Supporting information for:

Approaching the Hartree-Fock Limit Through the CABS Singles Correction and Auxiliary Basis Sets

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VnZ-F12/OptRI+ ABSs (n =D, T, Q) in MOLPRO Format

VDZ-F12/OptRI+

Hydrogen

spd, H, vdz-f12/optri
s, H, 1.88958225E+02, 1.19139490E+01

Helium

spd, He, vdz-f12/optri
s, He, 1.53254776E+03, 4.44924927E+02

Lithium

spdfg, Li, vdz-f12/optri
s, Li, 8.79687500E-02, 1.15820300E-02

Beryllium

spdfg, Be, vdz-f12/optri
s, Be, 6.20038600E-01, 4.22988600E-02

Boron

spdfg, B, vdz-f12/optri
s, B, 1.22111330E+01
p, B, 3.33423281E+01, 7.23665237E+00

Carbon

spdfg, C, vdz-f12/optri
s, C, 1.27500000E+00
p, C, 7.12736930E+01, 8.58446662E+00

Nitrogen

spdfg, N, vdz-f12/optri

s, N, 1.67093750E-01

p, N, 1.01595821E+02, 1.23743305E+01

Oxygen

spdfg, O, vdz-f12/optri

s, O, 2.15000000E-01

p, O, 1.07012096E+02, 1.93073067E+01

Fluorine

spdfg, F, vdz-f12/optri

s, F, 1.97500000E-01

p, F, 1.69144542E+02, 2.03049664E+01

Neon

spdfg, Ne, vdz-f12/optri

s, Ne, 4.07531250E+00

p, Ne, 1.99543177E+02, 2.61472558E+01

Sodium

spdfg, Na, vdz-f12/optri

s, Na, 8.64599370E-01, 3.67064900E-02

Magnesium

spdfg, Mg, vdz-f12/optri

s, Mg, 6.23168950E-01, 1.59001460E-01

Aluminium

spdfg, Al, vdz-f12/optri

s, Al, 8.34335940E-01

p, Al, 8.94738350E+00, 5.61410590E-01

Silicon

spdfg, Si, vdz-f12/optri
s, Si, 2.07812500E+00
p, Si, 1.43807876E+00, 6.16464840E-01

Phosphorous

spdfg, P, vdz-f12/optri
s, P, 2.62500000E+00
p, P, 2.93554115E+00, 1.61883260E-01

Sulfur

spdfg, S, vdz-f12/optri
s, S, 2.16709375E+00
p, S, 3.28315400E+00, 1.53598140E-01

Chlorine

spdfg, Cl, vdz-f12/optri
s, Cl, 4.52734375E+00
p, Cl, 2.48663783E+00, 1.82130400E-01

Argon

spdfg, Ar, vdz-f12/optri
s, Ar, 4.53125000E+00
p, Ar, 4.31267379E+00, 2.24786340E-01

VTZ-F12/OptRI+

Hydrogen

spdf, H, vtz-f12/optri
s, H, 5.54296875E+02, 1.63720703E+02

Helium

spdf, He, vtz-f12/optri
s, He, 4.25791626E+04, 4.85682137E+03

Lithium

spdfg, Li, vtz-f12/optri
s, Li, 8.60937500E-01, 1.77812500E-01

Beryllium

spdfg, Be, vtz-f12/optri
s, Be, 4.57321780E-01, 8.71118200E-02

Boron

spdfg, B, vtz-f12/optri
s, B, 8.18750000E-01
p, B, 8.93880930E+01 1.00070847E+01

Carbon

spdfg, C, vtz-f12/optri
s, C, 1.26875000E+00
p, C, 1.42117850E+02, 1.52888249E+01

Nitrogen

spdfg, N, vtz-f12/optri
s, N, 8.07812500E-01
p, N, 3.12951924E+02, 7.19422904E+00

Oxygen

spdfg, O, vtz-f12/optri
s, O, 1.11250000E+00
p, O, 2.62571009E+02, 2.82732220E+01

Fluorine

spdfg, F, vtz-f12/optri
s, F, 9.34375000E-01
p, F, 3.22111801E+02, 3.63535585E+01

Neon

spdfg, Ne, vtz-f12/optri
s, Ne, 4.00000000E+00
p, Ne, 6.31497291E+02, 9.93292809E+00

Sodium

spdfg, Na, vtz-f12/optri
s, Na, 9.80660200E-02, 7.41110000E-03

Magnesium

spdfg, Mg, vtz-f12/optri
s, Mg, 5.86105720E-01, 3.47512010E-01

Aluminium

spdfg, Al, vtz-f12/optri
s, Al, 1.40000000E+00
p, Al, 6.66394790E-01, 8.47839900E-02

Silicon

spdfg, Si, vtz-f12/optri
s, Si, 8.25000000E-01
p, Si, 6.29579600E-01, 1.14727890E-01

Phosphorous

spdfg, P, vtz-f12/optri
s, P, 1.03183594E+00
p, P, 8.68517180E-01, 8.71428571E-02

Sulfur

spdfg, S, vtz-f12/optri
s, S, 1.22500000E+00
p, S, 8.69031840E-01, 1.16732300E-01

Chlorine

spdfg, Cl, vtz-f12/optri
s, Cl, 1.43750000E+00
p, Cl, 1.00922971E+00, 6.86495000E-02

Argon

spdfg, Ar, vtz-f12/optri
s, Ar, 1.70000000E+00
p, Ar, 1.15647888E+00, 8.13977100E-02

VQZ-F12/OptRI+

Hydrogen

spdfg, H, vqz-f12/optri
s, H, 4.43041992E+03, 2.63564453E+02

Helium

spdfg, He, vqz-f12/optri
s, He, 7.85156250E+03, 2.18847656E+03

Lithium

spdfgh, Li, vqz-f12/optri
s, Li, 1.40625000E-01, 9.61875000E-03

Beryllium

spdfgh, Be, vqz-f12/optri
s, Be, 2.05100000E-01, 9.14332000E-03

Boron

spdfgh, B, vqz-f12/optri
s, B, 4.00000000E+00
p, B, 3.96421875E+02, 1.10332031E+01

Carbon

spdfgh, C, vqz-f12/optri
s, C, 1.24843750E-01
p, C, 5.90986328E+02, 1.71396484E+01

Nitrogen

spdfgh, N, vqz-f12/optri
s, N, 9.50000000E-02
p, N, 9.53906250E+02, 4.59062500E+00

Oxygen

spdfgh, O, vqz-f12/optri
s, O, 1.05000000E-01
p, O, 1.28904383E+03, 1.08109380E+01

Fluorine

spdfgh, F, vqz-f12/optri
s, F, 9.22753910E-01
p, F, 1.60001887E+03, 8.92267546E+00

Neon

spdfgh, Ne, vqz-f12/optri
s, Ne, 1.75000000E-01
p, Ne, 1.98167868E+03, 1.14522548E+01

Sodium

spdfgh, Na, vqz-f12/optri
s, Na, 1.65575700E-01, 3.99890000E-02

Magnesium

spdfgh, Mg, vqz-f12/optri
s, Mg, 6.71549200E-02, 7.71279000E-03

Aluminium

spdfgh, Al, vqz-f12/optri
s, Al, 1.02187500E-01
p, Al, 9.00239920E-01, 1.19556390E-01

Silicon

spdfgh, Si, vqz-f12/optri
s, Si, 1.97382812E+00
p, Si, 4.34663130E-01, 9.86530100E-02

Phosphorous

spdfgh, P, vqz-f12/optri
s, P, 1.55156250E+00
p, P, 8.20601320E-01, 1.26218280E-01

Sulfur

spdfgh, S, vqz-f12/optri
s, S, 1.80000000E+00
p, S, 5.95339020E-01, 2.23235790E-01

Chlorine

spdfgh, Cl, vqz-f12/optri
s, Cl, 2.15000000E+00
p, Cl, 4.97312940E-01, 1.67328990E-01

Argon

spdfgh, Ar, vqz-f12/optri
s, Ar, 1.97343750E+00
p, Ar, 6.11229680E-01, 1.95179140E-01

CCSD(T)/cc-pCVTZ Optimised Geometries for Group B Molecules

All coordinates are given in xyz format, in Angstrom.

CCl_2

CCSD(T)/CC-PCVTZ ENERGY=-957.39726052

C 0.0000000000 0.0000000000 -0.8539018056
Cl 0.0000000000 1.4063883802 0.1446452287
Cl 0.0000000000 -1.4063883802 0.1446452287

CClN

CCSD(T)/CC-PCVTZ ENERGY=-552.40717745

C 0.0000000000 -0.0000016535 -0.6801469737
Cl 0.0000000000 0.0000002326 0.9591116919
N 0.0000000000 0.0000008291 -1.8444131388

CH_2S

CCSD(T)/CC-PCVTZ ENERGY=-436.93983717

C 0.0000000000 0.0000012481 -1.1002860045
S 0.0000000000 0.0000007578 0.5175669632
H 0.0000000000 0.9229557052 -1.6755604066
H 0.0000000000 -0.9229946822 -1.6754938627

SiH_2

CCSD(T)/CC-PCVTZ ENERGY=-290.17251268

Si 0.0000000000 0.0000000000 -0.0704224494
H 0.0000000000 1.0964328130 0.9811346428
H 0.0000000000 -1.0964328130 0.9811346428

SiH_4

CCSD(T)/CC-PCVTZ ENERGY=-291.44025487

Si 0.0000000732 0.0000004227 -0.0000065945
H 0.0071862710 0.0555852411 1.4787710034
H 1.2407917082 0.6141404879 -0.5226848859
H -0.0754965990 -1.4108428386 -0.4401725199
H -1.1724834190 0.7411053304 -0.5157298477

SiHF

CCSD(T)/CC-PCVTZ ENERGY=-389.39671991

Si 0.0000000000 -0.0602881770 -0.6307117405
F 0.0000000000 0.0123129607 0.9795428020
H 0.0000000000 1.4478014611 -0.8888369555

SiHN

CCSD(T)/CC-PCVTZ ENERGY=-344.20576503

Si 0.0000000000 -0.0000009665 -0.4806612399
N 0.0000000000 0.0000009375 1.1053166202
H 0.0000000000 0.0000139042 -1.9666121505

$cis-H_2P_2$

CCSD(T)/CC-PCVTZ ENERGY=-682.99150055

P 0.0000000000 -1.0265932986 -0.0442247753
P 0.0000000000 1.0265932986 -0.0442247753
H 0.0000000000 -1.2452350960 1.3590169811
H 0.0000000000 1.2452350960 1.3590169811

CS_2

CCSD(T)/CC-PCVTZ ENERGY=-833.51733614

C 0.0000000000 -0.0000005987 0.0000000000
S 0.0000000000 0.0000001122 1.5609946759
S 0.0000000000 0.0000001122 -1.5609946759

CS

CCSD(T)/CC-PCVTZ ENERGY=-435.69816277

C 0.0000000000 0.0000000000 -1.1246850195
S 0.0000000000 0.0000000000 0.4213534551

Cl_2O

CCSD(T)/CC-PCVTZ ENERGY=-994.47192697

O 0.0000000000 0.0000000000 -0.7890499501

Cl 0.0000000000 1.4072170154 0.1780431243

Cl 0.0000000000 -1.4072170154 0.1780431243

Cl_2

CCSD(T)/CC-PCVTZ ENERGY=-919.43564066

Cl 0.0000000000 0.0000000000 -1.0037484281

Cl 0.0000000000 0.0000000000 1.0037484281

ClHO

CCSD(T)/CC-PCVTZ ENERGY=-535.40321497

O 0.0000000000 -0.0626557274 -1.1442594248

Cl 0.0000000000 0.0034813130 0.5557045330

H 0.0000000000 0.8721065279 -1.3829479615

ClH

CCSD(T)/CC-PCVTZ ENERGY=-460.34151872

H 0.0000000000 0.0000000000 -1.2396566626

Cl 0.0000000000 0.0000000000 0.0352438309

ClNO

CCSD(T)/CC-PCVTZ ENERGY=-589.45367898

N 0.0000000000 0.5307095520 -0.8395195494

O 0.0000000000 -0.3330781585 -1.5843793743

Cl 0.0000000000 -0.0593585534 1.0466820250

H_2S_2

CCSD(T)/CC-PCVTZ ENERGY=-796.67944710

S 1.0352918446 -0.0343159740 0.0285257621

S -1.0352918446 0.0343159740 0.0285257621

H 1.2518271068 0.9027003469 -0.9073317180

H -1.2518271068 -0.9027003469 -0.9073317180

H_2S

CCSD(T)/CC-PCVTZ ENERGY=-398.93922803

S 0.0000000000 0.0000000000 -0.0548483725
H 0.0000000000 0.9647540536 0.8722934008
H 0.0000000000 -0.9647540536 0.8722934008

HPO

CCSD(T)/CC-PCVTZ ENERGY=-416.61938037

P 0.0000000000 -0.0563374230 -0.4867384962
O 0.0000000000 0.0251724798 1.0010810671
H 0.0000000000 1.3316638361 -0.9331657253

iso−CClN

CCSD(T)/CC-PCVTZ ENERGY=-552.33787770

N 0.0000000000 -0.0000042105 -0.7091476384
Cl 0.0000000000 0.0000006995 0.9212190634
C 0.0000000000 0.0000028454 -1.8921955896

iso−CH_2S

CCSD(T)/CC-PCVTZ ENERGY=-436.86599161

C 0.0000000000 -0.1179279866 -1.1881041790
S 0.0000000000 0.0538588147 0.4668006564
H 0.0000000000 0.9368855122 -1.5254552609
H 0.0000000000 -1.2447218445 0.8356227819

iso−SiHN

CCSD(T)/CC-PCVTZ ENERGY=-344.31259639

N 0.0000000000 -0.0000004836 -0.9921791120
Si 0.0000000000 0.0000000943 0.5663234661
H 0.0000000000 0.0000040935 -1.9925020734

iso−H_2P_2

CCSD(T)/CC-PCVTZ ENERGY=-682.95636992

P 0.0000000000 0.0000000000 -0.9161389064
P 0.0000000000 0.0000000000 1.0332938640
H 0.0000000000 1.0970451108 -1.8000721954
H 0.0000000000 -1.0970451108 -1.8000721954

P_2O

CCSD(T)/CC-PCVTZ ENERGY=-756.92722052

P 0.0000000000 -0.0000002890 -0.4532953111
P 0.0000000000 0.0000001262 1.4498648899
O 0.0000000000 0.0000003151 -1.9292915332

PH_3

CCSD(T)/CC-PCVTZ ENERGY=-342.69575332

P -0.0000534660 -0.0681099898 -0.0000000000
H 1.1911195867 0.6969634889 -0.0000000000
H -0.5947382945 0.6980202679 1.0313219925
H -0.5947382945 0.6980202679 -1.0313219925

$trans-H_2P_2$

CCSD(T)/CC-PCVTZ ENERGY=-682.99695768

P 0.0000000000 -0.0515744134 -1.0203676959
P 0.0000000000 0.0515744134 1.0203676959
H 0.0000000000 1.3614116200 -1.1878477885
H 0.0000000000 -1.3614116200 1.1878477885

SiO

CCSD(T)/CC-PCVTZ ENERGY=-364.20248216

Si 0.0000000000 0.0000000000 -0.5516606033
O 0.0000000000 0.0000000000 0.9683903068

SiO_2

CCSD(T)/CC-PCVTZ ENERGY=-439.33734313

Si 0.0000000000 -0.0000007542 0.0000000000
O 0.0000000000 0.0000006619 1.5162936866
O 0.0000000000 0.0000006619 -1.5162936866

P_2

CCSD(T)/CC-PCVTZ ENERGY=-681.81210773

P 0.0000000000 0.0000000000 -0.9547754176
P 0.0000000000 0.0000000000 0.9547754176

Basis Set Compositions

Table S1: Compositions of the New[a] VnZ-F12/OptRI+ Sets and the Reference Even-Tempered RI and MP2FIT Sets

	H	He	Li - Be	B - Ne	Na-Mg	Al - Ar
DZ/OptRI+	$5s3p2d$	$6s4p2d$	$6s4p4d3f2g$	$5s6p4d3f1g$	$6s5p4d3f1g$	$5s6p4d3f1g$
TZ/OptRI+	$5s3p3d2f$	$6s3p3d2f$	$6s4p4d3f2g$	$5s6p4d3f2g$	$6s4p4d3f2g$	$5s6p4d3f2g$
QZ/OptRI+	$5s3p3d2f1g$	$6s3p3d2f1g$	$6s4p4d3f2g1h$	$5s6p4d3f2g1h$	$6s4p4d3f2g1h$	$5s6p4d3f2g1h$
Ref/MP2FIT	$24s18p14d12f10g8h6i$		$31s26p22d22f20g18h15i$		$32s27p23d20f18g17h15i$	
Ref/RI	$18s17p16d12f10g8h$		$18s17p16d12f10g8h7i$		$20s18p17d15f12g9h7i$	

[a] The original VnZ-F12/OptRI sets are the same, less $2s$ for H-Be, Na-Mg and $1s2p$ for B-Ne, Al-Ar.

Heats of Formation for Group A and B Molecules

Table S2: Reactions Used to Calculate Heats of Formation

Molecule	Reaction
FCN	$FCN + CO_2 \longrightarrow 2\,CO + 0.5\,N_2 + 0.5\,F_2$
iso-FCN	$iso-FCN + CO_2 \longrightarrow 2\,CO + 0.5\,N_2 + 0.5\,F_2$
CF_2	$CF_2{}^+CO_2 \longrightarrow 2\,CO^+F_2$
CHF	$CHF + CO_2 \longrightarrow 2\,CO + 0.5\,H_2 + 0.5\,F_2$
HCN	$HCN + CO_2 \longrightarrow 2\,CO + 0.5\,N_2 + 0.5\,H_2$
iso-HCN	$iso-HCN + CO_2 \longrightarrow 2\,CO + 0.5\,N_2 + 0.5\,H_2$
CH_2	$CH_2 + CO_2 \longrightarrow 2\,CO + H_2$
CH_2O	$CH_2O \longrightarrow CO + H_2$
$iso-CH_2O$	$iso-CH_2O \longrightarrow CO + H_2$
CH_4	$CH_4 + CO_2 \longrightarrow 2\,CO + 2\,H_2$
C_2H_2	$C_2H_2 + 2\,CO_2 \longrightarrow 4\,CO + H_2$
FH	$FH \longrightarrow 0.5\,F_2 + 0.5\,H_2$
FHO	$FHO + CO \longrightarrow CO_2 + 0.5\,F_2 + 0.5\,H_2$
FNO	$FNO + CO \longrightarrow CO_2 + 0.5\,F_2 + 0.5\,N_2$
F_2O	$F_2O + CO \longrightarrow CO_2 + F_2$
$cis-H_2N_2$	$cis-H_2N_2 \longrightarrow H_2 + N_2$
$trans-H_2N_2$	$trans-H_2N_2 \longrightarrow H_2 + N_2$
$iso-H_2N_2$	$iso-H_2N_2 \longrightarrow H_2 + N_2$
H_2O	$H_2O + CO \longrightarrow CO_2 + H_2$
H_2O_2	$H_2O_2 + 2\,CO \longrightarrow H_2 + 2\,CO_2$
HNO	$HNO + CO \longrightarrow CO_2 + 0.5\,H_2 + 0.5\,N_2$
NH_3	$NH_3 \longrightarrow 0.5\,N_2 + 1.5\,H_2$
N_2O	$N_2O + CO \longrightarrow CO_2 + N_2$

Molecule	Reaction
O_3	$O_3 + 3\,CO \longrightarrow 3\,CO_2$
CClN	$CClN + CO_2 \longrightarrow 2\,CO + 0.5\,N_2 + 0.5\,Cl_2$
iso−CClN	$\text{iso}-CClN + CO_2 \longrightarrow 2\,CO + 0.5\,N_2 + 0.5\,Cl_2$
CCl_2	$CCl_2 + CO_2 \longrightarrow 2\,CO + Cl_2$
SiHF	$SiHF + SiO_2 \longrightarrow 2\,SiO + 0.5\,H_2 + 0.5\,F_2$
SiHN	$SiHN + SiO_2 \longrightarrow 2\,SiO + 0.5\,N_2 + 0.5\,H_2$
iso−SiHN	$\text{iso}-SiHN + SiO_2 \longrightarrow 2\,SiO + 0.5\,N_2 + 0.5\,H_2$
SiH_2	$SiH_2 + SiO_2 \longrightarrow 2\,SiO + H_2$
CH_2S	$CH_2S \longrightarrow CS + H_2$
iso−CH_2S	$\text{iso}-CH_2S \longrightarrow CS + H_2$
SiH_4	$SiH_4 + SiO_2 \longrightarrow 2\,SiO + 2\,H_2$
ClH	$ClH \longrightarrow 0.5\,Cl_2 + 0.5\,H_2$
ClHO	$ClHO + CO \longrightarrow CO_2 + 0.5\,Cl_2 + 0.5\,H_2$
ClNO	$ClNO + CO \longrightarrow CO_2 + 0.5\,Cl_2 + 0.5\,N_2$
Cl_2O	$Cl_2O + CO \longrightarrow CO_2 + Cl_2$
cis−H_2P_2	$\text{cis}-H_2P_2 \longrightarrow H_2 + P_2$
trans−H_2P_2	$\text{trans}-H_2P_2 \longrightarrow H_2 + P_2$
iso−H_2P_2	$\text{iso}-H_2P_2 \longrightarrow H_2 + P_2$
H_2S	$H_2S + CS \longrightarrow CS_2 + H_2$
H_2S_2	$H_2S_2 + 2\,CS \longrightarrow H_2 + 2\,CS_2$
HPO	$HPO + CO \longrightarrow CO_2 + 0.5\,H_2 + 0.5\,P_2$
PH_3	$PH_3 + 0.5\,P_2 + 1.5\,H_2$
P_2O	$P_2O + CO \longrightarrow CO_2 + P_2$

Table S3: Heats of Formation (kJ mol^{-1}) at the HF + CABS level

	VnZ-F12/OptRI			VnZ-F12/OptRI+		
Molecule	DZ	TZ	QZ	DZ	TZ	QZ
FCN	307.09	306.63	306.39	306.03	306.27	306.38
iso-FCN	-228.79	-229.60	-229.78	-229.44	-229.84	-229.80
CF_2	40.61	39.91	39.73	39.66	39.63	39.71
CHF	-111.58	-111.67	-111.76	-111.86	-111.76	-111.77
HCN	411.52	411.61	411.56	411.29	411.51	411.56
iso-HCN	-80.51	-80.64	-80.79	-81.14	-80.87	-80.79
CH_2	123.81	123.53	123.38	123.34	123.36	123.37
CH_2O	176.22	175.99	175.86	175.65	175.80	175.86
iso$-CH_2O$	227.13	227.11	227.06	227.00	227.11	227.05
CH_4	37.65	37.82	37.90	38.08	37.98	37.90
C_2H_2	-109.31	-109.09	-109.10	-109.11	-108.97	-109.10
FH	-308.06	-308.22	-308.36	-308.48	-308.29	-308.37
FHO	-52.44	-52.15	-52.07	-51.86	-52.03	-52.07
FNO	-278.26	-278.18	-278.27	-278.24	-278.10	-278.27
F_2O	108.78	109.20	109.23	109.20	109.34	109.24
cis$-H_2N_2$	347.28	346.52	346.38	346.53	346.34	346.37
trans$-H_2N_2$	88.21	88.38	88.29	88.08	88.33	88.29
iso$-H_2N_2$	216.41	215.92	215.79	215.80	215.79	215.78
H_2O	276.88	276.61	276.40	276.51	276.58	276.40
H_2O_2	143.78	143.70	143.69	144.05	143.81	143.69
NH_3	-73.83	-73.89	-74.06	-74.15	-73.92	-74.06
N_2O	313.72	314.90	315.24	315.33	315.50	315.26
O_3	201.89	202.05	201.97	201.75	202.04	201.97

	VnZ-F12/OptRI			VnZ-F12/OptRI+		
Molecule	DZ	TZ	QZ	DZ	TZ	QZ
CClN	-294.60	-296.67	-297.01	-296.09	-297.00	-297.00
iso−CClN	283.06	284.04	284.28	283.16	284.06	284.30
CCl_2	202.28	202.27	202.26	201.71	202.13	202.26
SiHF	87.24	86.78	86.64	86.78	86.67	86.64
SiHN	279.89	279.83	279.91	280.01	279.84	279.91
iso−SiHN	18.67	18.44	18.64	18.83	18.46	18.64
SiH_2	-163.91	-165.23	-165.39	-164.11	-165.33	-165.39
CH_2S	612.38	612.43	612.39	612.69	612.44	612.39
iso−CH_2S	106.55	106.45	106.46	106.73	106.45	106.47
SiH_4	106.47	106.16	106.14	106.85	106.33	106.16
ClH	-107.97	-107.37	-107.22	-107.88	-107.36	-107.20
ClHO	117.29	118.38	118.69	118.06	118.55	118.70
ClNO	-52.36	-51.99	-52.08	-51.77	-51.93	-52.07
Cl_2O	-68.81	-68.24	-68.22	-68.44	-68.22	-68.21
cis−H_2P_2	-116.32	-117.10	-117.31	-115.93	-117.02	-117.30
trans−H_2P_2	369.12	368.67	368.54	368.57	368.56	368.54
iso−H_2P_2	259.84	259.58	259.50	259.72	259.52	259.50
H_2S	231.91	231.26	231.16	231.61	231.24	231.17
H_2S_2	189.75	189.60	189.63	189.92	189.60	189.63
HPO	-39.37	-40.23	-40.48	-38.96	-40.11	-40.47
PH_3	-45.55	-45.18	-45.08	-45.27	-45.18	-45.06
P_2O	92.02	92.02	92.05	92.22	92.03	92.06

Table S4: Heats of Formation (kJ mol^{-1}) at the CCSD-F12b level

	VnZ-F12/OptRI			VnZ-F12/OptRI+		
Molecule	DZ	TZ	QZ	DZ	TZ	QZ
FCN	210.85	202.09	200.12	209.67	201.73	200.12
iso-FCN	-209.76	-214.56	-216.38	-210.60	-214.81	-216.39
CF_2	3.45	-1.97	-3.45	2.30	-2.26	-3.47
CHF	-132.66	-135.21	-135.69	-132.95	-135.30	-135.69
HCN	412.39	407.25	406.47	412.17	407.14	406.47
iso-HCN	-122.68	-127.89	-128.96	-123.33	-128.12	-128.97
CH_2	131.30	126.47	125.12	130.76	126.29	125.11
CH_2O	122.00	117.26	116.32	121.37	117.08	116.31
iso$-CH_2O$	201.29	198.48	198.16	201.17	198.50	198.16
CH_4	32.87	35.08	35.79	33.26	35.26	35.79
C_2H_2	-96.26	-95.47	-95.29	-96.07	-95.34	-95.29
FH	-287.49	-288.71	-289.42	-288.00	-288.77	-289.43
FHO	-72.01	-68.89	-68.32	-71.43	-68.77	-68.32
FNO	-262.23	-261.88	-261.97	-262.17	-261.79	-261.96
F_2O	105.60	106.88	107.50	106.09	107.04	107.50
cis$-H_2N_2$	304.43	299.41	298.11	303.49	299.23	298.10
trans$-H_2N_2$	82.05	79.22	78.67	81.94	79.18	78.67
iso$-H_2N_2$	183.35	178.23	176.97	182.70	178.10	176.96
H_2O	280.99	276.83	275.87	280.63	276.83	275.87
H_2O_2	101.63	103.03	103.35	101.93	103.16	103.35
NH_3	-80.69	-84.08	-84.90	-81.01	-84.10	-84.91
N_2O	206.15	215.70	219.19	207.88	216.33	219.20
O_3	178.03	175.33	174.96	177.90	175.35	174.96

	VnZ-F12/OptRI			VnZ-F12/OptRI+		
Molecule	DZ	TZ	QZ	DZ	TZ	QZ
CClN	-350.29	-360.69	-363.71	-351.92	-361.17	-363.71
iso−CClN	232.32	232.77	232.88	232.39	232.75	232.89
CCl_2	134.87	132.99	132.57	134.18	132.81	132.57
SiHF	83.54	79.91	79.21	83.04	79.78	79.22
SiHN	291.67	285.15	284.46	291.78	285.08	284.45
iso−SiHN	35.19	28.45	27.47	35.34	28.38	27.46
SiH_2	-137.92	-145.08	-146.86	-138.21	-145.25	-146.86
CH_2S	505.07	497.99	497.15	505.38	497.94	497.15
iso−CH_2S	118.36	116.52	116.21	118.54	116.50	116.21
SiH_4	85.99	90.03	91.75	86.39	90.20	91.76
ClH	-98.91	-99.05	-99.18	-98.86	-99.04	-99.17
ClHO	78.13	82.57	83.85	78.95	82.75	83.85
ClNO	3.98	4.80	4.94	4.57	4.95	4.96
Cl_2O	-32.68	-32.42	-32.13	-32.29	-32.35	-32.11
cis−H_2P_2	-97.20	-94.21	-93.89	-96.79	-94.13	-93.88
trans−H_2P_2	316.78	314.61	314.15	316.11	314.47	314.15
iso−H_2P_2	271.43	268.78	268.21	271.31	268.71	268.21
H_2S	197.17	190.11	188.45	196.85	190.01	188.46
H_2S_2	208.25	205.04	204.12	208.42	205.01	204.12
HPO	-53.06	-52.41	-52.97	-52.65	-52.33	-52.96
PH_3	-19.40	-20.61	-20.62	-19.12	-20.62	-20.62
P_2O	103.54	102.02	101.77	103.74	102.00	101.77