Electronic Supplementary Information

for

The Diverse Mechanisms for the Oxidative Addition of C-Br bonds to $Pd(PR_3)$ and $Pd(PR_3)_2$ Complexes

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Summary

1.- Details of the mechanistic study
1.1 Table S1, SET mechanism.

We present in Table S1 the relative free energies of the lowest Single Electron Transfer transition states (SET) or in its defect the lowest SET intermediate $(PR_3)_2PdBr\cdot + \cdot R$ respect to PhBr or CH_3Br and palladium bis-and mono-phosphine. Energies presented corredpond to Gibbs free energies in kcal.mol^{-1}.

For bis-phosphines, the preferred type of TS is labelled in the table:

TSc states for cis bisphosphine transition state,
TSt states for trans bisphosphine transition states and
TSR1 for the monophosphine TSs.

In a large number of cases the open shell SET TS could not be located. In that cases we computed the energy of $(PR_3)_2PdBr\cdot + \cdot R$ intermediates. These energies should be taken as the minimum possible value for the bond cleavage through a SET mechanism, and are labelled in the Table with "I".

Table S1 Free energies of the lowest SET intermediates (I) or transition states (TSc,TSt orTSR1(see text) relative to separate reactants, in kcal.mol^{-1}

	Bis-phosphine						Mono-phosphine					
	Gas phase		THF		DMF		Gas phase		THF		DMF	
	PhBr	CH_3Br	PhBr	CH_3Br	PhBr	CH_3Br	PhBr	CH_3Br	PhBr	CH_3Br	PhBr	CH_3Br
PF_3	40.7^{I}	28.7^{I}	38.6^{I}	33.7^{TSc}	37.5^{I}	33.2^{TSc}	44.0^{I}	32.0^{I}	32.5^{I}	27.9^{TSR1}	30.8^{I}	27.4^{TSR1}
PH_3	32.9^{I}	26.4^{TSc}	24.6^{I}	22.8^{TSt}	22.6^{I}	22.8^{TSt}	27.1^{I}	15.1^{I}	26.4^{I}	35.1^{TSR1}	17.5^{I}	24.2^{TSR1}
PMe_3	23.9^{I}	21.5^{TSc}	15.7^{I}	16.5^{TSt}	17.1^{I}	17.1^{TSt}	22.8^{I}	10.9^{I}	14.9^{I}	19.8^{TSR1}	12.9^{I}	11.9^{TSR1}
PPh_3	26.4^{I}	14.4^{I}	22.4^{I}	24.6^{TSt}	19.4^{I}	25.6^{TSt}	18.9^{I}	6.9^{I}	12.1^{I}	15.4^{CTSR1}	10.1^{I}	14.7^{TSR1}

1.2 Benchmark study of the computational tools.

To check the validity of our computational approach we performed Single Point calculations with a variety of DFT functionals all of them including the dispersion correction D3 developed by Grimme et al.[1] See Table S2.

Table S2 Potential energies of the transition states (concerted and S_N) relative to separate reactants, for PhBr with mono and bis-trimethylphosphines, in DMF and in kcal.mol^{-1}.

Potential energies	$Pd(PMe_3)_2$		$Pd(PMe_3)$	
	S_N	Conc	Conc	S_N
B3LYP+DispGD2	**-5.3**	**3.7**	**-12.2**	**-9.1**
Singlet point calculations with different DFT-D3 methods				
B3LYP-D3	-1.9	5.7	-11.0	-6.7
B3PW91-D3	-5.5	2.6	-13.3	-8.3
B97D3	-4.7	2.7	-10.7	-9.1
BMK-D3	-8.7	1.6	-18.3	-14.4
BP86-D3	-11.6	-3.7	-17.9	-15.0
M06-D3	2.7	5.4	-12.3	-1.0
M06HF-D3	3.5	7.4	-9.8	-0.4
M06L-D3	-2.8	2.6	-12.5	-6.9
PBE0-D3	-2.3	4.8	-13.3	-5.9
PBE-D3	-7.7	-1.1	-17.2	-12.2
TPSS-D3	-10.5	-3.1	-17.4	-14.0

The results show that the different DFT-D3 methods show a similar behaviour. The approach we have used B3LYP+DispGD2 gives similar results to other functionals such as B97D3, B3PW91 or M06L. The different stability of the competing TSs holds as well as the relative energies.
A different behavior is observed for M06 and M06HF that give in all cases less stable TSs. As M06L, gives values similar to B3LYP+DispGD2 we believe its result is better than the ones of the two functionals of the same family. At the other end we find the results for TPSS and BP86, these functionals give smaller barriers, however they show exactly the same tendencies.

[1] S. Grimme, J. Antony, S. Ehrlich and H. Krieg, "A consistent and accurate ab initio parameterization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu," *J. Chem. Phys*., **132** (2010) 154104.

1.3 The adducts

In the main manuscript the energies presented correspond to the Gibbs free energies of the transition states respect to separate reactants. In the case of bis-phosphine systems this corresponds actually to the barrier of the addition, as adducts before the TS are known to be high in energy. However, in the case of mono-phosphines formation of stable adducts is expected. All barriers for the same palladium complex and substrate should be computed from the energy of the most stable adduct. Gibbs free energies of the mono-phosphine adducts respect to separate reactants are reported in Table S3.

Table S3 Free energies of the adducts relative to separate reactants, for PhBr with mono and bis-phosphines, and in kcal.mol^{-1}.

	Gas phase	THF	DMF	Water
$Pd(PF_3)$	-10.6	-3.1	-1.3	-1.0
$Pd(PH_3)$	-8.0	-6.2	-7.4	-7.2
$Pd(PMe_3)$	-9.8	-6.8	-6.3	-6.2
$Pd(PPh_3)$	-9.2	-6.2	-5.3	-4.7

2.- Coordinates (in Å) and Energies (in hartree) of the located species.

2.1 Non radical species optimized with B3LYP

2.1.1 Species Optimized in gas phase

gas_1PF3_conctransA
E=-2241470.136325709 kcal/mol
P 2.556974 -0.549330 -0.001953
Pd 0.307261 -0.207552 -0.007858
Br -0.692804 2.105876 0.003368
C -1.706712 -0.105327 -0.000768
C -2.280890 -0.464020 -1.227522
C -2.270591 -0.471727 1.228601
C -3.407802 -1.293441 -1.211199
H -1.867613 -0.101773 -2.162506
C -3.397670 -1.300850 1.216646
H -1.849326 -0.115421 2.162321
C -3.962234 -1.710873 0.003764
H -3.856692 -1.600195 -2.151713
H -3.838732 -1.613351 2.158974
H -4.846997 -2.340450 0.005534
F 3.182527 -1.796013 -0.788639
F 3.534660 0.571089 -0.582258
F 3.302179 -0.782824 1.393466

gas_1PF3_conctransB
E=-2241470.6298620156 kcal/mol
P 2.360387 0.215971 -0.000003
Pd 0.406453 -0.821716 -0.000020
Br -1.882892 -1.699057 0.000037
C -1.365543 0.496248 -0.000015
C -1.555648 1.141643 1.224805
C -1.555856 1.141627 -1.224811
C -1.869832 2.504693 1.210452
H -1.452910 0.604305 2.160323
C -1.870044 2.504676 -1.210423
H -1.453296 0.604275 -2.160341
C -2.023899 3.188321 0.000023
H -1.997664 3.026323 2.154769
H -1.998046 3.026291 -2.154725
H -2.277058 4.243979 0.000037
F 2.704865 1.218582 -1.199966
F 3.748077 -0.585973 -0.000250
F 2.705114 1.218273 1.200152

gas_1PH3_conctransA
E=-2054573.1276342494 kcal/mol
P -3.019689 -1.293795 0.000365
Pd -0.853395 -0.403883 -0.000681
Br -0.037109 2.031208 0.000333
C 1.126173 0.057641 0.000047
C 1.723770 -0.278969 1.226759
C 1.724407 -0.278356 -1.226504
C 2.900758 -1.034138 1.213000
H 1.282743 0.050247 2.161154
C 2.901398 -1.033549 -1.212495
H 1.283895 0.051366 -2.160962
C 3.489018 -1.411264 0.000308
H 3.362223 -1.317635 2.155098
H 3.363368 -1.316556 -2.154492
H 4.411251 -1.984707 0.000411
H -3.430091 -2.179767 -1.026040
H -4.154053 -0.448494 -0.053339
H -3.462168 -2.089409 1.085663

gas_1PH3_conctransB
E=-2054572.2982548005 kcal/mol
P -2.509809 -1.760741 0.001318
Pd -1.120479 0.059033 -0.001162
Br 0.370859 2.065074 0.000842
C 1.083881 0.041750 0.000805
C 1.571153 -0.441727 1.224121
C 1.570908 -0.440170 -1.223210
C 2.499928 -1.485873 1.209730
H 1.225540 -0.016902 2.159458
C 2.499602 -1.484412 -1.210396
H 1.225262 -0.014017 -2.157923
C 2.963394 -2.013494 -0.000729
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H 3.692999 -2.817587 -0.001318
H -2.533890 -2.631129 1.118451
H -2.348338 -2.764040 -0.985024
H -3.915819 -1.634719 -0.130086

gas_1PMe3_conctransA
E=-2128605.767072784 kcal/mol
Br 1.104634 2.085125 0.001410
P -2.644961 -0.449767 -0.001006
Pd -0.323393 -0.084565 -0.003886
C -3.720560 1.050085 -0.155087
H -4.785136 0.789223 -0.139530
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C -3.353851 -1.255866 1.510177
H -4.439851 -1.379982 1.428096
H -2.891056 -2.236635 1.653177
H -3.129130 -0.644538 2.388914
C 1.717368 -0.071580 0.000153
C 2.200987 -0.563129 1.226976
C 2.205302 -0.560744 -1.225863
C 3.126430 -1.611060 1.213791
H 1.865020 -0.126647 2.161192
C 3.130655 -1.608788 -1.211434

H 1.872701 -0.122402 -2.160408
C 3.592688 -2.133213 0.001477
H 3.491139 -2.011244 2.156140
H 3.498676 -2.007149 -2.153263
H 4.323570 -2.936483 0.002000

gas_1PMe3_conctransB
E=-2128604.4314499586 kcal/mol
P 2.525924 0.220908 0.000008
Pd 0.394535 -0.643953 -0.000095
Br -1.894443 -1.733057 0.000060
C -1.623272 0.327454 0.000009
C -1.805182 0.993072 1.223496
C -1.805271 0.993044 -1.223478
C -2.081481 2.362368 1.209959
H -1.720353 0.451169 2.158308
C -2.081568 2.362342 -1.209949
H -1.720511 0.451123 -2.158286
C -2.216017 3.053121 0.000002
H -2.199889 2.887073 2.154253
H -2.200043 2.887028 -2.154245
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C 2.960956 1.315031 1.431763
H 2.871383 0.749509 2.363570
H 3.981771 1.705823 1.344021
H 2.257297 2.151105 1.474791
C 2.961215 1.314916 -1.431755
H 2.257958 2.151342 -1.474583
H 3.982233 1.705214 -1.344177
H 2.871185 0.749512 -2.363587
C 3.958506 -0.957575 0.000194
H 4.917238 -0.424858 0.000567
H 3.902528 -1.598351 0.884638
H 3.903045 -1.598015 -0.884531

gas_1PPh3_conctransA
E=-2489532.165418429 kcal/mol
Pd 1.191769 -0.055928 -0.015577
P -1.157792 0.097518 -0.008910
Br 2.808201 -2.099145 -0.004332
C 3.228725 0.087021 -0.011335
C 3.661515 0.627483 1.214597
C 3.670035 0.617609 -1.238418
C 4.483787 1.757894 1.199141
H 3.365452 0.165476 2.150010
C 4.492752 1.747788 -1.226050
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H -1.371477 -0.828081 4.841055
H -3.298288 0.682513 5.287560

gas_2PF3_conccis
E=-2643700.470376028 kcal/mol
P -2.581841 -0.359016 0.503285
Pd -0.322802 -0.027679 -0.092870
P 0.054291 2.231861 -0.367408
Br 0.439785 -2.254126 -1.039909
C 1.733293 -0.680219 0.112210
C 2.773776 -0.127823 -0.642526
C 1.888784 -1.011746 1.460946
C 3.969273 0.180662 0.006761
H 2.646934 0.073728 -1.700015
C 3.095771 -0.678619 2.094889
H 1.106563 -1.528572 2.006358
C 4.132045 -0.084908 1.374625
H 4.775531 0.637143 -0.560614
H 3.221733 -0.914886 3.147693
H 5.070473 0.153273 1.865632
F 1.138931 2.753493 -1.426323
F 0.542657 3.109478 0.879046
F -1.154964 3.171831 -0.832193
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F -2.859012 -0.923501 1.975879
F -3.629633 0.850627 0.536394

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E=-2269905.790455915 kcal/mol
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Pd -0.833203 0.322605 0.005296
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Br 0.045968 -2.057511 -0.636307
H -4.092914 0.910234 0.709365
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C 2.174985 0.155947 -0.881670
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H 0.836658 -0.817657 2.116752
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P -2.648457 -0.265709 0.528503
Br 0.374255 -2.120650 -1.354204
C -3.742176 -0.614368 -0.928910
H -4.765602 -0.859483 -0.621226
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H -3.325404 -1.451479 -1.496556
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gas_2PPh3_conccis
E=-3139820.426537436 kcal/mol
Br -0.308101 -2.638395 -1.981896
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Pd 0.009908 -0.715486 -0.200635
P -2.224201 0.269515 0.104670
C 0.709073 -2.718794 0.021530
C 2.066595 -3.080886 -0.014375
C -0.136571 -3.212043 1.030885
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C 0.420120 -3.943855 2.089989
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C -2.633719 0.967394 1.769042
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H -5.080763 -3.579272 1.409859

H -6.279607 -3.713973 -0.769642
C -2.602491 1.632082 -1.091790
C -1.948851 1.592086 -2.334943
C -3.487256 2.689080 -0.828530
C -2.190766 2.572572 -3.298978
H -1.240365 0.793216 -2.539395
C -3.716907 3.677150 -1.788364
H -3.993395 2.751067 0.129340
C -3.074406 3.618613 -3.026943
H -1.677912 2.524270 -4.255914
H -4.400808 4.492553 -1.566645
H -3.256127 4.388176 -3.772559

gas_PhBr
E=-1758953.0652112688 kcal/mol
C 2.183766 1.209076 0.000002
C 0.785604 1.216597 0.000015
C 0.102580 0.000019 -0.000109
C 0.785595 -1.216591 -0.000007
C 2.183733 -1.209096 0.000024
C 2.885172 -0.000005 0.000000
H 2.720705 2.153307 0.000024
H 0.236387 2.151775 0.000034
H 0.236327 -2.151739 0.000010
H 2.720690 -2.153316 0.000049
H 3.971018 -0.000033 0.000015
Br -1.812680 0.000000 0.000009

2.2.1 Species Optimized in THF

thf_1PF3_conctransA
E= -2241476.3883545357 kcal/mol
Pd 0.336163 -0.159551 -0.000208
P 2.564649 -0.504889 -0.000099
Br -0.874770 2.115669 -0.000139
C -1.696684 -0.087736 -0.000067
C -2.221899 -0.508864 -1.229905
C -2.221939 -0.508531 1.229876
C -3.257783 -1.450442 -1.214292
H -1.841139 -0.113647 -2.165190
C -3.257838 -1.450074 1.214495
H -1.841161 -0.113101 2.165065
C -3.773316 -1.918282 0.000153
H -3.666392 -1.805506 -2.155987
H -3.666493 -1.804870 2.156271
H -4.588640 -2.635217 0.000240
F 3.151795 -2.000598 -0.067237
F 3.482775 0.106368 -1.166874
F 3.461464 -0.007973 1.235665

thf_1PF3_conctransB
E=-2241475.1058190237 kcal/mol
Pd -0.398101 -0.853876 -0.005803
P -2.347213 0.162661 -0.000519
Br 1.955244 -1.633452 0.005257
C 1.379340 0.507357 0.002002
C 1.537861 1.160138 -1.224273
C 1.526319 1.166076 1.226664
C 1.766592 2.540528 -1.212326
H 1.471829 0.616708 -2.159621
C 1.755341 2.546446 1.209772
H 1.451600 0.627269 2.164047
C 1.871229 3.235961 -0.002511
H 1.866950 3.066102 -2.157650
H 1.846686 3.076897 2.153292
H 2.057842 4.305320 -0.004292
F -2.899273 0.841295 1.351538
F -2.561551 1.450074 -0.941703
F -3.720029 -0.582718 -0.398835

thf_1PH3_conctransA
E=-2054577.650723504 kcal/mol
Pd -0.884214 -0.354102 -0.000172
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Br 0.156441 2.082805 0.000084
C 1.112754 0.085942 0.000010
C 1.663360 -0.326028 -1.229005
C 1.663178 -0.326165 1.229064
C 2.735452 -1.224839 -1.213528
H 1.268562 0.054384 -2.164690
C 2.735263 -1.224974 1.213657
H 1.268209 0.054106 2.164737
C 3.272430 -1.672142 0.000079
H 3.155992 -1.565698 -2.155606
H 3.155639 -1.565965 2.155760
H 4.115066 -2.356940 0.000106
H -3.447236 -2.102087 -1.045616
H -4.195910 -0.405493 -0.024616
H -3.462941 -2.061047 1.072480

thf_1PMe3_SN2cis
E=-2128599.9863726986 kcal/mol
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Br -0.480601 2.335591 -0.130957
C 3.205075 0.930490 -0.626945
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H 3.435102 0.594978 -1.641961
C 3.507271 -1.749933 0.412682
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H 4.432505 -1.385359 0.872383
H 3.095786 -2.556338 1.025702
C 2.154261 0.268462 1.982245
H 3.141582 0.577997 2.341369
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H 1.756333 -0.505002 2.644743
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C -1.716723 -0.271380 1.438317
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C -2.967159 -0.831936 1.690364
H -1.049616 -0.005738 2.249948
C -3.452990 -0.945867 -0.683101
H -1.961634 -0.061793 -1.987097
C -3.835126 -1.175201 0.635559
H -3.266686 -1.014226 2.719171
H -4.132530 -1.169433 -1.501181
H -4.808950 -1.602662 0.854566

thf_1PMe3_conctransA
E=-2128610.35233569 kcal/mol

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Br -1.294304 2.074266 -0.001077
C -1.715053 -0.065471 0.000113
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C -2.137298 -0.612108 -1.228965
C -2.939933 -1.758391 1.213071
H -1.863214 -0.137637 2.164593
C -2.935005 -1.761257 -1.214001
H -1.855344 -0.141926 -2.164733
C -3.339490 -2.332227 -0.000679
H -3.257111 -2.197646 2.155002
H -3.248384 -2.202563 -2.156242
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H 2.969106 -1.752744 1.999191
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H 3.535182 1.898753 0.133091
H 4.785899 0.786812 -0.487238
H 3.460014 1.338340 -1.546454
C 3.299460 -1.734610 -1.092960
H 3.018721 -1.530311 -2.130210
H 4.389983 -1.819073 -1.027008
H 2.847380 -2.685591 -0.796957

thf_1PPh3_conctransA

E=-2489538.3253037445 kcal/mol
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P 1.159741 -0.073567 -0.006768
Br -2.952527 2.107266 -0.012627
C -3.226949 -0.065292 -0.017798
C -3.627083 -0.631681 -1.244922
C -3.602805 -0.641277 1.212695
C -4.347693 -1.830661 -1.226955
H -3.386048 -0.140447 -2.181305
C -4.322726 -1.840775 1.200057
H -3.344133 -0.157051 2.148042
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H -4.643055 -2.286874 -2.167890
H -4.598369 -2.304735 2.143184
H -5.271440 -3.355686 -0.010033
C 1.851109 -0.573415 1.632698
C 1.227515 -0.068575 2.787173
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H 0.363262 0.584354 2.688221
C 3.419588 -1.774828 3.049514
H 3.443501 -1.839192 0.899402
C 2.798887 -1.260120 4.189582
H 1.211239 -0.002984 4.938640
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C 1.838781 -1.329748 -1.180580
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C 3.392754 3.848434 -1.161100
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H 3.896707 4.769273 -1.441291

thf_2PF3_conccis

E=-2643706.05654186 kcal/mol
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Pd 0.308385 -0.021783 -0.060572
P 0.024677 2.253573 -0.363723
C -1.749697 -0.649505 0.123396
C -1.856975 -1.114058 1.436256
C -2.801554 -0.003471 -0.533747
C -3.027271 -0.812441 2.152085
H -1.069134 -1.702744 1.893565
C -3.960509 0.269576 0.194714
H -2.712644 0.297485 -1.571159
C -4.073909 -0.125104 1.536827
H -3.117169 -1.148550 3.181004
H -4.775920 0.798759 -0.290135
H -4.984846 0.085752 2.088312
F 3.351981 -1.652887 -0.164451
F 3.698631 0.644366 0.450756
F 2.827189 -0.911169 2.069737
F -0.323809 3.204873 0.883618
F -1.092944 2.832884 -1.363731
F 1.255558 3.112214 -0.933886

thf_2PH3_SN2cis

E=-2269907.4305275767 kcal/mol
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Pd -0.950684 0.304992 -0.004892
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H 0.711248 1.010346 -1.917079
C 2.610717 2.686515 0.358839
H 3.104521 1.953767 2.336827
H 1.981359 3.131231 -1.655234
H 3.225392 3.576658 0.453373
H -3.476637 2.398626 -0.692378
H -3.591644 0.721440 -2.000674
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H -1.814802 -2.673343 0.974775

H -0.346730 -1.902235 2.328303

thf_2PH3_conccis
E=-2269909.616049415 kcal/mol
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P 0.766639 -2.242612 -1.313672
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H 2.987117 -0.386226 2.605563
H 0.208393 -2.209719 -2.617725
H 1.929976 -2.974427 -1.661896
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H -2.743060 -0.423781 3.022308
H -4.325543 -1.588507 1.491491

thf_2PMe3_SN2cis
E=-2417975.319085328 kcal/mol
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P -2.740259 0.742941 -0.372144
Br 2.908360 -0.768687 -1.124484
C -3.015624 2.444689 -1.044303
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H 0.881227 -2.045220 2.676117
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C 2.324399 2.293309 1.904779
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H 0.856450 1.774945 -1.648646
C 1.925939 3.410405 1.132871
H 2.767834 2.448450 2.885505
H 1.087115 4.067999 -0.737114
H 2.101248 4.414923 1.506812

thf_2PMe3_conccis
E=-2417971.432215515 kcal/mol
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Br 1.096908 -1.492750 -1.878887
C 0.789791 3.013208 -1.700605
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H 0.226579 2.699325 -2.584217
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H 1.930279 2.773459 1.216850
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C 2.838554 0.125173 0.081126
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C 3.411756 -0.723480 2.291393
H 2.140381 -2.285092 3.064316
H 4.535144 0.782318 1.211018
H 4.078911 -0.723346 3.148162

thf_2PMe3_conctrans
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Pd -0.196968 0.413144 0.054745
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H 3.038268 1.129128 -1.784325
H 1.859429 2.189717 -2.572109
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H 3.477829 3.085470 0.942284
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H 0.143347 3.962136 -1.004015
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H -3.380389 2.215936 0.993354
H -3.037794 2.767776 -0.655498
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H -4.189871 0.078960 -2.285094
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H -2.726532 -0.921225 -2.488064
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H 2.795946 -0.843733 0.332472
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H -0.156074 -3.749415 -2.416837
H 3.748429 -2.144776 -1.545529
H 2.278087 -3.599765 -2.941060

thf_2PPh3_conccis
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Br -0.280585 -2.645581 -1.992976
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Pd 0.011752 -0.659149 -0.191556
P -2.250300 0.293050 0.095227
C 0.610809 -2.700468 0.045231
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H -0.482715 -4.182307 2.906440
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H 3.707587 2.229370 -1.975987
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H 0.236734 2.767780 0.520428
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C -3.967288 1.292323 2.171331
C -1.587260 1.420855 2.570619
C -4.205863 1.892085 3.409098
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C -3.135646 2.264198 4.228216
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H -0.988705 2.299714 4.444132
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C -3.928488 -1.822897 0.916565
C -5.261070 -2.074472 -1.519794
H -4.091994 -0.390942 -2.168695
C -4.886386 -2.823197 0.744176
H -3.420145 -1.734218 1.873510
C -5.555311 -2.954473 -0.477152
H -5.777487 -2.163986 -2.471780
H -5.111401 -3.498308 1.565642
H -6.300264 -3.733676 -0.611518
C -2.640367 1.602312 -1.156831
C -1.968747 1.535553 -2.389494
C -3.560268 2.641731 -0.945870
C -2.224538 2.472008 -3.393968
H -1.235377 0.750414 -2.556455
C -3.804668 3.586418 -1.945546
H -4.084297 2.724405 0.000597
C -3.142239 3.501325 -3.172907
H -1.698530 2.402020 -4.342284
H -4.514856 4.388694 -1.763742
H -3.335605 4.236694 -3.949061

thf_PhBr
E=-1758954.7527854077 kcal/mol
C 2.185290 1.210023 0.000000
C 0.786294 1.218210 0.000021
C 0.106267 0.000017 -0.000110
C 0.786286 -1.218203 -0.000006
C 2.185259 -1.210042 0.000027
C 2.886314 -0.000005 -0.000003
H 2.721903 2.154193 0.000019
H 0.239198 2.154599 0.000040

H 0.239141 -2.154565 0.000011
H 2.721890 -2.154201 0.000051
H 3.972015 -0.000031 0.000009
Br -1.814526 0.000000 0.000008

2.2.3 Species Optimized in DMF

dmf_1PF3_conctransA
E=-2241477.932323101 kcal/mol
Pd 0.343126 -0.150924 -0.004068
P 2.565878 -0.490335 -0.001803
Br -0.921108 2.115956 0.001018
C -1.695228 -0.081787 -0.000207
C -2.206933 -0.518358 1.230537
C -2.210615 -0.516588 -1.229984
C -3.217768 -1.486799 1.215623
H -1.833010 -0.116070 2.165563
C -3.221365 -1.485237 -1.213314
H -1.839960 -0.112584 -2.165554
C -3.723247 -1.967069 0.001550
H -3.614404 -1.853951 2.157788
H -3.620917 -1.850976 -2.154793
H -4.519169 -2.705439 0.002247
F 3.201065 -1.726958 -0.812946
F 3.331759 -0.763826 1.385994
F 3.583309 0.625575 -0.556597

dmf_1PF3_conctransB
E=-2241476.202881521 kcal/mol
Pd -0.391504 -0.863691 0.000007
P -2.342487 0.139145 -0.000004
Br 1.984695 -1.607745 -0.000004
C 1.381112 0.514036 -0.000013
C 1.518857 1.173992 -1.225621
C 1.518840 1.173971 1.225609
C 1.713533 2.559705 -1.211189
H 1.460651 0.631656 -2.162155
C 1.713513 2.559685 1.211205
H 1.460622 0.631617 2.162133
C 1.806027 3.255067 0.000015
H 1.796188 3.089913 -2.155664
H 1.796152 3.089876 2.155691
H 1.965021 4.328901 0.000025
F -2.723051 1.149878 -1.197432
F -3.743502 -0.663629 -0.000168
F -2.723199 1.149641 1.197577

dmf_1PH3_SN2cis
E=-2054567.9433381208 kcal/mol
P 2.513850 -0.864510 0.811144
Pd 0.578828 -1.135857 -0.489922
Br 0.537486 2.168477 -0.137742
C -0.846337 0.079817 0.100510
C -1.364051 0.018519 1.407392
C -1.665032 -0.076051 -1.033889
C -2.714383 -0.289202 1.564454
H -0.723506 0.182538 2.266251
C -3.022758 -0.405508 -0.839580
H -1.288189 0.127272 -2.031940
C -3.544309 -0.506987 0.447777
H -3.123375 -0.373025 2.567872
H -3.663753 -0.537625 -1.706978
H -4.595017 -0.738962 0.592974
H 2.336153 -0.233806 2.059191
H 3.566004 -0.061769 0.321331
H 3.287037 -1.967750 1.241546

dmf_1PH3_conctransA
E=-2054578.5529944687 kcal/mol
Pd -0.890834 -0.345108 -0.000025
P -3.061752 -1.210625 0.000003
Br 0.201726 2.091321 0.000017
H -4.203463 -0.375018 -0.001949
H -3.469662 -2.053010 1.060776
H -3.468463 -2.056301 -1.058610
C 1.110515 0.087361 -0.000001
C 1.649867 -0.339780 1.229551
C 1.649920 -0.339736 -1.229544
C 2.698390 -1.266239 1.213819
H 1.265079 0.050112 2.165525
C 2.698443 -1.266194 -1.213800
H 1.265171 0.050190 -2.165520
C 3.224215 -1.726718 0.000012
H 3.109268 -1.618550 2.155903
H 3.109363 -1.618469 -2.155879
H 4.048859 -2.433013 0.000017

dmf_1PMe3_SN2cis
E=-2128603.023588227 kcal/mol
P 2.294310 -0.361371 0.244886
Pd 0.221446 -0.984103 -0.644608
Br -0.572979 2.329943 -0.130308
C 3.207609 0.943865 -0.686099
H 2.585120 1.840233 -0.741849
H 4.153634 1.184270 -0.188830
H 3.412854 0.594940 -1.701885
C 3.543472 -1.715310 0.392659
H 3.751468 -2.132758 -0.596482
H 4.476015 -1.336591 0.825311
H 3.149024 -2.511328 1.029997
C 2.216318 0.323990 1.953271
H 3.211236 0.634729 2.289459
H 1.543192 1.184925 1.960669
H 1.825880 -0.435569 2.636030
C -1.322108 -0.016314 0.097949
C -1.720764 -0.224078 1.435716
C -2.154245 -0.384837 -0.982740
C -2.928532 -0.872853 1.675555
H -1.087109 0.097526 2.254207
C -3.369496 -1.049810 -0.702631
H -1.927323 -0.074889 -1.998360
C -3.755321 -1.290452 0.612025
H -3.227908 -1.067979 2.702136
H -4.016926 -1.334414 -1.527946
H -4.697655 -1.787014 0.822785

dmf_1PMe3_conctransA
E=-2128611.340882951 kcal/mol
Pd 0.338146 -0.031503 -0.001964
P 2.667121 -0.360599 -0.000772
Br -1.342939 2.070738 0.000695

C 3.750629 1.132616 -0.157056
H 4.810971 0.856867 -0.145634
H 3.524314 1.650676 -1.093492
H 3.548582 1.817370 0.671639
C 3.330378 -1.445985 -1.346593
H 3.093117 -1.008791 -2.320736
H 4.416401 -1.562182 -1.260332
H 2.858189 -2.430775 -1.287598
C 3.364008 -1.172317 1.510552
H 4.448072 -1.304975 1.423088
H 3.147832 -0.557883 2.389198
H 2.893218 -2.149667 1.649906
C -1.712081 -0.073646 0.000164
C -2.120215 -0.630715 1.229663
C -2.122266 -0.629453 -1.229199
C -2.885672 -1.801867 1.214063
H -1.852136 -0.153186 2.165812
C -2.887667 -1.800665 -1.213524
H -1.855850 -0.150906 -2.165297
C -3.272577 -2.384507 0.000284
H -3.187314 -2.251491 2.156139
H -3.190891 -2.249304 -2.155560
H -3.880418 -3.284232 0.000339

dmf_1PPh3_SN2cis

E=-2489530.5568414745 kcal/mol
P 1.037166 -0.118549 -0.052703
Pd -0.952233 -0.591594 -1.234388
Br -2.474577 2.156792 -0.017654
C -2.644970 -0.326764 -0.266878
C -2.900360 -0.917181 0.984741
C -3.440398 -0.604968 -1.397458
C -3.922242 -1.859786 1.069947
H -2.296119 -0.664300 1.848289
C -4.456200 -1.578815 -1.280149
H -3.348922 -0.020451 -2.308228
C -4.698097 -2.197969 -0.057261
H -4.108991 -2.350764 2.021593
H -5.075606 -1.803068 -2.144489
H -5.495544 -2.929033 0.035658
C 0.959780 -0.286968 1.779234
C 1.675847 -1.274528 2.472850
C 0.111284 0.574835 2.499122
C 1.549592 -1.395549 3.860345
H 2.334860 -1.949976 1.937202
C -0.003737 0.455663 3.884993
H -0.463030 1.335414 1.976659
C 0.713089 -0.531759 4.569385
H 2.112330 -2.163334 4.383918
H -0.655301 1.133639 4.429553
H 0.620062 -0.624553 5.647676
C 2.341746 -1.307188 -0.590992
C 3.692925 -0.945769 -0.716293
C 1.957420 -2.624553 -0.899982
C 4.638078 -1.884196 -1.137936
H 4.010552 0.066736 -0.487963
C 2.906087 -3.562563 -1.311405
H 0.912072 -2.914820 -0.820090
C 4.248044 -3.192742 -1.433970
H 5.679692 -1.590614 -1.233366
H 2.594897 -4.577237 -1.543122
H 4.985416 -3.919628 -1.762432
C 1.771168 1.544929 -0.340242
C 1.544371 2.167223 -1.579208
C 2.565044 2.197894 0.616413
C 2.108274 3.412800 -1.860020
H 0.917416 1.678281 -2.321020
C 3.121342 3.448484 0.336050
H 2.747437 1.735543 1.581591
C 2.895508 4.056681 -0.901133
H 1.923893 3.883762 -2.821449
H 3.731607 3.944840 1.085292
H 3.327134 5.030149 -1.115887

dmf_1PPh3_conctransA

E=-2489539.821543929 kcal/mol
Pd 1.181854 -0.101183 -0.014808
P -1.164787 0.065700 -0.004674
Br 2.989715 -2.098583 0.019950
C 3.222268 0.071956 -0.015325
C 3.605560 0.628216 -1.252818
C 3.587884 0.674921 1.205651
C 4.297916 1.844103 -1.255161
H 3.373891 0.117469 -2.181097
C 4.279875 1.890745 1.171989
H 3.343654 0.199353 2.149304
C 4.637811 2.473327 -0.050535
H 4.579297 2.292920 -2.203847
H 4.547205 2.375401 2.106997
H 5.189118 3.408645 -0.064444
C -1.813690 1.523148 -0.937497
C -2.995270 1.495034 -1.694370
C -1.072547 2.716641 -0.881334
C -3.426033 2.636552 -2.377201
H -3.581346 0.583138 -1.756594
C -1.509864 3.858586 -1.553845
H -0.145916 2.746917 -0.312084
C -2.687499 3.819636 -2.306333
H -4.340889 2.598771 -2.962231
H -0.927567 4.774190 -1.497308
H -3.024221 4.705256 -2.837886
C -2.071241 -1.370460 -0.732345
C -3.291786 -1.850058 -0.232153
C -1.491913 -2.012915 -1.840252
C -3.919429 -2.946882 -0.830279
H -3.754390 -1.372528 0.626377
C -2.125783 -3.099769 -2.444082
H -0.536225 -1.662837 -2.224258
C -3.340585 -3.570972 -1.937554
H -4.861669 -3.310608 -0.429597
H -1.666671 -3.584271 -3.301431
H -3.830037 -4.423344 -2.400350
C -1.893231 0.255920 1.682154
C -1.280682 -0.434719 2.742507
C -3.014500 1.056158 1.952135
C -1.785931 -0.338164 4.040031
H -0.400899 -1.044148 2.548611
C -3.512982 1.159998 3.254013
H -3.499379 1.603155 1.149095
C -2.902425 0.462310 4.298631
H -1.302677 -0.879389 4.848825
H -4.379393 1.786046 3.449001
H -3.290950 0.545314 5.309780

dmf_2PF3_conccis
E=-2643707.596902245 kcal/mol
P -2.519692 -0.520841 0.564169
Pd -0.300885 -0.006817 -0.069740
P -0.062716 2.273838 -0.350876
Br 0.563611 -2.094854 -1.279657
C 1.758161 -0.640143 0.120864
C 2.814078 0.019902 -0.514843
C 1.852692 -1.127654 1.426384
C 3.964966 0.283528 0.230221
H 2.734179 0.339658 -1.547300
C 3.014543 -0.834681 2.159287
H 1.060211 -1.723228 1.866208
C 4.065814 -0.134347 1.566339
H 4.783774 0.823124 -0.237086
H 3.094096 -1.187033 3.183612
H 4.970478 0.069242 2.130765
F 1.185921 2.938490 -1.118715
F -1.215912 3.044815 -1.162661
F -0.035670 3.252989 0.925383
F -3.272766 -1.763826 -0.116923
F -2.781814 -0.934843 2.092922
F -3.725736 0.530943 0.432317

dmf_2PH3_SN2cis
E=-2269910.017831267 kcal/mol
P -1.305064 -1.767234 1.259551
Pd -0.994653 0.169531 -0.023548
P -3.269460 0.771819 -0.613276
Br 1.880291 -1.765091 -0.644219
C 0.982283 0.461041 0.141081
C 1.628250 0.802237 1.346859
C 0.937380 1.357738 -0.949044
C 2.155109 2.083053 1.476557
H 1.679201 0.094537 2.167180
C 1.479651 2.654966 -0.783085
H 0.621821 1.029236 -1.935832
C 2.082187 3.012882 0.416519
H 2.611510 2.374222 2.419179
H 1.464624 3.346185 -1.621628
H 2.512988 4.002295 0.537294
H -3.717104 2.090274 -0.373138
H -3.669795 0.673895 -1.964755
H -4.366039 0.091683 -0.039402
H -2.411096 -1.873359 2.133323
H -1.469609 -2.988319 0.571829
H -0.283938 -2.161152 2.149360

dmf_2PH3_conccis
E=-2269910.5211692736 kcal/mol
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Pd 0.840112 -0.266977 0.047673
P 0.826887 -2.171178 -1.396235
Br -0.275148 2.077968 -0.686108
H 4.061608 -0.778982 0.846659
H 3.558369 1.186853 1.422865
H 2.967644 -0.452460 2.620635
H 0.084078 -3.315428 -1.011846
H 0.300425 -2.090438 -2.711081
H 2.012024 -2.866223 -1.744064
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C -3.230682 -1.070906 -0.288835
H -2.017088 -0.298182 -1.898558
C -2.541090 -0.484972 1.958911
H -0.829434 0.838057 2.100893
C -3.420023 -1.148854 1.103595
H -3.920213 -1.575554 -0.960367
H -2.699866 -0.505520 3.033726
H -4.263523 -1.700785 1.506959

dmf_2PMe3_SN2cis
E=-2417977.8411280187 kcal/mol
P -0.421718 -2.086200 0.587620
Pd -0.401444 0.188447 -0.016260
P -2.719265 0.752208 -0.373353
Br 2.932449 -0.701135 -1.108542
C 1.525433 0.772153 0.180477
C 2.142050 0.984434 1.441667
C 1.096984 1.887358 -0.597734
C 2.252725 2.275902 1.934961
H 2.489648 0.139208 2.026548
C 1.253944 3.199044 -0.072281
H 0.863034 1.772192 -1.652873
C 1.814876 3.392089 1.179669
H 2.671151 2.429500 2.926864
H 0.971432 4.050537 -0.686773
H 1.937847 4.394941 1.578075
C -2.986833 2.468323 -1.011194
H -4.054048 2.681226 -1.136569
H -2.556119 3.188757 -0.310289
H -2.482656 2.581986 -1.975005
C -3.684827 -0.252547 -1.590190
H -3.711144 -1.299674 -1.276445
H -4.710939 0.120038 -1.679810
H -3.199134 -0.200032 -2.568870
C -1.908957 -2.755379 1.458762
H -2.795374 -2.648719 0.828000
H -1.770530 -3.815784 1.695809
H -2.072423 -2.202279 2.387906
C -0.243495 -3.240215 -0.843038
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H -0.225877 -4.281549 -0.503400
H -1.079849 -3.099551 -1.533057
C 0.942796 -2.618606 1.710263
H 1.900832 -2.362632 1.251459
H 0.856765 -2.092652 2.665386
H 0.899696 -3.698412 1.889561
C -3.806869 0.730446 1.122040
H -4.826045 1.043037 0.870476
H -3.835605 -0.276022 1.547002
H -3.399612 1.410125 1.876011

dmf_2PMe3_conctrans
E=-2417972.4572336343 kcal/mol
Br -0.120725 1.329988 2.167161
P 2.485060 -0.827826 -0.355299
Pd 0.105283 -0.453115 0.014503
P -1.882225 -1.795135 -0.221195
C -2.829219 -1.658574 -1.808409

H -3.678457 -2.350835 -1.820054
H -3.198702 -0.636741 -1.932483
H -2.167745 -1.888592 -2.648652
C -3.245731 -1.642927 1.028144
H -3.653654 -0.628146 1.020772
H -4.054599 -2.350706 0.814650
H -2.849248 -1.844680 2.027460
C -1.561616 -3.621347 -0.153861
H -1.100251 -3.876211 0.804631
H -2.490700 -4.191806 -0.267402
H -0.868912 -3.900417 -0.952939
C 3.012238 -2.596994 -0.170317
H 4.086313 -2.713165 -0.355837
H 2.784990 -2.942767 0.842273
H 2.456793 -3.219208 -0.877815
C 3.162947 -0.429279 -2.033676
H 4.230694 -0.667766 -2.095658
H 2.622591 -1.004834 -2.790787
H 3.021486 0.634065 -2.247022
C 3.718283 0.016011 0.743887
H 4.740818 -0.292685 0.499221
H 3.639873 1.101260 0.631864
H 3.508651 -0.234445 1.787780
C -0.416939 1.584220 -0.066362
C 0.611305 2.333506 -0.668429
C -1.760933 1.827007 -0.408163
C 0.300782 3.194387 -1.727525
H 1.632067 2.242275 -0.318386
C -2.051578 2.693417 -1.465778
H -2.560085 1.338662 0.136055
C -1.025605 3.371911 -2.137352
H 1.103627 3.739950 -2.216382
H -3.088500 2.845045 -1.753971
H -1.260812 4.051866 -2.950624

dmf_2PPh3_SN2cis

E=-3139829.5455447095 kcal/mol
P -2.206109 -0.012585 -0.082205
Pd 0.061373 0.907496 -0.002660
P 1.601829 -0.893015 0.185491
C -2.530706 -1.325990 -1.337304
C -1.805413 -1.260378 -2.540080
C -3.439959 -2.378013 -1.150757
C -1.997613 -2.215367 -3.540818
H -1.079450 -0.465140 -2.688702
C -3.621128 -3.340289 -2.147888
H -4.002000 -2.459273 -0.226566
C -2.904861 -3.259941 -3.344464
H -1.431709 -2.148304 -4.465703
H -4.323584 -4.153235 -1.986463
H -3.048453 -4.009684 -4.117278
C -2.902352 -0.622362 1.511644
C -4.286931 -0.756543 1.722091
C -2.024296 -0.935885 2.560722
C -4.775909 -1.211679 2.947217
H -4.986341 -0.494273 0.933715
C -2.515904 -1.387991 3.788551
H -0.954588 -0.819932 2.420175
C -3.891080 -1.529532 3.982277
H -5.847474 -1.312529 3.094706
H -1.823343 -1.624623 4.591391
H -4.274052 -1.879183 4.936867
C -3.394016 1.332709 -0.541906
C -3.690516 2.325282 0.409559
C -3.945790 1.443123 -1.827264
C -4.530686 3.391158 0.086328
H -3.268430 2.265416 1.409105
C -4.780235 2.517978 -2.151871
H -3.733292 0.690661 -2.579839
C -5.076977 3.492782 -1.197710
H -4.759808 4.141411 0.838258
H -5.203480 2.583818 -3.150401
H -5.731999 4.322344 -1.448333
C 3.064128 -0.468152 1.227265
C 2.832011 0.068286 2.506557
C 4.387942 -0.639445 0.796835
C 3.898528 0.397399 3.345764
H 1.813982 0.232635 2.850442
C 5.454661 -0.295351 1.632544
H 4.594584 -1.034456 -0.191835
C 5.214382 0.217877 2.909036
H 3.699755 0.798510 4.335794
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H 6.045070 0.479067 3.558396
C 2.271906 -1.464419 -1.434682
C 2.969292 -2.680484 -1.551213
C 2.063676 -0.687412 -2.583966
C 3.454128 -3.101648 -2.790150
H 3.130657 -3.303668 -0.676496
C 2.547134 -1.112997 -3.824598
H 1.530921 0.254448 -2.506147
C 3.242733 -2.319015 -3.929446
H 3.992935 -4.041970 -2.865358
H 2.376721 -0.501636 -4.706480
H 3.616581 -2.650743 -4.894050
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C 0.072670 -3.246005 0.190205
C 0.880235 -4.137207 2.705269
H 2.115574 -2.384145 2.776244
C -0.435483 -4.439216 0.704354
H -0.247576 -2.914794 -0.792359
C -0.035414 -4.887978 1.967009
H 1.205622 -4.480184 3.683554
H -1.143468 -5.016679 0.116619
H -0.431155 -5.816813 2.367825
C 1.111803 2.620425 0.148600
C 0.045901 3.242216 -0.548796
C 1.545825 3.119979 1.395780
C -0.617164 4.341772 0.050955
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C 0.865109 4.190316 1.965024
H 2.380604 2.656256 1.908445
C -0.213944 4.808645 1.294505
H -1.411613 4.842852 -0.495221
H 1.164045 4.546377 2.948006
H -0.715144 5.658623 1.748434
Br 3.179661 2.657476 -1.342024

dmf_2PPh3_conccis

E=-3139830.694339099 kcal/mol
Br -0.231947 -2.704824 -1.919737
P 2.035440 0.598090 -0.032146
Pd 0.005166 -0.672801 -0.122722

P -2.253644 0.282601 0.103919
C 0.674016 -2.698187 0.095603
C 2.037554 -3.045402 0.130862
C -0.209363 -3.151415 1.093220
C 2.531074 -3.723773 1.243204
H 2.697909 -2.753879 -0.676778
C 0.313768 -3.818186 2.212561
H -1.278150 -3.003996 0.990415
C 1.678009 -4.103382 2.294085
H 3.592348 -3.952735 1.294347
H -0.362792 -4.139440 3.000142
H 2.074817 -4.639258 3.151158
C 2.814437 0.744276 1.640671
C 3.770394 1.729405 1.944228
C 2.426590 -0.154123 2.647623
C 4.328924 1.807478 3.221694
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C 2.988585 -0.077497 3.925641
H 1.680194 -0.912880 2.430218
C 3.939791 0.903468 4.214746
H 5.065820 2.575271 3.441102
H 2.677333 -0.780182 4.693952
H 4.372931 0.967291 5.209085
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C 3.062503 -0.372927 -2.444606
C 4.685273 -0.339733 -0.654726
C 4.014876 -0.924499 -3.302773
H 2.054734 -0.192482 -2.810773
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H 4.961393 -0.120824 0.371451
C 5.305599 -1.196648 -2.836937
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H 6.045304 -1.633703 -3.501777
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C 0.992627 3.194291 0.131347
C 2.515136 4.287735 -1.931380
H 3.396942 2.337385 -2.122517
C 0.844135 4.539260 -0.206845
H 0.384548 2.776816 0.929259
C 1.603335 5.090366 -1.244552
H 3.112163 4.706293 -2.737200
H 0.131569 5.154998 0.335302
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C -4.350289 1.676666 3.421577
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C -1.988019 1.827753 3.911834
H -0.661572 1.122051 2.365539
C -3.316120 2.021485 4.297004
H -5.385927 1.818455 3.718084
H -1.179050 2.083563 4.590680
H -3.545985 2.431868 5.276316
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C -4.250282 -0.995565 -1.492596
C -3.934945 -1.895539 0.727066
C -5.188240 -1.998476 -1.761618
H -4.020122 -0.264341 -2.261278
C -4.875598 -2.891253 0.459254
H -3.458964 -1.865851 1.704107
C -5.504731 -2.948256 -0.789018
H -5.674520 -2.028965 -2.732956
H -5.118773 -3.620396 1.227526
H -6.236492 -3.723478 -0.997673
C -2.599403 1.656584 -1.090005
C -1.914216 1.635213 -2.317209
C -3.499699 2.704280 -0.838993
C -2.137836 2.624241 -3.278002
H -1.196431 0.843092 -2.515408
C -3.711663 3.701501 -1.794633
H -4.034157 2.752129 0.104131
C -3.036389 3.661616 -3.017239
H -1.602422 2.588497 -4.222910
H -4.406893 4.509109 -1.581976
H -3.204726 4.437480 -3.758875

dmf_PhBr
E=-1758955.1128880715 kcal/mol
C 2.185629 1.210232 0.000000
C 0.786445 1.218541 0.000022
C 0.106915 0.000017 -0.000110
C 0.786436 -1.218534 -0.000005
C 2.185599 -1.210251 0.000027
C 2.886590 -0.000005 -0.000004
H 2.722153 2.154409 0.000019
H 0.239876 2.155243 0.000041
H 0.239820 -2.155209 0.000011
H 2.722140 -2.154417 0.000051
H 3.972256 -0.000031 0.000008
Br -1.814912 0.000000 0.000008

2.2.4 Species Optimized in water

wat_1PF3_conctransA
E=-2241478.1804404 kcal/mol
Pd 0.343813 -0.152297 -0.000052
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Br -0.925280 2.115241 0.000038
C -1.695522 -0.079152 0.000008
C -2.207839 -0.516429 -1.230325
C -2.207728 -0.516543 1.230346
C -3.216101 -1.487596 -1.214476
H -1.836286 -0.112535 -2.165597
C -3.215993 -1.487710 1.214496
H -1.836094 -0.112734 2.165622
C -3.718668 -1.969863 0.000010
H -3.613137 -1.855156 -2.156310
H -3.612946 -1.855357 2.156330
H -4.512758 -2.710194 0.000010
F 3.599466 0.745221 -0.000832
F 3.259693 -1.300416 1.203581
F 3.259614 -1.301917 -1.202642

wat_1PF3_conctransB
E=-2241476.361396723 kcal/mol
P -2.341549 0.134746 -0.000016
Pd -0.390027 -0.865490 -0.000195
Br 1.989997 -1.603071 0.000178
C 1.380982 0.515595 0.000044

C 1.515767 1.176315 1.225674
C 1.516279 1.176166 -1.225601
C 1.704198 2.562906 1.211206
H 1.459598 0.633810 2.162237
C 1.704715 2.562751 -1.211230
H 1.460492 0.633540 -2.162116
C 1.793677 3.258678 -0.000036
H 1.784219 3.093545 2.155672
H 1.785149 3.093268 -2.155730
H 1.947569 4.333261 -0.000072
F -3.742448 -0.669018 -0.000313
F -2.724167 1.145061 1.197708
F -2.724066 1.145841 -1.197103

wat_1PH3_conctransA
E=-2054578.6810691797 kcal/mol
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Br -0.208561 2.092446 0.000020
H 4.204718 -0.370372 0.000047
H 3.471144 -2.050300 -1.059864
H 3.471228 -2.050587 1.059635
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C -1.647943 -0.341887 -1.229613
C -1.647887 -0.341953 1.229625
C -2.692971 -1.272320 -1.213835
H -1.264686 0.049416 -2.165630
C -2.692914 -1.272389 1.213845
H -1.264604 0.049316 2.165645
C -3.217074 -1.734767 0.000005
H -3.102469 -1.626222 -2.155917
H -3.102368 -1.626344 2.155926
H -4.039048 -2.444158 0.000003

wat_1PMe3_SN2cis
E=-2128603.450445363 kcal/mol
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H 4.156497 1.185693 -0.202481
H 3.409943 0.592254 -1.711070
C 3.548094 -1.710749 0.391370
H 3.752596 -2.132129 -0.596817
H 4.481956 -1.329902 0.819279
H 3.156012 -2.504265 1.033271
C 2.225482 0.333777 1.948639
H 3.221649 0.644222 2.281350
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H 1.835471 -0.422719 2.635043
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C -1.722387 -0.218743 1.435486
C -2.147469 -0.388305 -0.984240
C -2.924132 -0.879021 1.673098
H -1.094067 0.110133 2.255262
C -3.357325 -1.064266 -0.705880
H -1.921586 -0.077325 -1.999772
C -3.744368 -1.306373 0.608039
H -3.223991 -1.075879 2.699217
H -3.999580 -1.356901 -1.532451
H -4.682193 -1.812037 0.817258

wat_1PMe3_conctransA
E=-2128611.479757102 kcal/mol
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H 3.525284 1.652377 -1.094349
H 3.549662 1.819580 0.670885
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H 4.416109 -1.561230 -1.259959
H 2.857491 -2.429069 -1.286851
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H 4.448089 -1.302432 1.423521
H 3.148106 -0.554461 2.389271
H 2.893061 -2.146654 1.650801
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C -2.879672 -1.806337 1.214202
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C -2.881832 -1.805346 -1.213453
H -1.855443 -0.152369 -2.165525
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H -3.183589 -2.255083 -2.155427
H -3.869662 -3.292004 0.000636

wat_1PPh3_SN2cis
E=-2489531.1057806043 kcal/mol
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Pd -0.951815 -0.604265 -1.226172
Br -2.489656 2.147554 -0.010799
C -2.646118 -0.324371 -0.263790
C -2.906198 -0.916624 0.986867
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C -4.684987 -2.214204 -0.067264
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H -5.476340 -2.952464 0.020655
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H 2.136652 -2.125454 4.395224
H -0.654583 1.151649 4.425318
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H 0.923290 -2.914715 -0.817435
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C 3.095432 3.469205 0.306707
H 2.726403 1.768740 1.570777
C 2.873726 4.060264 -0.939467
H 1.917395 3.855611 -2.864392
H 3.696896 3.979354 1.053800
H 3.299643 5.034146 -1.163480

wat_1PPh3_conctransA
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Br 2.993869 -2.097433 0.022336
C 3.222062 0.072510 -0.015505
C 3.604246 0.628008 -1.253742
C 3.585967 0.677936 1.204827
C 4.293860 1.845481 -1.257512
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C 4.275186 1.895344 1.169645
H 3.342743 0.203093 2.149108
C 4.632107 2.477046 -0.053611
H 4.574372 2.293705 -2.206726
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C -2.996878 1.487497 -1.698222
C -1.074648 2.713253 -0.890044
C -3.428559 2.626324 -2.384990
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C -1.512890 3.852540 -1.566499
H -0.147915 2.746191 -0.321099
C -2.690716 3.810128 -2.318547
H -4.343621 2.585941 -2.969501
H -0.931212 4.768732 -1.513356
H -3.028158 4.693632 -2.853133
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wat_2PF3_conccis
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H 1.061172 -1.725287 1.865555
C 4.064371 -0.131074 1.568160
H 4.781949 0.828117 -0.234546
H 3.093252 -1.185762 3.184514
H 4.968136 0.074254 2.133403
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F -1.218046 3.043497 -1.164053
F -0.039834 3.254105 0.924675
F -3.268979 -1.770004 -0.112998
F -2.784181 -0.930677 2.094136
F -3.727966 0.525940 0.425633

wat_2PH3_SN2cis
E=-2269910.3854765957 kcal/mol
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P -3.268798 0.763085 -0.613496
Br 1.895545 -1.750954 -0.642352
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C 1.624178 0.804574 1.347221
C 0.929819 1.357718 -0.948591
C 2.135544 2.091044 1.480820
H 1.681731 0.095659 2.166087
C 1.457495 2.660702 -0.778594
H 0.620571 1.028140 -1.936979
C 2.053930 3.022680 0.422650
H 2.586442 2.385426 2.425096
H 1.435610 3.353712 -1.615519
H 2.472962 4.016736 0.546621
H -3.713590 2.085409 -0.389859
H -3.675220 0.646906 -1.961699
H -4.363535 0.092397 -0.025252
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H -0.287431 -2.170286 2.148260

wat_2PH3_conccis
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H 0.314294 -2.070634 -2.724910
H 2.022646 -2.850725 -1.755267
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wat_2PMe3_SN2cis
E=-2417978.19026809 kcal/mol
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P 2.716654 0.753192 -0.373265
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H 3.397629 1.402763 1.878378
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H 1.075108 -3.104146 -1.537326
C 1.910373 -2.760895 1.453166
H 1.770999 -3.820997 1.690951
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H -0.897627 -3.702677 1.888700
H -0.852321 -2.097281 2.665062
H -1.899624 -2.366216 1.253508
C -1.528686 0.769670 0.177953
C -2.141389 0.982597 1.441647
C -1.093858 1.885390 -0.597170
C -2.242345 2.272909 1.939426
H -2.492993 0.137764 2.024770
C -1.242508 3.196547 -0.067124
H -0.864123 1.772752 -1.653508
C -1.799501 3.389099 1.186474
H -2.657071 2.425848 2.932984
H -0.955825 4.048205 -0.679460
H -1.915338 4.391374 1.588448

wat_2PMe3_conctrans
E=-2417972.6905919076 kcal/mol
Br -0.124414 1.335498 2.166877
P 2.484308 -0.833331 -0.351782
Pd 0.104721 -0.453658 0.014327
P -1.885710 -1.792047 -0.220990
C -2.830218 -1.654984 -1.809572
H -3.680287 -2.346174 -1.821883
H -3.198343 -0.632791 -1.934682
H -2.167922 -1.886539 -2.648751
C -3.250240 -1.636469 1.026735
H -3.656564 -0.621058 1.018049
H -4.059973 -2.343061 0.812724
H -2.855309 -1.838455 2.026637
C -1.567391 -3.618472 -0.151786
H -1.108131 -3.873253 0.807736
H -2.497056 -4.187677 -0.266599
H -0.873665 -3.898973 -0.949470
C 3.005891 -2.603672 -0.163534
H 4.079678 -2.723250 -0.348365
H 2.777179 -2.946948 0.849571
H 2.448948 -3.225442 -0.870230
C 3.163810 -0.439030 -2.030466
H 4.230768 -0.681163 -2.091605
H 2.621944 -1.013993 -2.786950
H 3.026106 0.624535 -2.245188
C 3.718892 0.009083 0.746883
H 4.740777 -0.301759 0.502329
H 3.642610 1.094380 0.633909
H 3.509055 -0.240485 1.790959
C -0.413031 1.585703 -0.066511
C 0.618512 2.331809 -0.667057
C -1.755622 1.829841 -0.413119
C 0.312798 3.190209 -1.729600
H 1.638022 2.239726 -0.313607
C -2.041350 2.693782 -1.474140
H -2.557367 1.344187 0.129680
C -1.012013 3.368707 -2.144246
H 1.118174 3.732900 -2.217460
H -3.077057 2.846114 -1.766242
H -1.243439 4.046660 -2.960263

wat_2PPh3_SN2cis
E=-3139830.1569524216 kcal/mol
P -2.203795 -0.018306 -0.081554
Pd 0.061102 0.908805 -0.003457
P 1.607037 -0.889180 0.183982
C -2.523790 -1.329989 -1.339850
C -1.798804 -1.259153 -2.542532
C -3.429630 -2.385423 -1.155799
C -1.988124 -2.212329 -3.545604
H -1.075446 -0.461197 -2.689264
C -3.607856 -3.345868 -2.155237
H -3.991542 -2.470671 -0.231888
C -2.892029 -3.260275 -3.351737
H -1.422719 -2.141113 -4.470494
H -4.307703 -4.161421 -1.995697
H -3.033391 -4.008532 -4.126391
C -2.896588 -0.635992 1.510966
C -4.280502 -0.775436 1.722590
C -2.016356 -0.951260 2.557738

C -4.766596 -1.237109 2.946447
H -4.981773 -0.512408 0.936152
C -2.505039 -1.410022 3.784294
H -0.947176 -0.831805 2.416433
C -3.879565 -1.556512 3.979156
H -5.837659 -1.341961 3.094729
H -1.810736 -1.647905 4.585253
H -4.260295 -1.911276 4.932748
C -3.398409 1.322550 -0.537135
C -3.706022 2.307027 0.419181
C -3.943736 1.438547 -1.824818
C -4.550441 3.370354 0.098377
H -3.289551 2.242681 1.420770
C -4.782503 2.510787 -2.146936
H -3.722826 0.692397 -2.581254
C -5.090167 3.477537 -1.187970
H -4.788119 4.114119 0.854086
H -5.200670 2.580809 -3.147320
H -5.748654 4.304927 -1.436672
C 3.068366 -0.461401 1.226758
C 2.833795 0.079061 2.503953
C 4.393251 -0.633854 0.799740
C 3.898641 0.411990 3.343855
H 1.815136 0.243710 2.845666
C 5.458360 -0.285685 1.635919
H 4.602177 -1.033223 -0.186731
C 5.215452 0.232206 2.910075
H 3.697761 0.816158 4.332201
H 6.478398 -0.422922 1.287959
H 6.044778 0.496277 3.559999
C 2.280322 -1.456637 -1.436532
C 2.983599 -2.669217 -1.554370
C 2.067922 -0.679867 -2.585256
C 3.470340 -3.086896 -2.793789
H 3.147995 -3.292541 -0.680309
C 2.553313 -1.101859 -3.826405
H 1.529140 0.258571 -2.506577
C 3.254950 -2.304313 -3.932406
H 4.013634 -4.024544 -2.869940
H 2.379017 -0.491020 -4.707902
H 3.630062 -2.633481 -4.897382
C 1.006986 -2.480826 0.922325
C 1.406203 -2.941579 2.186125
C 0.086567 -3.247759 0.185049
C 0.894443 -4.137525 2.700622
H 2.123325 -2.379965 2.774054
C -0.418025 -4.443034 0.697991
H -0.234264 -2.916639 -0.797393
C -0.017730 -4.891110 1.960870
H 1.219702 -4.479754 3.679199
H -1.123423 -5.022659 0.109263
H -0.410716 -5.821513 2.360743
C 1.105212 2.627328 0.146639
C 0.031492 3.240283 -0.547808
C 1.532177 3.126544 1.397188
C -0.643429 4.330422 0.056497
H -0.166654 3.009161 -1.590744
C 0.838912 4.186020 1.970991
H 2.371578 2.670047 1.908810
C -0.246249 4.796128 1.302250
H -1.443097 4.825149 -0.487841
H 1.132622 4.540086 2.956265
H -0.756993 5.638442 1.759782
Br 3.157614 2.677891 -1.337034

wat_2PPh3_conccis
E=-3139831.054956321 kcal/mol
Br -0.224301 -2.710747 -1.916270
P 2.033121 0.599411 -0.031800
Pd 0.004434 -0.675441 -0.116830
P -2.253719 0.280881 0.104406
C 0.679850 -2.699454 0.098283
C 2.044266 -3.043568 0.134595
C -0.202985 -3.153133 1.096274
C 2.538852 -3.718937 1.248203
H 2.704317 -2.751599 -0.673159
C 0.321395 -3.816620 2.217133
H -1.272163 -3.009122 0.992763
C 1.686186 -4.098607 2.299529
H 3.600630 -3.945320 1.300237
H -0.354703 -4.138005 3.005033
H 2.083921 -4.632055 3.157665
C 2.820553 0.741980 1.637309
C 3.780770 1.724356 1.936547
C 2.434538 -0.155149 2.646050
C 4.345380 1.800736 3.211423
H 4.087413 2.435150 1.174299
C 3.002416 -0.080081 3.921608
H 1.684948 -0.911715 2.432101
C 3.957937 0.897967 4.206312
H 5.085607 2.566263 3.427429
H 2.692372 -0.781615 4.691446
H 4.395721 0.960557 5.198675
C 3.379735 -0.055417 -1.120300
C 3.047482 -0.363162 -2.453168
C 4.680837 -0.331911 -0.672967
C 3.995914 -0.909982 -3.318757
H 2.037314 -0.183520 -2.813042
C 5.627197 -0.893957 -1.537218
H 4.962863 -0.115532 0.352139
C 5.289992 -1.180771 -2.861512
H 3.722229 -1.132152 -4.346653
H 6.628858 -1.103151 -1.171457
H 6.026700 -1.613986 -3.532144
C 1.907859 2.380426 -0.539334
C 2.653143 2.947849 -1.584034
C 0.993850 3.195676 0.153806
C 2.487312 4.294490 -1.927195
H 3.366704 2.344926 -2.135629
C 0.840402 4.541467 -0.179006
H 0.396774 2.776265 0.959026
C 1.585023 5.095324 -1.225844
H 3.073129 4.715130 -2.740108
H 0.135574 5.155799 0.374730
H 1.460964 6.141536 -1.490855
C -2.728483 0.949348 1.760815
C -4.063321 1.139973 2.160714
C -1.702010 1.281473 2.659811
C -4.359080 1.663718 3.420720
H -4.876224 0.870563 1.492757
C -1.998173 1.810079 3.919345
H -0.667428 1.110035 2.374168
C -3.327357 2.003489 4.301023
H -5.395499 1.805466 3.714438
H -1.191191 2.062105 4.601944

H -3.559971 2.409798 5.281367
C -3.612996 -0.928132 -0.251512
C -4.250874 -0.987820 -1.500358
C -3.933720 -1.901642 0.713395
C -5.188621 -1.989500 -1.775048
H -4.021799 -0.251684 -2.264654
C -4.874282 -2.895947 0.440076
H -3.457236 -1.877928 1.690360
C -5.504186 -2.945440 -0.808194
H -5.675626 -2.013982 -2.746183
H -5.116783 -3.629824 1.204019
H -6.235867 -3.719542 -1.021175
C -2.594971 1.658939 -1.086081
C -1.914912 1.634939 -2.316222
C -3.486298 2.712852 -0.829286
C -2.134784 2.627702 -3.274019
H -1.204108 0.837751 -2.519401
C -3.694411 3.713766 -1.782029
H -4.016839 2.762660 0.115941
C -3.024281 3.671465 -3.007354
H -1.603667 2.589777 -4.221257
H -4.382650 4.526126 -1.564884
H -3.189615 4.450182 -3.746642

wat_PhBr
E=-1758955.1645572127 kcal/mol
C 2.185678 1.210262 0.000000
C 0.786466 1.218589 0.000022
C 0.107004 0.000017 -0.000110
C 0.786458 -1.218582 -0.000005
C 2.185648 -1.210281 0.000027
C 2.886630 -0.000005 -0.000004
H 2.722189 2.154440 0.000019
H 0.239976 2.155337 0.000041
H 0.239920 -2.155303 0.000011
H 2.722176 -2.154448 0.000051
H 3.972291 -0.000031 0.000008
Br -1.814967 0.000000 0.000008

2.2 Special species (other substrates) optimized with B3LYP

2.2.1 Species Optimized in gas phase

TS_cis with H2

Egas= -1051.39699923 h.

Ggas= -1051.204114 h.

Dispersion= -0.0425960094 h.

15	-2.003229	0.318784	-0.000104
46	0.000000	-0.954301	-0.000001
15	2.003230	0.318784	0.000101
1	-0.648868	-2.421883	-0.000228
1	0.648867	-2.421883	0.000224
6	-3.121518	-0.030783	1.437831
1	-4.066401	0.519850	1.359634
1	-3.327982	-1.103658	1.477990
1	-2.620113	0.250041	2.368840
6	-2.044379	2.179143	-0.008973
1	-3.071885	2.562507	-0.006380
1	-1.521392	2.563546	0.872043
1	-1.529238	2.554833	-0.898365
6	-3.130220	-0.044266	-1.427834
1	-3.337544	-1.117352	-1.456121
1	-4.074273	0.507794	-1.349696
1	-2.634005	0.226915	-2.364461
6	2.044376	2.179144	0.008779
1	1.529161	2.554926	0.898090
1	3.071882	2.562509	0.006232
1	1.521462	2.563455	-0.872320
6	3.130135	-0.044118	1.427936
1	4.074196	0.507927	1.349790
1	2.633869	0.227170	2.364506
1	3.337451	-1.117202	1.456353
6	3.121606	-0.030930	-1.437729
1	4.066480	0.519718	-1.359540
1	3.328081	-1.103808	-1.477759
1	2.620252	0.249786	-2.368799

TS_cis with CH3CH2Br

Egas= -3700.83417699 h.

Ggas= -3700.596982 h.

Dispersion= -0.0582764710 h.

15	-2.203667	-1.025802	0.138027
46	-0.061085	-0.074866	-0.108176
15	2.019533	-1.259576	-0.171329
35	0.765160	2.253575	0.718395
6	-0.349998	2.013791	-1.402865
1	0.542341	2.451974	-1.833707
1	-0.575862	1.040061	-1.859052
6	-1.523804	2.939543	-1.259711
1	-2.322421	2.493656	-0.663900
1	-1.240855	3.892753	-0.807885
1	-1.927949	3.140921	-2.265099
6	2.108181	-3.079328	-0.546170
1	1.683549	-3.269924	-1.536548
1	3.139024	-3.453701	-0.522159
1	1.513106	-3.631579	0.187724
6	3.288597	-0.614935	-1.367611
1	4.244672	-1.144886	-1.276744
1	2.917509	-0.724873	-2.391313
1	3.449249	0.450131	-1.176078
6	2.986638	-1.193627	1.412009
1	3.971802	-1.664251	1.308500
1	3.112135	-0.148340	1.708980
1	2.428009	-1.702663	2.203216
6	-3.786725	-0.152401	-0.315591
1	-3.784366	0.091624	-1.382718
1	-4.667903	-0.768588	-0.098297
1	-3.863765	0.782938	0.246993
6	-2.583580	-1.476411	1.900258
1	-2.573868	-0.572294	2.515711
1	-3.560831	-1.965965	1.992493
1	-1.808919	-2.148685	2.279598
6	-2.508757	-2.658141	-0.698666
1	-3.492061	-3.073662	-0.445651
1	-2.443981	-2.530494	-1.783640
1	-1.730642	-3.365734	-0.398541

TS_trans with CH3CH2Br

Egas= -3700.83439868 h.

Ggas= -3700.598008 h.

Dispersion= -0.0583246891 h.

15	2.176347	-1.112491	-0.096924
46	0.010698	-0.184969	0.117069
15	-2.227004	-1.029781	0.119668
35	-0.241377	2.232826	-0.868617
6	0.021977	1.790201	1.500160
1	-0.932304	2.284266	1.643114
1	0.039991	0.795124	1.972983
6	1.239296	2.620742	1.797252
1	2.150294	2.141715	1.430487
1	1.175105	3.623639	1.370877
1	1.331494	2.710155	2.891758
6	-2.645499	-2.749944	0.690929
1	-2.367713	-2.863113	1.743361
1	-3.714034	-2.972046	0.577551
1	-2.066700	-3.475285	0.111275
6	-3.499666	-0.054857	1.062823
1	-4.510700	-0.456257	0.923091
1	-3.258937	-0.069054	2.130629
1	-3.479076	0.984888	0.722206
6	-2.995553	-1.034198	-1.569438
1	-4.046310	-1.346760	-1.539051
1	-2.926774	-0.028241	-1.993088
1	-2.438364	-1.712851	-2.221869
6	3.591200	-0.015965	-0.604493
1	3.771305	0.738315	0.167586
1	4.514732	-0.585627	-0.764467
1	3.326485	0.509426	-1.526787
6	2.324500	-2.435995	-1.393266
1	2.022534	-2.029524	-2.362952
1	3.350245	-2.817724	-1.468706
1	1.650114	-3.261457	-1.148368
6	2.941454	-1.985567	1.355569
1	3.923855	-2.405411	1.106898
1	3.055843	-1.285091	2.188615
1	2.278604	-2.791848	1.682870

2.2.2 Species Optimized in THF

TS_cis with H2

ETHF= -1051.40411615 h.
GTHF= -1051.208650 h.
Dispersion= -0.0425628765 h.

15	1.940900	0.319860	-0.002937
46	0.003465	-1.084984	-0.011324
15	-1.930737	0.329921	-0.009977
6	-1.810270	2.072196	-0.636631
1	-1.481836	2.063565	-1.680298
1	-2.773257	2.591542	-0.570615
1	-1.069136	2.621448	-0.048757
6	-3.399531	-0.276574	-0.963888
1	-4.242546	0.419844	-0.888896
1	-3.126921	-0.396467	-2.016567
1	-3.702083	-1.253742	-0.577342
6	-2.673316	0.607051	1.665575
1	-3.571598	1.231513	1.603087
1	-2.935443	-0.356428	2.111655
1	-1.941849	1.096739	2.315052
6	3.599806	-0.506210	0.032855
1	3.700807	-1.153944	-0.842815
1	4.415880	0.225624	0.036218
1	3.673348	-1.131248	0.927556
6	2.105566	1.495113	1.422320
1	2.133701	0.930171	2.358756
1	3.018171	2.096316	1.340205
1	1.238680	2.161307	1.451924
6	2.149663	1.463145	-1.448082
1	3.063581	2.060561	-1.354095
1	2.199356	0.878216	-2.371257
1	1.287971	2.133108	-1.514377
1	0.579676	-2.598099	0.008084
1	-0.609853	-2.585796	-0.005788

TS_trans with CH3CH2Br
ETHF= -3700.84196439 h.
GTHF= -3700.604703 h.
Dispersion= -0.0579718883 h.

15	2.133319	-1.187736	-0.100833
46	-0.024030	-0.216204	0.028368
15	-2.298881	-0.944594	0.098266
35	-0.071709	2.309132	-0.848312
6	0.048636	1.754651	1.535655
1	-0.873021	2.314232	1.639564
1	-0.036089	0.731093	1.922285
6	1.312469	2.459526	1.919485
1	2.198419	1.912594	1.589294
1	1.359362	3.482761	1.542750
1	1.342559	2.492343	3.020809
6	-2.710663	-2.665030	0.665540
1	-2.361267	-2.804352	1.693068
1	-3.789663	-2.857182	0.624272
1	-2.193179	-3.389686	0.029948
6	-3.472717	0.042907	1.146852
1	-4.498844	-0.334959	1.069467
1	-3.156807	-0.000954	2.193812
1	-3.453123	1.089083	0.826898
6	-3.183052	-0.904891	-1.533437
1	-4.231659	-1.206708	-1.427388
1	-3.139243	0.107459	-1.945397
1	-2.685736	-1.580152	-2.235802
6	3.580753	-0.139474	-0.614698
1	3.727292	0.671893	0.104354
1	4.503062	-0.728926	-0.677500
1	3.375249	0.309071	-1.591177
6	2.304810	-2.585938	-1.310538
1	2.046472	-2.233647	-2.313482
1	3.327256	-2.982089	-1.323086
1	1.611586	-3.387859	-1.041673
6	2.817476	-1.976841	1.435100
1	3.807753	-2.412146	1.256185
1	2.896113	-1.228214	2.229332
1	2.135856	-2.762416	1.774189

2.3 Species for SET mechanism optimized with B3LYP

2.3.1 Species Optimized in gas phase

gas_set_Brpdph32
E=-2.1245689516091547E6 kcal.mol-1
1 P -3.8848 -1.5430 0.5755
2 Pd -1.8589 -0.5865 -0.0879
3 P -2.4023 1.4621 -1.1412
4 Br 0.5747 -0.2962 -0.4250
5 H -1.9291 1.6217 -2.4615
6 H -1.8271 2.6201 -0.5743
7 H -3.7107 1.9733 -1.3403
8 H -4.6868 -0.8837 1.5373
9 H -3.9188 -2.8285 1.1683
10 H -4.9031 -1.7639 -0.3821

gas_set_Brpdpf32trans
E=-2.4983502570608947E6 kcal.mol-1
1 P -1.3154 -2.6264 0.9048
2 Pd -1.7212 -0.5865 -0.1057
3 P -2.3581 1.4463 -1.0044
4 Br 0.5639 -0.5135 -1.1902
5 F -2.3750 1.5845 -2.5810
6 F -1.4863 2.7171 -0.6435
7 F -3.8020 2.0445 -0.6919
8 F -0.0881 -2.7248 1.8994
9 F -2.4282 -3.3041 1.8230
10 F -0.9894 -3.8604 -0.0312

gas_set_Brpdpme3cis
E=-1.9832574338584137E6 kcal.mol-1
1 Pd -1.6028 -0.3874 -0.2476
2 P -2.3944 1.5506 -1.1519
3 Br 0.8034 -0.8264 -0.2616
4 C -1.6896 3.0562 -0.3557
5 H -0.5986 2.9921 -0.3774
6 H -2.0138 3.9655 -0.8742
7 H -2.0065 3.1022 0.6896
8 C -4.2149 1.8756 -1.1448
9 H -4.7337 1.0838 -1.6926
10 H -4.5858 1.8825 -0.1160
11 H -4.4413 2.8403 -1.6129
12 C -1.9353 1.7535 -2.9257
13 H -2.2640 2.7259 -3.3095
14 H -0.8500 1.6695 -3.0253
15 H -2.3932 0.9562 -3.5172

gas_set_Brpdpph3trans
E=-2.344215401131098E6 kcal.mol-1
1 P 0.5377 0.0171 0.0036
2 Pd -1.7888 0.0669 0.0151
3 C 1.2437 -1.5225 0.7255
4 C 2.3893 -1.5303 1.5362
5 C 0.5885 -2.7361 0.4540
6 C 2.8755 -2.7332 2.0569
7 H 2.8992 -0.6007 1.7687
8 C 1.0803 -3.9366 0.9693
9 H -0.3107 -2.7421 -0.1572
10 C 2.2250 -3.9369 1.7728
11 H 3.7608 -2.7268 2.6865
12 H 0.5640 -4.8671 0.7524
13 H 2.6030 -4.8697 2.1811
14 C 1.3046 1.3911 0.9598
15 C 0.6952 1.7698 2.1687
16 C 2.4494 2.0776 0.5268
17 C 1.2312 2.8038 2.9380
18 H -0.2031 1.2589 2.5066
19 C 2.9801 3.1176 1.2959
20 H 2.9243 1.8088 -0.4114
21 C 2.3748 3.4805 2.5020
22 H 0.7498 3.0868 3.8695
23 H 3.8644 3.6446 0.9490
24 H 2.7872 4.2910 3.0959
25 C 1.2695 0.1352 -1.6817
26 C 2.4119 -0.5823 -2.0693
27 C 0.6400 0.9767 -2.6152
28 C 2.9202 -0.4510 -3.3650
29 H 2.9020 -1.2488 -1.3665
30 C 1.1537 1.1112 -3.9063
31 H -0.2567 1.5236 -2.3342
32 C 2.2950 0.3966 -4.2835
33 H 3.8025 -1.0143 -3.6552
34 H 0.6569 1.7641 -4.6178
35 H 2.6901 0.4943 -5.2906
36 Br -4.2307 0.1189 0.0263

gas_set_Brpdpph32
E=-2.9945449266724056E6 kcal.mol-1
1 P -2.2214 -1.8078 -0.0513
2 Pd 0.1028 -1.3253 -0.0313
3 P 2.4765 -1.4279 -0.0966
4 C 3.3649 0.0305 -0.7844
5 C 4.6289 0.4291 -0.3234
6 C 2.7519 0.7588 -1.8156
7 C 5.2750 1.5281 -0.8966
8 H 5.1078 -0.1097 0.4884
9 C 3.4028 1.8503 -2.3936
10 H 1.7551 0.4847 -2.1471
11 C 4.6658 2.2371 -1.9355
12 H 6.2509 1.8308 -0.5271
13 H 2.9150 2.4092 -3.1870
14 H 5.1667 3.0940 -2.3772
15 C 3.1025 -2.8521 -1.0967
16 C 2.4055 -4.0705 -1.0173
17 C 4.2187 -2.7664 -1.9436
18 C 2.8263 -5.1821 -1.7491
19 H 1.5256 -4.1477 -0.3834
20 C 4.6335 -3.8779 -2.6843
21 H 4.7642 -1.8326 -2.0324
22 C 3.9423 -5.0880 -2.5870
23 H 2.2764 -6.1160 -1.6739
24 H 5.4973 -3.7940 -3.3380
25 H 4.2653 -5.9494 -3.1646
26 C 3.2272 -1.6761 1.5717
27 C 4.2207 -2.6339 1.8263
28 C 2.7661 -0.8664 2.6257
29 C 4.7484 -2.7794 3.1135
30 H 4.5832 -3.2709 1.0258
31 C 3.3035 -1.0101 3.9061
32 H 1.9887 -0.1293 2.4410
33 C 4.2936 -1.9667 4.1547

34 H 5.5149 -3.5272 3.2981
35 H 2.9413 -0.3774 4.7116
36 H 4.7040 -2.0803 5.1543
37 C -2.4984 -3.4841 -0.7805
38 C -3.1445 -3.6820 -2.0101
39 C -1.9516 -4.5987 -0.1166
40 C -3.2494 -4.9652 -2.5584
41 H -3.5680 -2.8377 -2.5439
42 C -2.0664 -5.8784 -0.6596
43 H -1.4401 -4.4648 0.8334
44 C -2.7151 -6.0659 -1.8858
45 H -3.7527 -5.1002 -3.5117
46 H -1.6484 -6.7284 -0.1272
47 H -2.8004 -7.0616 -2.3117
48 C -3.2855 -0.6813 -1.0484
49 C -2.6692 0.2187 -1.9303
50 C -4.6872 -0.6958 -0.9533
51 C -3.4417 1.0744 -2.7211
52 H -1.5856 0.2658 -1.9756
53 C -5.4567 0.1623 -1.7410
54 H -5.1805 -1.3686 -0.2583
55 C -4.8350 1.0462 -2.6298
56 H -2.9517 1.7716 -3.3947
57 H -6.5398 0.1447 -1.6566
58 H -5.4351 1.7168 -3.2385
59 C -3.0575 -1.8899 1.5934
60 C -4.0395 -2.8456 1.9029
61 C -2.7025 -0.9329 2.5600
62 C -4.6562 -2.8446 3.1572
63 H -4.3208 -3.5987 1.1734
64 C -3.3282 -0.9323 3.8089
65 H -1.9397 -0.1924 2.3329
66 C -4.3033 -1.8871 4.1122
67 H -5.4116 -3.5918 3.3849
68 H -3.0459 -0.1864 4.5465
69 H -4.7830 -1.8874 5.0871
70 Br -0.0299 1.1252 0.8121

gas_set_Br
E=-1.6135569738282305E6 kcal.mol-1
1 Br 0.1256 -0.8094 -0.0106

gas_set_Brpdpf32
E=-2.498354874731282E6 kcal.mol-1
1 P -3.8325 -1.4744 0.5177
2 Pd -1.8448 -0.5453 -0.1241
3 P -2.4338 1.4512 -1.1075
4 Br 0.5747 -0.4969 -0.3456
5 F -2.0351 1.6869 -2.6255
6 F -1.8625 2.7941 -0.4835
7 F -3.9712 1.8676 -1.1988
8 F -3.8549 -2.8865 1.2497
9 F -4.7498 -0.6657 1.5355
10 F -4.9240 -1.7707 -0.6014

gas_set_Brpdpme3trans
E=-1.9832608552186366E6 kcal.mol-1
1 Pd -1.9318 -0.5794 -0.1242
2 P -4.2146 -0.8761 0.2093
3 Br 0.4621 -0.2675 -0.4776
4 C -5.0376 0.4076 1.2507
5 H -4.9069 1.3917 0.7918
6 H -6.1081 0.2025 1.3606
7 H -4.5739 0.4297 2.2409
8 C -4.6970 -2.4530 1.0394
9 H -4.3520 -3.3025 0.4432
10 H -4.2205 -2.5111 2.0221
11 H -5.7834 -2.5191 1.1630
12 C -5.2427 -0.8847 -1.3249
13 H -6.3028 -1.0326 -1.0917
14 H -5.1215 0.0654 -1.8529
15 H -4.9067 -1.6873 -1.9876

gas_set_Brpdpph3cis
E=-2.3442120408338737E6 kcal.mol-1
1 P -2.2145 -1.7637 0.0019
2 Pd -0.0383 -1.0898 0.2003
3 C -2.3764 -3.4032 -0.8217
4 C -3.0503 -3.5796 -2.0401
5 C -1.7252 -4.5052 -0.2355
6 C -3.0816 -4.8363 -2.6534
7 H -3.5515 -2.7412 -2.5127
8 C -1.7659 -5.7585 -0.8458
9 H -1.1889 -4.3828 0.7021
10 C -2.4439 -5.9272 -2.0586
11 H -3.6072 -4.9590 -3.5961
12 H -1.2638 -6.6010 -0.3790
13 H -2.4697 -6.9018 -2.5371
14 C -3.2602 -0.6089 -0.9769
15 C -2.6337 0.2584 -1.8853
16 C -4.6580 -0.5713 -0.8432
17 C -3.3938 1.1367 -2.6621
18 H -1.5500 0.2581 -1.9661
19 C -5.4148 0.3096 -1.6188
20 H -5.1568 -1.2195 -0.1295
21 C -4.7846 1.1624 -2.5310
22 H -2.8969 1.8074 -3.3569
23 H -6.4949 0.3340 -1.5054
24 H -5.3753 1.8511 -3.1283
25 C -3.0755 -1.9481 1.6177
26 C -4.0612 -2.9246 1.8370
27 C -2.7412 -1.0598 2.6541
28 C -4.7100 -3.0041 3.0722
29 H -4.3182 -3.6291 1.0518
30 C -3.3978 -1.1403 3.8841
31 H -1.9620 -0.3172 2.5035
32 C -4.3819 -2.1106 4.0958
33 H -5.4682 -3.7655 3.2329
34 H -3.1305 -0.4502 4.6789
35 H -4.8850 -2.1757 5.0564
36 Br 0.6698 0.9413 1.3655

gas_set_Brpdph3trans
E=-1.9092104138798027E6 kcal.mol-1
1 Pd -1.8008 -0.6020 -0.1402
2 P -4.1197 -0.8765 0.2005
3 Br 0.6044 -0.3385 -0.4701
4 H -4.9844 -0.8902 -0.9154
5 H -4.8162 0.0670 0.9863
6 H -4.5842 -2.0503 0.8323

gas_set_Brpdph32trans
E=-2.124568410507282E6 kcal.mol-1
1 P -1.3298 -2.6533 0.9543
2 Pd -1.8477 -0.5942 -0.0512
3 P -2.4165 1.4665 -1.0261

4 Br 0.4864 -0.5045 -1.1349
5 H -2.3155 1.5310 -2.4313
6 H -1.5747 2.5511 -0.7031
7 H -3.6630 2.1246 -0.8800
8 H -0.1983 -2.6567 1.7962
9 H -0.9436 -3.6862 0.0753
10 H -2.2024 -3.4037 1.7812

gas_set_Brpdpme32trans
E=-2.272639425773457E6 kcal.mol-1
Atom X Y Z
1 P -1.3445 -2.6723 0.9213
2 Pd -1.8361 -0.6066 -0.1048
3 P -2.4340 1.4672 -1.0550
4 Br 0.3404 -0.7206 -1.5412
5 C -1.1799 2.7930 -0.7825
6 H -0.2115 2.4291 -1.1355
7 H -1.4494 3.7122 -1.3147
8 H -1.0978 3.0063 0.2871
9 C -4.0103 2.2890 -0.5310
10 H -4.8582 1.6332 -0.7495
11 H -3.9902 2.4726 0.5473
12 H -4.1535 3.2423 -1.0526
13 C -2.5045 -3.3483 2.1985
14 H -3.4986 -3.4799 1.7612
15 H -2.1550 -4.3125 2.5853
16 H -2.5887 -2.6415 3.0293
17 C -1.1902 -4.0737 -0.2687
18 H -0.4625 -3.7942 -1.0350
19 H -0.8669 -4.9912 0.2356
20 H -2.1531 -4.2499 -0.7566
21 C 0.2784 -2.6952 1.7981
22 H 0.5142 -3.6964 2.1759
23 H 1.0518 -2.3695 1.0976
24 H 0.2532 -1.9903 2.6340
25 C -2.5958 1.4242 -2.8923
26 H -2.7757 2.4253 -3.2999
27 H -1.6730 1.0124 -3.3091
28 H -3.4232 0.7659 -3.1723

gas_set1_PhBrpdpf32
E=-2.6437231920027593E6 kcal.mol-1
1 P -0.1591 -1.0324 0.0251
2 Pd 0.0327 1.2076 -0.0593
3 P -1.6568 2.6785 -0.0871
4 Br 2.5215 2.2354 -0.1155
5 C 3.7649 0.7534 -0.0831
6 C 4.1864 0.2583 1.1483
7 C 4.2219 0.2352 -1.2922
8 C 5.0890 -0.8097 1.1617
9 H 3.8170 0.6860 2.0737
10 C 5.1246 -0.8325 -1.2589
11 H 3.8800 0.6455 -2.2359
12 C 5.5573 -1.3549 -0.0370
13 H 5.4224 -1.2121 2.1136
14 H 5.4858 -1.2524 -2.1929
15 H 6.2560 -2.1857 -0.0190
16 F -1.9270 3.5846 -1.3856
17 F -1.7739 3.8432 1.0139
18 F -3.1554 2.1288 0.0714
19 F -0.9877 -1.7595 -1.1393
20 F 1.0810 -2.0613 0.0382
21 F -0.9396 -1.6706 1.2721

gas_set_Ph
E=-145315.63718950746 kcal.mol-1
1 C 1.9266 -1.1397 0.2188
2 C 2.7289 -0.9478 -0.8863
3 C 2.3613 -1.2812 1.5200
4 C 4.1152 -0.8928 -0.6541
5 H 2.3242 -0.8430 -1.8891
6 C 3.7513 -1.2228 1.7277
7 H 1.6765 -1.4304 2.3501
8 C 4.6171 -1.0299 0.6451
9 H 4.7945 -0.7433 -1.4898
10 H 4.1491 -1.3285 2.7340
11 H 5.6890 -0.9862 0.8150

gas_set_Brpdph3cis
E=-1.9092201504065392E6 kcal.mol-1
1 Pd -1.6688 -0.3310 -0.2893
2 P -2.4939 1.6040 -1.1831
3 Br 0.7000 -0.8448 -0.1928
4 H -2.0103 2.8154 -0.6442
5 H -3.8745 1.9182 -1.1879
6 H -2.2233 1.8537 -2.5458

gas_set_PhBr
E=-1.758961133222163E6 kcal.mol-1
1 Br -0.8415 -0.9257 -0.1745
2 C 1.9607 -1.0155 0.2412
3 C 2.8158 -0.8726 -0.8448
4 C 2.4534 -1.2013 1.5273
5 C 4.2052 -0.9167 -0.6399
6 H 2.4126 -0.7278 -1.8459
7 C 3.8424 -1.2457 1.7346
8 H 1.7689 -1.3115 2.3670
9 C 4.7192 -1.1034 0.6505
10 H 4.8865 -0.8059 -1.4840
11 H 4.2412 -1.3910 2.7390
12 H 5.7952 -1.1377 0.8102

gas_set_pdpf32
E=-884553.6747640632 kcal.mol-1
1 P -3.7604 -1.3937 0.6380
2 Pd -1.7731 -0.3927 -0.0847
3 P -2.4579 1.4879 -1.2964
4 F -1.6575 1.8071 -2.6040
5 F -2.4164 2.8609 -0.5453
6 F -3.9344 1.4542 -1.8170
7 F -3.8115 -2.9583 0.5950
8 F -4.2037 -1.0933 2.1092
9 F -5.0448 -1.0025 -0.1678

gas_set_Me
E=-25004.07795232425 kcal.mol-1
Atom X Y Z
1 C -0.0000 1.3999 0.0000
2 H 1.0055 1.8030 -0.0000
3 H -0.8519 2.0691 -0.0000
4 H -0.1536 0.3276 -0.0000

gas_set_Brpdpf3trans
E=-2.0961161741254136E6 kcal.mol-1
1 P 2.1858 0.1843 0.0043

2 Pd -0.0280 0.6462 -0.0086
3 Br -2.3781 1.1308 -0.0219
4 F 3.2208 1.3861 -0.0866
5 F 2.8023 -0.5699 1.2592
6 F 2.7819 -0.7342 -1.1464

gas_set_Brpdpme32
E=-2.2726379255601997E6 kcal.mol-1
1 P -3.9683 -1.5159 0.5726
2 Pd -1.9833 -0.5160 -0.1350
3 P -2.5031 1.5576 -1.1646
4 Br 0.4878 -0.2981 -0.4690
5 C -1.6642 2.9752 -0.3308
6 H -0.5984 2.7458 -0.2546
7 H -1.8077 3.9077 -0.8889
8 H -2.0617 3.0951 0.6812
9 C -4.2378 2.1871 -1.3514
10 H -4.8259 1.4860 -1.9511
11 H -4.7077 2.2804 -0.3678
12 H -4.2543 3.1672 -1.8425
13 C -5.0422 -0.5524 1.7333
14 H -5.3652 0.3753 1.2526
15 H -5.9273 -1.1256 2.0319
16 H -4.4680 -0.2899 2.6264
17 C -5.1770 -2.0187 -0.7364
18 H -4.6917 -2.7093 -1.4318
19 H -6.0581 -2.5054 -0.3030
20 H -5.4976 -1.1387 -1.3012
21 C -3.7472 -3.1029 1.5036
22 H -4.7105 -3.5317 1.8042
23 H -3.2136 -3.8216 0.8755
24 H -3.1408 -2.9199 2.3952
25 C -1.8652 1.6600 -2.8939
26 H -1.9955 2.6669 -3.3070
27 H -0.8054 1.3932 -2.8844
28 H -2.3938 0.9396 -3.5248

gas_dosmet240ph3
E=-93212.81261807609 eV
1 P -0.6683 4.2834 -1.7129
2 H -1.1193 4.9115 -0.5315
3 H -1.6846 4.7322 -2.5841
4 H 0.3261 5.2304 -2.0693
5 C -5.2721 -1.1041 0.0010
6 Br -2.6739 1.4890 -0.9371
7 Pd -0.3348 1.9464 -1.6027
8 P 1.8979 1.5462 -2.1669
9 H 2.2085 0.6384 -3.2080
10 H 2.7793 1.0136 -1.1955
11 H 2.7363 2.6005 -2.6016
12 H -5.9519 -0.6751 0.7267
13 H -5.5912 -1.2371 -1.0251
14 H -4.2475 -1.3148 0.2777

gas_dostransph3
E=-93212.86431625499 eV
1 P 1.3295 -2.2906 0.0463
2 C -5.1344 -0.0464 0.2729
3 Br -1.4235 -0.1238 -0.2010
4 Pd 1.1373 0.0501 0.0407
5 P 1.0114 2.3950 0.0401
6 H -5.5138 -1.0598 0.2250
7 H -4.3221 0.1964 0.9451
8 H -5.5115 0.7016 -0.4137
9 H 0.1995 2.9690 1.0404
10 H 0.3989 2.9780 -1.0887
11 H 2.1182 3.2735 0.1480
12 H 0.6053 -2.9663 1.0505
13 H 0.7993 -2.9550 -1.0792
14 H 2.5458 -3.0098 0.1535

gas_dosmet240
E=-99632.84410445449 eV
1 P 1.3766 2.3186 -0.0397
2 C 0.2286 3.3402 0.9877
3 C 1.1015 2.9968 -1.7371
4 C 3.0241 3.0524 0.3957
5 H 0.3850 4.4119 0.8174
6 H 0.3857 3.1170 2.0469
7 H 1.2089 4.0878 -1.7547
8 H 0.0967 2.7172 -2.0637
9 H 3.8029 2.6182 -0.2385
10 H 3.2655 2.8294 1.4394
11 H -0.7991 3.0696 0.7323
12 H 1.8206 2.5528 -2.4316
13 H 3.0243 4.1403 0.2588
14 C -3.7105 -1.3775 -1.2091
15 Br -1.3771 0.1451 -0.6479
16 Pd 1.0013 0.0014 0.1315
17 P 2.8912 -1.1638 0.8823
18 C 4.4228 -1.0555 -0.1561
19 H 5.2384 -1.6548 0.2648
20 H 4.2031 -1.4102 -1.1671
21 H 4.7470 -0.0133 -0.2260
22 C 2.6988 -3.0017 1.0474
23 H 2.4266 -3.4266 0.0770
24 H 3.6212 -3.4766 1.4029
25 H 1.8886 -3.2201 1.7489
26 C 3.5515 -0.7205 2.5565
27 H 4.4159 -1.3384 2.8255
28 H 3.8494 0.3318 2.5677
29 H 2.7664 -0.8580 3.3056
30 H -4.1342 -1.2476 -0.2220
31 H -4.0336 -0.7334 -2.0165
32 H -3.1636 -2.2823 -1.4383

2.3.2 Species Optimized in THF

thf_set_Brpdpf32trans
E=-2.4983599549581152E6 kcal.mol-1
1 P -1.3208 -2.6919 0.8571
2 Pd -1.7157 -0.6707 -0.2418
3 P -2.3831 1.4013 -1.0920
4 Br 0.7394 -0.0678 -0.7063
5 F -2.0004 1.7558 -2.5930
6 F -1.8050 2.6999 -0.3833
7 F -3.9220 1.8231 -1.1379
8 F 0.1714 -3.1232 1.1771
9 F -1.9427 -2.9003 2.3096
10 F -1.8209 -4.0495 0.1897

thf_set_Brpdph32trans
E=-2.1245777872762596E6 kcal.mol-1

1 P -1.3355 -2.7506 0.7951
2 Pd -1.7717 -0.6373 -0.1823
3 P -2.4157 1.4064 -1.1950
4 Br 0.7085 0.1732 0.1645
5 H -1.7504 1.7643 -2.3858
6 H -2.1845 2.5863 -0.4585
7 H -3.7421 1.6682 -1.6070
8 H -0.3199 -3.5320 0.2066
9 H -2.3281 -3.7493 0.9184
10 H -0.8656 -2.7546 2.1246

thf_set_Brpdph32
E=-2.1245800941975 48E6 kcal.mol-1
1 P -3.8665 -1.4967 0.5433
2 Pd -1.7874 -0.6189 -0.1081
3 P -2.4332 1.4363 -1.1024
4 Br 0.7236 -0.4323 -0.4557
5 H -2.0259 1.6597 -2.4354
6 H -1.9216 2.6181 -0.5241
7 H -3.7838 1.8338 -1.2273
8 H -4.6921 -0.7226 1.3875
9 H -3.9415 -2.7181 1.2504
10 H -4.8183 -1.7838 -0.4594

thf_set_Brpdpme3cis
E=-1.9832702465144712E6 kcal.mol-1
1 Pd -1.6860 -0.4376 -0.2837
2 P -2.3825 1.5578 -1.1765
3 Br 0.8133 -0.8131 -0.1234
4 C -1.6724 3.0486 -0.3619
5 H -0.5815 3.0042 -0.4118
6 H -2.0216 3.9618 -0.8554
7 H -1.9711 3.0689 0.6894
8 C -4.2022 1.8621 -1.1366
9 H -4.7197 1.0700 -1.6848
10 H -4.5535 1.8571 -0.1012
11 H -4.4420 2.8290 -1.5924
12 C -1.9445 1.7797 -2.9522
13 H -2.2904 2.7524 -3.3179
14 H -0.8599 1.7136 -3.0700
15 H -2.4069 0.9858 -3.5446

thf_set_Brpdpph32
E=-2.9945568894038186E6 kcal.mol-1
1 P -2.2268 -1.8224 -0.0325
2 Pd 0.1125 -1.3577 0.0691
3 P 2.4967 -1.4382 -0.0168
4 C 3.3355 0.0182 -0.7714
5 C 4.5396 0.5439 -0.2796
6 C 2.7327 0.6202 -1.8886
7 C 5.1345 1.6475 -0.9004
8 H 5.0153 0.0993 0.5886
9 C 3.3331 1.7143 -2.5145
10 H 1.7861 0.2389 -2.2618
11 C 4.5354 2.2320 -2.0197
12 H 6.0640 2.0486 -0.5065
13 H 2.8558 2.1705 -3.3769
14 H 4.9971 3.0903 -2.4993
15 C 3.1057 -2.8737 -1.0082
16 C 2.4212 -4.0966 -0.8897
17 C 4.2050 -2.7935 -1.8780
18 C 2.8373 -5.2182 -1.6102
19 H 1.5574 -4.1718 -0.2336
20 C 4.6148 -3.9151 -2.6068
21 H 4.7436 -1.8584 -1.9921
22 C 3.9353 -5.1293 -2.4730
23 H 2.2996 -6.1561 -1.5050
24 H 5.4660 -3.8372 -3.2772
25 H 4.2549 -5.9987 -3.0402
26 C 3.3030 -1.6500 1.6297
27 C 4.3965 -2.5070 1.8340
28 C 2.7892 -0.9227 2.7183
29 C 4.9682 -2.6330 3.1043
30 H 4.8038 -3.0808 1.0076
31 C 3.3680 -1.0460 3.9838
32 H 1.9383 -0.2632 2.5718
33 C 4.4574 -1.9017 4.1806
34 H 5.8124 -3.3014 3.2492
35 H 2.9632 -0.4779 4.8166
36 H 4.9018 -2.0011 5.1668
37 C -2.5183 -3.4669 -0.8239
38 C -3.3250 -3.6408 -1.9586
39 C -1.8586 -4.5856 -0.2811
40 C -3.4720 -4.9073 -2.5361
41 H -3.8425 -2.7932 -2.3955
42 C -2.0156 -5.8498 -0.8513
43 H -1.2243 -4.4690 0.5942
44 C -2.8217 -6.0137 -1.9842
45 H -4.0993 -5.0253 -3.4152
46 H -1.5056 -6.7042 -0.4153
47 H -2.9389 -6.9961 -2.4325
48 C -3.2202 -0.6420 -1.0384
49 C -2.5992 -0.0227 -2.1358
50 C -4.5621 -0.3433 -0.7550
51 C -3.3113 0.8654 -2.9455
52 H -1.5536 -0.2282 -2.3490
53 C -5.2710 0.5531 -1.5606
54 H -5.0565 -0.8021 0.0953
55 C -4.6490 1.1562 -2.6582
56 H -2.8183 1.3382 -3.7899
57 H -6.3074 0.7804 -1.3278
58 H -5.2006 1.8547 -3.2809
59 C -3.1198 -1.9445 1.5792
60 C -4.1150 -2.9067 1.8183
61 C -2.7902 -1.0328 2.5975
62 C -4.7681 -2.9572 3.0537
63 H -4.3805 -3.6221 1.0467
64 C -3.4503 -1.0825 3.8282
65 H -2.0195 -0.2869 2.4247
66 C -4.4385 -2.0449 4.0605
67 H -5.5336 -3.7087 3.2260
68 H -3.1869 -0.3721 4.6067
69 H -4.9456 -2.0859 5.0203
70 Br -0.0643 1.1265 0.9770

thf_set_Brpdpph3trans
E=-2.3442303773914347E6 kcal.mol-1
1 P -1.3503 -2.9674 -0.4932
2 Pd -0.0662 -1.2453 0.3816
3 C -0.3557 -4.2487 -1.3600
4 C -0.8103 -4.9200 -2.5061
5 C 0.9176 -4.5515 -0.8466
6 C -0.0070 -5.8851 -3.1215
7 H -1.7856 -4.6910 -2.9238
8 C 1.7152 -5.5204 -1.4593

9 H 1.2862 -4.0255 0.0304
10 C 1.2541 -6.1882 -2.5990
11 H -0.3674 -6.3972 -4.0089
12 H 2.6968 -5.7458 -1.0531
13 H 1.8769 -6.9365 -3.0804
14 C -2.6118 -2.4132 -1.7121
15 C -2.2773 -1.3570 -2.5776
16 C -3.8854 -2.9973 -1.8034
17 C -3.1950 -0.9044 -3.5282
18 H -1.3006 -0.8852 -2.5062
19 C -4.8042 -2.5381 -2.7521
20 H -4.1651 -3.8060 -1.1356
21 C -4.4607 -1.4940 -3.6163
22 H -2.9250 -0.0879 -4.1915
23 H -5.7872 -2.9961 -2.8131
24 H -5.1771 -1.1375 -4.3506
25 C -2.2904 -3.8641 0.8089
26 C -2.4167 -5.2616 0.8361
27 C -2.8883 -3.1004 1.8275
28 C -3.1371 -5.8832 1.8614
29 H -1.9528 -5.8681 0.0649
30 C -3.6128 -3.7232 2.8455
31 H -2.7855 -2.0180 1.8257
32 C -3.7371 -5.1170 2.8648
33 H -3.2265 -6.9656 1.8742
34 H -4.0708 -3.1225 3.6258
35 H -4.2938 -5.6025 3.6611
36 Br 1.3102 0.6191 1.3711

thf_set_Brpdpme3trans
E=-1.9832754519232744E6 kcal.mol-1
1 Pd -1.9605 -0.5900 -0.1231
2 P -4.2353 -0.8818 0.2123
3 Br 0.5131 -0.2506 -0.4935
4 C -5.0347 0.4139 1.2504
5 H -4.9006 1.3928 0.7823
6 H -6.1051 0.2138 1.3657
7 H -4.5648 0.4337 2.2375
8 C -4.7027 -2.4564 1.0476
9 H -4.3576 -3.3048 0.4504
10 H -4.2243 -2.5056 2.0295
11 H -5.7887 -2.5220 1.1727
12 C -5.2453 -0.8895 -1.3297
13 H -6.3060 -1.0344 -1.0996
14 H -5.1183 0.0609 -1.8554
15 H -4.9067 -1.6965 -1.9851

thf_set_Brpdpme32trans
E=-2.272647713298027E6 kcal.mol-1
1 P -1.3050 -2.6999 0.8620
2 Pd -1.7000 -0.5758 -0.1170
3 P -2.3838 1.4358 -1.1741
4 Br 0.6725 0.4049 0.6008
5 C -2.4805 2.9013 -0.0568
6 H -1.5090 3.0496 0.4214
7 H -2.7561 3.8032 -0.6140
8 H -3.2255 2.7178 0.7224
9 C -4.0466 1.4306 -1.9836
10 H -4.0757 0.6588 -2.7581
11 H -4.8164 1.2038 -1.2406
12 H -4.2644 2.4029 -2.4391
13 C -1.0424 -2.6680 2.6882
14 H -1.9369 -2.2758 3.1799
15 H -0.8299 -3.6711 3.0732
16 H -0.2040 -2.0045 2.9152
17 C -2.6388 -3.9657 0.6629
18 H -2.8118 -4.1518 -0.4010
19 H -2.3628 -4.9073 1.1503
20 H -3.5678 -3.5937 1.1043
21 C 0.1902 -3.5877 0.2451
22 H 0.3278 -4.5369 0.7740
23 H 0.0833 -3.7838 -0.8254
24 H 1.0681 -2.9541 0.3954
25 C -1.2728 2.0185 -2.5263
26 H -1.6147 2.9764 -2.9325
27 H -0.2607 2.1290 -2.1288
28 H -1.2509 1.2744 -3.3275

thf_set_Brpdpph3cis
E=-2.3442251292617507E6 kcal.mol-1
1 P -2.2133 -1.7488 0.0301
2 Pd -0.0168 -1.1019 0.2333
3 C -2.3409 -3.3797 -0.8159
4 C -3.1489 -3.5955 -1.9433
5 C -1.5553 -4.4390 -0.3231
6 C -3.1784 -4.8514 -2.5593
7 H -3.7565 -2.7904 -2.3431
8 C -1.5937 -5.6927 -0.9352
9 H -0.9173 -4.2857 0.5437
10 C -2.4052 -5.9013 -2.0568
11 H -3.8087 -5.0061 -3.4303
12 H -0.9877 -6.5032 -0.5410
13 H -2.4308 -6.8753 -2.5366
14 C -3.2402 -0.5917 -0.9655
15 C -2.6195 0.1288 -1.9999
16 C -4.6120 -0.4068 -0.7285
17 C -3.3610 1.0055 -2.7952
18 H -1.5532 0.0114 -2.1749
19 C -5.3505 0.4762 -1.5219
20 H -5.1063 -0.9444 0.0743
21 C -4.7281 1.1809 -2.5569
22 H -2.8693 1.5578 -3.5906
23 H -6.4101 0.6144 -1.3275
24 H -5.3034 1.8694 -3.1691
25 C -3.1120 -1.9600 1.6214
26 C -4.0734 -2.9664 1.8110
27 C -2.8300 -1.0703 2.6725
28 C -4.7481 -3.0747 3.0307
29 H -4.2964 -3.6683 1.0136
30 C -3.5125 -1.1776 3.8866
31 H -2.0725 -0.3018 2.5442
32 C -4.4717 -2.1795 4.0686
33 H -5.4881 -3.8581 3.1671
34 H -3.2873 -0.4844 4.6918
35 H -4.9962 -2.2659 5.0159
36 Br 0.5374 0.9612 1.5808

thf_set_Brpdph3trans
E=-1.9092278288385277E6 kcal.mol-1
1 Pd -1.8033 -0.6530 -0.1543
2 P -4.1404 -0.8903 0.2042
3 Br 0.6744 -0.2896 -0.4716
4 H -5.0016 -0.8845 -0.9127
5 H -4.8019 0.0773 0.9875

6 H -4.6281 -2.0503 0.8403

thf_set_Ph
E=-145317.06705073622 kcal.mol-1
1 C 1.9268 -1.1395 0.2189
2 C 2.7283 -0.9475 -0.8878
3 C 2.3603 -1.2814 1.5211
4 C 4.1156 -0.8927 -0.6549
5 H 2.3252 -0.8428 -1.8911
6 C 3.7514 -1.2230 1.7286
7 H 1.6768 -1.4307 2.3523
8 C 4.6173 -1.0299 0.6452
9 H 4.7943 -0.7431 -1.4908
10 H 4.1487 -1.3286 2.7350
11 H 5.6892 -0.9862 0.8149

thf_set_Brpdpf3cis
E=-2.0961266256558693E6 kcal.mol-1
1 P 1.9247 0.7222 0.7263
2 Pd -0.0589 0.3733 -0.2026
3 Br -1.6086 1.9060 1.0270
4 F 2.4382 2.2274 0.8473
5 F 2.1390 0.3052 2.2520
6 F 3.2663 0.0792 0.1340

thf_set_Brpdpf32
E=-2.4983648209028337E6 kcal.mol-1
1 P -3.8821 -1.4990 0.5264
2 Pd -1.8497 -0.6175 -0.1227
3 P -2.4093 1.4179 -1.0824
4 Br 0.6006 -0.3134 -0.4902
5 F -1.9805 1.6484 -2.5978
6 F -1.7786 2.7364 -0.4531
7 F -3.9219 1.9171 -1.1954
8 F -3.9397 -2.8448 1.3773
9 F -4.8235 -0.6021 1.4454
10 F -4.9493 -1.8827 -0.5911

thf_set_Me
E=-25004.425119533455 kcal.mol-1
1 C -0.0000 1.3999 0.0000
2 H 1.0058 1.8032 0.0000
3 H -0.8522 2.0694 0.0000
4 H -0.1537 0.3272 0.0000

thf_set_Brpdpme32
E=-2.272649535034858E6 kcal.mol-1
1 P -3.9655 -1.4878 0.5722
2 Pd -1.9369 -0.4977 -0.0610
3 P -2.4949 1.5492 -1.1345
4 Br 0.6235 -0.3888 -0.2669
5 C -1.6546 3.0116 -0.3824
6 H -0.5772 2.8307 -0.3567
7 H -1.8599 3.9206 -0.9585
8 H -2.0069 3.1486 0.6437
9 C -4.2464 2.1261 -1.2629
10 H -4.8474 1.3805 -1.7907
11 H -4.6635 2.2657 -0.2617
12 H -4.3044 3.0762 -1.8055
13 C -5.0462 -0.5356 1.7297
14 H -5.3501 0.4060 1.2651
15 H -5.9415 -1.1101 1.9910
16 H -4.4886 -0.3056 2.6418
17 C -5.1292 -1.9441 -0.7880
18 H -4.6329 -2.6375 -1.4725
19 H -6.0316 -2.4187 -0.3878
20 H -5.4143 -1.0511 -1.3500
21 C -3.7631 -3.0968 1.4640
22 H -4.7364 -3.5268 1.7265
23 H -3.2191 -3.8002 0.8276
24 H -3.1823 -2.9383 2.3769
25 C -1.9272 1.6030 -2.8909
26 H -2.0977 2.5930 -3.3279
27 H -0.8610 1.3654 -2.9275
28 H -2.4688 0.8536 -3.4748

thf_onemetB
E=-87085.41333864459 eV
1 P -2.1294 0.1771 -0.1817
2 C -2.2728 1.9796 -0.5471
3 C -2.1467 0.1243 1.6621
4 C -3.7991 -0.4731 -0.6316
5 H -3.1371 2.4118 -0.0310
6 H -2.3841 2.1276 -1.6245
7 H -3.0118 0.6676 2.0577
8 H -1.2285 0.5757 2.0464
9 H -3.8710 -1.5275 -0.3510
10 H -3.9488 -0.3893 -1.7115
11 H -1.3630 2.4893 -0.2197
12 H -2.1881 -0.9152 1.9981
13 H -4.5850 0.0898 -0.1155
14 C 4.6434 0.4342 -0.2051
15 Br 1.8490 0.1672 -0.3539
16 Pd -0.3261 -0.8413 -1.1372
17 H 4.7871 -0.3358 0.5424
18 H 4.8353 0.1993 -1.2445
19 H 4.6294 1.4717 0.1049

thf_dostransph3new
E=-93213.11586562339 eV
1 P -1.3436 2.1304 1.0217
2 C 5.2544 0.0111 -0.0300
3 Br 1.4032 0.0021 -0.0021
4 Pd -1.2248 -0.0049 0.0120
5 P -1.3440 -2.1407 -0.9965
6 H 5.2405 -1.0542 -0.2240
7 H 5.2258 0.7119 -0.8550
8 H 5.2614 0.3754 0.9898
9 H -0.7133 -3.2059 -0.3210
10 H -0.7259 -2.2920 -2.2551
11 H -2.5740 -2.7735 -1.2875
12 H -0.7129 2.2847 2.2736
13 H -0.7252 3.1986 0.3395
14 H -2.5734 2.7572 1.3257

thf_dostransph3
E=-93213.11586562339 eV
1 P -1.4404 2.3630 0.0573
2 C 5.1584 -0.0048 0.0096
3 Br 1.3062 0.0021 0.0030
4 Pd -1.3219 0.0018 -0.0018
5 P -1.4413 -2.3594 -0.0614
6 H 5.1545 0.5537 -0.9183
7 H 5.1524 0.5196 0.9571
8 H 5.1320 -1.0872 -0.0101
9 H -0.8188 -3.0606 0.9920

10 H -0.8151 -3.0069 -1.1466
11 H -2.6713 -3.0555 -0.0810
12 H -0.8180 3.0102 1.1448
13 H -0.8137 3.0639 -0.9938
14 H -2.6703 3.0596 0.0723

thf_dostranspf3
E=-109421.7408281772 eV
1 P 2.2574 -1.0014 0.0159
2 C 0.4084 5.1709 0.0082
3 Br 0.1097 1.8091 -0.0036
4 Pd -0.0549 -0.7663 -0.0675
5 P -2.3758 -0.7636 0.0167
6 H 1.4696 4.9777 0.0990
7 H -0.0649 5.1352 -0.9647
8 H -0.1596 5.4820 0.8776
9 F -3.1686 -0.0130 -1.1401
10 F -3.0661 -0.0630 1.2661
11 F -3.2092 -2.1250 0.0228
12 F 3.1274 -0.2733 -1.0981
13 F 3.0078 -0.4442 1.3025
14 F 2.9492 -2.4387 -0.0548

thf_dostrans240b
E=-99633.85322438949 eV
1 P -2.2196 -1.2121 -0.1814
2 C -3.1607 -0.2530 -1.4474
3 C -3.1351 -0.8364 1.3772
4 C -2.7279 -2.9552 -0.5369
5 H -4.2332 -0.4679 -1.3883
6 H -2.7963 -0.5104 -2.4459
7 H -4.2080 -1.0224 1.2583
8 H -2.9728 0.2117 1.6415
9 H -2.3141 -3.6214 0.2255
10 H -2.3351 -3.2603 -1.5111
11 H -2.9919 0.8143 -1.2829
12 H -2.7490 -1.4609 2.1878
13 H -3.8190 -3.0539 -0.5442
14 C -0.5999 4.6934 0.9264
15 Br -0.2300 1.8106 0.3834
16 Pd 0.1025 -0.7781 -0.1105
17 P 2.4610 -0.6275 -0.0938
18 C 3.1974 0.0067 1.4759
19 H 4.2860 0.0961 1.3931
20 H 2.7660 0.9853 1.7012
21 H 2.9534 -0.6752 2.2955
22 C 3.1836 0.4983 -1.3662
23 H 2.7582 1.4973 -1.2405
24 H 4.2738 0.5499 -1.2729
25 H 2.9244 0.1357 -2.3649
26 C 3.3953 -2.2002 -0.3705
27 H 4.4767 -2.0254 -0.3484
28 H 3.1344 -2.9236 0.4073
29 H 3.1219 -2.6242 -1.3410
30 H -1.5421 4.7507 0.3967
31 H -0.5995 4.5704 2.0019
32 H 0.3131 4.9839 0.4227

thf_dosmet240trans
E=-99633.8653822643 eV
1 P -2.3590 -0.8884 -0.0005
2 C -3.1971 -0.0701 -1.4276
3 C -3.1919 -0.1187 1.4564
4 C -3.0861 -2.5895 -0.0278
5 H -4.2867 -0.1343 -1.3348
6 H -2.8860 -0.5517 -2.3589
7 H -4.2816 -0.1875 1.3689
8 H -2.8959 0.9315 1.5218
9 H -2.7442 -3.1494 0.8473
10 H -2.7523 -3.1166 -0.9262
11 H -2.8942 0.9794 -1.4638
12 H -2.8713 -0.6255 2.3710
13 H -4.1810 -2.5502 -0.0220
14 C 0.0010 4.8698 -0.0032
15 Br 0.0002 1.9130 0.0017
16 Pd -0.0001 -0.7432 -0.0001
17 P 2.3587 -0.8889 0.0000
18 C 3.1970 -0.0723 1.4279
19 H 4.2866 -0.1369 1.3353
20 H 2.8946 0.9774 1.4649
21 H 2.8855 -0.5545 2.3588
22 C 3.1918 -0.1179 -1.4561
23 H 2.8960 0.9323 -1.5206
24 H 4.2815 -0.1870 -1.3686
25 H 2.8712 -0.6240 -2.3712
26 C 3.0855 -2.5902 0.0255
27 H 4.1804 -2.5512 0.0201
28 H 2.7513 -3.1184 0.9231
29 H 2.7437 -3.1489 -0.8505
30 H -0.9365 4.9455 -0.5390
31 H 0.0060 4.9491 1.0764
32 H 0.9335 4.9452 -0.5476

thf_dosmet240ph3freq
E=-93212.9977943733 eV
1 P 1.3238 2.0638 0.0012
2 H 0.8898 2.9079 1.0487
3 H 0.9449 2.8896 -1.0817
4 H 2.6956 2.4061 0.0335
5 C -4.3302 -1.0140 0.0030
6 Br -1.8410 0.1808 -0.0013
7 Pd 0.6582 -0.1815 -0.0000
8 P 2.6272 -1.4839 0.0006
9 H 2.9472 -2.2761 -1.1271
10 H 2.8277 -2.4799 0.9858
11 H 3.8814 -0.8459 0.1334
12 H -4.3173 -1.3209 1.0414
13 H -4.8770 -0.1201 -0.2706
14 H -4.1187 -1.7508 -0.7617

thf_dosmet240ph3
E=-93212.9284144866 eV
1 P 1.3249 2.0739 -0.0064
2 H 0.8902 2.9219 1.0377
3 H 0.9388 2.8918 -1.0928
4 H 2.6951 2.4228 0.0198
5 C -4.3198 -1.0175 -0.0083
6 Br -1.8315 0.1799 0.0032
7 Pd 0.6691 -0.1743 0.0059
8 P 2.6432 -1.4687 0.0061
9 H 2.9646 -2.2606 -1.1214
10 H 2.8495 -2.4628 0.9919
11 H 3.8950 -0.8253 0.1361
12 H -4.4022 -1.1406 1.0644
13 H -4.8329 -0.1883 -0.4798
14 H -4.0466 -1.8734 -0.6125

thf_dosmet240
E=-99633.50161745299 eV
1 P 0.0919 2.1056 -0.0018
2 C 4.2043 -2.5402 -0.0097
3 Br 2.3644 -0.7104 -0.0033
4 Pd -0.1403 -0.2265 -0.0088
5 P -2.3664 -1.0379 -0.0010
6 H 4.5608 -2.4189 -1.0262
7 H 4.8274 -2.1560 0.7899
8 H 3.5901 -3.4068 0.2059
9 C -1.4434 3.1330 -0.1041
10 H -2.0934 2.9107 0.7464
11 H -1.1994 4.2015 -0.0984
12 H -1.9845 2.8948 -1.0240
13 C 1.1112 2.8180 -1.3712
14 H 1.1858 3.9076 -1.2803
15 H 2.1115 2.3790 -1.3371
16 H 0.6583 2.5680 -2.3348
17 C 0.9145 2.8059 1.5001
18 H 0.9981 3.8965 1.4305
19 H 0.3350 2.5463 2.3905
20 H 1.9118 2.3697 1.5988
21 C -3.7757 0.1622 0.0030
22 H -3.7132 0.7998 0.8892
23 H -3.7210 0.7988 -0.8842
24 H -4.7370 -0.3636 0.0079
25 C -2.8226 -2.1262 -1.4307
26 H -2.1417 -2.9811 -1.4701
27 H -3.8524 -2.4900 -1.3387
28 H -2.7229 -1.5660 -2.3648
29 C -2.8072 -2.1152 1.4419
30 H -3.8379 -2.4796 1.3641
31 H -2.1259 -2.9698 1.4810
32 H -2.6973 -1.5476 2.3705

thf_dosmet240pf3new
E=-109421.9890550825 eV
1 P 0.5155 1.9048 -0.0273
2 F -0.1101 2.7481 1.1688
3 F -0.1102 2.7172 -1.2445
4 F 1.9700 2.5632 -0.0358
5 C -6.6370 -1.6596 0.0229
6 Br -2.2556 -0.2976 0.0018
7 Pd 0.2417 -0.3923 0.0021
8 P 2.4111 -1.1861 0.0114
9 F 3.3702 -0.7964 -1.1982
10 F 2.6870 -2.7553 0.0317
11 F 3.3712 -0.7652 1.2097
12 H -6.5216 -2.5831 -0.5312
13 H -6.6119 -1.6709 1.1057
14 H -6.7656 -0.7232 -0.5060

thf_dostransPh240
E=-130938.3624611856 eV
1 C -0.3881 5.8244 -0.0582
2 Br -0.1349 2.7516 -0.0310
3 H 0.3631 5.9399 0.7122
4 H -0.1029 5.8781 -1.1009
5 H -1.4340 5.7659 0.2132
6 Pd 0.0064 0.1294 0.0273
7 P 2.3790 -0.2190 0.0117
8 P -2.3351 -0.2773 0.0187
9 C 2.9955 -1.0517 1.5419
10 C 3.5505 1.1861 -0.2197
11 C 2.8000 -1.3949 -1.3505
12 C -3.3382 0.5994 1.2921
13 C -2.6453 -2.0704 0.3414
14 C -3.2125 0.0447 -1.5744
15 C 4.3107 -0.9030 2.0122
16 C 2.1088 -1.8768 2.2548
17 C 3.4432 2.2846 0.6513
18 C 4.5252 1.2097 -1.2292
19 C 3.7164 -2.4478 -1.2010
20 C 2.1560 -1.2231 -2.5893
21 C -4.6759 0.9702 1.0831
22 C -2.7298 0.8997 2.5223
23 C -1.8806 -3.0080 -0.3773
24 C -3.5755 -2.5345 1.2842
25 C -4.1753 -0.8331 -2.0986
26 C -2.8953 1.2164 -2.2843
27 C 4.7294 -1.5694 3.1680
28 H 5.0102 -0.2651 1.4814
29 C 2.5305 -2.5498 3.4043
30 H 1.0834 -1.9898 1.9121
31 C 4.3087 3.3728 0.5280
32 H 2.6777 2.2941 1.4205
33 C 5.3830 2.3077 -1.3589
34 H 4.6224 0.3761 -1.9169
35 C 3.9868 -3.3080 -2.2705
36 H 4.2199 -2.6022 -0.2523
37 C 2.4346 -2.0770 -3.6592
38 H 1.4325 -0.4216 -2.7149
39 C -5.3941 1.6206 2.0916
40 H -5.1598 0.7572 0.1353
41 C -3.4511 1.5411 3.5319
42 H -1.6867 0.6420 2.6835
43 C -2.0548 -4.3775 -0.1696
44 H -1.1466 -2.6653 -1.1026
45 C -3.7415 -3.9075 1.4991
46 H -4.1727 -1.8303 1.8539
47 C -4.8132 -0.5424 -3.3089
48 H -4.4287 -1.7459 -1.5691
49 C -3.5405 1.5070 -3.4890
50 H -2.1445 1.8969 -1.8927
51 C 3.8422 -2.3954 3.8650
52 H 5.7487 -1.4419 3.5216
53 H 1.8328 -3.1845 3.9431
54 C 5.2802 3.3885 -0.4794
55 H 4.2160 4.2128 1.2104
56 H 6.1318 2.3127 -2.1460
57 C 3.3498 -3.1235 -3.5013
58 H 4.6955 -4.1209 -2.1395
59 H 1.9319 -1.9293 -4.6107
60 C -4.7851 1.9038 3.3179
61 H -6.4275 1.9061 1.9164
62 H -2.9680 1.7686 4.4778
63 C -2.9853 -4.8312 0.7728
64 H -1.4598 -5.0880 -0.7362
65 H -4.4644 -4.2512 2.2336
66 C -4.4992 0.6284 -4.0054
67 H -5.5545 -1.2314 -3.7040
68 H -3.2882 2.4165 -4.0268
69 H 4.1687 -2.9109 4.7636
70 H 5.9477 4.2396 -0.5800
71 H 3.5609 -3.7930 -4.3302

72 H -5.3436 2.4116 4.0990
73 H -3.1161 -5.8963 0.9409
74 H -4.9950 0.8528 -4.9456

thf_onemetBb
E=-87085.6820336641 eV
1 P -2.5038 1.0754 -0.0297
2 C 4.7167 0.2676 0.0826
3 Br 1.4116 0.2627 -0.0491
4 Pd -0.9432 -0.5898 -0.2634
5 H 4.6766 0.0143 1.1343
6 H 4.7761 -0.5167 -0.6612
7 H 4.7230 1.3058 -0.2242
8 H -2.4913 2.1246 -0.9724
9 H -3.8851 0.7782 -0.0546
10 H -2.4682 1.8438 1.1522

thf_onemetBpf3b
E=-91979.538802535 eV
1 P -2.0773 0.4576 -0.0100
2 C 5.8123 0.6721 0.0046
3 Br 1.5938 0.2730 -0.0048
4 Pd -0.5080 -1.1028 -0.0387
5 H 5.9033 0.0883 0.9124
6 H 5.7856 0.1764 -0.9580
7 H 5.7341 1.7509 0.0603
8 F -2.0924 1.4818 1.2141
9 F -2.0795 1.5381 -1.1846
10 F -3.6426 0.1168 -0.0265

thf_onemetBpPh3
E=-102737.55496472568 eV
1 C -6.2328 0.2401 -0.3765
2 Br -3.3747 0.0412 -0.4237
3 Pd -1.0877 -0.1529 -1.4416
4 H -6.2644 1.2341 -0.8042
5 H -6.4147 -0.6168 -1.0126
6 H -6.2909 0.1236 0.6983
7 P 0.6778 -0.0554 0.0085
8 C 0.8070 1.5066 0.9782
9 C 2.2836 -0.1817 -0.8909
10 C 0.7263 -1.3992 1.2677
11 C 2.0405 2.1114 1.2700
12 C -0.3774 2.1016 1.4461
13 C 2.4730 0.6474 -2.0125
14 C 3.2947 -1.0877 -0.5356
15 C 1.2684 -1.2136 2.5497
16 C 0.2052 -2.6570 0.9207
17 C 2.0883 3.2876 2.0250
18 H 2.9646 1.6712 0.9088
19 C -0.3248 3.2715 2.2076
20 H -1.3381 1.6538 1.2067
21 C 3.6556 0.5830 -2.7508
22 H 1.6927 1.3443 -2.3087
23 C 4.4755 -1.1571 -1.2832
24 H 3.1667 -1.7407 0.3214
25 C 1.2971 -2.2719 3.4631
26 H 1.6652 -0.2464 2.8412
27 C 0.2424 -3.7153 1.8317
28 H -0.2391 -2.8022 -0.0606
29 C 0.9073 3.8678 2.4976
30 H 3.0482 3.7476 2.2421
31 H -1.2465 3.7216 2.5651
32 C 4.6602 -0.3224 -2.3886
33 H 3.7895 1.2323 -3.6112
34 H 5.2495 -1.8638 -0.9978
35 C 0.7878 -3.5240 3.1056
36 H 1.7150 -2.1151 4.4535
37 H -0.1644 -4.6824 1.5508
38 H 0.9460 4.7822 3.0826
39 H 5.5773 -0.3787 -2.9676
40 H 0.8083 -4.3437 3.8180

2.3.3 Species Optimized in DMF

dmf_set_Brpdph32
E=-2.12458253406938E6 kcal.mol-1
1 P -3.8649 -1.4892 0.5377
2 Pd -1.7768 -0.6239 -0.1105
3 P -2.4384 1.4310 -1.0968
4 Br 0.7540 -0.4493 -0.4559
5 H -2.0467 1.6636 -2.4331
6 H -1.9341 2.6168 -0.5197
7 H -3.7947 1.8098 -1.2049
8 H -4.6912 -0.6984 1.3644
9 H -3.9474 -2.7012 1.2592
10 H -4.8065 -1.7835 -0.4717

dmf_set_Brpdpme3trans
E=-1.9832783704471842E6 kcal.mol-1
1 Pd -1.9653 -0.5903 -0.1250
2 P -4.2383 -0.8811 0.2126
3 Br 0.5257 -0.2489 -0.4995
4 C -5.0369 0.4146 1.2505
5 H -4.9053 1.3927 0.7801
6 H -6.1066 0.2119 1.3672
7 H -4.5652 0.4358 2.2367
8 C -4.7003 -2.4563 1.0489
9 H -4.3546 -3.3034 0.4504
10 H -4.2199 -2.5037 2.0300
11 H -5.7859 -2.5233 1.1758
12 C -5.2475 -0.8905 -1.3293
13 H -6.3078 -1.0366 -1.0982
14 H -5.1215 0.0602 -1.8545
15 H -4.9078 -1.6977 -1.9838

dmf_set_Brpdpme3cis
E=-1.983273348472104E6 kcal.mol-1
1 Pd -1.7077 -0.4430 -0.2738
2 P -2.3797 1.5590 -1.1772
3 Br 0.8152 -0.8185 -0.1115
4 C -1.6736 3.0534 -0.3646
5 H -0.5825 3.0176 -0.4211
6 H -2.0316 3.9645 -0.8557
7 H -1.9679 3.0710 0.6880
8 C -4.1995 1.8581 -1.1378
9 H -4.7130 1.0653 -1.6884
10 H -4.5503 1.8483 -0.1024
11 H -4.4409 2.8257 -1.5908
12 C -1.9411 1.7810 -2.9529
13 H -2.2921 2.7517 -3.3192
14 H -0.8560 1.7218 -3.0710
15 H -2.4000 0.9845 -3.5445

dmf_set_Brpdph32trans

E=-2.12458004319981E6 kcal.mol-1
1 P -1.3325 -2.7541 0.7969
2 Pd -1.7551 -0.6291 -0.1754
3 P -2.4157 1.4115 -1.1955
4 Br 0.7440 0.1862 0.1748
5 H -1.7725 1.7675 -2.3991
6 H -2.1878 2.6011 -0.4734
7 H -3.7510 1.6515 -1.5887
8 H -0.3359 -3.5524 0.1981
9 H -2.3448 -3.7318 0.9196
10 H -0.8537 -2.7757 2.1233

dmf_set_Brpdpme32trans
E=-2.2726499585037064E6 kcal.mol-1
1 P -1.3052 -2.6870 0.8928
2 Pd -1.6740 -0.5545 -0.0888
3 P -2.3589 1.4389 -1.1889
4 Br 0.6887 0.4505 0.7113
5 C -2.4744 2.9352 -0.1147
6 H -1.5035 3.1173 0.3532
7 H -2.7687 3.8147 -0.6971
8 H -3.2125 2.7624 0.6736
9 C -4.0220 1.3829 -1.9933
10 H -4.0397 0.5866 -2.7428
11 H -4.7857 1.1669 -1.2408
12 H -4.2559 2.3370 -2.4779
13 C -1.0489 -2.6778 2.7204
14 H -1.9348 -2.2657 3.2116
15 H -0.8674 -3.6904 3.0957
16 H -0.1925 -2.0420 2.9593
17 C -2.6651 -3.9206 0.6773
18 H -2.8366 -4.0942 -0.3888
19 H -2.4113 -4.8710 1.1593
20 H -3.5872 -3.5307 1.1176
21 C 0.1737 -3.6006 0.2733
22 H 0.2869 -4.5583 0.7922
23 H 0.0671 -3.7832 -0.7997
24 H 1.0666 -2.9911 0.4351
25 C -1.2593 1.9978 -2.5610
26 H -1.6243 2.9316 -3.0018
27 H -0.2492 2.1500 -2.1720
28 H -1.2206 1.2260 -3.3349

dmf_set_Brpdph3trans
E=-1.9092313437793169E6 kcal.mol-1
1 Pd -1.8047 -0.6203 -0.1221
2 P -4.1444 -0.8847 0.2082
3 Br 0.6949 -0.3125 -0.4974
4 H -4.9926 -0.8885 -0.9183
5 H -4.8324 0.0688 0.9866
6 H -4.6219 -2.0532 0.8363

dmf_set_Brpdpf32trans
E=-2.4983632674704534E6 kcal.mol-1
1 P -1.3269 -2.6943 0.8548
2 Pd -1.7113 -0.6942 -0.3024
3 P -2.3872 1.4051 -1.0907
4 Br 0.7616 -0.1108 -0.7600
5 F -2.0843 1.7751 -2.6096
6 F -1.7335 2.6850 -0.4079
7 F -3.9137 1.8690 -1.0400
8 F 0.1511 -3.0453 1.3230
9 F -2.0696 -2.9268 2.2469
10 F -1.6859 -4.0861 0.1650

dmf_set_Brpdpph32
E=-2.994560440859415E6 kcal.mol-1
1 P -2.2295 -1.8278 -0.0355
2 Pd 0.1129 -1.3639 0.0886
3 P 2.5003 -1.4394 0.0040
4 C 3.3269 0.0058 -0.7865
5 C 4.5162 0.5663 -0.2971
6 C 2.7274 0.5647 -1.9285
7 C 5.0990 1.6627 -0.9423
8 H 4.9913 0.1532 0.5867
9 C 3.3159 1.6515 -2.5783
10 H 1.7944 0.1534 -2.3048
11 C 4.5031 2.2050 -2.0844
12 H 6.0179 2.0896 -0.5507
13 H 2.8429 2.0724 -3.4609
14 H 4.9562 3.0564 -2.5839
15 C 3.1048 -2.8922 -0.9631
16 C 2.4285 -4.1155 -0.8074
17 C 4.1940 -2.8258 -1.8466
18 C 2.8428 -5.2513 -1.5067
19 H 1.5740 -4.1804 -0.1386
20 C 4.6017 -3.9618 -2.5541
21 H 4.7274 -1.8913 -1.9871
22 C 3.9302 -5.1762 -2.3845
23 H 2.3125 -6.1896 -1.3728
24 H 5.4454 -3.8952 -3.2351
25 H 4.2485 -6.0569 -2.9347
26 C 3.3216 -1.6162 1.6475
27 C 4.4424 -2.4380 1.8494
28 C 2.7934 -0.8991 2.7359
29 C 5.0258 -2.5396 3.1166
30 H 4.8623 -3.0034 1.0235
31 C 3.3831 -0.9977 3.9988
32 H 1.9219 -0.2666 2.5915
33 C 4.4995 -1.8187 4.1927
34 H 5.8910 -3.1808 3.2593
35 H 2.9664 -0.4383 4.8316
36 H 4.9529 -1.8995 5.1765
37 C -2.5239 -3.4547 -0.8598
38 C -3.3978 -3.6199 -1.9451
39 C -1.8078 -4.5696 -0.3860
40 C -3.5545 -4.8758 -2.5428
41 H -3.9600 -2.7741 -2.3268
42 C -1.9736 -5.8238 -0.9761
43 H -1.1220 -4.4577 0.4500
44 C -2.8462 -5.9794 -2.0599
45 H -4.2337 -4.9883 -3.3830
46 H -1.4184 -6.6761 -0.5950
47 H -2.9704 -6.9534 -2.5241
48 C -3.2123 -0.6244 -1.0258
49 C -2.6042 -0.0490 -2.1549
50 C -4.5287 -0.2617 -0.7009
51 C -3.3047 0.8577 -2.9536
52 H -1.5781 -0.3064 -2.4047
53 C -5.2255 0.6546 -1.4958
54 H -5.0145 -0.6879 0.1709
55 C -4.6174 1.2133 -2.6239
56 H -2.8229 1.2929 -3.8244
57 H -6.2425 0.9298 -1.2313
58 H -5.1599 1.9253 -3.2391
59 C -3.1289 -1.9796 1.5698

60 C -4.1557 -2.9174 1.7698
61 C -2.7694 -1.1235 2.6255
62 C -4.8111 -2.9972 3.0024
63 H -4.4439 -3.5910 0.9692
64 C -3.4308 -1.2021 3.8543
65 H -1.9730 -0.3986 2.4834
66 C -4.4515 -2.1393 4.0465
67 H -5.6014 -3.7289 3.1439
68 H -3.1435 -0.5354 4.6624
69 H -4.9601 -2.2035 5.0042
70 Br -0.0861 1.1403 1.0129

dmf_set_Brpdpph3trans
E=-2.3442335977162793E6 kcal.mol-1
1 P -1.3612 -2.9690 -0.4843
2 Pd -0.1083 -1.1900 0.3165
3 C -0.3539 -4.2455 -1.3441
4 C -0.8000 -4.9219 -2.4908
5 C 0.9193 -4.5388 -0.8250
6 C 0.0120 -5.8828 -3.1016
7 H -1.7757 -4.7006 -2.9117
8 C 1.7253 -5.5042 -1.4328
9 H 1.2812 -4.0076 0.0517
10 C 1.2729 -6.1771 -2.5734
11 H -0.3420 -6.3992 -3.9891
12 H 2.7066 -5.7232 -1.0223
13 H 1.9023 -6.9225 -3.0507
14 C -2.6201 -2.4305 -1.7135
15 C -2.2347 -1.4653 -2.6615
16 C -3.9361 -2.9178 -1.7281
17 C -3.1452 -1.0085 -3.6164
18 H -1.2223 -1.0692 -2.6510
19 C -4.8484 -2.4528 -2.6815
20 H -4.2552 -3.6553 -0.9987
21 C -4.4554 -1.5009 -3.6268
22 H -2.8348 -0.2646 -4.3442
23 H -5.8649 -2.8355 -2.6826
24 H -5.1662 -1.1403 -4.3645
25 C -2.2911 -3.8703 0.8218
26 C -2.4984 -5.2586 0.7876
27 C -2.8057 -3.1257 1.8977
28 C -3.2172 -5.8887 1.8084
29 H -2.1005 -5.8513 -0.0299
30 C -3.5290 -3.7567 2.9126
31 H -2.6382 -2.0526 1.9432
32 C -3.7350 -5.1400 2.8699
33 H -3.3710 -6.9633 1.7721
34 H -3.9228 -3.1707 3.7378
35 H -4.2917 -5.6320 3.6621
36 Br 1.2191 0.7866 1.1833

dmf_set_Brpdpph3cis
E=-2.3442286668807515E6 kcal.mol-1
1 P -2.1994 -1.7640 0.0604
2 Pd -0.0134 -1.1009 0.3335
3 C -2.3266 -3.3878 -0.7995
4 C -3.2563 -3.6406 -1.8204
5 C -1.4331 -4.4055 -0.4180
6 C -3.2976 -4.8933 -2.4416
7 H -3.9490 -2.8658 -2.1324
8 C -1.4818 -5.6574 -1.0346
9 H -0.6986 -4.2189 0.3617
10 C -2.4142 -5.9032 -2.0493
11 H -4.0215 -5.0774 -3.2302
12 H -0.7889 -6.4359 -0.7292
13 H -2.4481 -6.8747 -2.5336
14 C -3.2019 -0.5979 -0.9508
15 C -2.5824 0.0256 -2.0480
16 C -4.5451 -0.3061 -0.6659
17 C -3.2979 0.9127 -2.8548
18 H -1.5365 -0.1769 -2.2637
19 C -5.2575 0.5892 -1.4709
20 H -5.0387 -0.7706 0.1815
21 C -4.6375 1.1975 -2.5663
22 H -2.8077 1.3878 -3.6995
23 H -6.2954 0.8099 -1.2391
24 H -5.1919 1.8945 -3.1880
25 C -3.1351 -1.9771 1.6324
26 C -4.0774 -3.0026 1.8133
27 C -2.8919 -1.0747 2.6831
28 C -4.7700 -3.1188 3.0227
29 H -4.2743 -3.7125 1.0162
30 C -3.5918 -1.1894 3.8867
31 H -2.1526 -0.2876 2.5611
32 C -4.5310 -2.2122 4.0599
33 H -5.4950 -3.9174 3.1513
34 H -3.3970 -0.4857 4.6908
35 H -5.0691 -2.3046 4.9988
36 Br 0.2483 1.2269 1.3536

dmf_set_Ph
E=-145317.3885611323 kcal.mol-1
Atom X Y Z
1 C 1.9268 -1.1395 0.2189
2 C 2.7282 -0.9475 -0.8881
3 C 2.3601 -1.2814 1.5214
4 C 4.1156 -0.8927 -0.6551
5 H 2.3254 -0.8427 -1.8916
6 C 3.7514 -1.2230 1.7288
7 H 1.6769 -1.4308 2.3528
8 C 4.6173 -1.0300 0.6452
9 H 4.7943 -0.7431 -1.4911
10 H 4.1486 -1.3286 2.7352
11 H 5.6892 -0.9862 0.8150

dmf_set_Brpdpf32
E=-2.4983677101785024E6 kcal.mol-1
Atom X Y Z
1 P -3.8846 -1.4522 0.5988
2 Pd -1.8398 -0.5681 -0.0360
3 P -2.4115 1.3642 -1.1639
4 Br 0.6301 -0.2402 -0.3755
5 F -1.7869 1.6002 -2.6109
6 F -1.9901 2.7530 -0.5037
7 F -3.9270 1.7294 -1.5105
8 F -3.9941 -2.9963 0.9810
9 F -4.6314 -0.8439 1.8677
10 F -5.0986 -1.3858 -0.4305

dmf_set_Me
E=-25004.493371725373 kcal.mol-1
1 C -0.0000 1.3999 0.0000
2 H 1.0059 1.8032 0.0000
3 H -0.8522 2.0694 0.0000

4 H -0.1537 0.3271 0.0000

dmf_set_Brpdpf3trans
E=-2.0961231553624168E6 kcal.mol-1
1 P 2.2161 0.1989 0.0414
2 Pd -0.0433 0.6997 0.1610
3 Br -2.5276 1.0782 -0.1515
4 F 3.2969 1.3750 0.0317
5 F 2.8987 -0.7164 1.1587
6 F 2.7440 -0.5922 -1.2412

dmf_set_Brpdpf3cis
E=-2.0961309310145294E6 kcal.mol-1
1 P 1.9143 0.7253 0.6987
2 Pd -0.0476 0.3878 -0.2753
3 Br -1.5532 1.8654 1.1196
4 F 2.4441 2.2300 0.8123
5 F 2.0655 0.3465 2.2451
6 F 3.2776 0.0584 0.1835

dmf_set_Brpdpme32
E=-2.2726521084157177E6 kcal.mol-1
1 P -3.9633 -1.4807 0.5669
2 Pd -1.9224 -0.4525 0.0340
3 P -2.4904 1.5661 -1.0872
4 Br 0.6629 -0.3547 -0.0636
5 C -1.5435 3.0304 -0.4780
6 H -0.4737 2.8127 -0.5280
7 H -1.7656 3.9179 -1.0804
8 H -1.8086 3.2284 0.5644
9 C -4.2254 2.1984 -1.0943
10 H -4.8936 1.4548 -1.5368
11 H -4.5496 2.3947 -0.0688
12 H -4.2949 3.1267 -1.6716
13 C -5.1289 -0.5544 1.6596
14 H -5.4292 0.3795 1.1783
15 H -6.0223 -1.1526 1.8679
16 H -4.6305 -0.3134 2.6026
17 C -5.0329 -1.9614 -0.8604
18 H -4.4793 -2.6374 -1.5179
19 H -5.9426 -2.4627 -0.5129
20 H -5.3109 -1.0738 -1.4345
21 C -3.7727 -3.0844 1.4705
22 H -4.7500 -3.5348 1.6773
23 H -3.1790 -3.7760 0.8666
24 H -3.2494 -2.9122 2.4151
25 C -2.0724 1.5211 -2.8861
26 H -2.2712 2.4898 -3.3573
27 H -1.0149 1.2708 -3.0043
28 H -2.6692 0.7508 -3.3825

dmf_set_Brpdph3cis
E=-1.90923659278124E6 kcal.mol-1
1 Pd -1.7874 -0.2257 0.2325
2 P -2.4642 1.5737 -1.0408
3 Br 0.6935 -0.6547 -0.1012
4 H -2.0383 2.8597 -0.6478
5 H -3.8407 1.8399 -1.2102
6 H -2.0618 1.6113 -2.3914

dmf_dostranspf3
E=-109422.1069549033 eV
1 P -2.0807 -1.4278 0.0020
2 C 5.7670 -2.0104 0.0015
3 Br 2.4371 0.0288 -0.0019
4 Pd -0.0466 -0.3089 -0.0011
5 P -0.6018 1.9222 -0.0062
6 H 5.3764 -2.5650 0.8458
7 H 5.5620 -2.3455 -1.0078
8 H 6.3642 -1.1220 0.1665
9 F -0.0674 2.8251 -1.2071
10 F -0.0831 2.8228 1.2033
11 F -2.1208 2.4148 -0.0158
12 F -2.2559 -2.7223 -0.9125
13 F -2.6301 -2.0334 1.3702
14 F -3.3987 -0.6533 -0.4465

dmf_onemetB
E=-87085.38795894489 eV
1 P -1.9930 0.4174 -0.0373
2 C -2.0565 1.7630 -1.2988
3 C -2.0349 1.3465 1.5568
4 C -3.6858 -0.3161 -0.1315
5 H -2.9085 2.4265 -1.1145
6 H -2.1496 1.3254 -2.2964
7 H -2.8894 2.0315 1.5832
8 H -1.1100 1.9182 1.6699
9 H -3.8073 -1.0631 0.6575
10 H -3.8205 -0.8064 -1.0995
11 H -1.1312 2.3436 -1.2593
12 H -2.1118 0.6420 2.3893
13 H -4.4495 0.4607 -0.0123
14 C 4.6317 0.6122 -0.0745
15 Br 1.9499 0.2425 -0.1004
16 Pd -0.2481 -1.0290 -0.2617
17 H 4.8582 -0.0221 0.7741
18 H 4.8406 0.2340 -1.0679
19 H 4.6195 1.6853 0.0749

dmf_dostransph3
E=-93213.21174630299 eV
1 P -1.2390 2.3578 0.0008
2 C 4.6139 -0.0004 0.0043
3 Br 1.5392 -0.0002 -0.0024
4 Pd -1.1065 0.0001 0.0003
5 P -1.2400 -2.3574 0.0008
6 H 4.6707 0.9355 -0.5366
7 H 4.6665 0.0002 1.0856
8 H 4.6706 -0.9370 -0.5355
9 H -0.6268 -3.0479 1.0675
10 H -0.6331 -3.0482 -1.0692
11 H -2.4834 -3.0283 0.0045
12 H -0.6259 3.0479 1.0677
13 H -0.6314 3.0483 -1.0690
14 H -2.4821 3.0292 0.0041

dmf_onemetBpf3b
E=-91979.7202509252 eV
1 P -1.9764 0.4468 0.0046
2 C 5.5124 0.6957 -0.0175
3 Br 1.6901 0.2995 0.0020
4 Pd -0.4121 -1.1138 0.0033
5 H 5.5605 0.1210 0.8992
6 H 5.5365 0.1906 -0.9752
7 H 5.4412 1.7757 0.0236

8 F -2.0334 1.4624 1.2402
9 F -1.9346 1.5508 -1.1526
10 F -3.5447 0.1221 -0.0723

dmf_dosmet240b
E=-99633.25453885189 eV
1 P 1.3301 2.2204 0.0493
2 C -3.9663 -0.9579 -0.0820
3 Br -1.6868 0.2069 -0.0321
4 Pd 0.8587 -0.0728 -0.0106
5 P 2.7382 -1.5234 -0.0376
6 H -4.3268 -0.6956 0.9066
7 H -4.4145 -0.4444 -0.9255
8 H -3.6490 -1.9829 -0.2377
9 C 3.1062 2.7221 0.1659
10 H 3.6558 2.3346 -0.6961
11 H 3.2010 3.8136 0.1905
12 H 3.5477 2.3037 1.0745
13 C 0.5791 3.1688 1.4492
14 H 0.8453 4.2302 1.3910
15 H -0.5082 3.0637 1.4125
16 H 0.9338 2.7618 2.4004
17 C 0.7619 3.1847 -1.4239
18 H 1.0196 4.2449 -1.3215
19 H 1.2338 2.7868 -2.3267
20 H -0.3216 3.0826 -1.5261
21 C 4.4416 -0.8017 -0.0064
22 H 4.5819 -0.1518 -0.8744
23 H 4.5719 -0.2021 0.8985
24 H 5.1996 -1.5926 -0.0248
25 C 2.8304 -2.7334 1.3635
26 H 1.9243 -3.3457 1.3775
27 H 3.7047 -3.3867 1.2639
28 H 2.8945 -2.1925 2.3121
29 C 2.8471 -2.6464 -1.5083
30 H 3.7209 -3.3042 -1.4389
31 H 1.9418 -3.2571 -1.5695
32 H 2.9209 -2.0489 -2.4215

dmf_dosmet240pf3newc
E=-109422.1022528425 eV
1 P 0.6054 1.9268 0.0003
2 F 0.0800 2.8202 1.2123
3 F 0.0634 2.8287 -1.1980
4 F 2.1205 2.4315 -0.0084
5 C -5.7306 -2.0567 0.0008
6 Br -2.4183 0.0092 0.0013
7 Pd 0.0680 -0.3086 -0.0003
8 P 2.1110 -1.4111 -0.0013
9 F 2.2956 -2.7024 -0.9187
10 F 2.6666 -2.0151 1.3651
11 F 3.4223 -0.6253 -0.4496
12 H -5.3349 -2.6110 0.8429
13 H -6.3341 -1.1732 0.1693
14 H -5.5245 -2.3873 -1.0098

dmf_dostrans
E=-99633.955279245 eV
1 P -2.3592 -0.8709 -0.0014
2 C -3.2088 -0.1094 -1.4533
3 C -3.2189 -0.0835 1.4306
4 C -3.0455 -2.5881 0.0116
5 H -4.2962 -0.2084 -1.3680
6 H -2.8739 -0.6004 -2.3714
7 H -4.3060 -0.1799 1.3374
8 H -2.9500 0.9752 1.4729
9 H -2.6995 -3.1141 0.9059
10 H -2.6900 -3.1318 -0.8683
11 H -2.9435 0.9495 -1.5102
12 H -2.8938 -0.5611 2.3591
13 H -4.1409 -2.5732 0.0056
14 C 0.0006 4.8366 0.0341
15 Br 0.0004 1.9675 0.0049
16 Pd -0.0001 -0.7026 0.0015
17 P 2.3590 -0.8716 -0.0053
18 C 3.2212 -0.0847 1.4255
19 H 4.3081 -0.1814 1.3306
20 H 2.9526 0.9740 1.4684
21 H 2.8974 -0.5624 2.3545
22 C 3.2064 -0.1099 -1.4583
23 H 2.9412 0.9491 -1.5145
24 H 4.2940 -0.2090 -1.3748
25 H 2.8700 -0.6006 -2.3760
26 C 3.0450 -2.5890 0.0062
27 H 4.1403 -2.5742 -0.0015
28 H 2.7002 -3.1151 0.9009
29 H 2.6880 -3.1323 -0.8734
30 H -0.9334 4.9516 -0.5017
31 H 0.0024 4.9270 1.1131
32 H 0.9330 4.9513 -0.5046

dmf_dosmet240ph3
E=-93213.09187912689 eV
1 P 1.3059 2.0557 0.0289
2 H 0.8758 2.8927 1.0840
3 H 0.9335 2.8958 -1.0455
4 H 2.6794 2.3875 0.0664
5 C -4.2961 -0.9949 0.0041
6 Br -1.8611 0.1628 0.0171
7 Pd 0.6505 -0.1882 0.0013
8 P 2.6273 -1.4858 -0.0299
9 H 2.9524 -2.2464 -1.1776
10 H 2.8372 -2.5046 0.9295
11 H 3.8746 -0.8388 0.1179
12 H -4.4119 -1.0973 1.0762
13 H -4.8194 -0.1886 -0.4958
14 H -4.0366 -1.8749 -0.5717

dmf_onemetBpf3
E=-91979.7202509252 eV
1 P -1.9764 0.4468 0.0046
2 C 5.5124 0.6957 -0.0175
3 Br 1.6901 0.2995 0.0020
4 Pd -0.4121 -1.1138 0.0033
5 H 5.5605 0.1210 0.8992
6 H 5.5365 0.1906 -0.9752
7 H 5.4412 1.7757 0.0236
8 F -2.0334 1.4624 1.2402
9 F -1.9346 1.5508 -1.1526
10 F -3.5447 0.1221 -0.0723

dmf_onemetBph3
E=-83874.7456253376 eV
1 P -2.0273 0.3662 -0.0002
2 C 4.7825 0.6926 -0.0005
3 Br 1.9611 0.2517 0.0001

4 Pd -0.2178 -1.0207 0.0025
5 H 4.9714 0.1771 0.9326
6 H 4.9707 0.1789 -0.9348
7 H 4.6952 1.7719 0.0005
8 H -2.1785 1.2767 1.0676
9 H -2.1768 1.2747 -1.0700
10 H -3.3334 -0.1739 -0.0007

dmf_onemetBpPh3d
E=-102737.70580074089 eV
1 C -6.1093 0.1946 -0.3140
2 Br -3.3637 0.0699 -0.4276
3 Pd -1.0751 -0.1252 -1.4838
4 H -6.1960 1.2605 -0.4853
5 H -6.3169 -0.4820 -1.1338
6 H -6.1935 -0.1769 0.7001
7 P 0.6653 -0.0388 -0.0079
8 C 0.8067 1.5175 0.9718
9 C 2.2779 -0.1777 -0.8949
10 C 0.6955 -1.3867 1.2491
11 C 2.0423 2.1267 1.2447
12 C -0.3714 2.1072 1.4627
13 C 2.4546 0.6009 -2.0539
14 C 3.3088 -1.0404 -0.4907
15 C 1.2052 -1.2049 2.5449
16 C 0.1921 -2.6468 0.8831
17 C 2.0987 3.3008 2.0031
18 H 2.9619 1.6910 0.8675
19 C -0.3106 3.2739 2.2286
20 H -1.3346 1.6571 1.2380
21 C 3.6433 0.5300 -2.7824
22 H 1.6584 1.2617 -2.3881
23 C 4.4958 -1.1169 -1.2280
24 H 3.1919 -1.6547 0.3959
25 C 1.2182 -2.2680 3.4537
26 H 1.5913 -0.2377 2.8503
27 C 0.2140 -3.7099 1.7891
28 H -0.2239 -2.7909 -0.1109
29 C 0.9243 3.8746 2.4990
30 H 3.0605 3.7634 2.2051
31 H -1.2274 3.7188 2.6046
32 C 4.6671 -0.3320 -2.3717
33 H 3.7663 1.1392 -3.6732
34 H 5.2847 -1.7901 -0.9052
35 C 0.7262 -3.5217 3.0776
36 H 1.6123 -2.1141 4.4542
37 H -0.1772 -4.6788 1.4926
38 H 0.9697 4.7867 3.0871
39 H 5.5888 -0.3942 -2.9429
40 H 0.7357 -4.3452 3.7857

dmf_dostransPh240
E = -3.0195502923160377E6 kcal.mol-1
1 C 0.3254 5.0714 2.1433
2 Br 0.0772 2.3776 1.0786
3 H -0.5436 5.4607 1.6282
4 H 0.2351 4.7629 3.1771
5 H 1.3095 5.2367 1.7234
6 Pd -0.0093 -0.1044 0.1150
7 P -2.3751 -0.3521 0.1800
8 P 2.3418 -0.3470 -0.2064
9 C -2.8987 -1.8957 -0.6911
10 C -3.3302 0.9868 -0.6528
11 C -3.1431 -0.5148 1.8522
12 C 3.1540 1.0059 -1.1596
13 C 2.7270 -1.8746 -1.1729
14 C 3.3626 -0.5287 1.3228
15 C -3.9444 -1.9394 -1.6262
16 C -2.1925 -3.0783 -0.4050
17 C -2.7882 1.5512 -1.8208
18 C -4.5609 1.4626 -0.1748
19 C -4.2352 -1.3630 2.0997
20 C -2.6084 0.2377 2.9127
21 C 4.4308 1.5008 -0.8531
22 C 2.4490 1.5620 -2.2414
23 C 2.0500 -3.0572 -0.8240
24 C 3.6437 -1.9061 -2.2355
25 C 4.4697 -1.3905 1.3917
26 C 3.0103 0.2228 2.4579
27 C -4.2806 -3.1431 -2.2564
28 H -4.5007 -1.0395 -1.8671
29 C -2.5359 -4.2806 -1.0261
30 H -1.3705 -3.0577 0.3063
31 C -3.4727 2.5560 -2.5079
32 H -1.8242 1.2081 -2.1875
33 C -5.2402 2.4776 -0.8576
34 H -4.9935 1.0488 0.7303
35 C -4.7834 -1.4556 3.3828
36 H -4.6586 -1.9573 1.2963
37 C -3.1625 0.1474 4.1927
38 H -1.7597 0.8915 2.7339
39 C 4.9951 2.5261 -1.6204
40 H 4.9893 1.0932 -0.0167
41 C 3.0178 2.5769 -3.0137
42 H 1.4496 1.2039 -2.4749
43 C 2.2972 -4.2481 -1.5099
44 H 1.3263 -3.0457 -0.0130
45 C 3.8825 -3.0978 -2.9295
46 H 4.1746 -1.0056 -2.5264
47 C 5.2115 -1.4977 2.5724
48 H 4.7548 -1.9840 0.5290
49 C 3.7578 0.1184 3.6342
50 H 2.1521 0.8873 2.4179
51 C -3.5812 -4.3154 -1.9567
52 H -5.0917 -3.1613 -2.9789
53 H -1.9837 -5.1857 -0.7905
54 C -4.7009 3.0231 -2.0261
55 H -3.0425 2.9807 -3.4104
56 H -6.1902 2.8392 -0.4743
57 C -4.2499 -0.6999 4.4314
58 H -5.6262 -2.1177 3.5602
59 H -2.7399 0.7340 5.0036
60 C 4.2932 3.0629 -2.7033
61 H 5.9830 2.9021 -1.3698
62 H 2.4620 2.9946 -3.8483
63 C 3.2137 -4.2706 -2.5676
64 H 1.7692 -5.1535 -1.2249
65 H 4.5938 -3.1065 -3.7504
66 C 4.8588 -0.7427 3.6952
67 H 6.0635 -2.1704 2.6120
68 H 3.4752 0.7047 4.5040
69 H -3.8445 -5.2485 -2.4462
70 H -5.2297 3.8111 -2.5546
71 H -4.6754 -0.7741 5.4281
72 H 4.7328 3.8586 -3.2978

73 H 3.4012 -5.1945 -3.1070
74 H 5.4349 -0.8278 4.6122

3.- Table S4. Potential, Gibbs free energies and Dispersion correction (in hartree) of the located transition states.

In hartree	E (B3LYP)	G (B3LYP)	Disp. corr. D2	G (B3LYP+D2corr)
gas_1PF3_conctransA	-3572.00927	-3571.95383	-0.02527	-3571.979
gas_1PF3_conctransB	-3572.01006	-3571.95442	-0.02687	-3571.981
gas_1PH3_conctransA	-3274.16999	-3274.09196	-0.02328	-3274.115
gas_1PH3_conctransB	-3274.16867	-3274.09237	-0.02403	-3274.116
gas_1PMe3_conctransA	-3392.14849	-3391.99017	-0.03867	-3392.029
gas_1PMe3_conctransB	-3392.14636	-3391.98798	-0.03998	-3392.028
gas_1PPh3_conctransA	-3967.32119	-3967.01474	-0.08379	-3967.099
gas_2PF3_conccis	-4213.00397	-4212.95013	-0.03835	-4212.988
gas_2PH3_conccis	-3617.32436	-3617.22730	-0.03320	-3617.261
gas_2PMe3_conccis	-3853.27423	-3853.01390	-0.06970	-3853.084
gas_2PPh3_conccis	-5003.62128	-5003.06531	-0.17454	-5003.24
gas_PhBr	-2803.06954	-2803.00965	-0.01108	-2803.021
thf_1PF3_conctransA	-3572.01923	-3571.96489	-0.02516	-3571.99
thf_1PF3_conctransB	-3572.01719	-3571.96264	-0.02691	-3571.99
thf_1PH3_conctransA	-3274.17720	-3274.10069	-0.02331	-3274.124
thf_1PMe3_SN2cis	-3392.13927	-3391.98049	-0.04744	-3392.028
thf_1PMe3_conctransA	-3392.15579	-3391.99845	-0.03870	-3392.037
thf_1PPh3_conctransA	-3967.33101	-3967.02837	-0.08380	-3967.112
thf_2PF3_conccis	-4213.01287	-4212.95898	-0.03787	-4212.997
thf_2PH3_SN2cis	-3617.32697	-3617.22874	-0.03666	-3617.265
thf_2PH3_conccis	-3617.33046	-3617.23385	-0.03309	-3617.267
thf_2PMe3_SN2cis	-3853.28812	-3853.02465	-0.07563	-3853.1
thf_2PMe3_conccis	-3853.28193	-3853.02332	-0.06966	-3853.093
thf_2PMe3_conctrans	-3853.28108	-3853.02176	-0.06961	-3853.091
thf_2PPh3_conccis	-5003.63413	-5003.07816	-0.17343	-5003.252
thf_PhBr	-2803.07222	-2803.01242	-0.01109	-2803.024
dmf_1PF3_conctransA	-3572.02169	-3571.96675	-0.02516	-3571.992
dmf_1PF3_conctransB	-3572.01894	-3571.96501	-0.02692	-3571.992
dmf_1PH3_SN2cis	-3274.16173	-3274.08555	-0.02876	-3274.114
dmf_1PH3_conctransA	-3274.17864	-3274.10202	-0.02333	-3274.125
dmf_1PMe3_SN2cis	-3392.14411	-3391.98572	-0.04710	-3392.033
dmf_1PMe3_conctransA	-3392.15737	-3391.99949	-0.03872	-3392.038
dmf_1PPh3_SN2cis	-3967.31863	-3967.01408	-0.09314	-3967.107
dmf_1PPh3_conctransA	-3967.33339	-3967.03199	-0.08373	-3967.116
dmf_2PF3_conccis	-4213.01533	-4212.96100	-0.03767	-4212.999

dmf_2PH3_SN2cis	-3617.33110	-3617.23268	-0.03682	-3617.269
dmf_2PH3_conccis	-3617.33190	-3617.23502	-0.03307	-3617.268
dmf_2PMe3_SN2cis	-3853.29214	-3853.02831	-0.07543	-3853.104
dmf_2PMe3_conctrans	-3853.28356	-3853.02409	-0.06959	-3853.094
dmf_2PPh3_SN2cis	-5003.63581	-5003.07688	-0.18152	-5003.258
dmf_2PPh3_conccis	-5003.63764	-5003.08351	-0.17297	-5003.256
dmf_PhBr	-2803.07280	-2803.01302	-0.01109	-2803.024
wat_1PF3_conctransA	-3572.02209	-3571.96673	-0.02517	-3571.992
wat_1PF3_conctransB	-3572.01919	-3571.96524	-0.02693	-3571.992
wat_1PH3_conctransA	-3274.17884	-3274.10224	-0.02334	-3274.126
wat_1PMe3_SN2cis	-3392.14479	-3391.98655	-0.04705	-3392.034
wat_1PMe3_conctransA	-3392.15759	-3391.99977	-0.03872	-3392.038
wat_1PPh3_SN2cis	-3967.31950	-3967.01463	-0.09312	-3967.108
wat_1PPh3_conctransA	-3967.33374	-3967.03240	-0.08374	-3967.116
wat_2PF3_conccis	-4213.01571	-4212.96148	-0.03765	-4212.999
wat_2PH3_conccis	-3617.33211	-3617.23529	-0.03308	-3617.268
wat_2PH3_SN2cis	-3617.33168	-3617.23334	-0.03682	-3617.27
wat_2PMe3_SN2cis	-3853.29270	-3853.02890	-0.07541	-3853.104
wat_2PMe3_conctrans	-3853.28393	-3853.02425	-0.06958	-3853.094
wat_2PPh3_SN2cis	-5003.63678	-5003.07843	-0.18154	-5003.26
wat_2PPh3_conccis	-5003.63822	-5003.08275	-0.17292	-5003.256
wat_PhBr	-2803.07288	-2803.01311	-0.01109	-2803.024