Supplementary Material (ESI) for *PCCP*

Fluorine Substituent Effects on Dihydrogen Bonding of Transition Metal Hydrides

Heiko Jacobsen

Supplementary Material

NEt_3
BP86/N/n.log
Route: #P BP86/Gen/Auto Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

N	0.000010	-0.298169	-0.031212
C	-1.218703	-1.085014	0.193208
C	0.000013	0.992273	0.691099
C	1.218730	-1.085009	0.193192
C	-0.000055	2.211593	-0.234761
H	0.893874	2.212604	-0.890611
H	-0.893938	2.212483	-0.890673
H	-0.000146	3.154268	0.354077
H	-0.880098	1.037525	1.365956
H	0.880204	1.037565	1.365841
C	2.473228	-0.445405	-0.401860
H	3.349737	-1.109838	-0.253102
H	2.344879	-0.267072	-1.488867
H	2.713309	0.525348	0.078907
H	1.386200	-1.289066	1.283029
H	1.059303	-2.071847	-0.280124
C	-2.473218	-0.445458	-0.401859
H	-3.349778	-1.109738	-0.252717
H	-2.713103	0.525486	0.078617
H	-2.345042	-0.267522	-1.488952
H	-1.059260	-2.071866	-0.280073
H	-1.386177	-1.289033	1.283053

Energy E(RB-P86) -292.35270878 a.u.
                    -767572.04 kJ/mol

SCF Convergence: 0.4632D-09
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000027

ZPE-correction   :   0.197909 a.u.
                            519.61 kJ/mol

Energy (298K)   :   -292.145191 a.u.
                       -767027.20 kJ/mol
Enthalpy (298K)   :   -292.144247 a.u.
                       -767024.72 kJ/mol
Free Energy (298K):   -292.188798 a.u.
                       -767141.69 kJ/mol

Lowest Frequency   56.1247 cm-1
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1
BP86/Iso-N/iso-n.log
Route: #P BP86/Gen/Auto Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

C	2.542058	0.358688	-0.269136
O	1.595356	-0.718698	-0.241701
H	0.680367	-0.363407	-0.058991
C	2.707955	1.000795	1.114590
H	3.062665	0.246129	1.847636
H	3.439660	1.836547	1.087431
H	1.743079	1.408886	1.482498
C	3.854880	-0.212886	-0.799662
H	4.224047	-1.011803	-0.122893
H	4.633848	0.574155	-0.871799
H	3.707287	-0.656710	-1.804646
H	2.193582	1.146721	-0.979059
N	-1.173998	0.087970	-0.043267
C	-1.166769	1.543812	-0.316572
C	-1.660035	-0.689001	-1.205444
C	-1.866020	-0.256525	1.227543
C	-1.383443	-2.188908	-1.114834
H	-0.302763	-2.386198	-0.968248
H	-1.948571	-2.666964	-0.288793
H	-1.705002	-2.680740	-2.055974
H	-2.751823	-0.526035	-1.366229
H	-1.145271	-0.279098	-2.094745
H	-0.484242	1.708105	-1.172558
C	-2.518823	2.214945	-0.604941
H	-2.993668	1.815314	-1.523670
H	-3.233103	2.085403	0.234461
H	-2.373594	3.305211	-0.753090
H	-0.687748	2.031884	0.553213
C	-1.039012	-1.149654	2.155449
H	-1.608506	-1.368151	3.083881
H	-0.776911	-2.112939	1.677205
H	-0.089718	-0.653298	2.439947
H	-2.105613	0.683570	1.758878
H	-2.847615	-0.730401	1.010060

Energy E(RB-P86) -486.69707692 a.u.
                   -1277823.18 kJ/mol

SCF Convergence: 0.2338D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000014

ZPE-correction   :   0.304161 a.u.
                            798.57 kJ/mol

Energy (298K)   :   -486.376259 a.u.
                       -1276980.87 kJ/mol
Enthalpy (298K)   :   -486.375314 a.u.
                       -1276978.39 kJ/mol
Free Energy (298K):   -486.438187 a.u.
                       -1277143.46 kJ/mol

Lowest Frequency   24.3627 cm-1
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Isopropanol
BP86/Iso/iso.log
Route: #P BP86/Gen/Auto Opt Freq GFInput
Atom Coordinates (x,y,z) in Angstrom

O	-0.038252	1.383320	-0.161431
H	-0.893854	1.771571	0.092680
C	0.002564	0.035189	0.363327
H	-0.006096	0.078716	1.477063
C	-1.206394	-0.778882	-0.104165
H	-1.226689	-0.844770	-1.211951
H	-1.177004	-1.809021	0.309276
H	-2.158457	-0.314441	0.232687
C	1.330380	-0.559631	-0.090093
H	1.371084	-0.614039	-1.197807
H	1.462092	-1.582339	0.318530
H	2.175637	0.067703	0.256557

Energy E(RB-P86) -194.33571761 a.u.
                    -510228.43 kJ/mol
SCF Convergence: 0.6064D-09
Maximum Force: 0.000004

ZPE-correction   :   0.104191 a.u.
                            273.55 kJ/mol

Energy (298K)   :   -194.225967 a.u.
Enthalpy (298K)   :   -194.225023 a.u.
Free Energy (298K):   -194.258991 a.u.
Lowest Frequency 224.8565 cm-1
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H_2O
BP86/H2O/h2o.log
Route: #P BP86/Gen/Auto Opt Freq GFInput
Atom Coordinates (x,y,z) in Angstrom

O	0.000000	0.000000	0.119503
H	0.000000	0.766501	-0.478011
H	0.000000	-0.766501	-0.478011

Energy E(RB-P86)   -76.46073116 a.u.
                    -200747.65 kJ/mol

SCF Convergence: 0.4418D-09
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000043

ZPE-correction   :   0.020586 a.u.
                             54.05 kJ/mol

Energy (298K)   :   -76.437309 a.u.
                         -200686.15 kJ/mol
Enthalpy (298K)   :   -76.436365 a.u.
                         -200683.68 kJ/mol
Free Energy (298K):   -76.457820 a.u.
                         -200740.01 kJ/mol

Lowest Frequency 1568.3493 cm-1
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2
BP86/HFIP-N/hfip-n.log
Route: #P BP86/Gen/Auto Opt Freq GFInput
Atom Coordinates (x,y,z) in Angstrom

C	-1.260570	0.102972	-0.273662
O	-0.290611	0.652655	0.566354
H	0.654757	0.393670	0.257829
C	-1.624599	-1.341628	0.160067
F	-2.131315	-1.405290	1.403855
F	-2.499679	-1.924235	-0.690570
F	-0.487661	-2.101023	0.142472
C	-2.469524	1.066723	-0.300539
F	-2.957531	1.314563	0.928952
F	-3.477005	0.575351	-1.063494
F	-2.085492	2.244483	-0.845428
H	-0.930729	0.017915	-1.333209
N	2.273909	0.104155	-0.162088
C	2.895084	1.450205	-0.263373
C	2.930600	-0.772536	0.854708
C	2.195199	-0.553052	-1.496877
C	2.763650	2.308488	0.993169
H	1.705776	2.403410	1.309933
H	3.352123	1.902890	1.840669
H	3.154482	3.324967	0.782490
H	3.970411	1.363094	-0.537856
H	2.393441	1.961070	-1.106652
H	1.591674	0.112242	-2.144250
C	3.519626	-0.878321	-2.200401
H	4.106764	0.033173	-2.429573
H	4.156448	-1.556165	-1.595992
H	3.311543	-1.389572	-3.162767
H	1.603267	-1.475897	-1.358428
C	2.219645	-0.816202	2.208908
H	2.777958	-1.484101	2.897973
H	2.152260	0.181367	2.682087
H	1.189948	-1.208684	2.104531
H	2.959364	-1.796931	0.442030
H	3.991530	-0.467305	0.980886

Energy E(RB-P86) -1081.71477822 a.u.
                    -2840042.15 kJ/mol
SCF Convergence: 0.1804D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000052
ZPE-correction   :   0.259807 a.u.
                             682.12 kJ/mol
Energy (298K)   :   -1081.434578 a.u.
                         -2839306.48 kJ/mol
Enthalpy (298K)   :   -1081.433634 a.u.
                         -2839304.01 kJ/mol
Free Energy (298K):   -1081.506438 a.u.
                         -2839495.15 kJ/mol

Lowest Frequency   22.1586 cm-1
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HFIP

BP86/HFIP/hfip.log
Route: #P BP86/Gen/Auto Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

O	0.041113	1.874702	-0.016359
H	-0.799683	2.299729	-0.264934
C	0.004185	0.543045	-0.488795
C	1.312251	-0.135430	-0.027880
C	-1.285904	-0.172617	-0.022019
H	0.001009	0.485557	-1.599627
F	1.331985	-1.427910	-0.428628
F	2.364684	0.491775	-0.593418
F	1.465948	-0.100580	1.306613
F	-1.434559	-1.371955	-0.614716
F	-1.353291	-0.333399	1.308972
F	-2.342924	0.609525	-0.397979

Energy E(RB-P86) -789.34444586 a.u.
                   -2072423.84 kJ/mol

SCF Convergence: 0.3700D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000003

ZPE-correction   :   0.060008 a.u.
                             157.55 kJ/mol

Energy (298K)   :   -789.275066 a.u.
                        -2072241.69 kJ/mol
Enthalpy (298K)   :   -789.274122 a.u.
                        -2072239.21 kJ/mol
Free Energy (298K):   -789.319936 a.u.
                        -2072359.49 kJ/mol

Lowest Frequency   38.0356 cm-1
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5
BP86/W-CO/wco.log
Route: #P BP86/GenECP/Auto GFInput Opt(CalcFC) Freq

W	1.861100	0.137273	0.015361
H	2.176234	0.187316	-1.786945
C	3.573468	1.278418	0.095004
N	1.556374	0.093793	1.870825
C	0.247201	-0.979626	-0.496655
O	4.545156	1.920061	0.094928
O	1.369170	0.062356	3.048607
O	-0.670546	-1.635504	-0.832348
P	0.590714	2.227575	-0.588328
P	3.283914	-1.919611	-0.203887
C	-0.229358	3.085241	0.831427
C	1.588196	3.581978	-1.362838
C	-0.789032	2.032202	-1.804673
C	5.061681	-1.664678	-0.657028
C	2.738174	-3.136942	-1.487482
C	3.404196	-2.965007	1.320632
H	-0.960039	2.391727	1.290679
H	0.535836	3.337682	1.591822
H	-0.750854	4.009379	0.506253
H	2.383338	3.906188	-0.662993
H	0.950034	4.451758	-1.621965
H	2.071733	3.191664	-2.280015
H	-1.231503	3.014807	-2.068670
H	-1.581437	1.386670	-1.377560
H	-0.396243	1.547498	-2.720104
H	5.595375	-2.630929	-0.769136
H	5.559036	-1.060323	0.126935
H	5.111933	-1.102767	-1.610561
H	2.705598	-2.626940	-2.470342
H	1.715944	-3.490856	-1.248507
H	3.424907	-4.006864	-1.540420
H	2.386337	-3.281849	1.622416
H	4.037150	-3.861838	1.156332
H	3.830010	-2.357336	2.143477
H	-2.498254	-1.114439	-1.049393
O	-3.371311	-0.689809	-1.194175
C	-4.175787	-0.887907	-0.055408
H	-4.030165	-1.887510	0.404940
C	-5.648025	-0.842649	-0.523433
C	-3.828859	0.144557	1.048106
F	-5.879173	-1.868236	-1.370373
F	-5.944078	0.305118	-1.161093
F	-6.490827	-0.975339	0.527204
F	-4.034038	1.416951	0.654437
F	-2.504836	0.020239	1.349163
F	-4.524970	-0.072911	2.182047

Energy E(RB-P86) -2136.15010395 a.u.
                  -5608462.10 kJ/mol
SCF Convergence: 0.5671D-08
Maximum Force: 0.000033
ZPE-correction   :   0.312881 a.u.
Energy (298K)   :   -2135.801716 a.u.
Enthalpy (298K)   :   -2135.800771 a.u.
Free Energy (298K):   -2135.911817 a.u.
                       -5607836.48 kJ/mol
Lowest Frequency   9.9571 cm-1
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3’

BP86/W-H/wh.log
Route: #P BP86/GenECP/Auto GFInput Opt Freq

W	-1.553686	-0.085160	-0.071321
H	0.057285	0.332529	0.713634
C	-0.534143	-0.103913	-1.852513
N	-3.232539	-0.361894	-0.851834
C	-2.255656	-0.025172	1.858204
O	0.063585	-0.107066	-2.853170
O	-4.309281	-0.493004	-1.347553
O	-2.623889	0.007537	2.962578
P	-1.618291	2.431342	-0.148279
P	-0.974082	-2.513896	0.325727
C	-0.233903	3.272070	-1.045776
H	-0.366530	4.373704	-1.046260
H	-0.191081	2.907845	-2.091096
H	0.721331	3.020059	-0.545181
C	-3.123980	3.135714	-0.962290
H	-3.113504	4.245181	-0.951580
H	-3.171202	2.776466	-2.009332
H	-4.026778	2.768999	-0.435441
C	-1.592831	3.306703	1.482853
H	-1.582990	4.407456	1.345413
H	-0.691448	2.997326	2.047447
H	-2.486786	3.018373	2.070177
C	-0.224465	-2.919953	1.968372
H	-0.892745	-2.574085	2.781286
H	0.747218	-2.395881	2.060146
H	-0.060564	-4.012641	2.066914
C	0.201585	-3.335802	-0.842471
H	-0.182591	-3.248440	-1.877652
H	1.184072	-2.827547	-0.784219
H	0.330363	-4.407965	-0.587436
C	-2.455434	-3.623570	0.262114
H	-2.178199	-4.680813	0.454465
H	-2.928028	-3.540951	-0.736487
H	-3.192449	-3.291334	1.019551
H	1.373457	-0.237109	0.792545
O	2.312143	-0.593949	0.865552
C	3.124933	0.119552	-0.028821
C	3.705155	1.390372	0.643969
C	4.198229	-0.852714	-0.566524
H	2.567756	0.480639	-0.919671
F	4.486726	1.115378	1.702249
F	2.669466	2.159770	1.083266
F	4.414899	2.138932	-0.231546
F	4.909539	-1.428039	0.419903
F	3.591384	-1.840018	-1.273177
F	5.058221	-0.226716	-1.401838

Energy E(RB-P86) -2136.15731231 a.u.
                  -5608481.02 kJ/mol
SCF Convergence: 0.4132D-08
Maximum Force: 0.000342
ZPE-correction   :   0.312890 a.u.
                             821.49 kJ/mol
Energy (298K)   :   -2135.809105 a.u.
Enthalpy (298K)   :   -2135.808161 a.u.
Free Energy (298K):   -2135.918251 a.u.
Lowest Frequency   9.1652 cm-1

3
BP86/W-H/whfixbp86f.log
Route: # BP86/GenECP/Auto GFInput Int=UltraFine Freq

W	1.533643	-0.000374	-0.082876
H	-0.144191	0.001415	0.668581
C	0.538004	0.000559	-1.879073
N	3.245625	-0.001763	-0.839527
C	2.184708	-0.001229	1.863365
O	-0.052985	0.001041	-2.882996
O	4.335856	-0.002625	-1.322949
O	2.522934	-0.001743	2.978596
P	1.265147	-2.502682	0.090792
P	1.269617	2.502324	0.091259
C	0.383108	-3.370318	-1.286618
H	0.357537	-4.467544	-1.122966
H	0.893970	-3.152636	-2.245159
H	-0.654860	-2.988717	-1.346342
C	2.866289	-3.427490	0.188458
H	2.698633	-4.521648	0.266530
H	3.468968	-3.210472	-0.715743
H	3.435008	-3.077471	1.072510
C	0.343669	-3.101218	1.578584
H	0.324115	-4.209830	1.616698
H	-0.694369	-2.717013	1.536481
H	0.825466	-2.709552	2.496094
C	0.338656	3.101397	1.572939
H	0.812893	2.707722	2.493520
H	-0.699897	2.719511	1.522951
H	0.321265	4.210008	1.612073
C	0.399263	3.373062	-1.291606
H	0.916649	3.155404	-2.246646
H	-0.638933	2.993337	-1.359252
H	0.374490	4.470162	-1.127016
C	2.872104	3.423355	0.201432
H	2.706502	4.517823	0.279575
H	3.480734	3.205923	-0.698673
H	3.433612	3.070972	1.089146
H	-1.435061	0.002792	1.246727
O	-2.423996	0.002416	1.420521
C	-3.048168	0.001429	0.162920
C	-3.870231	-1.297997	-0.001871
C	-3.871534	1.299886	-0.002849
H	-2.312133	0.001577	-0.668476
F	-4.803114	-1.448120	0.954393
F	-3.023754	-2.363686	0.073409
F	-4.480044	-1.357234	-1.207669
F	-4.807681	1.447521	0.950640
F	-3.026742	2.366591	0.076242
F	-4.477611	1.359627	-1.210494

Energy E(RB-P86) -2136.15749326 a.u.
                  -5608481.50 kJ/mol
SCF Convergence: 0.2645D-08
Maximum Force: 0.000304
ZPE-correction   :   0.312149 a.u.
                             819.55 kJ/mol
Energy (298K)   :   -2135.809719 a.u.
Enthalpy (298K)   :   -2135.808775 a.u.
Free Energy (298K):   -2135.920261 a.u.
Lowest Frequency   5.6919 cm-1
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7

BP86/W-Iso/wiso.log
Route: #P BP86/GenECP/Auto Freq

W	0.707560	0.264579	-0.055543
H	-0.736530	-0.721058	0.528769
C	-0.006689	-0.140974	-1.938867
N	2.224816	1.193960	-0.641086
C	1.094423	0.488191	1.945268
O	-0.428185	-0.387252	-2.996238
O	3.205459	1.763024	-1.016458
O	1.283400	0.600914	3.090666
P	1.741878	-2.023467	0.044157
P	-0.836598	2.258844	0.112775
C	1.091375	-3.294138	-1.137075
H	1.585193	-4.277153	-0.991629
H	1.260703	-2.949327	-2.176312
H	-0.000384	-3.403719	-0.983950
C	3.564090	-2.072072	-0.282138
H	3.965415	-3.105056	-0.225548
H	3.761186	-1.652651	-1.288478
H	4.080402	-1.432468	0.460660
C	1.596787	-2.903730	1.667032
H	2.051053	-3.915284	1.626640
H	0.524549	-2.988454	1.931921
H	2.098539	-2.306921	2.454212
C	-1.927990	2.316643	1.605124
H	-1.310917	2.252232	2.522954
H	-2.616678	1.448457	1.570120
H	-2.520321	3.254838	1.624368
C	-2.049462	2.519840	-1.258265
H	-1.508487	2.600884	-2.221682
H	-2.721938	1.638345	-1.292675
H	-2.650668	3.437948	-1.093107
C	0.061524	3.876692	0.193812
H	-0.646441	4.728308	0.265594
H	0.688995	3.992673	-0.711928
H	0.730508	3.877631	1.077075
H	-2.337466	-0.594777	0.174428
O	-3.303656	-0.437785	0.021202
C	-3.963097	-1.714689	-0.096975
C	-3.880549	-2.504312	1.213803
C	-5.400448	-1.432745	-0.522956
H	-3.466347	-2.306087	-0.900235
H	-4.374656	-1.943199	2.034406
H	-2.823764	-2.678662	1.505398
H	-4.375606	-3.494150	1.116982
H	-5.919152	-0.827668	0.249898
H	-5.421407	-0.867398	-1.476206
H	-5.964013	-2.377969	-0.663826

Energy E(RB-P86) -1541.14174596 a.u.
                  -4046267.65 kJ/mol
SCF Convergence: 0.8273D-08
Maximum Force: 0.000098
ZPE-correction   :   0.357283 a.u.
Energy (298K)   :   -1540.752999 a.u.
Enthalpy (298K)   :   -1540.752055 a.u.
Free Energy (298K):   -1540.851773 a.u.
                       -4045506.33 kJ/mol
Lowest Frequency   11.2150 cm-1

4
BP86/W-NO/wno.log
Route: #P BP86/GenECP/Auto GFInput Opt Freq

W	-1.716953	0.169410	-0.019216
H	-3.067553	1.201074	0.656074
C	-1.405232	-0.064862	1.994126
N	-0.348684	-0.923412	-0.658762
C	-2.512541	0.779541	-1.804733
O	-1.294799	-0.154226	3.149310
O	0.528119	-1.662382	-1.056995
O	-3.015161	1.160462	-2.785823
P	-0.480447	2.373647	0.057616
P	-3.478839	-1.623143	0.057734
C	-1.543133	3.851806	-0.274919
H	-2.010878	3.751823	-1.274207
H	-2.351032	3.891511	0.481665
H	-0.947952	4.787546	-0.239675
C	0.362734	2.847052	1.636655
H	-0.374914	2.850756	2.463186
H	0.826765	3.851659	1.553911
H	1.149179	2.103034	1.868511
C	0.876932	2.546683	-1.185024
H	1.342028	3.552812	-1.131229
H	1.650917	1.774689	-0.999128
H	0.462852	2.386718	-2.200082
C	-5.226819	-1.025123	0.135614
C	-3.399877	-2.822557	1.467176
C	-3.490486	-2.751522	-1.411389
H	-5.944795	-1.871111	0.135683
H	-5.356904	-0.422101	1.055425
H	-5.426494	-0.368483	-0.733932
H	-4.193522	-3.594899	1.394517
H	-2.406933	-3.314613	1.465998
H	-3.510527	-2.272918	2.422831
H	-4.273825	-3.532527	-1.321314
H	-3.669577	-2.155342	-2.328088
H	-2.497777	-3.235469	-1.504056
H	2.117409	-0.874376	-1.172607
O	2.965180	-0.359754	-1.181935
C	3.854470	-0.935508	-0.257982
H	3.681239	-2.022938	-0.119168
C	5.282391	-0.800151	-0.834047
C	3.671873	-0.294862	1.141614
F	6.204292	-1.297674	0.024468
F	5.368307	-1.504553	-1.982863
F	5.604257	0.480329	-1.101234
F	4.473051	-0.859637	2.069218
F	3.898235	1.036449	1.136033
F	2.385002	-0.485212	1.542128

Energy E(RB-P86) -2136.15481743 a.u.
                  -5608474.47 kJ/mol
SCF Convergence: 0.7628D-08
Maximum Force: 0.000004
ZPE-correction   :   0.313067 a.u.
                             821.96 kJ/mol
Energy (298K)   :   -2135.806480 a.u.
Enthalpy (298K)   :   -2135.805536 a.u.
Free Energy (298K):   -2135.915661 a.u.
Lowest Frequency   7.5821 cm-1
==========

6
BP86/W-Water/ww.log
Route: #P BP86/GenECP/Auto GFInput Opt Freq

Atom Coordinates (x,y,z) in Angstrom

W	-0.082332	-0.163969	-0.094419
H	-0.041957	1.190444	1.152996
C	-0.039528	1.332023	-1.499973
N	-0.218553	-1.563321	-1.332259
C	-0.087558	-1.370724	1.564363
O	-0.022655	2.199673	-2.277661
O	-0.329619	-2.458713	-2.114536
O	-0.083362	-2.028125	2.527045
P	-2.535902	0.273105	0.236041
P	2.441826	-0.138918	0.044986
C	-3.111585	2.000972	-0.103607
H	-4.197058	2.114104	0.096706
H	-2.905464	2.258191	-1.161307
H	-2.542788	2.700728	0.539889
C	-3.676146	-0.740357	-0.814806
H	-4.740733	-0.500318	-0.613894
H	-3.449090	-0.549411	-1.882299
H	-3.495586	-1.814900	-0.614268
C	-3.199839	-0.012659	1.942050
H	-4.275431	0.251914	2.009781
H	-2.620906	0.602109	2.659272
H	-3.066118	-1.077992	2.215170
C	3.167987	0.050608	1.736119
H	2.766387	-0.736194	2.404591
H	2.883798	1.044001	2.137698
H	4.274445	-0.026845	1.699735
C	3.343940	1.162178	-0.910027
H	3.068553	1.093518	-1.980929
H	3.034139	2.151632	-0.516107
H	4.442414	1.047256	-0.801840
C	3.211557	-1.710706	-0.561603
H	4.318207	-1.672612	-0.488968
H	2.915834	-1.877534	-1.616233
H	2.831051	-2.559971	0.039742
H	1.006638	2.424597	1.238098
O	1.685241	3.133647	1.379297
H	1.177450	3.961514	1.351360

Energy E(RB-P86) -1423.26813600 a.u.
                    -3736790.49 kJ/mol
SCF Convergence: 0.5294D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000117

ZPE-correction   :   0.275054 a.u.
                             722.15 kJ/mol

Energy (298K)   :   -1422.965522 a.u.
                        -3735995.98 kJ/mol
Enthalpy (298K)   :   -1422.964578 a.u.
                        -3735993.50 kJ/mol
Free Energy (298K):   -1423.053640 a.u.
                        -3736227.33 kJ/mol
Lowest Frequency   13.1843 cm-1
==================================

$WH(CO)_2(NO)(PMe_3)_2$
BP86/W/w.log
Route: #P BP86/GenECP/Auto GFInput Opt Freq

Atom Coordinates (x,y,z) in Angstrom

W	-0.000031	0.000060	0.001041
H	0.000186	0.000468	-1.824747
C	-0.000117	-2.006604	-0.386649
C	-0.000221	2.006801	-0.386295
N	0.000579	-0.000253	1.880509
O	-0.000211	-3.131313	-0.700016
O	-0.000392	3.131515	-0.699642
O	0.001388	-0.000452	3.076849
P	-2.502994	-0.000027	-0.203986
P	2.502864	0.000022	-0.204353
C	-3.182573	0.000503	-1.925367
C	-3.375392	-1.438087	0.576081
C	-3.375477	1.437410	0.577126
C	3.375292	-1.437865	0.575997
C	3.182374	0.000195	-1.925753
C	3.375318	1.437636	0.576457
H	-4.477560	1.351496	0.477916
H	-3.104975	1.481819	1.651081
H	-3.035162	2.376416	0.097124
H	-4.477477	-1.352180	0.476885
H	-3.035000	-2.376721	0.095411
H	-3.104938	-1.483254	1.650016
H	-4.292344	0.000746	-1.926500
H	-2.807889	0.895758	-2.459421
H	-2.808318	-0.894755	-2.459724
H	4.292145	0.000556	-1.926925
H	2.808197	-0.895246	-2.459858
H	2.807565	0.895265	-2.460029
H	4.477377	-1.351963	0.476804
H	3.104818	-1.482831	1.649936
H	3.034919	-2.376597	0.095503
H	4.477405	1.351719	0.477310
H	3.035002	2.376529	0.096234
H	3.104771	1.482278	1.650391

Energy E(RB-P86) -1346.79699799 a.u.
-3536015.52 kJ/mol

SCF Convergence: 0.2594D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000009

ZPE-correction : 0.251668 a.u.
660.75 kJ/mol

Energy (298K) : -1346.521080 a.u.
-3535291.10 kJ/mol
Enthalpy (298K) : -1346.520135 a.u.
-3535288.61 kJ/mol
Free Energy (298K): -1346.601241 a.u.
-3535501.56 kJ/mol

Lowest Frequency 16.6303 cm-1
==========

NEt_3
PBE/N/n2.log
Route: #P PBEPBE/Gen/Auto Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

N	0.000067	-0.299387	-0.029446
C	-1.216199	-1.083549	0.190747
C	-0.000080	0.987564	0.690714
C	1.216474	-1.083309	0.190828
C	-0.000364	2.203967	-0.234018
H	0.892744	2.203693	-0.889638
H	-0.893621	2.203462	-0.889435
H	-0.000424	3.146503	0.353041
H	-0.879678	1.032916	1.365381
H	0.879655	1.033204	1.365177
C	2.467579	-0.440442	-0.400294
H	3.345007	-1.102230	-0.253322
H	2.339089	-0.258524	-1.485797
H	2.704334	0.528929	0.082928
H	1.384479	-1.291135	1.279461
H	1.058639	-2.068342	-0.285662
C	-2.467445	-0.440831	-0.400238
H	-3.344730	-1.102828	-0.253355
H	-2.704391	0.528408	0.083154
H	-2.339023	-0.258711	-1.485716
H	-1.058202	-2.068487	-0.285887
H	-1.384140	-1.291556	1.279357

Energy E(RPBE-PBE) -291.94878450 a.u.
                    -766511.53 kJ/mol

SCF Convergence: 0.2181D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000046

ZPE-correction   :   0.198468 a.u.
                            521.08 kJ/mol

Energy (298K)   :   -291.740762 a.u.
                       -765965.37 kJ/mol
Enthalpy (298K)   :   -291.739818 a.u.
                       -765962.89 kJ/mol
Free Energy (298K):   -291.784184 a.u.
                       -766079.38 kJ/mol

Lowest Frequency   60.3791 cm-1
==================================

1
PBE/Iso-N/iso-n2.log
Route: #P PBEPBE/Gen/Auto Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

C	2.523104	0.362272	-0.282453
O	1.585772	-0.717570	-0.316491
H	0.673224	-0.374656	-0.107871
C	2.639525	0.966761	1.120060
H	2.971769	0.194096	1.843610
H	3.367892	1.804154	1.140092
H	1.662064	1.362192	1.465716
C	3.854695	-0.182982	-0.784162
H	4.210737	-0.993139	-0.115248
H	4.626345	0.612455	-0.814196
H	3.742318	-0.604527	-1.802180
H	2.193553	1.169046	-0.980650
N	-1.170206	0.083003	-0.045090
C	-1.155697	1.532350	-0.328053
C	-1.677949	-0.700971	-1.187654
C	-1.830786	-0.250755	1.240194
C	-1.401319	-2.197400	-1.087180
H	-0.318540	-2.394756	-0.963502
H	-1.946269	-2.665024	-0.242870
H	-1.745035	-2.699450	-2.013681
H	-2.771934	-0.538407	-1.330302
H	-1.179591	-0.300542	-2.090070
H	-0.483664	1.685762	-1.194099
C	-2.504233	2.208890	-0.601413
H	-2.994084	1.804920	-1.509232
H	-3.206611	2.089257	0.248304
H	-2.355490	3.296174	-0.759670
H	-0.660209	2.023346	0.530539
C	-0.972054	-1.113742	2.163082
H	-1.519689	-1.332650	3.103218
H	-0.698795	-2.075924	1.690458
H	-0.028355	-0.596169	2.424960
H	-2.079463	0.692310	1.761294
H	-2.806622	-0.745463	1.048406

Energy E(RPBE-PBE) -486.04554638 a.u.
                   -1276112.58 kJ/mol

SCF Convergence: 0.2169D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000003

ZPE-correction   :   0.304923 a.u.
                            800.58 kJ/mol

Energy (298K)   :   -485.724038 a.u.
                       -1275268.46 kJ/mol
Enthalpy (298K)   :   -485.723093 a.u.
                       -1275265.98 kJ/mol
Free Energy (298K):   -485.785510 a.u.
                       -1275429.86 kJ/mol

Lowest Frequency   29.7667 cm-1
==================================

Isopropanol

PBE/Iso/iso2.log
Route: #P PBEPBE/Gen/Auto Opt Freq GFInput
Atom Coordinates (x,y,z) in Angstrom

O	-0.040777	1.380521	-0.160610
H	-0.899093	1.763588	0.088289
C	0.002515	0.036626	0.362688
H	-0.005899	0.077978	1.476228
C	-1.201837	-0.779747	-0.103847
H	-1.220618	-0.845201	-1.210813
H	-1.168838	-1.808808	0.309275
H	-2.154369	-0.318108	0.232336
C	1.328446	-0.556331	-0.090041
H	1.367234	-0.610758	-1.196966
H	1.460553	-1.577916	0.318490
H	2.172498	0.071775	0.255242

Energy E(RPBE-PBE) -194.08504439 a.u.
                    -509570.28 kJ/mol
SCF Convergence: 0.2482D-08

  Maximum Force: 0.000104
ZPE-correction   :   0.104478 a.u.
                            274.31 kJ/mol
Energy (298K)   :   -193.975025 a.u.
Enthalpy (298K)   :   -193.974081 a.u.
Free Energy (298K):   -194.008008 a.u.
Lowest Frequency 227.3083 cm-1

H_2O

PBE/H2O/h2o.log
Route: #P PBEPBE/Gen/Auto Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

O	0.000000	0.000000	0.119418
H	0.000000	0.765591	-0.477671
H	0.000000	-0.765591	-0.477671

Energy E(RPBE-PBE)   -76.37435885 a.u.
                    -200520.88 kJ/mol

SCF Convergence: 0.2950D-09
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000048

ZPE-correction   :   0.020662 a.u.
                             54.25 kJ/mol

Energy (298K)   :   -76.350860 a.u.
                         -200459.18 kJ/mol
Enthalpy (298K)   :   -76.349916 a.u.
                         -200456.70 kJ/mol
Free Energy (298K):   -76.371369 a.u.
                         -200513.03 kJ/mol

Lowest Frequency 1570.3895 cm-1

2
PBE/HFIP-N/hfip-n2.log
Route: #P PBEPBE/Gen/Auto Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

C	1.261770	0.122298	0.291435
O	0.297170	0.714552	-0.520135
H	-0.647608	0.429505	-0.237241
C	1.563049	-1.329527	-0.156574
F	2.013345	-1.403717	-1.419449
F	2.451643	-1.940738	0.654208
F	0.405048	-2.053591	-0.094970
C	2.506152	1.035151	0.293515
F	2.987660	1.247979	-0.943465
F	3.499213	0.508912	1.048246
F	2.178879	2.230890	0.828814
H	0.956213	0.043680	1.359314
N	-2.261382	0.122559	0.165756
C	-2.896947	1.460184	0.215284
C	-2.892957	-0.795612	-0.823251
C	-2.180225	-0.484189	1.519256
C	-2.770853	2.272284	-1.068571
H	-1.713908	2.363434	-1.387275
H	-3.354387	1.831821	-1.900659
H	-3.169130	3.291828	-0.895557
H	-3.971773	1.371322	0.489722
H	-2.404397	2.007158	1.040585
H	-1.588773	0.211509	2.145052
C	-3.500869	-0.802791	2.225735
H	-4.103784	0.106346	2.416228
H	-4.122440	-1.512441	1.643834
H	-3.291659	-1.273468	3.207189
H	-1.574826	-1.402596	1.416297
C	-2.177661	-0.867273	-2.171199
H	-2.721387	-1.565299	-2.840197
H	-2.126492	0.115260	-2.674959
H	-1.142481	-1.238744	-2.053052
H	-2.902361	-1.806775	-0.379456
H	-3.959349	-0.517629	-0.963268

Energy E(RPBE-PBE) -1080.55032758 a.u.
                    -2836984.89 kJ/mol

SCF Convergence: 0.4869D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000019

ZPE-correction   :   0.260566 a.u.
                             684.12 kJ/mol

Energy (298K)   :   -1080.269468 a.u.
                        -2836247.49 kJ/mol
Enthalpy (298K)   :   -1080.268524 a.u.
                        -2836245.01 kJ/mol
Free Energy (298K):   -1080.341075 a.u.
                        -2836435.49 kJ/mol

Lowest Frequency   18.4397 cm-1
==================================

HFIP
PBE/HFIP/hfip2.log
Route: #P PBEPBE/Gen/Auto Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

O	0.040318	1.873137	-0.020331
H	-0.806986	2.291078	-0.255195
C	0.004101	0.543736	-0.490127
C	1.308369	-0.134854	-0.028112
C	-1.281530	-0.172605	-0.022488
H	0.001402	0.483700	-1.600709
F	1.327199	-1.424889	-0.430120
F	2.360994	0.492011	-0.588346
F	1.456251	-0.101671	1.305313
F	-1.427948	-1.370194	-0.614261
F	-1.344214	-0.333058	1.307002
F	-2.339237	0.606965	-0.394819

Energy E(RPBE-PBE) -788.58046027 a.u.
                   -2070418.00 kJ/mol

SCF Convergence: 0.6051D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000073

ZPE-correction   :   0.060288 a.u.
                             158.29 kJ/mol

Energy (298K)   :   -788.510849 a.u.
                        -2070235.23 kJ/mol
Enthalpy (298K)   :   -788.509905 a.u.
                        -2070232.76 kJ/mol
Free Energy (298K):   -788.555581 a.u.
                        -2070352.68 kJ/mol

Lowest Frequency   39.0761 cm-1
==========

5
PBE/W-CO/wcopbe.log
Route: #P PBEPBE/GenECP/Auto Opt(CalcFC) Freq

W	1.795217	0.152720	0.000003
H	2.180608	0.322643	-1.782478
C	3.478702	1.315791	0.184220
N	1.400537	0.003189	1.829860
C	0.256560	-0.973729	-0.676438
O	4.441757	1.967771	0.228350
O	1.149248	-0.091298	2.990228
O	-0.608175	-1.637919	-1.118235
P	0.503391	2.242220	-0.525242
P	3.248698	-1.870530	-0.221848
C	-0.367245	3.001623	0.915073
C	1.497187	3.649627	-1.192721
C	-0.839775	2.089933	-1.782371
C	5.079611	-1.616928	-0.247424
C	2.979839	-2.872418	-1.749850
C	3.040735	-3.116955	1.126918
H	-1.108871	2.277154	1.301390
H	0.370146	3.206108	1.715193
H	-0.882622	3.941574	0.631244
H	2.266569	3.942744	-0.452551
H	0.854075	4.523431	-1.420645
H	2.012889	3.317012	-2.114243
H	-1.284126	3.079060	-2.013355
H	-1.635422	1.419904	-1.402904
H	-0.418895	1.649461	-2.706770
H	5.620755	-2.576836	-0.370546
H	5.395711	-1.135937	0.698419
H	5.338725	-0.938062	-1.082832
H	3.170457	-2.230340	-2.631175
H	1.923889	-3.203275	-1.788258
H	3.646463	-3.757893	-1.778138
H	1.983194	-3.443800	1.153337
H	3.698424	-3.997466	0.978650
H	3.274558	-2.638410	2.097840
H	-2.461412	-1.133871	-1.237259
O	-3.331478	-0.686527	-1.298753
C	-4.064028	-0.932381	-0.125159
H	-3.964849	-1.977833	0.235340
C	-5.554933	-0.741787	-0.473810
C	-3.567391	-0.034745	1.034255
F	-5.921379	-1.665293	-1.384182
F	-5.802145	0.476312	-0.985749
F	-6.328619	-0.908981	0.620977
F	-3.676932	1.279545	0.752707
F	-2.247803	-0.294510	1.242684
F	-4.218436	-0.283603	2.184451

Energy E(RPBE-PBE) -2134.19864160 a.u.
                    -5603338.53 kJ/mol
SCF Convergence: 0.6192D-08
Maximum Force: 0.000113
ZPE-correction   :   0.313485 a.u.
                             823.05 kJ/mol
Energy (298K)   :   -2133.849669 a.u.
Enthalpy (298K)   :   -2133.848725 a.u.
Free Energy (298K):   -2133.959211 a.u.
Lowest Frequency   8.3774 cm-1
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3’

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PBE/W-H/wh.log
Route:   #P PBEPBE/GenECP/Auto GFInput Opt Freq
---------------------------------
 W   -1.523521  -0.086352  -0.072907
 H    0.008322   0.377117   0.835876
 C   -0.391042  -0.078940  -1.778802
 N   -3.151150  -0.376903  -0.946826
 C   -2.321217  -0.060730   1.815784
 O    0.280571  -0.067166  -2.731325
 O   -4.201841  -0.506594  -1.491720
 O   -2.737084  -0.051977   2.902996
 P   -1.618029   2.418541  -0.147511
 P   -0.934502  -2.503375   0.332986
 C   -0.174411   3.272028  -0.922590
 H   -0.312929   4.372051  -0.925491
 H   -0.052919   2.915095  -1.963766
 H    0.741259   3.018900  -0.354234
 C   -3.051204   3.094965  -1.094846
 H   -3.059065   4.203580  -1.091980
 H   -2.996017   2.727161  -2.137832
 H   -3.990974   2.714967  -0.649418
 C   -1.749679   3.281885   1.479205
 H   -1.748943   4.383624   1.355858
 H   -0.894358   2.979325   2.113791
 H   -2.683833   2.968309   1.984066
 C   -0.206417  -2.902572   1.982084
 H   -0.877593  -2.536737   2.783002
 H    0.771265  -2.391575   2.076095
 H   -0.059974  -3.995782   2.093127
 C    0.246706  -3.324648  -0.822920
 H   -0.133963  -3.239584  -1.859024
 H    1.226919  -2.813668  -0.762418
 H    0.375079  -4.395161  -0.564173
 C   -2.416518  -3.604313   0.256454
 H   -2.148120  -4.662041   0.454194
 H   -2.877629  -3.519632  -0.746729
 H   -3.158243  -3.263587   1.004585
 H    1.317142  -0.240566   0.826729
 O    2.250060  -0.614649   0.860867
 C    3.050321   0.131275  -0.014165
 C    3.633183   1.375819   0.696610
 C    4.118366  -0.815372  -0.596475
 H    2.484401   0.520904  -0.887230
 F    4.409119   1.062565   1.745367
 F    2.598470   2.132838   1.159241
 F    4.345437   2.149293  -0.150493
 F    4.852782  -1.408116   0.360326
 F    3.505995  -1.788708  -1.314388
 F    4.954256  -0.160664  -1.430366
---------------------------------
Energy E(RPBE-PBE)  -2134.20630098 a.u.
                    -5603358.64 kJ/mol
SCF Convergence: 0.8862D-08
Maximum Force: 0.000013
ZPE-correction    :        0.313898 a.u.
                             824.14 kJ/mol
Energy (298K)     :    -2133.857334 a.u.
Enthalpy (298K)   :    -2133.856390 a.u.
Free Energy (298K):    -2133.964611 a.u.
Lowest Frequency    11.1632 cm-1
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3

PBE/W-H/whfixf.log
Route: # PBEPBE/GenECP/Auto GFInput Int=UltraFine Freq
Atom Coordinates (x,y,z) in Angstrom

W	-1.510338	0.000114	-0.088812
H	0.141155	-0.000035	0.711616
C	-0.471090	-0.000121	-1.855810
N	-3.200551	0.000079	-0.888601
C	-2.205331	0.000374	1.837855
O	0.147072	-0.000246	-2.842680
O	-4.277011	-0.000014	-1.396842
O	-2.564646	0.000522	2.945971
P	-1.232043	2.489440	0.098667
P	-1.232722	-2.489237	0.099129
C	-0.292666	3.352796	-1.237450
H	-0.266713	4.448262	-1.067833
H	-0.767195	3.141708	-2.215120
H	0.743737	2.964316	-1.256465
C	-2.828242	3.418977	0.135897
H	-2.658611	4.511441	0.220731
H	-3.395541	3.203151	-0.790394
H	-3.431140	3.069901	0.996569
C	-0.367768	3.077995	1.619699
H	-0.343428	4.185640	1.660430
H	0.668399	2.687675	1.615690
H	-0.887600	2.686602	2.515536
C	-0.366029	-3.077532	1.618876
H	-0.883951	-2.685299	2.515452
H	0.670383	-2.687907	1.612760
H	-0.342371	-4.185171	1.660162
C	-0.296003	-3.353363	-1.238343
H	-0.772144	-3.142360	-2.215247
H	0.740484	-2.965199	-1.259246
H	-0.270120	-4.448789	-1.068466
C	-2.829252	-3.418057	0.139503
H	-2.660008	-4.510562	0.224581
H	-3.398050	-3.202413	-0.785914
H	-3.430493	-3.068268	1.001043
H	1.409149	-0.000150	1.326175
O	2.400781	-0.000444	1.472943
C	2.977330	-0.000154	0.195437
C	3.790662	1.296079	-0.001279
C	3.790111	-1.296606	-0.002112
H	2.209867	0.000262	-0.606943
F	4.754856	1.446870	0.920165
F	2.946456	2.360391	0.103233
F	4.355595	1.353797	-1.226100
F	4.754109	-1.448486	0.919358
F	2.945420	-2.360626	0.101511
F	4.355188	-1.353694	-1.226894

Energy E(RPBE-PBE) -2134.20667871 a.u.
                    -5603359.63 kJ/mol
SCF Convergence: 0.3208D-08
Maximum Force: 0.000387
ZPE-correction   :   0.313094 a.u.
Energy (298K)   :   -2133.858144 a.u.
Enthalpy (298K)   :   -2133.857200 a.u.
Free Energy (298K):   -2133.967240 a.u.
Lowest Frequency   5.4410 cm-1
==========

7
PBE/W-Iso/wiso.log
Route: #P PBEPBE/GenECP/Auto Freq

W	0.697545	0.251553	-0.063191
H	-0.696001	-0.628793	0.759471
C	-0.228112	-0.242895	-1.822892
N	2.188351	1.056797	-0.856921
C	1.286255	0.579761	1.869470
O	-0.777269	-0.544491	-2.804987
O	3.157277	1.542835	-1.352705
O	1.583019	0.751714	2.983063
P	1.596863	-2.079190	0.075945
P	-0.724978	2.320936	0.110254
C	0.544233	-3.405922	-0.664731
H	1.007796	-4.405757	-0.543234
H	0.393821	-3.197657	-1.741811
H	-0.446186	-3.394187	-0.169879
C	3.223866	-2.347801	-0.759708
H	3.563010	-3.399310	-0.665794
H	3.125561	-2.083248	-1.830434
H	3.978774	-1.673594	-0.310616
C	1.902190	-2.742696	1.773801
H	2.274336	-3.786793	1.743840
H	0.956884	-2.701697	2.349066
H	2.644459	-2.101684	2.287749
C	-1.670076	2.530883	1.681796
H	-0.976223	2.478209	2.542965
H	-2.406141	1.707115	1.762885
H	-2.203766	3.502693	1.694572
C	-2.037399	2.562757	-1.164010
H	-1.578006	2.556603	-2.171293
H	-2.748380	1.715798	-1.084328
H	-2.576721	3.519087	-1.008293
C	0.259062	3.881045	0.001232
H	-0.390642	4.776370	0.078730
H	0.802438	3.898335	-0.963471
H	1.008616	3.894230	0.816215
H	-2.298896	-0.436755	0.466820
O	-3.270105	-0.290353	0.347430
C	-3.862748	-1.533781	-0.061908
C	-3.689179	-2.611818	1.009750
C	-5.326881	-1.250435	-0.369686
H	-3.367127	-1.882632	-0.997483
H	-4.172896	-2.295257	1.956573
H	-2.614475	-2.792517	1.218960
H	-4.140799	-3.572896	0.686981
H	-5.847437	-0.888587	0.540728
H	-5.418065	-0.471664	-1.152283
H	-5.839613	-2.166303	-0.726173

Energy E(RPBE-PBE) -1539.70279858 a.u.
                    -4042489.70 kJ/mol
SCF Convergence: 0.8193D-08
Maximum Force: 0.000447
ZPE-correction   :   0.358413 a.u.
                             941.01 kJ/mol
Energy (298K)   :   -1539.313148 a.u.
Enthalpy (298K)   :   -1539.312204 a.u.
Free Energy (298K):   -1539.410511 a.u.
Lowest Frequency   19.8195 cm-1
==========

4
PBE/W-NO/wno.log
Route: #P PBEPBE/GenECP/Auto GFInput Opt Freq

W	-1.660976	0.158766	-0.023728
H	-2.980550	1.167288	0.749509
C	-1.270912	-0.149619	1.963068
N	-0.339847	-0.928479	-0.758381
C	-2.511213	0.854499	-1.747252
O	-1.115774	-0.274823	3.108928
O	0.500008	-1.671450	-1.216211
O	-3.045002	1.290047	-2.687881
P	-0.413990	2.345880	0.095441
P	-3.461172	-1.576634	0.061879
C	-1.476236	3.831177	-0.179205
H	-1.963187	3.755313	-1.170892
H	-2.268815	3.853353	0.593330
H	-0.877399	4.763258	-0.132531
C	0.454049	2.772674	1.669151
H	-0.266234	2.733972	2.509261
H	0.901324	3.785911	1.612532
H	1.255599	2.033164	1.855069
C	0.917280	2.546308	-1.165410
H	1.384070	3.550065	-1.095983
H	1.692736	1.769260	-1.013315
H	0.480800	2.411080	-2.174058
C	-5.183477	-0.953083	-0.162929
C	-3.604146	-2.581292	1.606586
C	-3.314180	-2.874557	-1.245052
H	-5.919561	-1.782086	-0.139264
H	-5.405999	-0.228709	0.644039
H	-5.255485	-0.420820	-1.131253
H	-4.416750	-3.332387	1.532738
H	-2.641259	-3.095558	1.793696
H	-3.804589	-1.905985	2.461153
H	-4.122270	-3.630070	-1.166039
H	-3.355715	-2.390843	-2.240407
H	-2.329697	-3.373010	-1.148260
H	2.106291	-0.899009	-1.325934
O	2.961459	-0.400824	-1.301456
C	3.774822	-0.950581	-0.299902
H	3.606464	-2.039013	-0.160526
C	5.241715	-0.799990	-0.755113
C	3.472091	-0.297967	1.070598
F	6.092213	-1.279740	0.179780
F	5.432043	-1.506612	-1.886524
F	5.565082	0.482138	-1.000950
F	4.201931	-0.837241	2.064985
F	3.680402	1.036476	1.063469
F	2.161057	-0.499707	1.367860

Energy E(RPBE-PBE) -2134.20344491 a.u.
                    -5603351.14 kJ/mol
SCF Convergence: 0.3255D-08
Maximum Force: 0.000361
ZPE-correction   :   0.313809 a.u.
                             823.91 kJ/mol
Energy (298K)   :   -2133.854469 a.u.
Enthalpy (298K)   :   -2133.853524 a.u.
Free Energy (298K):   -2133.962599 a.u.
Lowest Frequency   12.8958 cm-1
==========

6
PBE/W-Water/ww.log
Route: #P PBEPBE/GenECP/Auto GFInput Freq

Atom Coordinates (x,y,z) in Angstrom

W	-0.083130	-0.157716	-0.094919
H	-0.058252	1.171827	1.179916
C	-0.030566	1.373543	-1.456084
N	-0.229777	-1.530483	-1.357531
C	-0.089191	-1.381639	1.545673
O	-0.006293	2.266386	-2.203516
O	-0.356766	-2.408332	-2.153829
O	-0.084009	-2.043568	2.504666
P	-2.527313	0.268343	0.238049
P	2.432664	-0.151920	0.040463
C	-3.111875	1.987425	-0.108073
H	-4.197057	2.095754	0.091688
H	-2.905489	2.240386	-1.166047
H	-2.545655	2.691325	0.532020
C	-3.657726	-0.756362	-0.804783
H	-4.723401	-0.523043	-0.606405
H	-3.429606	-0.569963	-1.872157
H	-3.468135	-1.827442	-0.597844
C	-3.182085	-0.014208	1.943400
H	-4.258437	0.242729	2.014045
H	-2.603477	0.607110	2.654084
H	-3.038211	-1.076720	2.219689
C	3.164568	-0.000568	1.728328
H	2.752270	-0.791550	2.384133
H	2.894901	0.989929	2.144836
H	4.268787	-0.093329	1.687190
C	3.342984	1.150498	-0.896556
H	3.056972	1.102846	-1.965074
H	3.047130	2.135561	-0.483337
H	4.439741	1.019249	-0.799011
C	3.174119	-1.720792	-0.595736
H	4.280733	-1.702725	-0.526850
H	2.870047	-1.862156	-1.651033
H	2.779970	-2.572975	-0.008779
H	1.016614	2.395122	1.261599
O	1.711889	3.087312	1.393562
H	1.220443	3.924339	1.392297

Energy E(RPBE-PBE) -1421.99280299 a.u.
                    -3733442.10 kJ/mol
SCF Convergence: 0.9386D-08
<S**2>:   0.0000
Charge: 0.0000
  Maximum Force: 0.000012

ZPE-correction   :   0.275754 a.u.
                             723.99 kJ/mol
Energy (298K)   :   -1421.689588 a.u.
                        -3732646.01 kJ/mol
Enthalpy (298K)   :   -1421.688644 a.u.
                        -3732643.53 kJ/mol
Free Energy (298K):   -1421.777161 a.u.
                        -3732875.94 kJ/mol

Lowest Frequency   16.1319 cm-1
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$WH(CO)_2(NO)(PMe_3)_2$
PBE/W/w2.log
Route: #P PBEPBE/GenECP/Auto GFInput Opt Freq

Atom Coordinates (x,y,z) in Angstrom

W	-0.000029	0.000078	0.001010
H	0.000084	0.000298	-1.825902
C	-0.000137	-2.000243	-0.397725
C	-0.000125	2.000523	-0.397226
N	0.000483	-0.000284	1.878340
O	-0.000250	-3.121988	-0.719685
O	-0.000191	3.122287	-0.719116
O	0.001137	-0.000586	3.072446
P	-2.492806	-0.000029	-0.200033
P	2.492691	-0.000032	-0.200338
C	-3.174104	0.000482	-1.915941
C	-3.358254	-1.435880	0.581587
C	-3.358323	1.435293	0.582479
C	3.358109	-1.435890	0.581306
C	3.173953	0.000431	-1.916252
C	3.358225	1.435287	0.582151
H	-4.460067	1.352543	0.486355
H	-3.083293	1.477231	1.654685
H	-3.015221	2.372432	0.102337
H	-4.460000	-1.353161	0.485445
H	-3.015070	-2.372710	0.100911
H	-3.083300	-1.478393	1.653788
H	-4.283004	0.000433	-1.914875
H	-2.799326	0.895277	-2.449144
H	-2.799248	-0.893964	-2.449683
H	4.282852	0.000429	-1.915203
H	2.799130	-0.894063	-2.449937
H	2.799121	0.895176	-2.449499
H	4.459859	-1.353215	0.485171
H	3.083146	-1.478374	1.653506
H	3.014891	-2.372716	0.100645
H	4.459970	1.352512	0.486061
H	3.015151	2.372421	0.101977
H	3.083165	1.477257	1.654349

Energy E(RPBE-PBE) -1345.60505260 a.u.
                    -3532886.07 kJ/mol

SCF Convergence: 0.6769D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000009

ZPE-correction   :   0.252176 a.u.
                             662.09 kJ/mol

Energy (298K)   :   -1345.328656 a.u.
                        -3532160.39 kJ/mol
Enthalpy (298K)   :   -1345.327712 a.u.
                        -3532157.91 kJ/mol
Free Energy (298K):   -1345.408817 a.u.
                        -3532370.85 kJ/mol

Lowest Frequency   16.7143 cm-1
==================================

NEt_3
B3LYP/N/n.log
Route: #P B3LYP/Gen Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

N	0.000010	-0.297620	-0.016672
C	-1.215987	-1.080174	0.197040
C	-0.000015	0.991906	0.693427
C	1.216033	-1.080135	0.197047
C	-0.000061	2.202435	-0.236735
H	0.887593	2.199418	-0.887084
H	-0.887719	2.199361	-0.887078
H	-0.000089	3.140715	0.343648
H	-0.872682	1.043394	1.360669
H	0.872667	1.043444	1.360645
C	2.462794	-0.445731	-0.409061
H	3.332744	-1.106073	-0.263675
H	2.326983	-0.276958	-1.488248
H	2.704627	0.520943	0.059080
H	1.390860	-1.276717	1.275929
H	1.058371	-2.060047	-0.268119
C	-2.462769	-0.445798	-0.409056
H	-3.332701	-1.106160	-0.263654
H	-2.704616	0.520872	0.059085
H	-2.326978	-0.277025	-1.488245
H	-1.058297	-2.060075	-0.268138
H	-1.390809	-1.276772	1.275920

Energy E(RB+HF-LYP) -292.36995391 a.u.
                    -767617.31 kJ/mol

SCF Convergence: 0.2529D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000004

ZPE-correction   :   0.203951 a.u.
                            535.47 kJ/mol

Energy (298K)   :   -292.156603 a.u.
                        -767057.16 kJ/mol
Enthalpy (298K)   :   -292.155659 a.u.
                        -767054.68 kJ/mol
Free Energy (298K):   -292.199843 a.u.
                        -767170.69 kJ/mol

Lowest Frequency   57.2479 cm-1
==================================

1
B3LYP/Iso-N/iso-n.log
Route: #P B3LYP/Gen Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

C	2.561083	0.359464	-0.266811
O	1.618366	-0.710115	-0.290577
H	0.718078	-0.377820	-0.088836
C	2.702661	0.951577	1.135218
H	3.043636	0.179226	1.843188
H	3.428887	1.781113	1.145258
H	1.738585	1.344499	1.496708
C	3.876787	-0.192354	-0.795107
H	4.235824	-1.005386	-0.143981
H	4.648379	0.592951	-0.831888
H	3.743184	-0.600668	-1.808018
H	2.223865	1.161776	-0.948507
N	-1.202976	0.083789	-0.043453
C	-1.167675	1.530534	-0.317885
C	-1.686369	-0.693731	-1.196401
C	-1.879100	-0.252958	1.228426
C	-1.402360	-2.188478	-1.106173
H	-0.327984	-2.380056	-0.970409
H	-1.952152	-2.663893	-0.279565
H	-1.728193	-2.679160	-2.036959
H	-2.770050	-0.540775	-1.352183
H	-1.183364	-0.289990	-2.083240
H	-0.486823	1.683690	-1.164963
C	-2.502911	2.222256	-0.612999
H	-2.976389	1.829508	-1.525369
H	-3.217417	2.108263	0.217404
H	-2.338043	3.301227	-0.763245
H	-0.690109	2.011301	0.544726
C	-1.035908	-1.117159	2.162365
H	-1.595758	-1.335379	3.087099
H	-0.758061	-2.072407	1.696122
H	-0.104037	-0.601810	2.439210
H	-2.132707	0.678984	1.747392
H	-2.842693	-0.745710	1.025036

Energy E(RB+HF-LYP) -486.72235138 a.u.
                    -1277889.53 kJ/mol

SCF Convergence: 0.3492D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000013

ZPE-correction   :   0.313413 a.u.
                            822.87 kJ/mol

Energy (298K)   :   -486.392568 a.u.
                       -1277023.69 kJ/mol
Enthalpy (298K)   :   -486.391623 a.u.
                       -1277021.21 kJ/mol
Free Energy (298K):   -486.454049 a.u.
                       -1277185.11 kJ/mol

Lowest Frequency   25.5533 cm-1
==================================

Isopropanol
B3LYP/Iso/iso.log
Route: #P B3LYP/Gen Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

O	-0.048499	1.373987	-0.162294
H	-0.885379	1.773670	0.098531
C	0.002488	0.036909	0.360759
H	-0.006575	0.083603	1.463666
C	-1.197639	-0.782553	-0.102993
H	-1.217082	-0.850719	-1.202238
H	-1.160726	-1.803268	0.310705
H	-2.144314	-0.324381	0.230182
C	1.329148	-0.550617	-0.089038
H	1.371033	-0.604301	-1.188394
H	1.462727	-1.565363	0.317117
H	2.164320	0.076432	0.256414

Energy E(RB+HF-LYP) -194.34383692 a.u.
                     -510249.74 kJ/mol

SCF Convergence: 0.2600D-08
Maximum Force: 0.000032

ZPE-correction   :   0.107287 a.u.
                             281.68 kJ/mol
Energy (298K)   :   -194.231105 a.u.
                         -509953.77 kJ/mol
Enthalpy (298K)   :   -194.230161 a.u.
                         -509951.29 kJ/mol
Free Energy (298K):   -194.263926 a.u.
                         -510039.94 kJ/mol

Lowest Frequency   229.0518 cm-1
==================================

H_2O
B3LYP/H2O/h2o.log
Route: #P B3LYP/Gen Opt Freq GFInput
Atom Coordinates (x,y,z) in Angstrom

O	0.000000	0.000000	0.117175
H	0.000000	0.764021	-0.468700
H	0.000000	-0.764021	-0.468700

Energy E(RB+HF-LYP)   -76.46062200 a.u.
                     -200747.36 kJ/mol
SCF Convergence: 0.1195D-09
Maximum Force: 0.000101

ZPE-correction   :   0.021174 a.u.
                              55.59 kJ/mol
Energy (298K)   :   -76.436612 a.u.
                         -200684.32 kJ/mol
Enthalpy (298K)   :   -76.435668 a.u.
                         -200681.85 kJ/mol
Free Energy (298K):   -76.457093 a.u.
                         -200738.10 kJ/mol

Lowest Frequency 1604.1424 cm-1
==================================

2
B3LYP/HFIP-N/hfip-n.log
Route: #P B3LYP/Gen Opt Geom=Check Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

C	1.274385	0.113090	0.284093
O	0.314829	0.692129	-0.534648
H	-0.612535	0.418253	-0.266552
C	1.594642	-1.328341	-0.162697
F	2.126856	-1.388410	-1.383100
F	2.422499	-1.943488	0.692015
F	0.444227	-2.039494	-0.183463
C	2.501469	1.038960	0.296586
F	2.966627	1.284783	-0.928475
F	3.498622	0.508664	1.023841
F	2.166384	2.207841	0.859529
H	0.955938	0.032239	1.335808
N	-2.293345	0.108371	0.159208
C	-2.899784	1.452489	0.259401
C	-2.948781	-0.763654	-0.850043
C	-2.194011	-0.542685	1.485952
C	-2.762438	2.308082	-0.993819
H	-1.711741	2.395844	-1.307318
H	-3.346977	1.907887	-1.835465
H	-3.144682	3.319321	-0.784433
H	-3.966768	1.377691	0.530164
H	-2.399931	1.959643	1.093351
H	-1.578648	0.110676	2.118165
C	-3.503739	-0.853650	2.214404
H	-4.071610	0.057596	2.453115
H	-4.154642	-1.518307	1.625847
H	-3.282465	-1.364063	3.165010
H	-1.621013	-1.465609	1.343401
C	-2.230941	-0.826231	-2.195680
H	-2.793079	-1.480581	-2.881824
H	-2.141002	0.161088	-2.667386
H	-1.218493	-1.237907	-2.083085
H	-2.994397	-1.777337	-0.438417
H	-3.994925	-0.449490	-0.989954

Energy E(RB+HF-LYP) -1081.72260509 a.u.
                    -2840062.70 kJ/mol

SCF Convergence: 0.2379D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000013

ZPE-correction   :   0.268648 a.u.
                             705.34 kJ/mol

Energy (298K)   :   -1081.434055 a.u.
                        -2839305.11 kJ/mol
Enthalpy (298K)   :   -1081.433111 a.u.
                        -2839302.63 kJ/mol
Free Energy (298K):   -1081.504770 a.u.
                        -2839490.77 kJ/mol

Lowest Frequency   22.8818 cm-1
==================================

HFIP
B3LYP/HFIP/hfip.log
Route: #P B3LYP/Gen Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

O	0.043770	1.864947	-0.011233
H	-0.763426	2.317949	-0.281740
C	0.003809	0.545407	-0.485392
C	1.302204	-0.135546	-0.028289
C	-1.279022	-0.169107	-0.022844
H	0.000509	0.493857	-1.585459
F	1.298542	-1.425668	-0.394826
F	2.345694	0.459045	-0.615656
F	1.470160	-0.072680	1.290932
F	-1.437340	-1.341537	-0.640477
F	-1.323054	-0.367666	1.292647
F	-2.326134	0.617849	-0.357486

Energy E(RB+HF-LYP) -789.33513004 a.u.
                    -2072399.38 kJ/mol

SCF Convergence: 0.1429D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000050

ZPE-correction   :   0.062429 a.u.
                             163.91 kJ/mol

Energy (298K)   :   -789.263581 a.u.
                        -2072211.53 kJ/mol
Enthalpy (298K)   :   -789.262636 a.u.
                        -2072209.05 kJ/mol
Free Energy (298K):   -789.307881 a.u.
                        -2072327.84 kJ/mol

Lowest Frequency   40.4075 cm-1
==================================

5
B3LYP/W-CO/wco.log
Route: #N B3LYP/GenECP Freq

W	1.841208	0.144843	0.002229
H	2.199943	0.239464	-1.793679
C	3.523551	1.338252	0.193403
N	1.494869	0.052894	1.834288
C	0.255366	-1.013138	-0.532692
O	4.460795	1.997957	0.271165
O	1.282314	-0.010308	2.996777
O	-0.638388	-1.678462	-0.859347
P	0.515210	2.223350	-0.588729
P	3.339712	-1.876794	-0.218431
C	-0.396754	2.998427	0.813335
C	1.493817	3.631951	-1.270018
C	-0.798062	2.018649	-1.866877
C	5.108300	-1.560789	-0.641656
C	2.851967	-3.094169	-1.515909
C	3.470617	-2.925451	1.294341
H	-1.122832	2.273969	1.207168
H	0.313323	3.246139	1.615621
H	-0.926704	3.910009	0.494992
H	2.235933	3.960967	-0.528168
H	0.841932	4.480517	-1.530005
H	2.030599	3.294502	-2.168481
H	-1.261613	2.985886	-2.116487
H	-1.578438	1.338231	-1.497036
H	-0.353613	1.582040	-2.772859
H	5.668908	-2.501963	-0.753412
H	5.573726	-0.954785	0.149219
H	5.155878	-0.993717	-1.582616
H	2.823734	-2.583875	-2.489411
H	1.843963	-3.477120	-1.299797
H	3.558598	-3.937596	-1.561522
H	2.469182	-3.284252	1.573329
H	4.136596	-3.788275	1.134753
H	3.854478	-2.315334	2.124946
H	-2.518108	-1.200775	-1.091355
O	-3.379182	-0.771406	-1.209204
C	-4.154923	-0.930108	-0.056986
H	-4.037269	-1.922625	0.401998
C	-5.628364	-0.828417	-0.482584
C	-3.744956	0.090022	1.024260
F	-5.927887	-1.851798	-1.289621
F	-5.887904	0.307233	-1.131307
F	-6.434650	-0.896010	0.587125
F	-3.961270	1.354356	0.649514
F	-2.421858	-0.041859	1.254830
F	-4.381226	-0.126588	2.178169

Energy E(RB+HF-LYP) -2135.97770970 a.u.
                    -5608009.48 kJ/mol
SCF Convergence: 0.9023D-08
Maximum Force: 0.000068
ZPE-correction   :   0.322300 a.u.
                             846.20 kJ/mol
Energy (298K)   :   -2135.620520 a.u.
Enthalpy (298K)   :   -2135.619576 a.u.
Free Energy (298K):   -2135.728871 a.u.
Lowest Frequency   11.6201 cm-1
==========

3′

B3LYP/W-H/wh.log
Route: #N B3LYP/GenECP Freq

W	-1.553003	-0.086269	-0.069731
H	0.039186	0.302052	0.774251
C	-0.500973	-0.064146	-1.841359
N	-3.193795	-0.364009	-0.896369
C	-2.344003	-0.072505	1.837392
O	0.102080	-0.044210	-2.821044
O	-4.244975	-0.507729	-1.420489
O	-2.769156	-0.068873	2.905036
P	-1.625663	2.446428	-0.104727
P	-0.954619	-2.533138	0.293869
C	-0.212139	3.300585	-0.927258
H	-0.343142	4.393882	-0.908747
H	-0.135242	2.964350	-1.971655
H	0.719970	3.039695	-0.406140
C	-3.092216	3.148033	-0.974624
H	-3.089294	4.249046	-0.951248
H	-3.090579	2.804130	-2.019301
H	-4.009534	2.773448	-0.497603
C	-1.679751	3.287667	1.535871
H	-1.676895	4.383163	1.424302
H	-0.806377	2.979574	2.128773
H	-2.588213	2.981202	2.074647
C	-0.225825	-2.956239	1.934134
H	-0.901642	-2.628675	2.737478
H	0.734483	-2.432425	2.046894
H	-0.057978	-4.041065	2.020620
C	0.238440	-3.320529	-0.870946
H	-0.133292	-3.223245	-1.901299
H	1.210554	-2.812322	-0.797923
H	0.373401	-4.387636	-0.634227
C	-2.421603	-3.646487	0.188616
H	-2.142002	-4.698427	0.357078
H	-2.882866	-3.544549	-0.804578
H	-3.163398	-3.340681	0.940706
H	1.416030	-0.220284	0.895264
O	2.348966	-0.543498	0.963301
C	3.122812	0.108957	0.005210
C	3.700835	1.424444	0.563955
C	4.191106	-0.879759	-0.485352
H	2.541893	0.394096	-0.884899
F	4.563387	1.231791	1.561436
F	2.685136	2.176786	1.034953
F	4.312245	2.136052	-0.393595
F	4.913184	-1.385089	0.514313
F	3.588894	-1.901416	-1.119309
F	5.027435	-0.299049	-1.357030

Energy E(RB+HF-LYP) -2135.98446237 a.u.
                    -5608027.21 kJ/mol
SCF Convergence: 0.8611D-08
Maximum Force: 0.000314
ZPE-correction   :   0.322483 a.u.
                             846.68 kJ/mol
Energy (298K)   :   -2135.627275 a.u.
Enthalpy (298K)   :   -2135.626330 a.u.
Free Energy (298K):   -2135.735075 a.u.
Lowest Frequency   6.9454 cm-1

3
B3LYP/W-H/whfixb3lypf.log
Route: # B3LYP/GenECP/Auto GFInput Int=UltraFine Freq

W	-1.528302	0.000171	-0.080893
H	0.138915	-0.000169	0.694412
C	-0.534719	-0.000066	-1.888915
N	-3.215897	0.000443	-0.858528
C	-2.247918	0.000339	1.851474
O	0.036384	-0.000186	-2.886610
O	-4.289560	0.000501	-1.355718
O	-2.632581	0.000365	2.935171
P	-1.246670	2.516492	0.096251
P	-1.247785	-2.516275	0.096447
C	-0.274495	3.366712	-1.221913
H	-0.247576	4.455316	-1.057089
H	-0.724521	3.159708	-2.203685
H	0.754684	2.979957	-1.218724
C	-2.838334	3.448818	0.086032
H	-2.667730	4.534123	0.161973
H	-3.382123	3.228119	-0.844176
H	-3.460126	3.117304	0.930470
C	-0.417490	3.118303	1.629144
H	-0.390353	4.218819	1.658061
H	0.610924	2.730041	1.656391
H	-0.954589	2.744867	2.513108
C	-0.421009	-3.118552	1.630466
H	-0.959225	-2.745040	2.513719
H	0.607505	-2.730675	1.659203
H	-0.394303	-4.219082	1.659297
C	-0.274097	-3.366743	-1.220434
H	-0.722653	-3.159495	-2.202828
H	0.755211	-2.980395	-1.215733
H	-0.247826	-4.455369	-1.055663
C	-2.839772	-3.448009	0.083928
H	-2.669686	-4.533381	0.160061
H	-3.382153	-3.227058	-0.847040
H	-3.462641	-3.116300	0.927496
H	1.471237	-0.000440	1.313982
O	2.448565	-0.000012	1.448565
C	3.036820	-0.000238	0.184578
C	3.849615	1.291659	0.000499
C	3.849126	-1.292453	0.000146
H	2.286757	0.000054	-0.619259
F	4.805084	1.433743	0.918009
F	3.014453	2.346483	0.104976
F	4.416585	1.350699	-1.212352
F	4.805811	-1.434214	0.916482
F	3.014000	-2.347091	0.106323
F	4.414501	-1.352270	-1.213435

Energy E(RB+HF-LYP) -2135.98481060 a.u.
                    -5608028.12 kJ/mol
SCF Convergence: 0.7513D-08
Maximum Force: 0.000218
ZPE-correction   :   0.322051 a.u.
                             845.54 kJ/mol
Energy (298K)   :   -2135.627825 a.u.
Enthalpy (298K)   :   -2135.626881 a.u.
Free Energy (298K):   -2135.737180 a.u.
Lowest Frequency   4.7093 cm-1
==========

7
B3LYP/W-Iso/wisob3.log
Route: #P B3LYP/GenECP Freq

W	0.726907	0.274053	-0.021859
H	-0.763076	-0.785504	0.227630
C	0.336523	0.064004	-2.036910
N	2.282725	1.259899	-0.274419
C	0.830357	0.313648	2.036345
O	0.106623	-0.066100	-3.155885
O	3.290644	1.861402	-0.438265
O	0.868781	0.324781	3.186147
P	1.800474	-2.013706	-0.014376
P	-0.894100	2.233028	0.080986
C	1.214404	-3.201383	-1.300446
H	1.717026	-4.176802	-1.206379
H	1.411815	-2.787678	-2.300161
H	0.128489	-3.338258	-1.194495
C	3.627097	-2.011032	-0.271584
H	4.041068	-3.031498	-0.261446
H	3.854162	-1.532424	-1.235313
H	4.101620	-1.414469	0.521074
C	1.611843	-3.007839	1.529528
H	2.083499	-3.998178	1.430595
H	0.541300	-3.132635	1.747511
H	2.072285	-2.469842	2.370959
C	-2.043857	2.271007	1.521569
H	-1.469091	2.238572	2.458588
H	-2.698850	1.388846	1.470762
H	-2.661703	3.182640	1.505661
C	-2.052053	2.454432	-1.336026
H	-1.479891	2.558130	-2.269425
H	-2.694904	1.564218	-1.404408
H	-2.680974	3.347455	-1.193958
C	-0.044235	3.867613	0.183055
H	-0.769974	4.695371	0.219576
H	0.610108	3.991797	-0.692068
H	0.585972	3.893957	1.083925
H	-2.435561	-0.694525	-0.006492
O	-3.388371	-0.522082	-0.129386
C	-4.091209	-1.767806	-0.194908
C	-3.973801	-2.537179	1.118943
C	-5.532132	-1.446668	-0.558196
H	-3.655536	-2.382076	-1.002114
H	-4.410887	-1.954150	1.945360
H	-2.918294	-2.738038	1.363406
H	-4.498489	-3.504872	1.058513
H	-5.992061	-0.819760	0.222462
H	-5.577031	-0.897350	-1.510488
H	-6.125854	-2.368781	-0.658995

Energy E(RB+HF-LYP) -1540.98556231 a.u.
                    -4045857.59 kJ/mol
SCF Convergence: 0.9291D-08
Maximum Force: 0.000005
ZPE-correction   :   0.367655 a.u.
                             965.28 kJ/mol
Energy (298K)   :   -1540.586953 a.u.
Enthalpy (298K)   :   -1540.586009 a.u.
Free Energy (298K):   -1540.684775 a.u.
Lowest Frequency   12.9973 cm-1
==========

4
B3LYP/W-NO/wno.log
Route: #P B3LYP/GenECP GFInput Freq

W	-1.680135	0.166761	-0.022118
H	-3.019735	1.171847	0.727841
C	-1.239079	-0.200142	1.962691
N	-0.351239	-0.908552	-0.726354
C	-2.448246	0.814998	-1.819983
O	-1.031888	-0.376140	3.077577
O	0.500679	-1.641371	-1.162708
O	-2.903069	1.200350	-2.803883
P	-0.423975	2.374591	0.115691
P	-3.524311	-1.560623	0.066345
C	-1.480043	3.861412	-0.155757
H	-1.961423	3.794737	-1.142298
H	-2.269097	3.885940	0.609140
H	-0.883253	4.785524	-0.104772
C	0.436525	2.785133	1.695029
H	-0.283157	2.757799	2.526093
H	0.895978	3.784802	1.645238
H	1.221220	2.039528	1.884575
C	0.914842	2.579924	-1.133021
H	1.383660	3.573237	-1.051276
H	1.680443	1.803913	-0.986602
H	0.491542	2.459690	-2.140932
C	-5.192508	-0.971962	-0.453628
C	-3.882612	-2.337534	1.701540
C	-3.245147	-3.025206	-1.020059
H	-5.937472	-1.780799	-0.394394
H	-5.495984	-0.141096	0.199068
H	-5.145369	-0.597468	-1.486481
H	-4.706514	-3.064774	1.629391
H	-2.980218	-2.847376	2.069160
H	-4.152791	-1.553258	2.423629
H	-4.069792	-3.750989	-0.941277
H	-3.152306	-2.689431	-2.063222
H	-2.300362	-3.511262	-0.736056
H	2.102020	-0.866118	-1.281296
O	2.950067	-0.375434	-1.250293
C	3.785750	-0.948766	-0.292330
H	3.602215	-2.024814	-0.159009
C	5.232850	-0.821090	-0.794737
C	3.544844	-0.304312	1.087074
F	6.099113	-1.307222	0.108103
F	5.374580	-1.528718	-1.920712
F	5.567717	0.445362	-1.051299
F	4.269690	-0.886053	2.048073
F	3.811272	1.008100	1.094532
F	2.244736	-0.450754	1.412158

Energy E(RB+HF-LYP) -2135.98411537 a.u.
                    -5608026.29 kJ/mol
SCF Convergence: 0.8445D-08
Maximum Force: 0.000040
ZPE-correction   :   0.322561 a.u.
                             846.88 kJ/mol
Energy (298K)   :   -2135.626886 a.u.
Enthalpy (298K)   :   -2135.625942 a.u.
Free Energy (298K):   -2135.735181 a.u.
Lowest Frequency   6.4944 cm-1
==========

6
B3LYP/W-Water/wwb3.log
Route: #P B3LYP/GenECP Freq

Atom Coordinates (x,y,z) in Angstrom

W	-0.087188	-0.158047	-0.080268
H	-0.022044	1.291190	1.061202
C	-0.031252	1.224299	-1.611608
N	-0.243443	-1.625773	-1.209456
C	-0.104074	-1.271206	1.653620
O	-0.005404	2.006532	-2.453508
O	-0.366324	-2.561310	-1.926357
O	-0.108858	-1.871472	2.635096
P	-2.555936	0.304436	0.215802
P	2.456432	-0.155451	0.026597
C	-3.160353	1.946992	-0.372937
H	-4.238006	2.071648	-0.183460
H	-2.969216	2.042909	-1.451677
H	-2.604492	2.741631	0.145566
C	-3.685530	-0.869504	-0.650745
H	-4.743100	-0.609962	-0.485910
H	-3.468517	-0.852617	-1.728728
H	-3.498285	-1.889514	-0.284731
C	-3.187773	0.267599	1.949649
H	-4.260836	0.511113	1.993823
H	-2.621453	0.993311	2.551085
H	-3.025048	-0.732467	2.377365
C	3.212738	0.050003	1.695386
H	2.819680	-0.716863	2.378629
H	2.949567	1.044657	2.084192
H	4.309161	-0.039824	1.640988
C	3.352743	1.115989	-0.962384
H	3.068572	1.027234	-2.021132
H	3.064560	2.112160	-0.595171
H	4.443194	0.993654	-0.866700
C	3.191574	-1.738931	-0.570967
H	4.291543	-1.713747	-0.521367
H	2.875437	-1.917454	-1.609016
H	2.817072	-2.569521	0.044931
H	1.086538	2.536162	1.191683
O	1.793914	3.196090	1.331038
H	1.339162	4.007249	1.578202

Energy E(RB+HF-LYP) -1423.10340153 a.u.
                    -3736357.98 kJ/mol

SCF Convergence: 0.7732D-08
Maximum Force: 0.000566

ZPE-correction   :   0.282592 a.u.
                             741.95 kJ/mol

Energy (298K)   :   -1422.793487 a.u.
                        -3735544.30 kJ/mol
Enthalpy (298K)   :   -1422.792543 a.u.
                        -3735541.82 kJ/mol
Free Energy (298K):   -1422.881482 a.u.
                        -3735775.33 kJ/mol

Lowest Frequency   9.8647 cm-1
==================================

$WH(CO)_2(NO)(PMe_3)_2$
B3LYP/W/w.log
Route: #P B3LYP/GenECP Freq

Atom Coordinates (x,y,z) in Angstrom

W	0.000003	0.025119	0.022029
H	-0.000054	0.034256	-1.810381
C	-0.000054	2.067188	-0.254483
C	0.000054	-2.018076	-0.203946
N	0.000000	0.044735	1.885675
O	-0.000111	3.198218	-0.463661
O	0.000107	-3.157124	-0.378015
O	-0.000031	0.067180	3.071788
P	2.510394	-0.019290	-0.275993
P	-2.510391	-0.019339	-0.275993
C	3.116774	-0.808103	-1.828910
C	3.396709	1.601185	-0.292220
C	3.426024	-0.942522	1.034978
C	-3.396765	1.601105	-0.292241
C	-3.116748	-0.808166	-1.828910
C	-3.425985	-0.942592	1.034987
H	4.513685	-0.920026	0.862265
H	3.202145	-0.494038	2.014100
H	3.081652	-1.986896	1.052161
H	4.483382	1.467437	-0.412338
H	3.013819	2.217836	-1.118607
H	3.197489	2.130667	0.651026
H	4.217280	-0.813037	-1.874708
H	2.744434	-1.841569	-1.882753
H	2.711688	-0.256579	-2.689175
H	-4.217255	-0.813194	-1.874673
H	-2.711742	-0.256576	-2.689171
H	-2.744320	-1.841598	-1.882802
H	-4.483426	1.467309	-0.412410
H	-3.197617	2.130594	0.651016
H	-3.013867	2.217779	-1.118607
H	-4.513652	-0.920089	0.862310
H	-3.081613	-1.986966	1.052138
H	-3.202070	-0.494130	2.014110

Energy E(RB+HF-LYP) -1346.63146137 a.u.
                    -3535580.90 kJ/mol

SCF Convergence: 0.9767D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000298

ZPE-correction   :   0.258455 a.u.
                             678.57 kJ/mol

Energy (298K)   :   -1346.349059 a.u.
                        -3534839.45 kJ/mol
Enthalpy (298K)   :   -1346.348115 a.u.
                        -3534836.98 kJ/mol
Free Energy (298K):   -1346.429077 a.u.
                        -3535049.54 kJ/mol

Lowest Frequency   12.0426 cm-1
==================================

NEt_3
TPSS/N/n.log
Route: #P TPSSTPSS/Gen Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

N	0.000039	-0.296085	-0.038068
C	-1.218303	-1.085146	0.197158
C	-0.000034	0.993225	0.692539
C	1.218451	-1.085027	0.197189
C	-0.000206	2.211673	-0.234661
H	0.890522	2.209671	-0.885207
H	-0.890998	2.209511	-0.885118
H	-0.000266	3.147858	0.354108
H	-0.879166	1.033783	1.359740
H	0.879197	1.033945	1.359594
C	2.471087	-0.446489	-0.403954
H	3.344148	-1.103530	-0.243227
H	2.342326	-0.285818	-1.487678
H	2.699509	0.526946	0.064134
H	1.382980	-1.273410	1.283723
H	1.057686	-2.069351	-0.268315
C	-2.471015	-0.446708	-0.403927
H	-3.343994	-1.103863	-0.243218
H	-2.699544	0.526670	0.064226
H	-2.342303	-0.285962	-1.487646
H	-1.057450	-2.069433	-0.268394
H	-1.382804	-1.273593	1.283687

Energy E(RTPSS-TPSS) -292.41764802 a.u.
                     -767742.53 kJ/mol

SCF Convergence: 0.2627D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000033

ZPE-correction   :   0.201522 a.u.
                             529.10 kJ/mol

Energy (298K)   :   -292.206556 a.u.
                        -767188.31 kJ/mol
Enthalpy (298K)   :   -292.205612 a.u.
                        -767185.83 kJ/mol
Free Energy (298K):   -292.250107 a.u.
                        -767302.66 kJ/mol

Lowest Frequency   57.9195 cm-1
==================================

1
TPSS/Iso-N/iso-n.log
Route: #P TPSSTPSS/Gen Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

C	2.559875	0.364901	-0.278378
O	1.615438	-0.716733	-0.250930
H	0.704081	-0.363952	-0.074897
C	2.719234	1.007342	1.105910
H	3.068915	0.256154	1.835923
H	3.448737	1.837600	1.076772
H	1.756710	1.413934	1.464477
C	3.872923	-0.210055	-0.803878
H	4.237414	-1.002117	-0.126278
H	4.645891	0.575395	-0.875408
H	3.724733	-0.652719	-1.802984
H	2.209914	1.143700	-0.987442
N	-1.177753	0.085076	-0.045518
C	-1.190829	1.540083	-0.334826
C	-1.677753	-0.704744	-1.195427
C	-1.863220	-0.247596	1.234986
C	-1.393585	-2.202622	-1.086289
H	-0.316004	-2.391263	-0.951930
H	-1.943793	-2.663268	-0.247693
H	-1.726721	-2.703741	-2.011938
H	-2.766960	-0.548971	-1.339694
H	-1.175401	-0.304401	-2.089618
H	-0.524122	1.699970	-1.197150
C	-2.555705	2.188702	-0.616231
H	-3.026327	1.776504	-1.524771
H	-3.254592	2.050041	0.227112
H	-2.424954	3.274541	-0.769296
H	-0.715711	2.038902	0.524183
C	-1.014791	-1.112637	2.170626
H	-1.577078	-1.327305	3.097801
H	-0.739406	-2.070830	1.702740
H	-0.080776	-0.593597	2.442743
H	-2.110223	0.694791	1.747771
H	-2.830452	-0.741270	1.026694

Energy E(RTPSS-TPSS) -486.79577910 a.u.
                     -1278082.32 kJ/mol

SCF Convergence: 0.1486D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000003

ZPE-correction   :   0.309576 a.u.
                             812.79 kJ/mol

Energy (298K)   :   -486.469587 a.u.
                        -1277225.90 kJ/mol
Enthalpy (298K)   :   -486.468643 a.u.
                        -1277223.42 kJ/mol
Free Energy (298K):   -486.531361 a.u.
                        -1277388.09 kJ/mol

Lowest Frequency   23.4194 cm-1
==================================

Isopropanol
TPSS/Iso/iso.log
Route: #P TPSSTPSS/Gen Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

O	-0.031595	1.381561	-0.162609
H	-0.877286	1.779658	0.098821
C	0.002278	0.032815	0.364909
H	-0.006823	0.080886	1.471962
C	-1.211019	-0.773425	-0.104950
H	-1.228366	-0.837341	-1.206888
H	-1.184827	-1.797848	0.308048
H	-2.153448	-0.302205	0.230825
C	1.328123	-0.564889	-0.090480
H	1.365528	-0.618197	-1.192394
H	1.452936	-1.582926	0.317357
H	2.168758	0.058469	0.256267

Energy E(RTPSS-TPSS) -194.36886528 a.u.
                      -510315.46 kJ/mol
SCF Convergence: 0.2204D-08
Maximum Force: 0.000026

ZPE-correction   :   0.105990 a.u.
                             278.28 kJ/mol

Energy (298K)   :   -194.257327 a.u.
                         -510022.61 kJ/mol
Enthalpy (298K)   :   -194.256383 a.u.
                         -510020.13 kJ/mol
Free Energy (298K):   -194.290346 a.u.
                         -510109.30 kJ/mol

Lowest Frequency   223.7991 cm-1
==================================

H_2O
TPSS/H2O/h2o.log
Route: #P TPSSTPSS/Gen/Auto Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

O	0.000000	0.000000	0.119007
H	0.000000	0.765320	-0.476030
H	0.000000	-0.765320	-0.476030

Energy E(RTPSS-TPSS)   -76.46175897 a.u.
                      -200750.35 kJ/mol
SCF Convergence: 0.3471D-09
Maximum Force: 0.000082

ZPE-correction   :   0.020791 a.u.
                              54.59 kJ/mol
Energy (298K)   :   -76.438132 a.u.
                        -200688.32 kJ/mol
Enthalpy (298K)   :   -76.437188 a.u.
                        -200685.84 kJ/mol
Free Energy (298K):   -76.458635 a.u.
                        -200742.15 kJ/mol
Lowest Frequency 1609.7323 cm-1
==================================

2
TPSS/HFIP-N/hfip-n.log
Route: #P TPSSTPSS/Gen Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

C	-1.272561	0.102756	-0.279562
O	-0.306344	0.661475	0.560196
H	0.631276	0.391472	0.265050
C	-1.628885	-1.338925	0.159445
F	-2.164805	-1.399255	1.388963
F	-2.477145	-1.937183	-0.704910
F	-0.486053	-2.083611	0.174782
C	-2.482433	1.058897	-0.300913
F	-2.958076	1.318565	0.928049
F	-3.494346	0.552114	-1.044767
F	-2.112154	2.230332	-0.863522
H	-0.941955	0.019185	-1.331666
N	2.280490	0.102131	-0.159375
C	2.895914	1.451300	-0.278856
C	2.953933	-0.758781	0.863066
C	2.215820	-0.571064	-1.489234
C	2.758041	2.320080	0.970545
H	1.704241	2.410883	1.281231
H	3.344504	1.921406	1.815490
H	3.144658	3.329914	0.749304
H	3.966888	1.365018	-0.547395
H	2.391394	1.945531	-1.123379
H	1.610530	0.078591	-2.141688
C	3.549768	-0.883342	-2.181774
H	4.117261	0.032483	-2.416062
H	4.188152	-1.538723	-1.564682
H	3.352033	-1.407561	-3.132972
H	1.643955	-1.498764	-1.341528
C	2.240473	-0.799554	2.216746
H	2.808480	-1.448027	2.907699
H	2.158170	0.198301	2.673780
H	1.223890	-1.209681	2.111967
H	2.993405	-1.780323	0.458137
H	4.003241	-0.433278	0.986638

Energy E(RTPSS-TPSS) -1081.83618221 a.u.
                     -2840360.90 kJ/mol

SCF Convergence: 0.4924D-08
<S**2>:   0.0000
Charge: 0.0000
  Maximum Force: 0.000090

ZPE-correction   :   0.263993 a.u.
                             693.11 kJ/mol

Energy (298K)   :   -1081.551815 a.u.
                        -2839614.29 kJ/mol
Enthalpy (298K)   :   -1081.550871 a.u.
                        -2839611.81 kJ/mol
Free Energy (298K):   -1081.623772 a.u.
                        -2839803.21 kJ/mol

Lowest Frequency   21.9793 cm-1
==================================

HFIP
TPSS/HFIP/hfip.log
Route: #P TPSSTPSS/Gen Opt Freq GFInput

Atom Coordinates (x,y,z) in Angstrom

O	0.044006	1.872149	-0.015583
H	-0.794629	2.297365	-0.260877
C	0.004871	0.541307	-0.490921
C	1.309100	-0.135068	-0.028308
C	-1.282921	-0.171320	-0.022722
H	0.000452	0.487695	-1.595267
F	1.304098	-1.440061	-0.381741
F	2.358869	0.455560	-0.632803
F	1.487449	-0.055735	1.298237
F	-1.460023	-1.345903	-0.652538
F	-1.327595	-0.379558	1.300651
F	-2.334373	0.635500	-0.350417

Energy E(RTPSS-TPSS) -789.40023733 a.u.
                  -2072570.32 kJ/mol

SCF Convergence: 0.1385D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000004

ZPE-correction   :   0.060509 a.u.
                            158.87 kJ/mol

Energy (298K)   :   -789.330356 a.u.
                       -2072386.85 kJ/mol
Enthalpy (298K)   :   -789.329412 a.u.
                       -2072384.37 kJ/mol
Free Energy (298K):   -789.375216 a.u.
                       -2072504.63 kJ/mol

Lowest Frequency   40.6905 cm-1
==========

5
TPSS/W-CO/wco.log
Route: #N TPSSTPSS/GenECP Freq

W	1.851784	0.136424	0.009833
H	2.208710	0.218090	-1.782924
C	3.547293	1.301261	0.187992
N	1.495057	0.060260	1.853543
C	0.255279	-1.003692	-0.530149
O	4.506008	1.953208	0.255067
O	1.271019	0.008264	3.022303
O	-0.650319	-1.669798	-0.865200
P	0.578382	2.222922	-0.600330
P	3.309224	-1.895673	-0.209757
C	-0.257091	3.085832	0.806852
C	1.583450	3.574353	-1.368121
C	-0.790633	2.027098	-1.828414
C	5.089698	-1.606526	-0.626784
C	2.806059	-3.099605	-1.521881
C	3.419988	-2.963969	1.298607
H	-0.995157	2.400467	1.252756
H	0.495449	3.335282	1.572756
H	-0.765242	4.006996	0.471023
H	2.363646	3.901190	-0.661334
H	0.948262	4.436331	-1.636993
H	2.075472	3.180587	-2.272442
H	-1.222330	3.007064	-2.097115
H	-1.583449	1.390514	-1.404209
H	-0.392054	1.539923	-2.733244
H	5.633281	-2.559985	-0.746277
H	5.561796	-1.014357	0.174193
H	5.145836	-1.029974	-1.564615
H	2.787210	-2.576404	-2.491771
H	1.789961	-3.469493	-1.307515
H	3.504405	-3.953336	-1.571648
H	2.407821	-3.304901	1.571579
H	4.071212	-3.839712	1.129200
H	3.816946	-2.364511	2.134319
H	-2.525405	-1.191397	-1.052651
O	-3.399132	-0.778918	-1.202419
C	-4.184609	-0.916044	-0.041676
H	-4.065294	-1.901477	0.441481
C	-5.658409	-0.828661	-0.486211
C	-3.783266	0.134344	1.022029
F	-5.951483	-1.884301	-1.271615
F	-5.918556	0.293884	-1.176461
F	-6.482438	-0.867474	0.584900
F	-3.980724	1.400627	0.609823
F	-2.453997	-0.004363	1.279250
F	-4.441660	-0.045616	2.182191

Energy E(RTPSS-TPSS) -2136.18135171 a.u.
                    -5608544.14 kJ/mol
SCF Convergence: 0.4698D-08
Maximum Force: 0.000083
ZPE-correction   :   0.317771 a.u.
                             834.31 kJ/mol
Energy (298K)   :   -2135.828124 a.u.
Enthalpy (298K)   :   -2135.827180 a.u.
Free Energy (298K):   -2135.937917 a.u.
Lowest Frequency   10.8126 cm-1
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3’

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TPSS/W-H/wh.log
Route:   #N TPSSTPSS/GenECP Freq
---------------------------------
 W   -1.550865  -0.075501  -0.075509
 H    0.057868   0.290984   0.733596
 C   -0.526224  -0.087222  -1.859766
 N   -3.220254  -0.331198  -0.881474
 C   -2.305839  -0.030949   1.839725
 O    0.067944  -0.086898  -2.858979
 O   -4.287246  -0.462125  -1.393906
 O   -2.714461  -0.009010   2.926888
 P   -1.570592   2.442800  -0.111975
 P   -1.004085  -2.514667   0.304146
 C   -0.213866   3.280201  -1.052772
 H   -0.327925   4.377883  -1.017565
 H   -0.232368   2.944566  -2.102671
 H    0.754838   3.001185  -0.608101
 C   -3.094732   3.187088  -0.852517
 H   -3.053872   4.290240  -0.833681
 H   -3.194945   2.838641  -1.893576
 H   -3.976131   2.840560  -0.288381
 C   -1.460649   3.282684   1.532784
 H   -1.460746   4.380740   1.418923
 H   -0.531750   2.964645   2.033883
 H   -2.316383   2.978914   2.157685
 C   -0.283621  -2.943468   1.953268
 H   -0.959875  -2.599207   2.752782
 H    0.686826  -2.433116   2.064473
 H   -0.135778  -4.033839   2.041560
 C    0.173507  -3.345449  -0.855462
 H   -0.197790  -3.244455  -1.888416
 H    1.159068  -2.858055  -0.782727
 H    0.278429  -4.416011  -0.606471
 C   -2.498175  -3.603624   0.212157
 H   -2.236778  -4.660139   0.398846
 H   -2.953187  -3.506466  -0.787247
 H   -3.234759  -3.267841   0.960424
 H    1.389977  -0.238889   0.858356
 O    2.329444  -0.577220   0.943583
 C    3.119834   0.083917  -0.009561
 C    3.696147   1.400867   0.564001
 C    4.194987  -0.911246  -0.486755
 H    2.547381   0.373483  -0.908485
 F    4.567565   1.206054   1.566523
 F    2.669437   2.151082   1.047037
 F    4.306647   2.133038  -0.394401
 F    4.883356  -1.451620   0.531393
 F    3.597628  -1.920835  -1.166227
 F    5.074274  -0.321620  -1.326447
---------------------------------
Energy E(RTPSS-TPSS)  -2136.18914435 a.u.
                     -5608564.60 kJ/mol
SCF Convergence: 0.5722D-08
Maximum Force: 0.000039
ZPE-correction    :        0.318220 a.u.
                             835.49 kJ/mol
Energy (298K)     :    -2135.835810 a.u.
Enthalpy (298K)   :    -2135.834866 a.u.
Free Energy (298K):    -2135.943540 a.u.
Lowest Frequency    13.8072 cm-1
=================================
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3
TPSS/W-H/whfixtpssf.log
Route: # TPSSTPSS/GenECP/Auto GFInput Int=UltraFine Freq

W	-1.524760	-0.000140	-0.083977
H	0.145806	0.000174	0.675929
C	-0.529172	-0.000078	-1.886449
N	-3.229212	-0.000783	-0.855723
C	-2.214565	-0.000128	1.854185
O	0.055911	-0.000047	-2.890215
O	-4.312748	-0.001313	-1.349675
O	-2.580614	-0.000127	2.957356
P	-1.262368	2.503103	0.094265
P	-1.261180	-2.503232	0.094778
C	-0.357984	3.379152	-1.262938
H	-0.336954	4.469131	-1.087888
H	-0.854978	3.171251	-2.224654
H	0.675605	2.999987	-1.310213
C	-2.866843	3.423707	0.162736
H	-2.699837	4.512098	0.244074
H	-3.447962	3.206906	-0.748767
H	-3.446361	3.073869	1.032859
C	-0.375224	3.104292	1.601472
H	-0.355347	4.207651	1.632641
H	0.657045	2.718967	1.586989
H	-0.881623	2.720378	2.502264
C	-0.372477	-3.103630	1.601372
H	-0.878188	-2.719612	2.502506
H	0.659644	-2.717958	1.585838
H	-0.352208	-4.206972	1.632847
C	-0.357606	-3.379236	-1.262990
H	-0.855476	-3.171710	-2.224334
H	0.675803	-2.999695	-1.311189
H	-0.336030	-4.469171	-1.087733
C	-2.865237	-3.424450	0.164867
H	-2.697755	-4.512761	0.246313
H	-3.447257	-3.208091	-0.746169
H	-3.444116	-3.074630	1.035421
H	1.442419	0.000418	1.265731
O	2.428035	-0.000826	1.431353
C	3.040649	0.000098	0.166776
C	3.861390	1.296767	0.000767
C	3.862296	-1.295826	-0.000353
H	2.299667	0.000189	-0.650834
F	4.803126	1.444145	0.946039
F	3.018428	2.361644	0.087078
F	4.459492	1.360762	-1.209199
F	4.803614	-1.443709	0.945261
F	3.020009	-2.361357	0.084196
F	4.461114	-1.357943	-1.210057

Energy E(RTPSS-TPSS) -2136.19565256 a.u.
                     -5608581.69 kJ/mol
SCF Convergence: 0.7416D-08
Maximum Force: 0.000247
ZPE-correction   :   0.317411 a.u.
                             833.36 kJ/mol
Energy (298K)   :   -2135.842773 a.u.
Enthalpy (298K)   :   -2135.841829 a.u.
Free Energy (298K):   -2135.951985 a.u.
Lowest Frequency   11.1304 cm-1
==========

7
TPSS/W-Iso/wisotp.log
Route: #P TPSSTPSS/GenECP/Auto Freq

W	0.711666	0.242375	-0.050990
H	-0.736985	-0.604432	0.702081
C	-0.148548	-0.198700	-1.867609
N	2.243174	1.029258	-0.786879
C	1.276071	0.548469	1.903190
O	-0.648945	-0.462251	-2.883147
O	3.233702	1.506598	-1.248356
O	1.568361	0.712965	3.016307
P	1.570897	-2.116079	0.064691
P	-0.690252	2.339652	0.101291
C	0.481680	-3.414569	-0.681932
H	0.925380	-4.419771	-0.573027
H	0.330253	-3.194901	-1.751610
H	-0.499102	-3.387564	-0.179748
C	3.186468	-2.411898	-0.790900
H	3.498192	-3.468105	-0.710497
H	3.085162	-2.135681	-1.853300
H	3.957090	-1.764686	-0.340728
C	1.882317	-2.813211	1.751912
H	2.222377	-3.862381	1.697481
H	0.951437	-2.757057	2.339814
H	2.649537	-2.205613	2.259282
C	-1.620533	2.588981	1.680080
H	-0.918628	2.566651	2.529859
H	-2.347543	1.768234	1.793315
H	-2.155874	3.554646	1.669782
C	-2.016472	2.571844	-1.166040
H	-1.568058	2.550482	-2.172979
H	-2.731607	1.737236	-1.069658
H	-2.542300	3.531533	-1.017589
C	0.302126	3.895481	-0.045548
H	-0.342252	4.789542	0.024216
H	0.830593	3.895192	-1.013095
H	1.056394	3.919903	0.758213
H	-2.357988	-0.453686	0.476683
O	-3.321219	-0.279387	0.351706
C	-3.955798	-1.506377	-0.064512
C	-3.873041	-2.570104	1.035910
C	-5.393491	-1.153747	-0.433610
H	-3.440695	-1.887899	-0.968524
H	-4.383737	-2.217355	1.949073
H	-2.820397	-2.785755	1.292213
H	-4.346408	-3.513744	0.708377
H	-5.924400	-0.747449	0.445179
H	-5.411080	-0.393494	-1.232380
H	-5.934416	-2.048428	-0.788454

Energy E(RTPSS-TPSS) -1541.15143229 a.u.
                     -4046293.09 kJ/mol
SCF Convergence: 0.8632D-08
Maximum Force: 0.000271
ZPE-correction   :   0.363805 a.u.
                             955.17 kJ/mol
Energy (298K)   :   -1540.756346 a.u.
Enthalpy (298K)   :   -1540.755402 a.u.
Free Energy (298K):   -1540.854424 a.u.
Lowest Frequency   16.4767 cm-1
==========

4
TPSS/W-NO/wno.log
Route: #P TPSSTPSS/GenECP GFInput Freq

W	-1.693569	0.154672	-0.023028
H	-3.050617	1.156071	0.687623
C	-1.289196	-0.169041	1.971101
N	-0.334958	-0.927171	-0.696692
C	-2.443691	0.771977	-1.833803
O	-1.102489	-0.319907	3.106101
O	0.532709	-1.662644	-1.113119
O	-2.896780	1.147237	-2.837056
P	-0.482459	2.369217	0.099903
P	-3.522236	-1.565665	0.064639
C	-1.566867	3.834138	-0.215995
H	-2.023987	3.741029	-1.214653
H	-2.373386	3.847717	0.534610
H	-0.987305	4.772283	-0.163191
C	0.343591	2.830721	1.690586
H	-0.394756	2.800946	2.508486
H	0.780814	3.842531	1.626890
H	1.142156	2.103655	1.907231
C	0.877921	2.588424	-1.132421
H	1.317247	3.598758	-1.058906
H	1.661315	1.833735	-0.954640
H	0.471194	2.437403	-2.145760
C	-5.196411	-0.968756	-0.447337
C	-3.879481	-2.354343	1.701073
C	-3.255278	-3.032370	-1.032977
H	-5.943887	-1.778795	-0.385012
H	-5.490494	-0.136424	0.212177
H	-5.148920	-0.591585	-1.481902
H	-4.705391	-3.082883	1.623338
H	-2.971984	-2.865191	2.062506
H	-4.148984	-1.569822	2.427107
H	-4.088131	-3.752839	-0.953196
H	-3.163521	-2.688236	-2.076230
H	-2.311051	-3.525815	-0.749868
H	2.136139	-0.878389	-1.248969
O	2.988530	-0.379090	-1.243557
C	3.841922	-0.943856	-0.280031
H	3.672582	-2.025672	-0.143124
C	5.285435	-0.794825	-0.800286
C	3.601240	-0.294918	1.103716
F	6.176794	-1.262611	0.103567
F	5.428777	-1.515282	-1.930681
F	5.600737	0.483010	-1.074944
F	4.354629	-0.859323	2.067966
F	3.837352	1.033154	1.104732
F	2.298301	-0.471725	1.446864

Energy E(RTPSS-TPSS) -2136.18627706 a.u.
                     -5608557.07 kJ/mol
SCF Convergence: 0.7007D-08
Maximum Force: 0.000489
ZPE-correction   :   0.318297 a.u.
                             835.69 kJ/mol
Energy (298K)   :   -2135.832874 a.u.
Enthalpy (298K)   :   -2135.831930 a.u.
Free Energy (298K):   -2135.940551 a.u.
Lowest Frequency   14.9277 cm-1
==========

6
TPSS/W-Water/wwtp.log
Route: #P TPSSTPSS/GenECP/Auto GFInput Opt(CalcFC) Freq

Atom Coordinates (x,y,z) in Angstrom

W	-0.081293	-0.160093	-0.093379
H	-0.047901	1.187038	1.158762
C	-0.034632	1.334401	-1.508270
N	-0.213423	-1.550817	-1.340135
C	-0.091953	-1.396930	1.549374
O	-0.014049	2.191886	-2.292371
O	-0.322619	-2.439139	-2.127851
O	-0.091757	-2.073458	2.494917
P	-2.535732	0.270763	0.236672
P	2.442785	-0.135731	0.051106
C	-3.121182	1.987587	-0.136391
H	-4.200778	2.096742	0.067480
H	-2.923463	2.220342	-1.195615
H	-2.554816	2.698591	0.487136
C	-3.679009	-0.769831	-0.782384
H	-4.736580	-0.525620	-0.580043
H	-3.459590	-0.603854	-1.849860
H	-3.496190	-1.833056	-0.555926
C	-3.184836	0.020593	1.952951
H	-4.255885	0.280740	2.019860
H	-2.605917	0.652781	2.646025
H	-3.044605	-1.032779	2.246251
C	3.167291	0.028829	1.744991
H	2.766255	-0.765913	2.395147
H	2.883947	1.009838	2.160094
H	4.268093	-0.048945	1.706304
C	3.352698	1.170392	-0.888957
H	3.081075	1.108909	-1.955660
H	3.048827	2.153588	-0.492376
H	4.444451	1.046931	-0.778506
C	3.208711	-1.702074	-0.572440
H	4.309714	-1.666205	-0.496787
H	2.915342	-1.852973	-1.624280
H	2.826151	-2.551652	0.016833
H	0.988758	2.439404	1.267408
O	1.659182	3.152063	1.402071
H	1.148403	3.974594	1.364712

Energy E(RTPSS-TPSS) -1423.24506792 a.u.
                    -3736729.93 kJ/mol

SCF Convergence: 0.2892D-08
Maximum Force: 0.000176

ZPE-correction   :   0.279800 a.u.
                             734.61 kJ/mol

Energy (298K)   :   -1422.937743 a.u.
                        -3735923.04 kJ/mol
Enthalpy (298K)   :   -1422.936798 a.u.
                        -3735920.56 kJ/mol
Free Energy (298K):   -1423.026669 a.u.
                        -3736156.52 kJ/mol

Lowest Frequency   8.6518 cm-1
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$WH(CO)_2(NO)(PMe_3)_2$
TPSS/W/w.log
Route: #P TPSSTPSS/GenECP Freq

Atom Coordinates (x,y,z) in Angstrom

W	0.000000	0.026710	0.030602
H	0.000058	0.034501	-1.797144
C	-0.000006	2.058923	-0.274578
C	0.000005	-2.008707	-0.221605
N	-0.000015	0.046549	1.907534
O	0.000023	3.196566	-0.514547
O	-0.000012	-3.155592	-0.424608
O	-0.000006	0.068895	3.101217
P	2.493377	-0.019126	-0.271624
P	-2.493376	-0.019117	-0.271628
C	3.087547	-0.777088	-1.851385
C	3.393249	1.600392	-0.255039
C	3.419991	-0.981087	1.012420
C	-3.393479	1.600247	-0.252950
C	-3.087475	-0.775167	-1.852335
C	-3.419830	-0.982832	1.011216
H	4.508326	-0.959826	0.826091
H	3.207710	-0.550443	2.004965
H	3.065832	-2.025050	1.006346
H	4.480589	1.459728	-0.386348
H	3.005152	2.238585	-1.066010
H	3.201075	2.106507	0.705438
H	4.190655	-0.786174	-1.902755
H	2.705511	-1.808728	-1.923178
H	2.677407	-0.199776	-2.695587
H	-4.190586	-0.784488	-1.903626
H	-2.677561	-0.196648	-2.695821
H	-2.705158	-1.806605	-1.925499
H	-4.480807	1.459580	-0.384347
H	-3.201299	2.105187	0.708143
H	-3.005542	2.239510	-1.063155
H	-4.508179	-0.961424	0.824984
H	-3.065580	-2.026755	1.003762
H	-3.207530	-0.553456	2.004308

Energy E(RTPSS-TPSS) -1346.77048293 a.u.
                     -3535945.90 kJ/mol

SCF Convergence: 0.4803D-08
<S**2>: 0.0000
Charge: 0.0000
  Maximum Force: 0.000133

ZPE-correction   :   0.256056 a.u.
                             672.28 kJ/mol

Energy (298K)   :   -1346.490258 a.u.
                        -3535210.17 kJ/mol
Enthalpy (298K)   :   -1346.489314 a.u.
                        -3535207.69 kJ/mol
Free Energy (298K):   -1346.569818 a.u.
                        -3535419.06 kJ/mol

Lowest Frequency   21.8402 cm-1
==================================

O–H bond lengths (in pm) of isopropanol and HFIP in compounds 1, 2, 3, 3′, 4 and 5:

	BP86	PBE	B3LYP	TPSS
Isopropanol	97.3	97.2	96.3	97.1
HFIP	97.4	97.3	96.4	97.2
1	99.8	99.7	98.1	99.3
2	103	103	100	102
3	100	100	98.7	99.9
3′	101	101	99.0	100
4	99.2	99.0	98.7	98.8
5	98.1	98.0	96.9	97.8