotropy = 122.2601

XX= 30.1786 YX= -30.2107 ZX= 8.9762

XY= -38.3598 YY= 34.8817 ZY= 48.5411

XZ= 8.8212 YZ= 38.1519 ZZ= 129.2053

Eigenvalues: -11.6629 59.6666 146.2619

8 H Isotropic = 25.3746 Anisotropy = 8.7389

XX= 26.2013 YX= -3.8729 ZX= 2.0156

XY= -3.0143 YY= 27.0105 ZY= -1.9653

XZ= 1.4547 YZ= -3.1207 ZZ= 22.9121

Eigenvalues: 21.6926 23.2307 31.2005

9 C Isotropic = 48.1985 Anisotropy = 169.6880

XX= 33.5381 YX= 22.4608 ZX= -15.1991

XY= 28.7096 YY= -16.1407 ZY= 78.9304

XZ= -12.4328 YZ= 76.5869 ZZ= 127.1980

Eigenvalues: -59.2717 42.5434 161.3238

10 H Isotropic = 24.9791 Anisotropy = 4.1846

XX= 27.4538 YX= 0.9669 ZX= -0.1769

XY= 0.9280 YY= 24.9042 ZY= -0.7443

XZ= 0.6624 YZ= -0.1594 ZZ= 22.5794

Eigenvalues: 22.4582 24.7103 27.7688

11 C Isotropic = 53.9316 Anisotropy = 177.3492

XX= -32.2637 YX= -1.4544 ZX= -12.7495

XY= 24.9480 YY= 66.4919 ZY= 49.6767

XZ= 4.9889 YZ= 87.5159 ZZ= 127.5667

Eigenvalues: -34.8330 24.4635 172.1644

12 H Isotropic = 23.8736 Anisotropy = 10.2604

XX= 23.4217 YX= 5.4287 ZX= -0.4925

XY= 5.4460 YY= 25.8496 ZY= -1.6824

XZ= 1.1511 YZ= -4.0096 ZZ= 22.3494

Eigenvalues: 18.0251 22.8818 30.7139

13 C Isotropic = 20.3729 Anisotropy = 146.1705

XX= -41.3814 YX= 6.1442 ZX= -15.7163

XY= -5.3697 YY= 8.9915 ZY= 45.4448

XZ= -3.2627 YZ= 56.2712 ZZ= 93.5085

Eigenvalues: -42.5199 -14.1814 117.8199

14 C Isotropic = 33.6931 Anisotropy = 119.5808

XX= 23.3025 YX= 5.9373 ZX= -8.4155

XY= -7.8948 YY= -19.2306 ZY= 59.4562

XZ= -12.7363 YZ= 30.0112 ZZ= 97.0073

Eigenvalues: -34.5604 22.2260 113.4136

15 H Isotropic = 21.6017 Anisotropy = 8.6932

XX= 27.1444 YX= 1.5920 ZX= -1.0842

XY= 0.3025 YY= 22.5401 ZY= 0.8100

XZ= -0.6370 YZ= -1.3514 ZZ= 15.1207

Eigenvalues: 15.0539 22.3541 27.3972

16 C Isotropic = 18.2350 Anisotropy = 172.6647

XX= -62.9685 YX= -24.1474 ZX= -15.8014

XY= -14.0957 YY= 120.0719 ZY= 38.4232

XZ= -13.6079 YZ= 37.1042 ZZ= -2.3983

Eigenvalues: -66.9875 -11.6522 133.3448

17 C Isotropic = 48.7677 Anisotropy = 153.0315

XX= 36.8731 YX= -10.5494 ZX= -24.7594

XY= -20.3445 YY= 135.1529 ZY= 42.3738

XZ= -30.6546 YZ= 46.0064 ZZ= -25.7229

Eigenvalues: -43.8264 39.3409 150.7888

18 H Isotropic = 24.7263 Anisotropy = 5.3045

XX= 27.5367 YX= 0.5862 ZX= -2.0211

XY= 0.2514 YY= 23.5720 ZY= 0.7948

XZ= -1.8526 YZ= 0.7750 ZZ= 23.0702

Eigenvalues: 21.8856 24.0306 28.2627

19 C Isotropic = 43.9298 Anisotropy = 182.5929

XX= -4.7034 YX= -40.2763 ZX= 45.1130

XY= -38.2837 YY= 146.2957 ZY= 46.3020

XZ= 41.0625 YZ= 55.9320 ZZ= -9.8029

Eigenvalues: -69.5141 35.6451 165.6584

20 H Isotropic = 24.2112 Anisotropy = 4.4680

XX= 26.2692 YX= -0.8392 ZX= 1.6459

XY= -0.6754 YY= 22.3490 ZY= -0.6525

XZ= 1.4173 YZ= -0.0791 ZZ= 24.0154

Eigenvalues: 22.2027 23.2411 27.1899

21 C Isotropic = 56.1065 Anisotropy = 168.8791

XX= -35.3909 YX= -25.7071 ZX= -25.1989

XY= -25.8211 YY= 157.7895 ZY= 24.4356

XZ= -30.7384 YZ= 28.8335 ZZ= 45.9210

Eigenvalues: -45.5317 45.1587 168.6926

22 H Isotropic = 24.7478 Anisotropy = 2.7295

XX= 25.5037 YX= -0.1953 ZX= -0.2382

XY= -0.2787 YY= 22.8895 ZY= -1.7111

XZ= -0.4203 YZ= -1.4227 ZZ= 25.8502

Eigenvalues: 22.1777 25.4982 26.5675

23 C Isotropic = 45.6774 Anisotropy = 180.9314

XX= 31.1129 YX= -12.7946 ZX= -32.6242

XY= -9.7908 YY= 151.4771 ZY= 48.4632

XZ= -29.2647 YZ= 52.9840 ZZ= -45.5579

Eigenvalues: -65.7282 36.4620 166.2983

24 H Isotropic = 24.3943 Anisotropy = 4.5334

XX= 27.3131 YX= 0.4915 ZX= -0.3947

XY= 0.8893 YY= 22.6952 ZY= -0.9928

XZ= 0.5244 YZ= -1.2341 ZZ= 23.1745

Eigenvalues: 21.7353 24.0310 27.4165

25 C Isotropic = 58.6658 Anisotropy = 171.8607

XX= -2.1466 YX= -33.2951 ZX= 18.9216

XY= -5.3685 YY= 152.4449 ZY= 53.7077

XZ= 51.2213 YZ= 56.4500 ZZ= 25.6991

Eigenvalues: -38.3926 41.1504 173.2396

26 H Isotropic = 24.0120 Anisotropy = 8.4927

XX= 27.0093 YX= 0.9201 ZX= 5.0589

XY= 1.0957 YY= 23.0067 ZY= -1.1574

XZ= 3.9438 YZ= -1.1359 ZZ= 22.0200

Eigenvalues: 18.8290 23.5332 29.6738

27 N Isotropic = -0.7543 Anisotropy = 278.8725

XX= -122.0707 YX= 27.5577 ZX= -26.0694

XY= 9.7330 YY= -22.9358 ZY= 95.3952

XZ= -14.1599 YZ= 91.5053 ZZ= 142.7437

Eigenvalues: -131.9556 -55.4680 185.1607

28 N Isotropic = 14.1676 Anisotropy = 261.6630

XX= -144.1962 YX= -72.6392 ZX= -22.1453

XY= 15.9158 YY= 78.6782 ZY= 71.3743

XZ= 58.9196 YZ= 116.7487 ZZ= 108.0208

Eigenvalues: -151.7433 5.6364 188.6096

29 H Isotropic = 31.8916 Anisotropy = 11.2895

XX= 33.1868 YX= -4.8465 ZX= -0.4780

XY= -4.7831 YY= 35.6751 ZY= -1.6122

XZ= -1.8512 YZ= -1.2421 ZZ= 26.8130

Eigenvalues: 25.8960 30.3609 39.4180

30 H Isotropic = 30.8715 Anisotropy = 5.5041

XX= 28.2448 YX= 0.4726 ZX= 0.6671

XY= -1.4114 YY= 32.9862 ZY= 1.0876

XZ= 0.9700 YZ= 3.3410 ZZ= 31.3834

Eigenvalues: 27.8072 30.2663 34.5409

31 H Isotropic = 31.1398 Anisotropy = 7.4199

XX= 29.0070 YX= 0.4942 ZX= -2.0292

XY= -0.7414 YY= 33.1927 ZY= -2.7894

XZ= -2.8474 YZ= -4.1203 ZZ= 31.2199

Eigenvalues: 26.6842 30.6489 36.0864

32 H Isotropic = 26.5831 Anisotropy = 8.3506

XX= 25.9526 YX= -1.0625 ZX= 0.1659

XY= -1.4036 YY= 31.6178 ZY= -0.7722

XZ= 0.2486 YZ= -2.5276 ZZ= 22.1790

Eigenvalues: 21.8989 25.7003 32.1502

33 C Isotropic = 112.9977 Anisotropy = 62.5878

XX= 141.5265 YX= -26.2033 ZX= -11.4384

XY= -23.0569 YY= 102.0559 ZY= 0.5473

XZ= -7.0185 YZ= 2.6315 ZZ= 95.4106

Eigenvalues: 88.9645 95.3057 154.7229

34 C Isotropic = 155.8948 Anisotropy = 34.8000

XX= 150.6880 YX= -4.4610 ZX= 12.7241

XY= -6.1442 YY= 147.2630 ZY= -5.8528

XZ= 13.2407 YZ= -9.8656 ZZ= 169.7335

Eigenvalues: 143.1496 145.4400 179.0949

35 C Isotropic = 158.1303 Anisotropy = 34.6273

XX= 153.5294 YX= 6.4564 ZX= -9.9874

XY= 7.0892 YY= 157.4402 ZY= -17.8690

XZ= -9.1959 YZ= -13.2192 ZZ= 163.4212

Eigenvalues: 144.4374 148.7382 181.2152

36 H Isotropic = 30.5079 Anisotropy = 8.4785

XX= 28.0745 YX= 0.4441 ZX= 0.9887

XY= 0.0310 YY= 28.7428 ZY= -4.2240

XZ= 0.7796 YZ= -2.1704 ZZ= 34.7065

Eigenvalues: 27.0251 28.3384 36.1603

37 H Isotropic = 30.5428 Anisotropy = 7.6916

XX= 33.6760 YX= -1.7282 ZX= -3.4510

XY= -0.7278 YY= 30.0647 ZY= -2.0341

XZ= -4.2507 YZ= -0.1105 ZZ= 27.8877

Eigenvalues: 25.4661 30.4919 35.6705

38 H Isotropic = 30.6706 Anisotropy = 7.7213

XX= 28.7931 YX= 1.9789 ZX= -0.6547

XY= 1.8507 YY= 35.2894 ZY= 0.9718

XZ= -2.0628 YZ= 0.2239 ZZ= 27.9292

Eigenvalues: 26.6189 29.5747 35.8181

39 C Isotropic = 64.7560 Anisotropy = 122.2776

XX= 30.2060 YX= -30.2797 ZX= -8.7933

XY= -38.4166 YY= 34.4071 ZY= -48.1270

XZ= -8.5670 YZ= -37.6139 ZZ= 129.6549

Eigenvalues: -11.6738 59.6673 146.2744

40 H Isotropic = 25.3747 Anisotropy = 8.7400

XX= 26.2033 YX= -3.8760 ZX= -2.0061

XY= -3.0185 YY= 27.0269 ZY= 1.9533

XZ= -1.4462 YZ= 3.1103 ZZ= 22.8938

Eigenvalues: 21.6893 23.2334 31.2013

41 C Isotropic = 48.1813 Anisotropy = 169.7057

XX= 33.5314 YX= 22.5222 ZX= 15.1868

XY= 28.7680 YY= -16.8023 ZY= -78.3244

XZ= 12.3976 YZ= -76.0439 ZZ= 127.8148

Eigenvalues: -59.3261 42.5516 161.3185

42 H Isotropic = 24.9799 Anisotropy = 4.1868

XX= 27.4549 YX= 0.9703 ZX= 0.1717

XY= 0.9273 YY= 24.9055 ZY= 0.7351

XZ= -0.6682 YZ= 0.1519 ZZ= 22.5792

Eigenvalues: 22.4605 24.7080 27.7710

43 C Isotropic = 53.9498 Anisotropy = 177.3843

XX= -32.2574 YX= -1.3621 ZX= 12.8456

XY= 25.0719 YY= 66.0501 ZY= -49.4785

XZ= -5.4619 YZ= -87.3216 ZZ= 128.0567

Eigenvalues: -34.8314 24.4748 172.2060

44 H Isotropic = 23.8759 Anisotropy = 10.2675

XX= 23.4258 YX= 5.4283 ZX= 0.4747

XY= 5.4560 YY= 25.8688 ZY= 1.6819

XZ= -1.1878 YZ= 4.0004 ZZ= 22.3331

Eigenvalues: 18.0135 22.8933 30.7209

45 C Isotropic = 20.3423 Anisotropy = 146.1771

XX= -41.4061 YX= 6.2925 ZX= 15.4920

XY= -5.3225 YY= 8.6094 ZY= -45.2626

XZ= 3.1761 YZ= -55.9350 ZZ= 93.8237

Eigenvalues: -42.5270 -14.2398 117.7937

46 C Isotropic = 33.6824 Anisotropy = 119.5605

XX= 23.2106 YX= 5.9589 ZX= 8.3123

XY= -7.7529 YY= -19.5074 ZY= -58.8113

XZ= 12.3514 YZ= -29.8633 ZZ= 97.3441

Eigenvalues: -34.5306 22.1885 113.3894

47 H Isotropic = 21.6021 Anisotropy = 8.6815

XX= 27.1379 YX= 1.5886 ZX= 1.0650

XY= 0.2908 YY= 22.5681 ZY= -0.7772

XZ= 0.6509 YZ= 1.3953 ZZ= 15.1003

Eigenvalues: 15.0316 22.3849 27.3898

48 C Isotropic = 18.2385 Anisotropy = 172.6945

XX= -63.0351 YX= -23.9581 ZX= 15.7026

XY= -13.8976 YY= 119.9631 ZY= -38.7043

XZ= 13.5237 YZ= -37.4109 ZZ= -2.2126

Eigenvalues: -66.9819 -11.6708 133.3681

49 C Isotropic = 48.7885 Anisotropy = 152.9752

XX= 36.8356 YX= -10.3618 ZX= 24.8341

XY= -20.1353 YY= 135.0032 ZY= -42.7091

XZ= 30.7285 YZ= -46.3225 ZZ= -25.4733

Eigenvalues: -43.8065 39.4000 150.7720

50 H Isotropic = 24.7264 Anisotropy = 5.3060

XX= 27.5329 YX= 0.5820 ZX= 2.0242

XY= 0.2495 YY= 23.5720 ZY= -0.8003

XZ= 1.8623 YZ= -0.7735 ZZ= 23.0743

Eigenvalues: 21.8840 24.0314 28.2637

51 C Isotropic = 43.9432 Anisotropy = 182.5936

XX= -4.6179 YX= -40.1684 ZX= -45.0648

XY= -38.1892 YY= 146.1735 ZY= -46.6278

XZ= -41.0453 YZ= -56.2476 ZZ= -9.7259

Eigenvalues: -69.5128 35.6702 165.6723

52 H Isotropic = 24.2105 Anisotropy = 4.4767

XX= 26.2775 YX= -0.8464 ZX= -1.6432

XY= -0.6839 YY= 22.3502 ZY= 0.6571

XZ= -1.4144 YZ= 0.0842 ZZ= 24.0039

Eigenvalues: 22.2009 23.2357 27.1950

53 C Isotropic = 56.1307 Anisotropy = 168.8323

XX= -35.4800 YX= -25.4768 ZX= 25.1020

XY= -25.5292 YY= 157.7195 ZY= -24.7382

XZ= 30.5982 YZ= -29.0919 ZZ= 46.1525

Eigenvalues: -45.4810 45.1875 168.6855

54 H Isotropic = 24.7485 Anisotropy = 2.7290

XX= 25.5047 YX= -0.1968 ZX= 0.2353

XY= -0.2740 YY= 22.8937 ZY= 1.7147

XZ= 0.4139 YZ= 1.4298 ZZ= 25.8473

Eigenvalues: 22.1776 25.5002 26.5679

55 C Isotropic = 45.7072 Anisotropy = 180.8892

XX= 31.0502 YX= -12.5763 ZX= 32.6943

XY= -9.5894 YY= 151.2977 ZY= -48.8701

XZ= 29.3532 YZ= -53.3950 ZZ= -45.2262

Eigenvalues: -65.6715 36.4932 166.3000

56 H Isotropic = 24.3940 Anisotropy = 4.5327

XX= 27.3136 YX= 0.4900 ZX= 0.3957

XY= 0.8826 YY= 22.6924 ZY= 0.9996

XZ= -0.5210 YZ= 1.2336 ZZ= 23.1760

Eigenvalues: 21.7321 24.0341 27.4158

57 C Isotropic = 58.6528 Anisotropy = 171.7677

XX= -2.0532 YX= -33.1891 ZX= -18.9388

XY= -5.4225 YY= 152.2147 ZY= -53.8097

XZ= -51.2414 YZ= -56.7158 ZZ= 25.7969

Eigenvalues: -38.3845 41.1783 173.1646

58 H Isotropic = 24.0154 Anisotropy = 8.4889

XX= 27.0183 YX= 0.9024 ZX= -5.0516

XY= 1.0815 YY= 23.0068 ZY= 1.1529

XZ= -3.9396 YZ= 1.1380 ZZ= 22.0210

Eigenvalues: 18.8422 23.5293 29.6746

59 N Isotropic = -0.7452 Anisotropy = 278.8903

XX= -122.1412 YX= 27.6555 ZX= 26.0951

XY= 9.8202 YY= -23.7238 ZY= -94.6468

XZ= 14.1088 YZ= -90.6687 ZZ= 143.6295

Eigenvalues: -132.0307 -55.3865 185.1817

60 N Isotropic = 14.0625 Anisotropy = 261.8467

XX= -144.3572 YX= -72.3711 ZX= 21.9263

XY= 16.0860 YY= 78.3017 ZY= -71.1798

XZ= -59.6760 YZ= -117.0696 ZZ= 108.2429

Eigenvalues: -151.9590 5.5195 188.6270

61 H Isotropic = 31.8902 Anisotropy = 11.2800

XX= 33.1870 YX= -4.8523 ZX= 0.4861

XY= -4.7770 YY= 35.6646 ZY= 1.6148

XZ= 1.8648 YZ= 1.2181 ZZ= 26.8191

Eigenvalues: 25.8991 30.3613 39.4102

62 H Isotropic = 30.8703 Anisotropy = 5.4896

XX= 28.2473 YX= 0.4731 ZX= -0.6640

XY= -1.4043 YY= 32.9663 ZY= -1.0773

XZ= -0.9638 YZ= -3.3465 ZZ= 31.3972

Eigenvalues: 27.8148 30.2660 34.5300

63 H Isotropic = 31.1391 Anisotropy = 7.4217

XX= 29.0033 YX= 0.4966 ZX= 2.0261

XY= -0.7344 YY= 33.2031 ZY= 2.7910

XZ= 2.8479 YZ= 4.1129 ZZ= 31.2108

Eigenvalues: 26.6847 30.6457 36.0869

64 H Isotropic = 26.5812 Anisotropy = 8.3744

XX= 25.9485 YX= -1.0644 ZX= -0.1684

XY= -1.4184 YY= 31.6315 ZY= 0.7630

XZ= -0.2485 YZ= 2.5270 ZZ= 22.1636

Eigenvalues: 21.8859 25.6936 32.1641

## BETAINE dimer\_iso2 (gas-phase) – PBE0/IGLO-III level

64

C -2.67201 -2.22598 -0.31674

C -3.37269 -2.04059 1.01697

C -3.38185 -3.20840 -1.23044

H -2.83168 -3.34418 -2.16024

H -4.36773 -2.80899 -1.46523

H -3.51552 -4.17982 -0.75635

C -0.97964 -3.83369 0.46234

H -1.81100 -4.46883 0.71564

C 0.35849 -4.16103 0.67122

H 0.58981 -5.12769 1.09731

C 1.37413 -3.28576 0.34552

H 2.40373 -3.57519 0.50241

C 1.08224 -2.00100 -0.23976

C -0.30658 -1.75512 -0.44765

H -0.67317 -0.82604 -0.86794

C 3.26610 -1.11818 -0.28467

C 4.23037 -0.70079 -1.22178

H 3.89280 -0.46795 -2.22457

C 5.57573 -0.59136 -0.88129

H 6.29177 -0.27419 -1.62889

C 6.00334 -0.89266 0.41251

H 7.04792 -0.80907 0.67890

C 5.06349 -1.30645 1.35741

H 5.37683 -1.53309 2.36870

C 3.71801 -1.41648 1.01712

H 2.99616 -1.69937 1.77362

N -1.25930 -2.63403 -0.09895

N 1.92787 -1.06525 -0.64816

H -4.34987 -1.58962 0.84288

H -2.80274 -1.36782 1.65547

H -3.51018 -2.99209 1.53106

H -2.60069 -1.25864 -0.80763

C 2.67238 2.22495 -0.31504

C 3.37287 2.04224 1.01905

C 3.38245 3.20518 -1.23084

H 2.83212 3.33938 -2.16073

H 4.36800 2.80489 -1.46515

H 3.51695 4.17757 -0.75873

C 0.97971 3.83536 0.45749

H 1.81082 4.47210 0.70769

C -0.35861 4.16300 0.66560

H -0.59029 5.13126 1.08771

C -1.37391 3.28592 0.34390

H -2.40349 3.57585 0.49951

C -1.08179 1.99937 -0.23731

C 0.30730 1.75238 -0.44293

H 0.67433 0.82169 -0.85914

C -3.26612 1.11746 -0.28280

C -4.22933 0.69906 -1.22050

H -3.89054 0.46409 -2.22240

C -5.57524 0.59114 -0.88169

H -6.29042 0.27325 -1.62969

C -6.00435 0.89536 0.41092

H -7.04939 0.81288 0.67603

C -5.06565 1.31007 1.35631

H -5.38031 1.53903 2.36672

C -3.71972 1.41869 1.01780

H -2.99863 1.70279 1.77470

N 1.25969 2.63329 -0.09842

N -1.92744 1.06292 -0.64421

H 4.35024 1.59127 0.84614

H 2.80295 1.37046 1.65875

H 3.50979 2.99475 1.53146

H 2.60123 1.25662 -0.80415

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 119.9161 Anisotropy = 62.6318

XX= 148.6831 YX= -25.8099 ZX= 11.5577

XY= -22.7487 YY= 109.2052 ZY= -1.0036

XZ= 7.0454 YZ= -3.0082 ZZ= 101.8600

Eigenvalues: 96.4724 101.6052 161.6706

2 C Isotropic = 161.3399 Anisotropy = 33.0303

XX= 156.6555 YX= -4.5511 ZX= -11.8107

XY= -6.2270 YY= 153.1808 ZY= 5.4323

XZ= -13.0173 YZ= 9.4653 ZZ= 174.1835

Eigenvalues: 149.0247 151.6349 183.3601

3 C Isotropic = 163.2402 Anisotropy = 33.1706

XX= 159.2269 YX= 5.8660 ZX= 9.5259

XY= 6.9274 YY= 162.5822 ZY= 17.4039

XZ= 9.1111 YZ= 12.6395 ZZ= 167.9114

Eigenvalues: 149.7705 154.5961 185.3539

4 H Isotropic = 30.4881 Anisotropy = 8.8498

XX= 28.0250 YX= 0.4144 ZX= -1.2561

XY= 0.1117 YY= 28.5566 ZY= 4.3850

XZ= -0.7632 YZ= 2.2580 ZZ= 34.8827

Eigenvalues: 26.7835 28.2928 36.3880

5 H Isotropic = 30.5423 Anisotropy = 8.2460

XX= 34.0046 YX= -1.8357 ZX= 3.6092

XY= -0.8584 YY= 29.9908 ZY= 2.0575

XZ= 4.4196 YZ= 0.0798 ZZ= 27.6316

Eigenvalues: 25.1882 30.3991 36.0397

6 H Isotropic = 30.6592 Anisotropy = 8.3500

XX= 28.6025 YX= 2.0757 ZX= 0.6367

XY= 2.0264 YY= 35.6513 ZY= -1.1464

XZ= 2.0908 YZ= -0.4540 ZZ= 27.7238

Eigenvalues: 26.3430 29.4088 36.2259

7 C Isotropic = 66.5206 Anisotropy = 129.6869

XX= 29.6973 YX= -32.5128 ZX= 9.6246

XY= -39.9840 YY= 35.3559 ZY= 51.4052

XZ= 9.9275 YZ= 41.3540 ZZ= 134.5086

Eigenvalues: -14.5124 61.0957 152.9785

8 H Isotropic = 25.1756 Anisotropy = 9.1442

XX= 26.1569 YX= -3.8629 ZX= 2.0695

XY= -2.9308 YY= 27.0816 ZY= -2.2907

XZ= 1.4975 YZ= -3.3833 ZZ= 22.2882

Eigenvalues: 20.9601 23.2949 31.2717

9 C Isotropic = 50.4478 Anisotropy = 177.3824

XX= 35.2760 YX= 23.1030 ZX= -15.8386

XY= 29.2874 YY= -16.9975 ZY= 82.3715

XZ= -13.4847 YZ= 80.1502 ZZ= 133.0647

Eigenvalues: -61.7703 44.4109 168.7027

10 H Isotropic = 24.7365 Anisotropy = 4.4210

XX= 27.3709 YX= 1.0342 ZX= -0.1599

XY= 0.8612 YY= 24.8114 ZY= -0.9830

XZ= 0.6930 YZ= -0.4142 ZZ= 22.0272

Eigenvalues: 21.8188 24.7069 27.6838

11 C Isotropic = 56.1568 Anisotropy = 182.6676

XX= -32.4682 YX= -0.7546 ZX= -13.1004

XY= 26.2336 YY= 67.2276 ZY= 51.7530

XZ= 4.7684 YZ= 88.0754 ZZ= 133.7108

Eigenvalues: -35.4073 25.9424 177.9352

12 H Isotropic = 23.6943 Anisotropy = 10.8418

XX= 23.4256 YX= 5.4696 ZX= -0.4774

XY= 5.6269 YY= 25.9558 ZY= -1.9965

XZ= 1.1643 YZ= -4.1396 ZZ= 21.7016

Eigenvalues: 17.6907 22.4701 30.9222

13 C Isotropic = 20.6759 Anisotropy = 159.3429

XX= -47.6249 YX= 6.8513 ZX= -17.1613

XY= -4.6870 YY= 8.4438 ZY= 50.0238

XZ= -3.4518 YZ= 59.1300 ZZ= 101.2087

Eigenvalues: -48.9529 -15.9239 126.9045

14 C Isotropic = 35.4091 Anisotropy = 127.2972

XX= 22.9819 YX= 5.7191 ZX= -8.8533

XY= -6.9902 YY= -18.8310 ZY= 62.5122

XZ= -12.8336 YZ= 34.5712 ZZ= 102.0763

Eigenvalues: -36.0618 22.0151 120.2739

15 H Isotropic = 21.3828 Anisotropy = 9.1593

XX= 27.1976 YX= 1.7331 ZX= -1.1221

XY= 0.3491 YY= 22.4390 ZY= 0.6579

XZ= -0.6941 YZ= -1.5244 ZZ= 14.5120

Eigenvalues: 14.4311 22.2284 27.4891

16 C Isotropic = 19.6546 Anisotropy = 183.0488

XX= -67.3037 YX= -25.0069 ZX= -16.9345

XY= -15.1854 YY= 127.8072 ZY= 40.1940

XZ= -14.9299 YZ= 39.1238 ZZ= -1.5398

Eigenvalues: -71.6194 -11.1039 141.6871

17 C Isotropic = 51.3317 Anisotropy = 159.1373

XX= 38.4236 YX= -11.1941 ZX= -26.4232

XY= -19.3768 YY= 141.6096 ZY= 43.3111

XZ= -31.7085 YZ= 48.0683 ZZ= -26.0381

Eigenvalues: -45.0253 41.5971 157.4232

18 H Isotropic = 24.5423 Anisotropy = 5.6678

XX= 27.5690 YX= 0.6600 ZX= -2.0553

XY= 0.2392 YY= 23.0304 ZY= 0.6892

XZ= -1.9126 YZ= 0.6040 ZZ= 23.0276

Eigenvalues: 21.8051 23.5010 28.3209

19 C Isotropic = 45.9546 Anisotropy = 189.6978

XX= -4.8818 YX= -41.7112 ZX= 46.4728

XY= -39.8745 YY= 151.9147 ZY= 49.6439

XZ= 42.1602 YZ= 57.8353 ZZ= -9.1691

Eigenvalues: -71.5562 37.0003 172.4198

20 H Isotropic = 24.0564 Anisotropy = 4.6225

XX= 26.2713 YX= -0.7911 ZX= 1.6021

XY= -0.6250 YY= 21.9111 ZY= -0.7004

XZ= 1.3735 YZ= -0.2013 ZZ= 23.9867

Eigenvalues: 21.7724 23.2587 27.1380

21 C Isotropic = 59.1222 Anisotropy = 174.4923

XX= -35.7659 YX= -26.5250 ZX= -26.2371

XY= -26.8975 YY= 163.9586 ZY= 26.0522

XZ= -31.0521 YZ= 29.7284 ZZ= 49.1738

Eigenvalues: -46.0460 47.9621 175.4504

22 H Isotropic = 24.6386 Anisotropy = 2.8467

XX= 25.6330 YX= -0.1377 ZX= -0.1968

XY= -0.1957 YY= 22.4732 ZY= -1.7997

XZ= -0.3050 YZ= -1.5485 ZZ= 25.8096

Eigenvalues: 21.7618 25.6175 26.5364

23 C Isotropic = 47.5454 Anisotropy = 188.1756

XX= 32.2981 YX= -13.3520 ZX= -34.0916

XY= -10.5388 YY= 157.7803 ZY= 49.6770

XZ= -30.6406 YZ= 54.8230 ZZ= -47.4423

Eigenvalues: -68.2873 37.9277 172.9958

24 H Isotropic = 24.2394 Anisotropy = 4.7127

XX= 27.2767 YX= 0.5376 ZX= -0.3632

XY= 0.9058 YY= 22.3294 ZY= -1.1546

XZ= 0.5734 YZ= -1.3811 ZZ= 23.1122

Eigenvalues: 21.3239 24.0131 27.3813

25 C Isotropic = 59.9939 Anisotropy = 178.0561

XX= -2.9214 YX= -34.7125 ZX= 20.7109

XY= -5.5405 YY= 158.5059 ZY= 53.5286

XZ= 52.5231 YZ= 57.3273 ZZ= 24.3970

Eigenvalues: -40.7731 42.0567 178.6979

26 H Isotropic = 23.9083 Anisotropy = 8.9505

XX= 27.0204 YX= 0.9512 ZX= 5.1669

XY= 1.2900 YY= 22.6533 ZY= -1.2553

XZ= 4.2562 YZ= -1.2970 ZZ= 22.0511

Eigenvalues: 18.5302 23.3193 29.8753

27 N Isotropic = -1.2350 Anisotropy = 298.7936

XX= -133.5278 YX= 30.0700 ZX= -28.3235

XY= 10.8453 YY= -22.9642 ZY= 101.4325

XZ= -17.0725 YZ= 97.1401 ZZ= 152.7870

Eigenvalues: -144.1969 -57.4689 197.9608

28 N Isotropic = 29.4604 Anisotropy = 257.9662

XX= -127.6980 YX= -68.4279 ZX= -23.7615

XY= 18.7212 YY= 94.7168 ZY= 70.1884

XZ= 55.0180 YZ= 114.5741 ZZ= 121.3624

Eigenvalues: -133.4414 20.3847 201.4378

29 H Isotropic = 32.0168 Anisotropy = 12.0008

XX= 33.5094 YX= -5.1441 ZX= -0.4728

XY= -5.0920 YY= 35.9581 ZY= -1.7511

XZ= -1.8791 YZ= -1.4452 ZZ= 26.5829

Eigenvalues: 25.6147 30.4184 40.0174

30 H Isotropic = 30.9411 Anisotropy = 5.7244

XX= 28.2579 YX= 0.6513 ZX= 0.8638

XY= -1.4871 YY= 33.1396 ZY= 1.1756

XZ= 0.8360 YZ= 3.4607 ZZ= 31.4259

Eigenvalues: 27.8157 30.2503 34.7574

31 H Isotropic = 31.1705 Anisotropy = 8.1698

XX= 28.8328 YX= 0.5670 ZX= -2.0695

XY= -0.7014 YY= 33.5060 ZY= -3.1223

XZ= -3.0470 YZ= -4.4900 ZZ= 31.1726

Eigenvalues: 26.3863 30.5081 36.6170

32 H Isotropic = 26.6103 Anisotropy = 9.1423

XX= 25.9477 YX= -1.0895 ZX= 0.1871

XY= -1.5562 YY= 32.1182 ZY= -0.8569

XZ= 0.2443 YZ= -2.8462 ZZ= 21.7651

Eigenvalues: 21.4439 25.6819 32.7052

33 C Isotropic = 119.9544 Anisotropy = 62.6192

XX= 148.7129 YX= -25.8084 ZX= -11.5251

XY= -22.7768 YY= 109.2895 ZY= 0.9655

XZ= -6.9808 YZ= 2.9580 ZZ= 101.8606

Eigenvalues: 96.5066 101.6560 161.7005

34 C Isotropic = 161.3187 Anisotropy = 33.0244

XX= 156.6387 YX= -4.5313 ZX= 11.8118

XY= -6.1661 YY= 153.1329 ZY= -5.3467

XZ= 13.0562 YZ= -9.4552 ZZ= 174.1845

Eigenvalues: 149.0182 151.6030 183.3350

35 C Isotropic = 163.2579 Anisotropy = 33.1410

XX= 159.2370 YX= 5.8340 ZX= -9.5344

XY= 6.8702 YY= 162.5424 ZY= -17.3824

XZ= -9.0993 YZ= -12.6349 ZZ= 167.9943

Eigenvalues: 149.7904 154.6313 185.3519

36 H Isotropic = 30.4914 Anisotropy = 8.8467

XX= 28.0268 YX= 0.4132 ZX= 1.2573

XY= 0.1069 YY= 28.5517 ZY= -4.3719

XZ= 0.7617 YZ= -2.2446 ZZ= 34.8959

Eigenvalues: 26.7931 28.2920 36.3892

37 H Isotropic = 30.5457 Anisotropy = 8.2395

XX= 34.0009 YX= -1.8519 ZX= -3.6062

XY= -0.8745 YY= 30.0045 ZY= -2.0555

XZ= -4.4164 YZ= -0.0758 ZZ= 27.6316

Eigenvalues: 25.1884 30.4100 36.0387

38 H Isotropic = 30.6591 Anisotropy = 8.3545

XX= 28.6064 YX= 2.0756 ZX= -0.6384

XY= 2.0231 YY= 35.6564 ZY= 1.1333

XZ= -2.0914 YZ= 0.4424 ZZ= 27.7145

Eigenvalues: 26.3426 29.4059 36.2288

39 C Isotropic = 66.5218 Anisotropy = 129.7009

XX= 29.7278 YX= -32.5854 ZX= -9.4273

XY= -40.0431 YY= 34.8551 ZY= -50.9661

XZ= -9.6765 YZ= -40.8020 ZZ= 134.9825

Eigenvalues: -14.5217 61.0981 152.9891

40 H Isotropic = 25.1757 Anisotropy = 9.1452

XX= 26.1592 YX= -3.8668 ZX= -2.0605

XY= -2.9343 YY= 27.1008 ZY= 2.2758

XZ= -1.4907 YZ= 3.3685 ZZ= 22.2671

Eigenvalues: 20.9570 23.2976 31.2725

41 C Isotropic = 50.4299 Anisotropy = 177.3979

XX= 35.2653 YX= 23.1669 ZX= 15.8271

XY= 29.3564 YY= -17.6894 ZY= -81.7379

XZ= 13.4458 YZ= -79.5642 ZZ= 133.7139

Eigenvalues: -61.8224 44.4170 168.6952

42 H Isotropic = 24.7373 Anisotropy = 4.4233

XX= 27.3720 YX= 1.0377 ZX= 0.1544

XY= 0.8609 YY= 24.8146 ZY= 0.9723

XZ= -0.6982 YZ= 0.4058 ZZ= 22.0253

Eigenvalues: 21.8209 24.7048 27.6861

43 C Isotropic = 56.1775 Anisotropy = 182.6958

XX= -32.4615 YX= -0.6640 ZX= 13.1968

XY= 26.3618 YY= 66.7755 ZY= -51.5352

XZ= -5.2247 YZ= -87.8471 ZZ= 134.2185

Eigenvalues: -35.4084 25.9662 177.9747

44 H Isotropic = 23.6966 Anisotropy = 10.8494

XX= 23.4301 YX= 5.4693 ZX= 0.4595

XY= 5.6362 YY= 25.9764 ZY= 1.9935

XZ= -1.2000 YZ= 4.1291 ZZ= 21.6834

Eigenvalues: 17.6789 22.4814 30.9296

45 C Isotropic = 20.6462 Anisotropy = 159.3506

XX= -47.6562 YX= 7.0108 ZX= 16.9226

XY= -4.6281 YY= 8.0507 ZY= -49.8091

XZ= 3.3317 YZ= -58.7838 ZZ= 101.5442

Eigenvalues: -48.9648 -15.9765 126.8800

46 C Isotropic = 35.4048 Anisotropy = 127.2799

XX= 22.9028 YX= 5.7470 ZX= 8.7518

XY= -6.8447 YY= -19.1348 ZY= -61.8424

XZ= 12.4755 YZ= -34.4013 ZZ= 102.4463

Eigenvalues: -36.0275 21.9838 120.2580

47 H Isotropic = 21.3821 Anisotropy = 9.1466

XX= 27.1899 YX= 1.7282 ZX= 1.1035

XY= 0.3357 YY= 22.4696 ZY= -0.6292

XZ= 0.7051 YZ= 1.5662 ZZ= 14.4869

Eigenvalues: 14.4033 22.2632 27.4798

48 C Isotropic = 19.6563 Anisotropy = 183.0762

XX= -67.3799 YX= -24.8036 ZX= 16.8269

XY= -14.9774 YY= 127.6892 ZY= -40.4946

XZ= 14.8412 YZ= -39.4388 ZZ= -1.3404

Eigenvalues: -71.6185 -11.1196 141.7071

49 C Isotropic = 51.3532 Anisotropy = 159.0826

XX= 38.3818 YX= -10.9974 ZX= 26.5017

XY= -19.1632 YY= 141.4559 ZY= -43.6568

XZ= 31.7824 YZ= -48.3988 ZZ= -25.7779

Eigenvalues: -45.0039 41.6553 157.4083

50 H Isotropic = 24.5429 Anisotropy = 5.6681

XX= 27.5654 YX= 0.6551 ZX= 2.0584

XY= 0.2366 YY= 23.0321 ZY= -0.6938

XZ= 1.9212 YZ= -0.6018 ZZ= 23.0311

Eigenvalues: 21.8048 23.5022 28.3217

51 C Isotropic = 45.9666 Anisotropy = 189.6971

XX= -4.7957 YX= -41.5988 ZX= -46.4251

XY= -39.7755 YY= 151.7827 ZY= -49.9772

XZ= -42.1419 YZ= -58.1612 ZZ= -9.0872

Eigenvalues: -71.5552 37.0237 172.4313

52 H Isotropic = 24.0564 Anisotropy = 4.6308

XX= 26.2796 YX= -0.7985 ZX= -1.5995

XY= -0.6341 YY= 21.9135 ZY= 0.7051

XZ= -1.3711 YZ= 0.2071 ZZ= 23.9760

Eigenvalues: 21.7715 23.2541 27.1436

53 C Isotropic = 59.1486 Anisotropy = 174.4449

XX= -35.8547 YX= -26.2864 ZX= 26.1326

XY= -26.6014 YY= 163.8877 ZY= -26.3584

XZ= 30.9063 YZ= -29.9944 ZZ= 49.4130

Eigenvalues: -45.9913 47.9920 175.4452

54 H Isotropic = 24.6396 Anisotropy = 2.8462

XX= 25.6345 YX= -0.1399 ZX= 0.1938

XY= -0.1925 YY= 22.4780 ZY= 1.8042

XZ= 0.2990 YZ= 1.5562 ZZ= 25.8063

Eigenvalues: 21.7614 25.6204 26.5371

55 C Isotropic = 47.5767 Anisotropy = 188.1307

XX= 32.2318 YX= -13.1245 ZX= 34.1641

XY= -10.3251 YY= 157.5957 ZY= -50.1045

XZ= 30.7290 YZ= -55.2507 ZZ= -47.0973

Eigenvalues: -68.2265 37.9594 172.9972

56 H Isotropic = 24.2394 Anisotropy = 4.7116

XX= 27.2772 YX= 0.5359 ZX= 0.3641

XY= 0.8981 YY= 22.3276 ZY= 1.1616

XZ= -0.5697 YZ= 1.3816 ZZ= 23.1135

Eigenvalues: 21.3208 24.0170 27.3805

57 C Isotropic = 59.9813 Anisotropy = 177.9713

XX= -2.8270 YX= -34.6031 ZX= -20.7274

XY= -5.5847 YY= 158.2762 ZY= -53.6548

XZ= -52.5465 YZ= -57.6092 ZZ= 24.4948

Eigenvalues: -40.7678 42.0829 178.6288

58 H Isotropic = 23.9113 Anisotropy = 8.9460

XX= 27.0295 YX= 0.9328 ZX= -5.1597

XY= 1.2736 YY= 22.6535 ZY= 1.2525

XZ= -4.2512 YZ= 1.3000 ZZ= 22.0509

Eigenvalues: 18.5432 23.3153 29.8753

59 N Isotropic = -1.2271 Anisotropy = 298.8105

XX= -133.5917 YX= 30.1683 ZX= 28.3439

XY= 10.9272 YY= -23.7955 ZY= -100.6294

XZ= 17.0387 YZ= -96.2975 ZZ= 153.7058

Eigenvalues: -144.2650 -57.3963 197.9799

60 N Isotropic = 29.3588 Anisotropy = 258.1473

XX= -127.8699 YX= -68.1592 ZX= 23.5499

XY= 18.9015 YY= 94.3333 ZY= -70.0068

XZ= -55.7510 YZ= -114.8650 ZZ= 121.6131

Eigenvalues: -133.6550 20.2745 201.4570

61 H Isotropic = 32.0147 Anisotropy = 11.9907

XX= 33.5098 YX= -5.1501 ZX= 0.4811

XY= -5.0841 YY= 35.9471 ZY= 1.7535

XZ= 1.8944 YZ= 1.4200 ZZ= 26.5871

Eigenvalues: 25.6164 30.4191 40.0084

62 H Isotropic = 30.9404 Anisotropy = 5.7095

XX= 28.2608 YX= 0.6510 ZX= -0.8616

XY= -1.4781 YY= 33.1193 ZY= -1.1652

XZ= -0.8285 YZ= -3.4664 ZZ= 31.4410

Eigenvalues: 27.8243 30.2501 34.7467

63 H Isotropic = 31.1698 Anisotropy = 8.1718

XX= 28.8292 YX= 0.5689 ZX= 2.0659

XY= -0.6932 YY= 33.5175 ZY= 3.1232

XZ= 3.0483 YZ= 4.4822 ZZ= 31.1626

Eigenvalues: 26.3869 30.5049 36.6176

64 H Isotropic = 26.6095 Anisotropy = 9.1695

XX= 25.9438 YX= -1.0923 ZX= -0.1897

XY= -1.5707 YY= 32.1356 ZY= 0.8471

XZ= -0.2462 YZ= 2.8457 ZZ= 21.7493

Eigenvalues: 21.4308 25.6753 32.7226

## BETAINE dimer\_iso2 (IEFPCM solvent = tetrahydrofuran) – BP86/IGLO-III level

64

C -2.67201 -2.22598 -0.31674

C -3.37269 -2.04059 1.01697

C -3.38185 -3.20840 -1.23044

H -2.83168 -3.34418 -2.16024

H -4.36773 -2.80899 -1.46523

H -3.51552 -4.17982 -0.75635

C -0.97964 -3.83369 0.46234

H -1.81100 -4.46883 0.71564

C 0.35849 -4.16103 0.67122

H 0.58981 -5.12769 1.09731

C 1.37413 -3.28576 0.34552

H 2.40373 -3.57519 0.50241

C 1.08224 -2.00100 -0.23976

C -0.30658 -1.75512 -0.44765

H -0.67317 -0.82604 -0.86794

C 3.26610 -1.11818 -0.28467

C 4.23037 -0.70079 -1.22178

H 3.89280 -0.46795 -2.22457

C 5.57573 -0.59136 -0.88129

H 6.29177 -0.27419 -1.62889

C 6.00334 -0.89266 0.41251

H 7.04792 -0.80907 0.67890

C 5.06349 -1.30645 1.35741

H 5.37683 -1.53309 2.36870

C 3.71801 -1.41648 1.01712

H 2.99616 -1.69937 1.77362

N -1.25930 -2.63403 -0.09895

N 1.92787 -1.06525 -0.64816

H -4.34987 -1.58962 0.84288

H -2.80274 -1.36782 1.65547

H -3.51018 -2.99209 1.53106

H -2.60069 -1.25864 -0.80763

C 2.67238 2.22495 -0.31504

C 3.37287 2.04224 1.01905

C 3.38245 3.20518 -1.23084

H 2.83212 3.33938 -2.16073

H 4.36800 2.80489 -1.46515

H 3.51695 4.17757 -0.75873

C 0.97971 3.83536 0.45749

H 1.81082 4.47210 0.70769

C -0.35861 4.16300 0.66560

H -0.59029 5.13126 1.08771

C -1.37391 3.28592 0.34390

H -2.40349 3.57585 0.49951

C -1.08179 1.99937 -0.23731

C 0.30730 1.75238 -0.44293

H 0.67433 0.82169 -0.85914

C -3.26612 1.11746 -0.28280

C -4.22933 0.69906 -1.22050

H -3.89054 0.46409 -2.22240

C -5.57524 0.59114 -0.88169

H -6.29042 0.27325 -1.62969

C -6.00435 0.89536 0.41092

H -7.04939 0.81288 0.67603

C -5.06565 1.31007 1.35631

H -5.38031 1.53903 2.36672

C -3.71972 1.41869 1.01780

H -2.99863 1.70279 1.77470

N 1.25969 2.63329 -0.09842

N -1.92744 1.06292 -0.64421

H 4.35024 1.59127 0.84614

H 2.80295 1.37046 1.65875

H 3.50979 2.99475 1.53146

H 2.60123 1.25662 -0.80415

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 112.2538 Anisotropy = 62.9361

XX= 140.8854 YX= -26.2655 ZX= 11.7846

XY= -23.1529 YY= 101.3001 ZY= -0.4736

XZ= 7.3752 YZ= -2.6886 ZZ= 94.5758

Eigenvalues: 88.0143 94.5358 154.2112

2 C Isotropic = 156.1412 Anisotropy = 34.6725

XX= 151.5635 YX= -4.6521 ZX= -12.5791

XY= -6.5935 YY= 147.2415 ZY= 5.6709

XZ= -13.5576 YZ= 9.7246 ZZ= 169.6187

Eigenvalues: 143.2325 145.9350 179.2562

3 C Isotropic = 158.3512 Anisotropy = 34.5351

XX= 154.2953 YX= 6.2977 ZX= 10.1080

XY= 7.0534 YY= 157.6342 ZY= 17.8817

XZ= 9.7519 YZ= 13.1551 ZZ= 163.1239

Eigenvalues: 144.3293 149.3496 181.3746

4 H Isotropic = 30.4534 Anisotropy = 8.4844

XX= 28.0468 YX= 0.4598 ZX= -1.0165

XY= 0.0711 YY= 28.6749 ZY= 4.2644

XZ= -0.7153 YZ= 2.1908 ZZ= 34.6386

Eigenvalues: 26.9341 28.3164 36.1097

5 H Isotropic = 30.5448 Anisotropy = 7.7796

XX= 33.7325 YX= -1.6896 ZX= 3.4633

XY= -0.6800 YY= 30.0258 ZY= 2.0403

XZ= 4.3083 YZ= 0.1145 ZZ= 27.8763

Eigenvalues: 25.4485 30.4549 35.7312

6 H Isotropic = 30.5165 Anisotropy = 7.8835

XX= 28.5656 YX= 2.0089 ZX= 0.6222

XY= 1.9159 YY= 35.2267 ZY= -1.0323

XZ= 2.0633 YZ= -0.2864 ZZ= 27.7572

Eigenvalues: 26.4139 29.3635 35.7722

7 C Isotropic = 61.7172 Anisotropy = 128.3292

XX= 25.6358 YX= -29.1436 ZX= 8.2267

XY= -37.1802 YY= 30.4246 ZY= 51.1110

XZ= 8.6402 YZ= 40.5901 ZZ= 129.0913

Eigenvalues: -15.6110 53.4926 147.2701

8 H Isotropic = 25.0656 Anisotropy = 8.7895

XX= 25.9640 YX= -3.8334 ZX= 2.0145

XY= -2.9960 YY= 26.7495 ZY= -2.0322

XZ= 1.4609 YZ= -3.1386 ZZ= 22.4833

Eigenvalues: 21.2593 23.0123 30.9252

9 C Isotropic = 47.4054 Anisotropy = 173.4275

XX= 30.4740 YX= 21.6731 ZX= -15.1674

XY= 27.5315 YY= -16.7080 ZY= 79.8446

XZ= -12.1821 YZ= 77.6650 ZZ= 128.4501

Eigenvalues: -59.9176 39.1100 163.0237

10 H Isotropic = 24.7521 Anisotropy = 4.2155

XX= 27.2319 YX= 0.9772 ZX= -0.1741

XY= 0.9480 YY= 24.7563 ZY= -0.8372

XZ= 0.6345 YZ= -0.2632 ZZ= 22.2680

Eigenvalues: 22.1145 24.5793 27.5624

11 C Isotropic = 54.2401 Anisotropy = 177.3856

XX= -32.1236 YX= -1.0479 ZX= -12.8567

XY= 23.5752 YY= 66.6114 ZY= 49.9942

XZ= 5.0934 YZ= 86.8413 ZZ= 128.2326

Eigenvalues: -34.5142 24.7374 172.4972

12 H Isotropic = 23.8110 Anisotropy = 10.2023

XX= 23.3730 YX= 5.3362 ZX= -0.4692

XY= 5.3483 YY= 25.8566 ZY= -1.7468

XZ= 1.1559 YZ= -3.9866 ZZ= 22.2033

Eigenvalues: 18.0311 22.7893 30.6125

13 C Isotropic = 20.2443 Anisotropy = 147.7750

XX= -41.7658 YX= 3.9715 ZX= -14.9351

XY= -6.4633 YY= 8.2045 ZY= 46.2145

XZ= -2.4487 YZ= 56.6591 ZZ= 94.2943

Eigenvalues: -42.4491 -15.5789 118.7610

14 C Isotropic = 34.7086 Anisotropy = 118.5297

XX= 25.4252 YX= 5.3003 ZX= -7.9722

XY= -7.3992 YY= -18.4466 ZY= 59.2573

XZ= -12.9053 YZ= 30.5681 ZZ= 97.1473

Eigenvalues: -33.9432 24.3407 113.7284

15 H Isotropic = 21.5701 Anisotropy = 8.7774

XX= 27.1927 YX= 1.5128 ZX= -1.0608

XY= 0.2871 YY= 22.5027 ZY= 0.7969

XZ= -0.6198 YZ= -1.3675 ZZ= 15.0148

Eigenvalues: 14.9505 22.3381 27.4216

16 C Isotropic = 18.1584 Anisotropy = 173.1543

XX= -63.1558 YX= -24.0881 ZX= -15.4926

XY= -13.8667 YY= 120.1981 ZY= 39.1085

XZ= -13.6033 YZ= 37.1400 ZZ= -2.5670

Eigenvalues: -67.0901 -12.0293 133.5946

17 C Isotropic = 48.9147 Anisotropy = 151.9046

XX= 37.4735 YX= -10.6038 ZX= -25.2477

XY= -19.3586 YY= 135.0058 ZY= 41.3724

XZ= -30.7205 YZ= 45.5983 ZZ= -25.7353

Eigenvalues: -43.7254 40.2851 150.1844

18 H Isotropic = 24.7057 Anisotropy = 5.3634

XX= 27.5373 YX= 0.5654 ZX= -2.0543

XY= 0.1248 YY= 23.5464 ZY= 0.8105

XZ= -1.8961 YZ= 0.7361 ZZ= 23.0335

Eigenvalues: 21.8649 23.9709 28.2814

19 C Isotropic = 43.8229 Anisotropy = 183.8909

XX= -5.2412 YX= -40.1685 ZX= 44.6171

XY= -38.8655 YY= 147.0118 ZY= 46.3590

XZ= 40.4836 YZ= 56.0056 ZZ= -10.3019

Eigenvalues: -69.5525 34.6045 166.4169

20 H Isotropic = 24.1228 Anisotropy = 4.4374

XX= 26.1877 YX= -0.8022 ZX= 1.6229

XY= -0.6211 YY= 22.2553 ZY= -0.6898

XZ= 1.3975 YZ= -0.1087 ZZ= 23.9255

Eigenvalues: 22.1162 23.1712 27.0811

21 C Isotropic = 56.6857 Anisotropy = 169.0106

XX= -34.7375 YX= -25.7006 ZX= -24.9590

XY= -26.6065 YY= 158.3541 ZY= 24.4156

XZ= -30.6206 YZ= 28.8562 ZZ= 46.4406

Eigenvalues: -44.8622 45.5599 169.3594

22 H Isotropic = 24.6911 Anisotropy = 2.6751

XX= 25.4895 YX= -0.1743 ZX= -0.2095

XY= -0.2898 YY= 22.8130 ZY= -1.7061

XZ= -0.3873 YZ= -1.4089 ZZ= 25.7709

Eigenvalues: 22.1116 25.4873 26.4745

23 C Isotropic = 45.6863 Anisotropy = 181.9997

XX= 30.5940 YX= -13.1083 ZX= -32.2256

XY= -9.9602 YY= 152.3005 ZY= 47.9895

XZ= -28.9836 YZ= 53.2508 ZZ= -45.8356

Eigenvalues: -65.7356 35.7751 167.0194

24 H Isotropic = 24.3043 Anisotropy = 4.5077

XX= 27.2073 YX= 0.4857 ZX= -0.3790

XY= 0.8888 YY= 22.5950 ZY= -1.0301

XZ= 0.5341 YZ= -1.2406 ZZ= 23.1106

Eigenvalues: 21.6265 23.9769 27.3095

25 C Isotropic = 57.7444 Anisotropy = 173.6363

XX= -3.7289 YX= -33.4496 ZX= 19.1026

XY= -3.8088 YY= 153.2325 ZY= 53.0220

XZ= 51.0142 YZ= 56.6328 ZZ= 23.7296

Eigenvalues: -39.6223 39.3536 173.5020

26 H Isotropic = 23.9230 Anisotropy = 8.5553

XX= 26.8734 YX= 0.8813 ZX= 5.0728

XY= 1.2020 YY= 22.9350 ZY= -1.1907

XZ= 4.0836 YZ= -1.1223 ZZ= 21.9605

Eigenvalues: 18.6730 23.4694 29.6265

27 N Isotropic = -2.8980 Anisotropy = 282.9873

XX= -125.6412 YX= 25.3720 ZX= -25.0169

XY= 8.8930 YY= -25.8173 ZY= 96.9988

XZ= -14.1348 YZ= 92.7418 ZZ= 142.7646

Eigenvalues: -134.4769 -59.9772 185.7602

28 N Isotropic = 20.8680 Anisotropy = 251.2728

XX= -129.8529 YX= -70.2750 ZX= -21.1852

XY= 18.2383 YY= 84.5850 ZY= 69.1277

XZ= 59.7913 YZ= 113.6575 ZZ= 107.8718

Eigenvalues: -137.2490 11.4697 188.3832

29 H Isotropic = 31.9867 Anisotropy = 11.2126

XX= 33.3106 YX= -4.7892 ZX= -0.4790

XY= -4.7626 YY= 35.7348 ZY= -1.5972

XZ= -1.9020 YZ= -1.2178 ZZ= 26.9149

Eigenvalues: 25.9993 30.4992 39.4618

30 H Isotropic = 30.9265 Anisotropy = 5.4280

XX= 28.3553 YX= 0.4895 ZX= 0.6547

XY= -1.4479 YY= 32.9837 ZY= 1.0698

XZ= 0.8504 YZ= 3.3331 ZZ= 31.4406

Eigenvalues: 27.9446 30.2898 34.5452

31 H Isotropic = 30.9627 Anisotropy = 7.5979

XX= 28.7647 YX= 0.5358 ZX= -1.9999

XY= -0.7106 YY= 33.1043 ZY= -2.8505

XZ= -2.9048 YZ= -4.1997 ZZ= 31.0190

Eigenvalues: 26.4512 30.4088 36.0280

32 H Isotropic = 26.6400 Anisotropy = 8.2936

XX= 26.0858 YX= -1.0147 ZX= 0.1654

XY= -1.3505 YY= 31.6547 ZY= -0.7739

XZ= 0.2136 YZ= -2.5228 ZZ= 22.1795

Eigenvalues: 21.9010 25.8501 32.1691

33 C Isotropic = 112.2906 Anisotropy = 62.9236

XX= 140.9131 YX= -26.2645 ZX= -11.7511

XY= -23.1822 YY= 101.3846 ZY= 0.4363

XZ= -7.3107 YZ= 2.6370 ZZ= 94.5742

Eigenvalues: 88.0480 94.5842 154.2397

34 C Isotropic = 156.1193 Anisotropy = 34.6624

XX= 151.5452 YX= -4.6329 ZX= 12.5824

XY= -6.5286 YY= 147.1956 ZY= -5.5808

XZ= 13.5946 YZ= -9.7103 ZZ= 169.6172

Eigenvalues: 143.2279 145.9024 179.2276

35 C Isotropic = 158.3692 Anisotropy = 34.5061

XX= 154.3066 YX= 6.2626 ZX= -10.1171

XY= 6.9937 YY= 157.5920 ZY= -17.8613

XZ= -9.7412 YZ= -13.1521 ZZ= 163.2089

Eigenvalues: 144.3465 149.3878 181.3732

36 H Isotropic = 30.4568 Anisotropy = 8.4818

XX= 28.0485 YX= 0.4585 ZX= 1.0174

XY= 0.0664 YY= 28.6701 ZY= -4.2521

XZ= 0.7143 YZ= -2.1781 ZZ= 34.6519

Eigenvalues: 26.9433 28.3158 36.1114

37 H Isotropic = 30.5485 Anisotropy = 7.7721

XX= 33.7293 YX= -1.7050 ZX= -3.4604

XY= -0.6958 YY= 30.0390 ZY= -2.0378

XZ= -4.3051 YZ= -0.1106 ZZ= 27.8772

Eigenvalues: 25.4494 30.4662 35.7299

38 H Isotropic = 30.5161 Anisotropy = 7.8875

XX= 28.5692 YX= 2.0086 ZX= -0.6239

XY= 1.9123 YY= 35.2307 ZY= 1.0204

XZ= -2.0636 YZ= 0.2762 ZZ= 27.7483

Eigenvalues: 26.4134 29.3604 35.7744

39 C Isotropic = 61.7188 Anisotropy = 128.3446

XX= 25.6637 YX= -29.2099 ZX= -8.0441

XY= -37.2356 YY= 29.9314 ZY= -50.6755

XZ= -8.3904 YZ= -40.0365 ZZ= 129.5612

Eigenvalues: -15.6194 53.4939 147.2819

40 H Isotropic = 25.0657 Anisotropy = 8.7907

XX= 25.9661 YX= -3.8367 ZX= -2.0053

XY= -2.9999 YY= 26.7665 ZY= 2.0196

XZ= -1.4531 YZ= 3.1273 ZZ= 22.4644

Eigenvalues: 21.2558 23.0150 30.9261

41 C Isotropic = 47.3885 Anisotropy = 173.4437

XX= 30.4691 YX= 21.7347 ZX= 15.1607

XY= 27.5895 YY= -17.3799 ZY= -79.2309

XZ= 12.1505 YZ= -77.1099 ZZ= 129.0764

Eigenvalues: -59.9719 39.1199 163.0176

42 H Isotropic = 24.7528 Anisotropy = 4.2177

XX= 27.2329 YX= 0.9806 ZX= 0.1688

XY= 0.9475 YY= 24.7585 ZY= 0.8272

XZ= -0.6405 YZ= 0.2555 ZZ= 22.2671

Eigenvalues: 22.1168 24.5772 27.5646

43 C Isotropic = 54.2617 Anisotropy = 177.4082

XX= -32.1129 YX= -0.9549 ZX= 12.9516

XY= 23.6884 YY= 66.1729 ZY= -49.7930

XZ= -5.5318 YZ= -86.6305 ZZ= 128.7249

Eigenvalues: -34.5089 24.7601 172.5338

44 H Isotropic = 23.8134 Anisotropy = 10.2092

XX= 23.3775 YX= 5.3358 ZX= 0.4518

XY= 5.3575 YY= 25.8758 ZY= 1.7455

XZ= -1.1906 YZ= 3.9770 ZZ= 22.1867

Eigenvalues: 18.0203 22.8002 30.6195

45 C Isotropic = 20.2131 Anisotropy = 147.7774

XX= -41.7913 YX= 4.1226 ZX= 14.7199

XY= -6.4131 YY= 7.8218 ZY= -46.0249

XZ= 2.3607 YZ= -56.3196 ZZ= 94.6088

Eigenvalues: -42.4574 -15.6348 118.7314

46 C Isotropic = 34.7008 Anisotropy = 118.5079

XX= 25.3388 YX= 5.3243 ZX= 7.8769

XY= -7.2539 YY= -18.7224 ZY= -58.6171

XZ= 12.5225 YZ= -30.4224 ZZ= 97.4859

Eigenvalues: -33.9125 24.3088 113.7060

47 H Isotropic = 21.5702 Anisotropy = 8.7648

XX= 27.1855 YX= 1.5092 ZX= 1.0420

XY= 0.2751 YY= 22.5308 ZY= -0.7650

XZ= 0.6337 YZ= 1.4121 ZZ= 14.9943

Eigenvalues: 14.9279 22.3693 27.4134

48 C Isotropic = 18.1593 Anisotropy = 173.1848

XX= -63.2220 YX= -23.9011 ZX= 15.3930

XY= -13.6685 YY= 120.0858 ZY= -39.3899

XZ= 13.5167 YZ= -37.4461 ZZ= -2.3859

Eigenvalues: -67.0847 -12.0533 133.6158

49 C Isotropic = 48.9302 Anisotropy = 151.8694

XX= 37.4207 YX= -10.4212 ZX= 25.3208

XY= -19.1560 YY= 134.8643 ZY= -41.7135

XZ= 30.7906 YZ= -45.9182 ZZ= -25.4942

Eigenvalues: -43.7121 40.3263 150.1765

50 H Isotropic = 24.7051 Anisotropy = 5.3648

XX= 27.5324 YX= 0.5612 ZX= 2.0571

XY= 0.1230 YY= 23.5458 ZY= -0.8160

XZ= 1.9060 YZ= -0.7345 ZZ= 23.0371

Eigenvalues: 21.8628 23.9708 28.2816

51 C Isotropic = 43.8343 Anisotropy = 183.8945

XX= -5.1585 YX= -40.0599 ZX= -44.5714

XY= -38.7687 YY= 146.8903 ZY= -46.6849

XZ= -40.4655 YZ= -56.3253 ZZ= -10.2290

Eigenvalues: -69.5553 34.6276 166.4306

52 H Isotropic = 24.1221 Anisotropy = 4.4458

XX= 26.1956 YX= -0.8095 ZX= -1.6203

XY= -0.6296 YY= 22.2568 ZY= 0.6944

XZ= -1.3948 YZ= 0.1136 ZZ= 23.9140

Eigenvalues: 22.1145 23.1658 27.0860

53 C Isotropic = 56.7137 Anisotropy = 168.9565

XX= -34.8216 YX= -25.4707 ZX= 24.8619

XY= -26.3135 YY= 158.2846 ZY= -24.7169

XZ= 30.4835 YZ= -29.1122 ZZ= 46.6782

Eigenvalues: -44.8066 45.5964 169.3514

54 H Isotropic = 24.6923 Anisotropy = 2.6741

XX= 25.4909 YX= -0.1759 ZX= 0.2067

XY= -0.2855 YY= 22.8180 ZY= 1.7095

XZ= 0.3811 YZ= 1.4157 ZZ= 25.7681

Eigenvalues: 22.1123 25.4896 26.4751

55 C Isotropic = 45.7206 Anisotropy = 181.9495

XX= 30.5409 YX= -12.8875 ZX= 32.2979

XY= -9.7557 YY= 152.1216 ZY= -48.3992

XZ= 29.0709 YZ= -53.6619 ZZ= -45.5008

Eigenvalues: -65.6746 35.8160 167.0203

56 H Isotropic = 24.3043 Anisotropy = 4.5067

XX= 27.2078 YX= 0.4842 ZX= 0.3799

XY= 0.8818 YY= 22.5929 ZY= 1.0369

XZ= -0.5308 YZ= 1.2402 ZZ= 23.1122

Eigenvalues: 21.6237 23.9804 27.3088

57 C Isotropic = 57.7353 Anisotropy = 173.5407

XX= -3.6299 YX= -33.3418 ZX= -19.1195

XY= -3.8623 YY= 153.0030 ZY= -53.1294

XZ= -51.0443 YZ= -56.9049 ZZ= 23.8330

Eigenvalues: -39.6130 39.3899 173.4291

58 H Isotropic = 23.9264 Anisotropy = 8.5515

XX= 26.8828 YX= 0.8640 ZX= -5.0657

XY= 1.1871 YY= 22.9355 ZY= 1.1864

XZ= -4.0794 YZ= 1.1246 ZZ= 21.9609

Eigenvalues: 18.6859 23.4659 29.6274

59 N Isotropic = -2.8901 Anisotropy = 283.0029

XX= -125.7098 YX= 25.4620 ZX= 25.0590

XY= 8.9765 YY= -26.6147 ZY= -96.2321

XZ= 14.0932 YZ= -91.9074 ZZ= 143.6541

Eigenvalues: -134.5519 -59.8970 185.7784

60 N Isotropic = 20.7400 Anisotropy = 251.4972

XX= -130.0748 YX= -70.0364 ZX= 20.9773

XY= 18.3769 YY= 84.2064 ZY= -68.9548

XZ= -60.4985 YZ= -113.9771 ZZ= 108.0884

Eigenvalues: -137.5334 11.3486 188.4048

61 H Isotropic = 31.9852 Anisotropy = 11.2033

XX= 33.3105 YX= -4.7951 ZX= 0.4871

XY= -4.7563 YY= 35.7243 ZY= 1.5998

XZ= 1.9159 YZ= 1.1942 ZZ= 26.9208

Eigenvalues: 26.0020 30.4995 39.4541

62 H Isotropic = 30.9246 Anisotropy = 5.4138

XX= 28.3569 YX= 0.4900 ZX= -0.6518

XY= -1.4401 YY= 32.9633 ZY= -1.0596

XZ= -0.8442 YZ= -3.3385 ZZ= 31.4537

Eigenvalues: 27.9513 30.2887 34.5338

63 H Isotropic = 30.9625 Anisotropy = 7.5995

XX= 28.7617 YX= 0.5380 ZX= 1.9966

XY= -0.7033 YY= 33.1154 ZY= 2.8519

XZ= 2.9053 YZ= 4.1920 ZZ= 31.0103

Eigenvalues: 26.4525 30.4062 36.0288

64 H Isotropic = 26.6385 Anisotropy = 8.3173

XX= 26.0821 YX= -1.0164 ZX= -0.1680

XY= -1.3648 YY= 31.6690 ZY= 0.7646

XZ= -0.2135 YZ= 2.5220 ZZ= 22.1645

Eigenvalues: 21.8884 25.8438 32.1834

## BETAINE dimer\_iso2 (IEFPCM solvent = tetrahydrofuran) – PBE0/IGLO-III level

64

C -2.67201 -2.22598 -0.31674

C -3.37269 -2.04059 1.01697

C -3.38185 -3.20840 -1.23044

H -2.83168 -3.34418 -2.16024

H -4.36773 -2.80899 -1.46523

H -3.51552 -4.17982 -0.75635

C -0.97964 -3.83369 0.46234

H -1.81100 -4.46883 0.71564

C 0.35849 -4.16103 0.67122

H 0.58981 -5.12769 1.09731

C 1.37413 -3.28576 0.34552

H 2.40373 -3.57519 0.50241

C 1.08224 -2.00100 -0.23976

C -0.30658 -1.75512 -0.44765

H -0.67317 -0.82604 -0.86794

C 3.26610 -1.11818 -0.28467

C 4.23037 -0.70079 -1.22178

H 3.89280 -0.46795 -2.22457

C 5.57573 -0.59136 -0.88129

H 6.29177 -0.27419 -1.62889

C 6.00334 -0.89266 0.41251

H 7.04792 -0.80907 0.67890

C 5.06349 -1.30645 1.35741

H 5.37683 -1.53309 2.36870

C 3.71801 -1.41648 1.01712

H 2.99616 -1.69937 1.77362

N -1.25930 -2.63403 -0.09895

N 1.92787 -1.06525 -0.64816

H -4.34987 -1.58962 0.84288

H -2.80274 -1.36782 1.65547

H -3.51018 -2.99209 1.53106

H -2.60069 -1.25864 -0.80763

C 2.67238 2.22495 -0.31504

C 3.37287 2.04224 1.01905

C 3.38245 3.20518 -1.23084

H 2.83212 3.33938 -2.16073

H 4.36800 2.80489 -1.46515

H 3.51695 4.17757 -0.75873

C 0.97971 3.83536 0.45749

H 1.81082 4.47210 0.70769

C -0.35861 4.16300 0.66560

H -0.59029 5.13126 1.08771

C -1.37391 3.28592 0.34390

H -2.40349 3.57585 0.49951

C -1.08179 1.99937 -0.23731

C 0.30730 1.75238 -0.44293

H 0.67433 0.82169 -0.85914

C -3.26612 1.11746 -0.28280

C -4.22933 0.69906 -1.22050

H -3.89054 0.46409 -2.22240

C -5.57524 0.59114 -0.88169

H -6.29042 0.27325 -1.62969

C -6.00435 0.89536 0.41092

H -7.04939 0.81288 0.67603

C -5.06565 1.31007 1.35631

H -5.38031 1.53903 2.36672

C -3.71972 1.41869 1.01780

H -2.99863 1.70279 1.77470

N 1.25969 2.63329 -0.09842

N -1.92744 1.06292 -0.64421

H 4.35024 1.59127 0.84614

H 2.80295 1.37046 1.65875

H 3.50979 2.99475 1.53146

H 2.60123 1.25662 -0.80415

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 119.2683 Anisotropy = 62.9990

XX= 148.1420 YX= -25.8993 ZX= 11.8685

XY= -22.8774 YY= 108.5802 ZY= -0.8768

XZ= 7.3546 YZ= -2.9939 ZZ= 101.0826

Eigenvalues: 95.5704 100.9668 161.2676

2 C Isotropic = 161.5986 Anisotropy = 32.8994

XX= 157.5056 YX= -4.7127 ZX= -11.6459

XY= -6.5697 YY= 153.1434 ZY= 5.2002

XZ= -13.2829 YZ= 9.3568 ZZ= 174.1470

Eigenvalues: 149.1411 152.1233 183.5316

3 C Isotropic = 163.5190 Anisotropy = 33.0711

XX= 160.0226 YX= 5.6723 ZX= 9.6426

XY= 6.8226 YY= 162.7520 ZY= 17.4173

XZ= 9.5956 YZ= 12.6023 ZZ= 167.7824

Eigenvalues: 149.7061 155.2845 185.5664

4 H Isotropic = 30.4379 Anisotropy = 8.8621

XX= 27.9956 YX= 0.4287 ZX= -1.2873

XY= 0.1437 YY= 28.4853 ZY= 4.4160

XZ= -0.7073 YZ= 2.2690 ZZ= 34.8328

Eigenvalues: 26.6991 28.2686 36.3460

5 H Isotropic = 30.5471 Anisotropy = 8.3251

XX= 34.0581 YX= -1.8131 ZX= 3.6191

XY= -0.8263 YY= 29.9628 ZY= 2.0633

XZ= 4.4709 YZ= 0.0806 ZZ= 27.6205

Eigenvalues: 25.1708 30.3734 36.0972

6 H Isotropic = 30.4934 Anisotropy = 8.5246

XX= 28.3645 YX= 2.1048 ZX= 0.6031

XY= 2.0871 YY= 35.5853 ZY= -1.1984

XZ= 2.0892 YZ= -0.5084 ZZ= 27.5303

Eigenvalues: 26.1254 29.1784 36.1764

7 C Isotropic = 63.2489 Anisotropy = 136.0002

XX= 24.8484 YX= -31.4011 ZX= 8.8533

XY= -38.7156 YY= 30.6196 ZY= 54.0757

XZ= 9.6326 YZ= 43.8723 ZZ= 134.2788

Eigenvalues: -18.6889 54.5200 153.9157

8 H Isotropic = 24.8439 Anisotropy = 9.1959

XX= 25.8895 YX= -3.8227 ZX= 2.0662

XY= -2.9190 YY= 26.7975 ZY= -2.3565

XZ= 1.5035 YZ= -3.4057 ZZ= 21.8448

Eigenvalues: 20.5087 23.0486 30.9745

9 C Isotropic = 49.6465 Anisotropy = 181.0603

XX= 32.0691 YX= 22.2813 ZX= -15.7849

XY= 27.9787 YY= -17.4395 ZY= 83.1963

XZ= -13.1831 YZ= 81.1417 ZZ= 134.3100

Eigenvalues: -62.2254 40.8115 170.3534

10 H Isotropic = 24.4941 Anisotropy = 4.4516

XX= 27.1305 YX= 1.0415 ZX= -0.1574

XY= 0.8870 YY= 24.6552 ZY= -1.0822

XZ= 0.6678 YZ= -0.5240 ZZ= 21.6967

Eigenvalues: 21.4497 24.5708 27.4618

11 C Isotropic = 56.2273 Anisotropy = 183.0579

XX= -32.7178 YX= -0.3093 ZX= -13.2317

XY= 24.7768 YY= 67.1101 ZY= 52.1475

XZ= 5.0435 YZ= 87.5860 ZZ= 134.2897

Eigenvalues: -35.4420 25.8580 178.2659

12 H Isotropic = 23.6244 Anisotropy = 10.7680

XX= 23.3491 YX= 5.3695 ZX= -0.4549

XY= 5.5249 YY= 25.9608 ZY= -2.0557

XZ= 1.1864 YZ= -4.1164 ZZ= 21.5633

Eigenvalues: 17.6748 22.3953 30.8031

13 C Isotropic = 20.6231 Anisotropy = 160.7487

XX= -47.6296 YX= 4.1755 ZX= -16.0909

XY= -6.1303 YY= 7.5576 ZY= 50.7940

XZ= -2.5430 YZ= 59.5206 ZZ= 101.9413

Eigenvalues: -48.3741 -17.5456 127.7889

14 C Isotropic = 36.5451 Anisotropy = 126.0521

XX= 25.4338 YX= 4.9626 ZX= -8.3457

XY= -6.5737 YY= -18.0213 ZY= 62.3009

XZ= -12.9516 YZ= 35.0692 ZZ= 102.2227

Eigenvalues: -35.3913 24.4466 120.5798

15 H Isotropic = 21.3631 Anisotropy = 9.2402

XX= 27.2598 YX= 1.6449 ZX= -1.0955

XY= 0.3303 YY= 22.4110 ZY= 0.6454

XZ= -0.6823 YZ= -1.5326 ZZ= 14.4186

Eigenvalues: 14.3398 22.2263 27.5233

16 C Isotropic = 19.5570 Anisotropy = 183.5801

XX= -67.5587 YX= -24.9612 ZX= -16.6489

XY= -14.8392 YY= 127.9586 ZY= 40.8399

XZ= -14.9040 YZ= 39.1887 ZZ= -1.7290

Eigenvalues: -71.7819 -11.4908 141.9437

17 C Isotropic = 51.5598 Anisotropy = 157.9507

XX= 39.0661 YX= -11.2395 ZX= -26.9447

XY= -18.2293 YY= 141.4586 ZY= 42.5942

XZ= -31.7009 YZ= 47.6049 ZZ= -25.8454

Eigenvalues: -44.7880 42.6071 156.8603

18 H Isotropic = 24.5193 Anisotropy = 5.7198

XX= 27.5634 YX= 0.6388 ZX= -2.0894

XY= 0.1236 YY= 22.9984 ZY= 0.7059

XZ= -1.9523 YZ= 0.5599 ZZ= 22.9960

Eigenvalues: 21.7915 23.4339 28.3325

19 C Isotropic = 45.7837 Anisotropy = 191.1595

XX= -5.5681 YX= -41.5922 ZX= 45.8396

XY= -40.5185 YY= 152.6391 ZY= 49.8206

XZ= 41.4791 YZ= 57.9143 ZZ= -9.7198

Eigenvalues: -71.6072 35.7351 173.2234

20 H Isotropic = 23.9525 Anisotropy = 4.5938

XX= 26.1786 YX= -0.7494 ZX= 1.5756

XY= -0.5689 YY= 21.7950 ZY= -0.7374

XZ= 1.3506 YZ= -0.2358 ZZ= 23.8839

Eigenvalues: 21.6563 23.1861 27.0150

21 C Isotropic = 59.6310 Anisotropy = 174.8069

XX= -35.1598 YX= -26.5465 ZX= -25.9517

XY= -27.7987 YY= 164.5507 ZY= 26.0398

XZ= -30.9437 YZ= 29.8260 ZZ= 49.5020

Eigenvalues: -45.4362 48.1602 176.1689

22 H Isotropic = 24.5674 Anisotropy = 2.7920

XX= 25.6110 YX= -0.1131 ZX= -0.1656

XY= -0.2098 YY= 22.3755 ZY= -1.7957

XZ= -0.2725 YZ= -1.5352 ZZ= 25.7156

Eigenvalues: 21.6732 25.6002 26.4287

23 C Isotropic = 47.4857 Anisotropy = 189.4365

XX= 31.5796 YX= -13.7249 ZX= -33.6277

XY= -10.8025 YY= 158.6417 ZY= 49.2148

XZ= -30.3096 YZ= 55.1350 ZZ= -47.7642

Eigenvalues: -68.3205 37.0010 173.7767

24 H Isotropic = 24.1325 Anisotropy = 4.6892

XX= 27.1557 YX= 0.5328 ZX= -0.3430

XY= 0.9029 YY= 22.2038 ZY= -1.1946

XZ= 0.5857 YZ= -1.3888 ZZ= 23.0380

Eigenvalues: 21.1918 23.9470 27.2586

25 C Isotropic = 59.1605 Anisotropy = 179.7670

XX= -4.3430 YX= -34.8110 ZX= 20.8525

XY= -4.1090 YY= 159.2900 ZY= 52.8725

XZ= 52.1678 YZ= 57.5100 ZZ= 22.5346

Eigenvalues: -41.8195 40.2959 179.0052

26 H Isotropic = 23.8149 Anisotropy = 9.0015

XX= 26.8777 YX= 0.9110 ZX= 5.1710

XY= 1.3932 YY= 22.5709 ZY= -1.2908

XZ= 4.3846 YZ= -1.2843 ZZ= 21.9962

Eigenvalues: 18.3810 23.2479 29.8159

27 N Isotropic = -3.3072 Anisotropy = 302.6991

XX= -137.1322 YX= 27.6177 ZX= -27.1189

XY= 9.8727 YY= -25.5805 ZY= 102.8728

XZ= -16.8888 YZ= 98.2888 ZZ= 152.7911

Eigenvalues: -146.5832 -61.8306 198.4922

28 N Isotropic = 36.7686 Anisotropy = 246.6538

XX= -112.0791 YX= -66.2107 ZX= -22.4079

XY= 20.6311 YY= 100.9642 ZY= 67.6283

XZ= 56.1829 YZ= 111.1866 ZZ= 121.4207

Eigenvalues: -117.8388 26.9402 201.2045

29 H Isotropic = 32.1179 Anisotropy = 11.9210

XX= 33.6371 YX= -5.0867 ZX= -0.4734

XY= -5.0676 YY= 36.0247 ZY= -1.7365

XZ= -1.9225 YZ= -1.4220 ZZ= 26.6919

Eigenvalues: 25.7272 30.5613 40.0653

30 H Isotropic = 31.0049 Anisotropy = 5.6469

XX= 28.3742 YX= 0.6680 ZX= 0.8521

XY= -1.5223 YY= 33.1462 ZY= 1.1542

XZ= 0.7288 YZ= 3.4536 ZZ= 31.4944

Eigenvalues: 27.9570 30.2882 34.7696

31 H Isotropic = 30.9815 Anisotropy = 8.3559

XX= 28.5749 YX= 0.6083 ZX= -2.0413

XY= -0.6695 YY= 33.4117 ZY= -3.1866

XZ= -3.1005 YZ= -4.5702 ZZ= 30.9578

Eigenvalues: 26.1400 30.2523 36.5520

32 H Isotropic = 26.6736 Anisotropy = 9.0793

XX= 26.0851 YX= -1.0429 ZX= 0.1850

XY= -1.5051 YY= 32.1571 ZY= -0.8559

XZ= 0.2111 YZ= -2.8399 ZZ= 21.7786

Eigenvalues: 21.4593 25.8350 32.7265

33 C Isotropic = 119.3047 Anisotropy = 62.9867

XX= 148.1687 YX= -25.8996 ZX= -11.8351

XY= -22.9086 YY= 108.6640 ZY= 0.8396

XZ= -7.2872 YZ= 2.9436 ZZ= 101.0815

Eigenvalues: 95.6008 101.0176 161.2959

34 C Isotropic = 161.5769 Anisotropy = 32.8941

XX= 157.4882 YX= -4.6949 ZX= 11.6498

XY= -6.5099 YY= 153.0974 ZY= -5.1139

XZ= 13.3236 YZ= -9.3449 ZZ= 174.1451

Eigenvalues: 149.1340 152.0903 183.5063

35 C Isotropic = 163.5369 Anisotropy = 33.0424

XX= 160.0332 YX= 5.6387 ZX= -9.6496

XY= 6.7639 YY= 162.7121 ZY= -17.3992

XZ= -9.5819 YZ= -12.6011 ZZ= 167.8655

Eigenvalues: 149.7231 155.3224 185.5652

36 H Isotropic = 30.4414 Anisotropy = 8.8589

XX= 27.9975 YX= 0.4277 ZX= 1.2884

XY= 0.1384 YY= 28.4807 ZY= -4.4030

XZ= 0.7058 YZ= -2.2555 ZZ= 34.8461

Eigenvalues: 26.7091 28.2678 36.3473

37 H Isotropic = 30.5509 Anisotropy = 8.3179

XX= 34.0548 YX= -1.8290 ZX= -3.6159

XY= -0.8423 YY= 29.9770 ZY= -2.0614

XZ= -4.4675 YZ= -0.0768 ZZ= 27.6210

Eigenvalues: 25.1715 30.3851 36.0962

38 H Isotropic = 30.4927 Anisotropy = 8.5293

XX= 28.3678 YX= 2.1050 ZX= -0.6050

XY= 2.0837 YY= 35.5901 ZY= 1.1851

XZ= -2.0898 YZ= 0.4966 ZZ= 27.5203

Eigenvalues: 26.1245 29.1748 36.1789

39 C Isotropic = 63.2510 Anisotropy = 136.0120

XX= 24.8794 YX= -31.4709 ZX= -8.6563

XY= -38.7729 YY= 30.0993 ZY= -53.6145

XZ= -9.3861 YZ= -43.3028 ZZ= 134.7744

Eigenvalues: -18.6958 54.5231 153.9257

40 H Isotropic = 24.8442 Anisotropy = 9.1970

XX= 25.8919 YX= -3.8267 ZX= -2.0573

XY= -2.9224 YY= 26.8172 ZY= 2.3410

XZ= -1.4972 YZ= 3.3899 ZZ= 21.8233

Eigenvalues: 20.5056 23.0514 30.9755

41 C Isotropic = 49.6288 Anisotropy = 181.0743

XX= 32.0602 YX= 22.3451 ZX= 15.7794

XY= 28.0470 YY= -18.1414 ZY= -82.5555

XZ= 13.1478 YZ= -80.5447 ZZ= 134.9677

Eigenvalues: -62.2778 40.8192 170.3450

42 H Isotropic = 24.4951 Anisotropy = 4.4537

XX= 27.1315 YX= 1.0451 ZX= 0.1517

XY= 0.8869 YY= 24.6593 ZY= 1.0704

XZ= -0.6731 YZ= 0.5153 ZZ= 21.6944

Eigenvalues: 21.4521 24.5689 27.4642

43 C Isotropic = 56.2518 Anisotropy = 183.0736

XX= -32.7059 YX= -0.2180 ZX= 13.3264

XY= 24.8950 YY= 66.6614 ZY= -51.9253

XZ= -5.4690 YZ= -87.3423 ZZ= 134.7998

Eigenvalues: -35.4383 25.8928 178.3008

44 H Isotropic = 23.6270 Anisotropy = 10.7752

XX= 23.3540 YX= 5.3693 ZX= 0.4373

XY= 5.5333 YY= 25.9816 ZY= 2.0519

XZ= -1.2201 YZ= 4.1054 ZZ= 21.5454

Eigenvalues: 17.6642 22.4063 30.8105

45 C Isotropic = 20.5923 Anisotropy = 160.7525

XX= -47.6624 YX= 4.3378 ZX= 15.8637

XY= -6.0693 YY= 7.1641 ZY= -50.5722

XZ= 2.4250 YZ= -59.1712 ZZ= 102.2753

Eigenvalues: -48.3881 -17.5955 127.7607

46 C Isotropic = 36.5430 Anisotropy = 126.0334

XX= 25.3593 YX= 4.9923 ZX= 8.2527

XY= -6.4255 YY= -18.3245 ZY= -61.6361

XZ= 12.5953 YZ= -34.9003 ZZ= 102.5941

Eigenvalues: -35.3566 24.4203 120.5652

47 H Isotropic = 21.3622 Anisotropy = 9.2267

XX= 27.2516 YX= 1.6398 ZX= 1.0772

XY= 0.3166 YY= 22.4417 ZY= -0.6174

XZ= 0.6934 YZ= 1.5751 ZZ= 14.3935

Eigenvalues: 14.3119 22.2615 27.5134

48 C Isotropic = 19.5557 Anisotropy = 183.6093

XX= -67.6351 YX= -24.7599 ZX= 16.5402

XY= -14.6314 YY= 127.8372 ZY= -41.1413

XZ= 14.8125 YZ= -39.5038 ZZ= -1.5350

Eigenvalues: -71.7819 -11.5130 141.9619

49 C Isotropic = 51.5753 Anisotropy = 157.9180

XX= 39.0080 YX= -11.0478 ZX= 27.0214

XY= -18.0229 YY= 141.3125 ZY= -42.9443

XZ= 31.7702 YZ= -47.9390 ZZ= -25.5946

Eigenvalues: -44.7742 42.6462 156.8540

50 H Isotropic = 24.5190 Anisotropy = 5.7202

XX= 27.5588 YX= 0.6339 ZX= 2.0921

XY= 0.1210 YY= 22.9991 ZY= -0.7104

XZ= 1.9610 YZ= -0.5576 ZZ= 22.9990

Eigenvalues: 21.7906 23.4339 28.3324

51 C Isotropic = 45.7935 Anisotropy = 191.1625

XX= -5.4854 YX= -41.4787 ZX= -45.7944

XY= -40.4167 YY= 152.5078 ZY= -50.1553

XZ= -41.4596 YZ= -58.2448 ZZ= -9.6419

Eigenvalues: -71.6107 35.7561 173.2352

52 H Isotropic = 23.9523 Anisotropy = 4.6022

XX= 26.1865 YX= -0.7568 ZX= -1.5732

XY= -0.5780 YY= 21.7972 ZY= 0.7422

XZ= -1.3484 YZ= 0.2416 ZZ= 23.8731

Eigenvalues: 21.6551 23.1814 27.0204

53 C Isotropic = 59.6612 Anisotropy = 174.7534

XX= -35.2440 YX= -26.3083 ZX= 25.8471

XY= -27.5009 YY= 164.4808 ZY= -26.3459

XZ= 30.8013 YZ= -30.0904 ZZ= 49.7467

Eigenvalues: -45.3769 48.1970 176.1635

54 H Isotropic = 24.5685 Anisotropy = 2.7914

XX= 25.6129 YX= -0.1155 ZX= 0.1629

XY= -0.2068 YY= 22.3804 ZY= 1.8002

XZ= 0.2666 YZ= 1.5430 ZZ= 25.7123

Eigenvalues: 21.6728 25.6033 26.4295

55 C Isotropic = 47.5218 Anisotropy = 189.3839

XX= 31.5231 YX= -13.4948 ZX= 33.7022

XY= -10.5857 YY= 158.4582 ZY= -49.6452

XZ= 30.3971 YZ= -55.5629 ZZ= -47.4157

Eigenvalues: -68.2549 37.0426 173.7778

56 H Isotropic = 24.1327 Anisotropy = 4.6878

XX= 27.1563 YX= 0.5309 ZX= 0.3438

XY= 0.8950 YY= 22.2024 ZY= 1.2018

XZ= -0.5822 YZ= 1.3896 ZZ= 23.0393

Eigenvalues: 21.1888 23.9514 27.2579

57 C Isotropic = 59.1520 Anisotropy = 179.6791

XX= -4.2440 YX= -34.7000 ZX= -20.8685

XY= -4.1525 YY= 159.0610 ZY= -53.0039

XZ= -52.2008 YZ= -57.7974 ZZ= 22.6389

Eigenvalues: -41.8129 40.3307 178.9381

58 H Isotropic = 23.8180 Anisotropy = 8.9972

XX= 26.8872 YX= 0.8929 ZX= -5.1640

XY= 1.3763 YY= 22.5713 ZY= 1.2883

XZ= -4.3797 YZ= 1.2874 ZZ= 21.9954

Eigenvalues: 18.3937 23.2441 29.8161

59 N Isotropic = -3.3014 Anisotropy = 302.7157

XX= -137.1961 YX= 27.7076 ZX= 27.1577

XY= 9.9506 YY= -26.4221 ZY= -102.0538

XZ= 16.8653 YZ= -97.4474 ZZ= 153.7140

Eigenvalues: -146.6532 -61.7601 198.5091

60 N Isotropic = 36.6429 Anisotropy = 246.8759

XX= -112.3119 YX= -65.9735 ZX= 22.2094

XY= 20.7780 YY= 100.5793 ZY= -67.4691

XZ= -56.8652 YZ= -111.4787 ZZ= 121.6614

Eigenvalues: -118.1223 26.8242 201.2268

61 H Isotropic = 32.1156 Anisotropy = 11.9112

XX= 33.6372 YX= -5.0928 ZX= 0.4817

XY= -5.0597 YY= 36.0137 ZY= 1.7390

XZ= 1.9381 YZ= 1.3971 ZZ= 26.6960

Eigenvalues: 25.7286 30.5619 40.0564

62 H Isotropic = 31.0033 Anisotropy = 5.6325

XX= 28.3760 YX= 0.6678 ZX= -0.8501

XY= -1.5126 YY= 33.1253 ZY= -1.1440

XZ= -0.7214 YZ= -3.4592 ZZ= 31.5087

Eigenvalues: 27.9645 30.2871 34.7583

63 H Isotropic = 30.9813 Anisotropy = 8.3576

XX= 28.5719 YX= 0.6100 ZX= 2.0374

XY= -0.6612 YY= 33.4240 ZY= 3.1873

XZ= 3.1018 YZ= 4.5620 ZZ= 30.9481

Eigenvalues: 26.1412 30.2497 36.5530

64 H Isotropic = 26.6732 Anisotropy = 9.1066

XX= 26.0816 YX= -1.0454 ZX= -0.1876

XY= -1.5193 YY= 32.1750 ZY= 0.8460

XZ= -0.2129 YZ= 2.8393 ZZ= 21.7630

Eigenvalues: 21.4465 25.8289 32.7442

# References

[1] D. V. Waterhous, D. D. Muccio, *Magn. Reson. Chem.* **1990**, *28*, 223-226.

[2] M. Suenaga, *J. Comput. Chem Jpn.* **2005**, *4*, 25-32.

[3] <http://jmol.sourceforge.net/> ed.