**Supplementary Information**

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

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

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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

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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

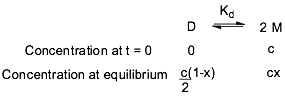
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**VT NMR:** NMR data were acquired in tubes sealed with a Young’s Teflon stopcock. Samples were prepared by extracting (*via* microsyringe) a known volume from thf-d8 stock solutions of **1** (26.9 mM (3.4 mg in 0.6 mL)) and **2** (120 mM (15.3 mg 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



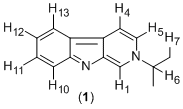
Under fast exchange the observed chemical shift of H(1) (obs) is a number weighted average of the dimer (D) and monomer (M) chemical shift.



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.

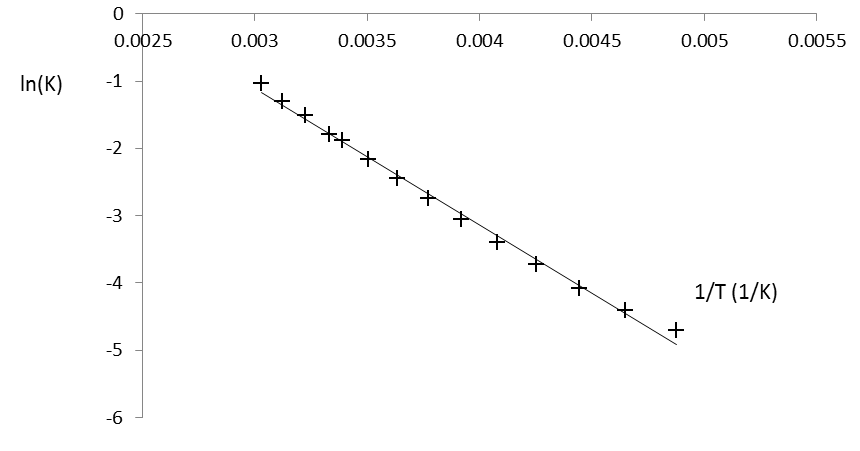




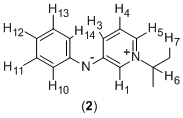
# Fig. S1 VT NMR of 1 in thf-d8 (13.5 mM)



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

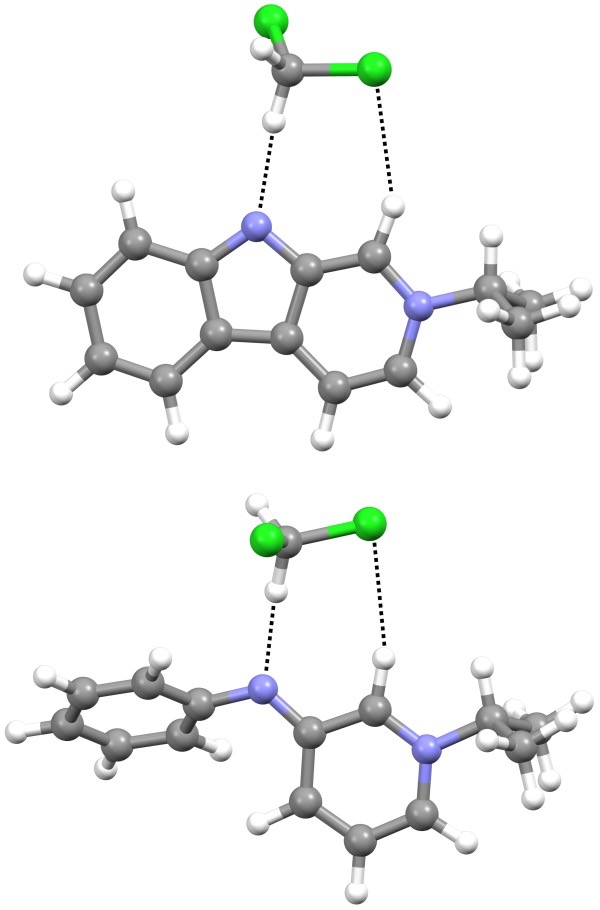


Fig. S8. Optimised structures of **1**.CH2Cl2 and **2**.CH2Cl2 (at the (RI-)PBE0/def2-TZVPP level), where each substrate forms two hydrogen bonding interactions (C-H…N and C-H…Cl) to a molecule of CH2Cl2 to form a 7-membered ring structure. The C-H…N bonds in these structures (3.25 and 3.23 Å for the 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

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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:

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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

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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

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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:

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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

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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

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9 a 30.13 1.76802 YES YES

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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

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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:

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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

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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

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