Electronic Supplementary Information for Dalton Transactions

A DFT study on the Pd-Mediated Decarboxylation Process of Aryl Carboxylic Acids

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Electronic Supplementary Information

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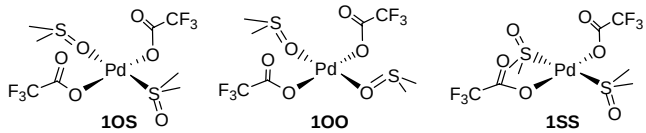
Summary of Additional Computational Results

A. B3PW91 versus B3LYP

Scheme S1 shows the relative stability of the three DMSO linkage isomers (**1OS, 1OO and 1SS**) of *trans*-$Pd(OOCCF_3)_2(DMSO)_2$ at both the B3PW91 and B3LYP levels. As we mentioned in the text, the isomer **1OS** was the one characterized by single crystal X-ray diffraction studies in experiment. Therefore, we feel that the results from the B3PW91 method are more reasonable in the prediction of the relative stability.

Scheme S1



	1OS	**1OO**	**1SS**
Results from the B3PW91 calculation	0.0	1.1	5.8
Results from the B3LYP calculation	0.0	-2.5	8.9

The calculated relative free energies in the gas phase are given in kcal/mol.

B. Other less favorable pathways are listed here.

i. Pathways in which the $OOCCF_3^-$ ligand is just a spectator ligand.

Fig. S1a is Fig. 1 discussed in the main text. It is again presented here for the purpose of comparison.

Fig. S1b shows the energy profile calculated for a direct conversion from **4** to **5** by rotating the phenyl carboxylate ligand around one of the two C-O bonds.

Fig. S1c shows the energy profile calculated for a similar direct conversion by rotating the phenyl carboxylate ligand around the other C-O bond in **4** leading to **8**, an isomer of **5**.

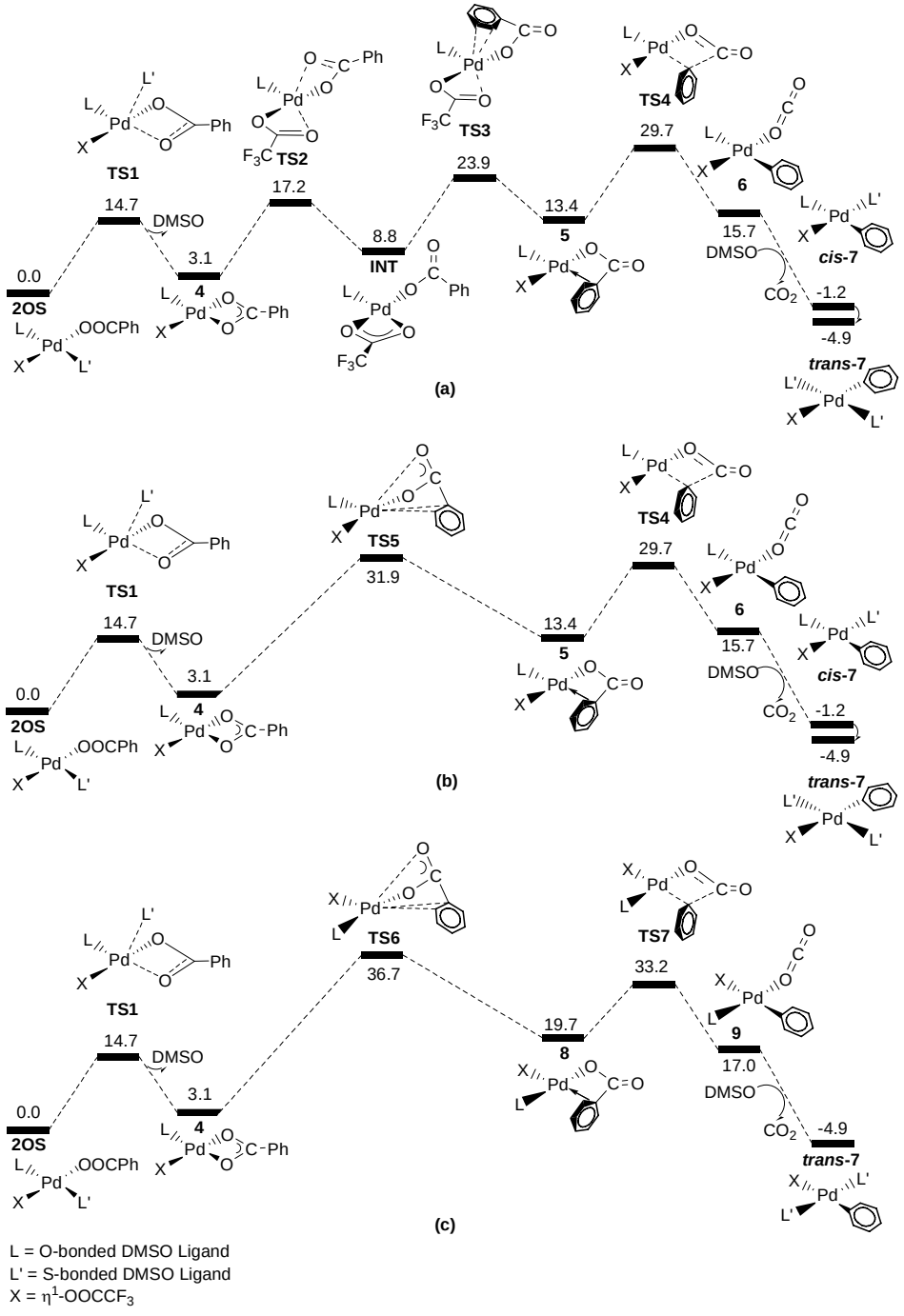


Fig. S1. Energy profiles calculated for various possible pathways for the conversion of **2OS** → ***trans*-7**. The calculated relative free energies in the gas phase are given in kcal/mol.

ii. Pathway that involves dissociation of the O-bonded DMSO ligand

The most favorable pathway discussed in the main text involves dissociation of the S-bonded DMSO ligand as the first step. Fig. S2 shows the possible pathway that involves dissociation of the O-bonded DMSO ligand as the first step.

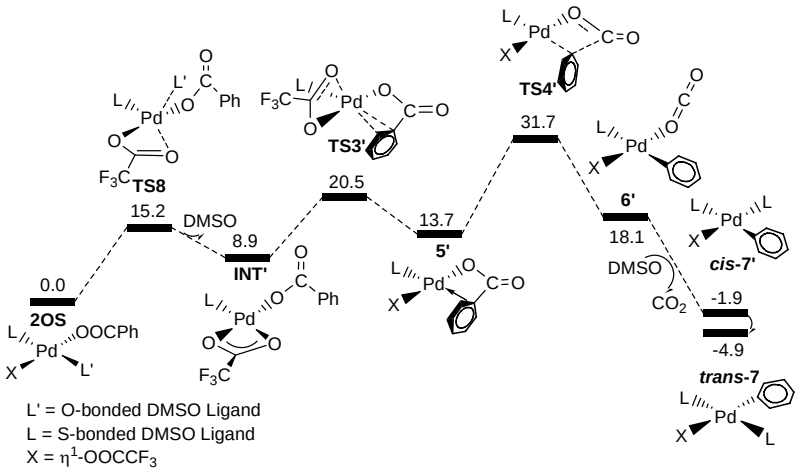


Fig. S2 Energy profile calculated for reaction of **2OS** → ***trans*-7** via the O-bonded DMSO ligand dissociation as the first step. The calculated relative free energies in the gas phase are given in kcal/mol.

C. Barriers calculated for insertion of styrene into a Pd-Ar$_R$ bond (R = OMe, NO$_2$)

The OMe and NO_2 substituents when they are in an *ortho* position have a significant effect to lower the decarboxylation barriers. For these two substituted systems, we examined the possibility of their styrene insertion steps, which are immediately followed their decarboxylation steps, becoming rate-determining in the catalytic cycle. The calculated results were presented in Fig. S3. For each system, there are two possible pathways starting from **10R** and **11R** in consideration of the different possible styrene coordination isomers. When we take **trans-7$_R$** as the energy reference point, the overall barriers caclualted for the styrene insertion are much lower than those of the decarboxylation steps.

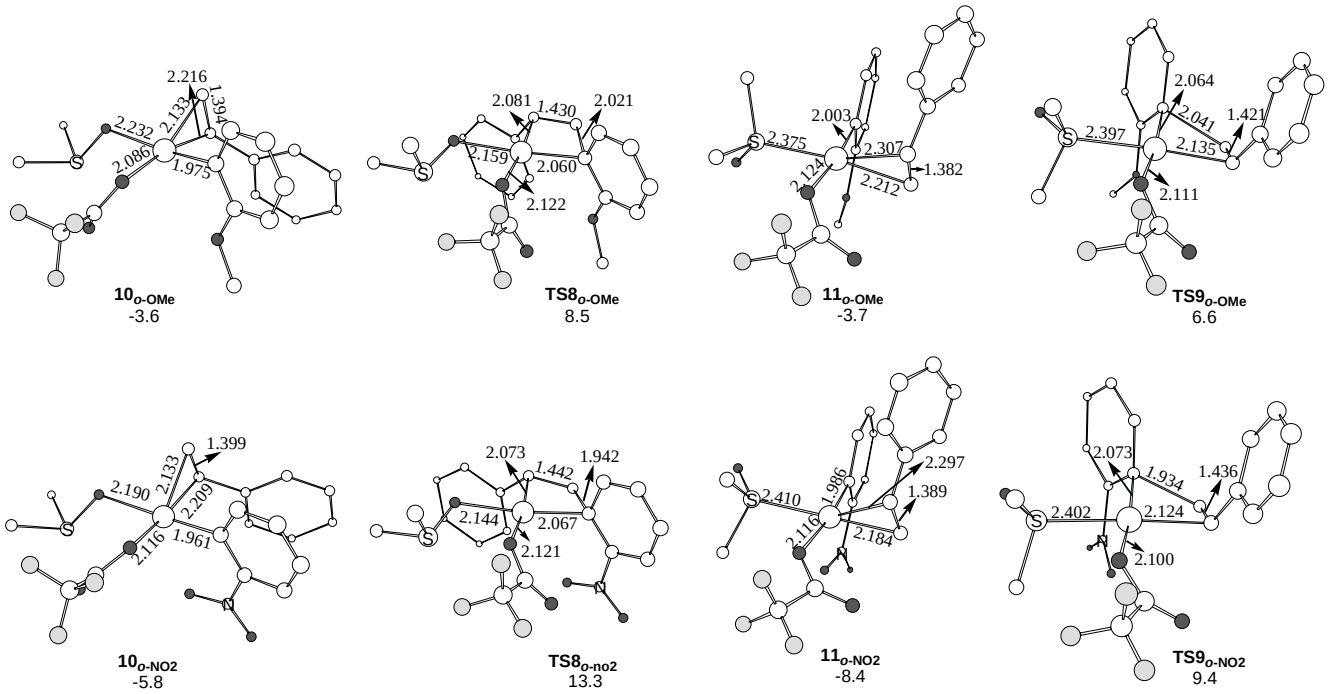


Fig. S3 The calculated relative free energies in the gas phase are given in kcal/mol and the selected bond distances (Å) calculated for **10**$_{o\text{-OMe}}$, **TS8**$_{o\text{-OMe}}$, **11**$_{o\text{-OMe}}$, **TS9**$_{o\text{-OMe}}$, **10**$_{o\text{-NO2}}$, **TS8**$_{o\text{-OMe}}$, **11**$_{o\text{-NO2}}$ and **TS9**$_{o\text{-NO2}}$. For clarity, the hydrogen atoms associated with the phenyl rings and the methyl groups were omitted. The dark spheres represent oxygen atoms and the grey sphere represent flourine atoms. In calculating the relative energies, we included the energies calculated for free styrene, DMSO and CO_2 whenever necessary in order to make the energies comparable for all the species.

D. Basis set effect

Examining the basis set dependence, we also performed single-point energy calculations with a much larger basis set. Table S1 gives the calculated results. The results suggest that the conclusions made in the main text should be valid with the use of the basis set chosen for this study.

Table S1. Computed relative electronic energies and single point relative electronic energies (kcal/mol) in the gas phase for selected sturctues.[a]

	ΔE	ΔE_{sp}
2OS	0.0	0.0
TS2+ DMSO	32.1	31.3
TS3+ DMSO	38.2	36.6
TS4+ DMSO	46.1	43.6

[a] Single point energy calculations were carried out base on the optimized structures calculated with the lower basis set (6-31G* for C, H and O, 6-31G+* for S and SDDAll for Pd). The large basis set we selected is SDDAll for Pd and 6-311+G(2d, p) for the others.

Results of calculations that include solvation effects

Table S2. Computed relative free energies and relative electronic energies (kcal/mol) in the gas phase and in DMF for selected steps that are crucial.

$$\Delta G_{sol} = \Delta E_{sol} + (\Delta G - \Delta E)$$

	Gas Phase		In DMF	
	ΔE	ΔG	ΔE_{sol}	ΔG_{sol}
2OS	0.0	0.0	0.0	0.0
TS4 + DMSO	46.1	29.7	43.7	27.3
***trans*-7 + CO_2**	7.0	-4.9	6.2	-5.7
2OS$_{o\text{-OMe}}$	0.0	0.0	0.0	0.0
TS4$_{o\text{-OMe}}$ + DMSO	38.1	22.0	37.2	21.1
***trans*-7$_{o\text{-OMe}}$ + CO_2**	3.3	-8.6	2.0	-9.9
2OS$_{p\text{-OMe}}$	0.0	0.0	0.0	0.0
TS4$_{p\text{-OMe}}$ + DMSO	43.4	26.9	41.8	25.3
***trans*-7$_{p\text{-OMe}}$ + CO_2**	10.6	-1.2	8.4	-3.4
2OS$_{m\text{-OMe}}$	0.0	0.0	0.0	0.0
TS4$_{m\text{-OMe}}$ + DMSO	46.0	29.8	44.0	27.8
***trans*-7$_{m\text{-OMe}}$ + CO_2**	8.1	-3.5	6.5	-5.1
2OS$_{o\text{-NO2}}$	0.0	0.0	0.0	0.0
TS4$_{o\text{-NO2}}$ + DMSO	44.9	28.1	41.8	25.0
***trans*-7$_{o\text{-NO2}}$ + CO_2**	2.7	-9.4	-0.3	-12.4
2OS$_{p\text{-NO2}}$	0.0	0.0	0.0	0.0
TS4$_{p\text{-NO2}}$ + DMSO	49.3	33.1	47.0	30.7
***trans*-7$_{p\text{-NO2}}$ + CO_2**	8.8	-2.9	5.5	-6.2
2OS$_{m\text{-NO2}}$	0.0	0.0	0.0	0.0
TS4$_{m\text{-NO2}}$ + DMSO	48.6	32.5	46.4	30.3

***trans*-7$_{m\text{-NO2}}$ + CO$_2$**	8.7	-3.0	6.4	-5.3
2OS$_{o\text{-Me}}$	0.0	0.0	0.0	0.0
TS4$_{o\text{-Me}}$ + DMSO	42.0	25.9	40.0	23.9
***trans*-7$_{o\text{-Me}}$ + CO$_2$**	7.7	-4.7	3.4	-9.0
2OS$_{p\text{-Me}}$	0.0	0.0	0.0	0.0
TS4$_{p\text{-Me}}$ + DMSO	45.0	28.7	43.4	27.1
***trans*-7$_{p\text{-Me}}$ + CO$_2$**	9.3	-2.4	9.0	-2.7
2OS$_{m\text{-Me}}$	0.0	0.0	0.0	0.0
TS4$_{m\text{-Me}}$ + DMSO	45.5	29.9	43.5	27.9
***trans*-7$_{m\text{-Me}}$ + CO$_2$**	9.0	-1.2	7.1	-3.1
2OS$_{o\text{-CN}}$	0.0	0.0	0.0	0.0
TS4$_{o\text{-CN}}$ + DMSO	48.3	31.3	44.5	27.5
***trans*-7$_{o\text{-CN}}$ + CO$_2$**	6.5	-6.4	3.6	-9.3
2OS$_{p\text{-CN}}$	0.0	0.0	0.0	0.0
TS4$_{p\text{-CN}}$ + DMSO	48.7	32.4	46.3	30.0
***trans*-7$_{p\text{-CN}}$ + CO$_2$**	9.2	-2.6	6.1	-5.7
2OS$_{m\text{-CN}}$	0.0	0.0	0.0	0.0
TS4$_{m\text{-CN}}$ + DMSO	48.8	33.1	46.3	30.6
***trans*-7$_{m\text{-CN}}$ + CO$_2$**	9.2	-2.3	6.6	-4.9

Cartesian coordinates for all the species calculated at the B3PW91 level in this study

10S
E = -2286.194065 a.u.

Pd	0.042317	-0.265112	-0.471024
S	-0.120003	-2.493691	-0.116355
S	-0.366879	2.691765	0.155777
F	4.647457	0.393630	-1.021000
F	4.525728	-1.213278	0.440208
F	4.922006	0.820886	1.087445
F	-4.849081	-0.329076	1.372206
F	-4.646730	-0.341105	-0.785830
F	-4.186265	1.462215	0.339727
O	2.059522	-0.457031	-0.447812
O	0.216042	1.744968	-0.942848
O	-1.951830	0.024019	-0.546528
O	-1.364899	-3.204495	-0.515768
O	2.279064	1.132447	1.160760
O	-2.243964	-0.862999	1.520858
C	1.276028	-3.288830	-0.938984
C	0.250306	-2.826853	1.615139
C	2.705761	0.316979	0.358023
C	4.230242	0.084601	0.217164
C	0.926996	3.931838	0.349678
C	-1.601172	3.653756	-0.743306
C	-2.628934	-0.318805	0.498745
C	-4.109278	0.107198	0.354903
H	2.199582	-2.771646	-0.673523
H	1.281551	-4.340171	-0.638504
H	1.092863	-3.206684	-2.012856
H	1.222672	-2.393629	1.863793
H	-0.548084	-2.346094	2.183007
H	0.244056	-3.911560	1.757232
H	0.568448	4.718862	1.020119
H	1.773534	3.404940	0.796010
H	1.195910	4.337492	-0.629488
H	-1.948821	4.474242	-0.107818
H	-1.165394	4.029591	-1.673096
H	-2.427342	2.972120	-0.955324

100
E = -2286.191642 a.u.

Pd	-0.000035	0.000016	0.661523
S	-0.188682	-2.745320	-0.574486
S	0.188443	2.745381	-0.574447
F	-4.666271	0.219100	1.162266
F	-4.373943	-1.241724	-0.422723
F	-4.961417	0.790422	-0.907307
O	-2.008326	-0.237112	0.645411
O	-0.135006	2.029565	0.781003
O	2.008275	0.237102	0.645743
O	0.134803	-2.029558	0.780980
O	-2.358108	1.276601	-1.017853
O	2.358000	-1.276394	-1.017725
C	-1.664166	-3.706617	-0.168170
C	1.034597	-4.067767	-0.624373
C	-2.706722	0.442901	-0.190956
C	-4.204579	0.059166	-0.086708
C	-1.034800	4.067863	-0.624140
C	1.663977	3.706620	-0.168165
C	2.706662	-0.442856	-0.190682
H	-1.910483	-4.361464	-1.010147
H	-1.489356	-4.284692	0.743412
H	-2.467224	-2.984114	-0.007293
H	0.795546	-4.741344	-1.452944
H	1.993272	-3.574963	-0.796331
H	1.030899	-4.599077	0.331269
H	-0.795788	4.741513	-1.452661
H	-1.993498	3.575098	-0.796080
H	-1.031028	4.599081	0.331553
H	1.910335	4.361397	-1.010186
H	1.489198	4.284766	0.743377
H	2.466998	2.984089	-0.007228
C	4.204546	-0.059257	-0.086340
F	4.961377	-0.790627	-0.906846
F	4.374053	1.241594	-0.422420
F	4.666142	-0.219160	1.162672

1SS
E = -2286.184891 a.u.

Pd	-0.086929	0.097539	-0.325783
S	-0.000286	-2.203388	-0.716790
F	4.583380	0.776774	-0.918898
F	4.313494	-1.161764	0.033729
F	4.936964	0.553703	1.209462
F	-4.817749	-1.129232	1.454207
F	-4.657511	-1.011637	-0.706608
F	-4.584107	0.801354	0.490106
O	1.933933	0.089185	-0.514099
O	-2.100705	0.108623	-0.357424
O	-1.199342	-2.868570	-1.298415
O	2.330259	1.060815	1.496889
O	-2.157921	-1.347621	1.372523
C	1.418560	-2.574797	-1.769438
C	0.480859	-3.015021	0.819968
C	2.668192	0.497355	0.472455
C	4.157791	0.171427	0.202569
C	-2.679126	-0.623604	0.543552
C	-4.217280	-0.492807	0.450670
H	2.319520	-2.122678	-1.353633
H	1.492956	-3.663471	-1.840494
H	1.201568	-2.150197	-2.752212
H	1.410276	-2.571175	1.186895
H	-0.337441	-2.834159	1.519310
H	0.600922	-4.082783	0.614239
S	-0.385515	2.387722	0.014440
O	-0.974776	2.838958	1.304165
C	1.096135	3.354464	-0.333008
H	1.784156	3.167299	0.493077
H	1.532734	3.029315	-1.281217
H	0.806647	4.408563	-0.364914
C	-1.457652	2.913010	-1.338853
H	-2.375844	2.329316	-1.248935
H	-1.657385	3.980961	-1.212237
H	-0.968237	2.707191	-2.295262

(DMSO)AgOOCPh
E = -1120.221193 a.u.

Ag	-0.908686	-0.118953	-0.308732
O	1.029310	0.848690	-0.205448
O	1.244597	-1.365802	-0.031380
C	1.736440	-0.215729	-0.071071
O	-3.028535	-0.643254	-0.343890
S	-4.073885	0.466073	-0.106289
C	-4.153063	0.708833	1.687680
H	-4.976789	1.390189	1.922939
H	-4.283322	-0.256199	2.186068
H	-3.205104	1.159990	1.992540
C	-5.653302	-0.390489	-0.321145
H	-5.718584	-0.679480	-1.372725
H	-5.670366	-1.282966	0.310682
H	-6.473943	0.288608	-0.070891
C	3.222216	-0.036681	0.040336
C	3.798773	1.236687	-0.014942
C	4.042280	-1.158791	0.198243
C	5.180002	1.384972	0.086169
H	3.148871	2.097188	-0.138991
C	5.422820	-1.009871	0.300024
H	3.574232	-2.137587	0.237407
C	5.993957	0.262418	0.243756
H	5.623782	2.376868	0.041355
H	6.055712	-1.885761	0.422412
H	7.072549	0.378943	0.322117

2OS
E = -2180.252629 a.u.

Pd	0.349018	-0.237913	-0.515071
S	0.205836	-2.474271	-0.187615
S	0.103095	2.689090	0.279837
F	4.993636	0.363958	-1.046473
F	4.816309	-1.203481	0.451200
F	5.265614	0.833074	1.053447
O	2.375166	-0.419240	-0.447132
O	0.503135	1.790727	-0.933650
O	-1.639955	-0.010431	-0.655960
O	-1.021565	-3.209226	-0.599792
O	2.639799	1.256578	1.066195
O	-1.842718	-0.804006	1.441335
C	1.621433	-3.246683	-1.000622
C	0.568861	-2.812560	1.544498
C	3.038998	0.378405	0.315093
C	4.557498	0.096377	0.195848
C	1.336953	4.002962	0.237073
C	-1.328335	3.598734	-0.345122
C	-2.328551	-0.356160	0.400362
H	2.534164	-2.715095	-0.726288
H	1.642006	-4.298661	-0.702998
H	1.445678	-3.165138	-2.075786
H	1.535790	-2.371236	1.799970
H	-0.237429	-2.337963	2.106368
H	0.572123	-3.897934	1.681672
H	1.050988	4.782148	0.950257
H	2.276546	3.536872	0.539825
H	1.406890	4.402056	-0.778629
H	-1.626252	4.353394	0.389564
H	-1.084913	4.057796	-1.307346
H	-2.125695	2.862802	-0.471776
C	-3.806754	-0.133872	0.265223
C	-4.621138	-0.355974	1.380907
C	-4.382449	0.288609	-0.938842
C	-5.995301	-0.152091	1.296402
H	-4.154676	-0.691577	2.301985
C	-5.758461	0.489480	-1.021759
C	-6.565889	0.271941	0.095240
H	-6.623786	-0.326445	2.166255
H	-6.202956	0.811022	-1.960477
H	-7.639934	0.428319	0.028629
H	-3.744765	0.442767	-1.803639

(DMSO)AgOOCCF$_3$

E = -1226.162458 a.u.

Ag	-0.876633	-0.081286	-0.161370
O	1.102448	0.704571	-0.358852
O	1.370562	-1.424353	0.315912
C	1.792893	-0.315181	-0.018898
O	-2.973152	-0.590099	0.025470
S	-4.059418	0.503614	-0.074308
C	-4.321355	1.094000	1.617697
H	-5.176971	1.776429	1.632141
H	-4.483406	0.242349	2.284682
H	-3.417987	1.633095	1.914321
C	-5.587968	-0.442907	-0.264426
H	-5.537730	-0.936495	-1.237789
H	-5.651967	-1.191985	0.529766
H	-6.443527	0.238589	-0.237193
C	3.315054	-0.056513	-0.040929
F	3.709689	0.374349	-1.252201
F	3.641379	0.890506	0.859155
F	4.016219	-1.156788	0.250910

3OS

E = -2074.310469 a.u.

Pd	0.033142	-0.274355	-0.557138
S	-0.165170	-2.488955	-0.153650
S	-0.201833	2.650845	0.180488
O	2.053553	-0.476244	-0.516806
O	0.227843	1.746935	-1.016909
O	-1.955071	0.007573	-0.698359
O	-1.403447	-3.218752	-0.545063
O	2.174198	1.069920	1.121911
O	-2.205991	-0.751302	1.407649
C	1.236669	-3.327709	-0.922981
C	0.181892	-2.767416	1.592723
C	2.697034	0.305874	0.304001
C	1.111097	3.884332	0.260733
C	-1.520763	3.659132	-0.534695
C	-2.662100	-0.294701	0.357001
H	2.154747	-2.793442	-0.672946
H	1.241724	-4.363482	-0.572614
H	1.063365	-3.297507	-2.001183
H	1.151747	-2.326440	1.838208
H	-0.621592	-2.259302	2.128799
H	0.168748	-3.846557	1.772355
H	0.825166	4.663563	0.973990
H	1.991212	3.344313	0.616212
H	1.281408	4.301957	-0.735533
H	-1.816712	4.431228	0.182467
H	-1.180480	4.102478	-1.474741
H	-2.356371	2.980207	-0.719906
C	-4.130109	-0.010245	0.210083
C	-4.679702	0.425401	-1.001358
C	-4.960875	-0.185736	1.321739
C	-6.045180	0.685270	-1.095746
H	-4.029806	0.543297	-1.862839
C	-6.324435	0.077030	1.226295
H	-4.514622	-0.532337	2.248759
C	-6.868660	0.514016	0.017595
H	-6.469181	1.016935	-2.040525
H	-6.965352	-0.061261	2.093659
H	-7.934444	0.716594	-0.057718
C	4.193826	0.203972	0.200608
C	4.815648	-0.490314	-0.843478
C	4.979290	0.826632	1.176677
C	6.205305	-0.560087	-0.908516
H	4.201073	-0.960407	-1.604679
C	6.367767	0.749721	1.115289
H	4.479238	1.362969	1.977504
C	6.983215	0.056515	0.071903
H	6.682953	-1.094978	-1.725764
H	6.972082	1.230754	1.880476
H	8.067867	-0.001344	0.021884

TS1

E = -2180.226553 a.u.

Pd	0.007845	0.218260	-0.023392
S	0.040900	-2.511844	-0.702949
S	0.595853	3.220348	-0.153543
F	4.596476	-0.663980	0.339969
F	3.755065	-1.342648	2.226148
F	4.811341	0.550944	2.125751
O	1.856353	-0.359396	0.513933
O	0.733311	1.912119	-0.998474
O	-1.913383	0.638772	-0.412536
O	-1.055638	-3.294533	-1.380245
O	2.481100	1.628641	1.420920
O	-1.689712	-0.800820	1.233071
C	1.583799	-2.811909	-1.613067
C	0.486543	-3.368195	0.832230
C	2.646566	0.455173	1.118547
C	3.978960	-0.254421	1.465584
C	2.157101	4.074548	-0.448191
C	-0.488649	4.235992	-1.186313
C	-2.447266	-0.143639	0.476342
H	2.402192	-2.296904	-1.104333
H	1.759787	-3.890111	-1.676787
H	1.445822	-2.399857	-2.615879
H	1.355134	-2.873431	1.274358
H	-0.374456	-3.280823	1.498104
H	0.690282	-4.419539	0.606959
H	2.086726	5.089451	-0.044937
H	2.913333	3.503722	0.093249
H	2.365840	4.088693	-1.521484
H	-0.567243	5.238260	-0.753382
H	-0.099360	4.277285	-2.207358
H	-1.466878	3.749469	-1.180031
C	-3.921873	-0.225362	0.562664

C	-4.505534	-1.010131	1.563597
C	-4.730487	0.472345	-0.342095
C	-5.890827	-1.092928	1.660068
H	-3.860569	-1.547018	2.252212
C	-6.115638	0.385448	-0.242558
C	-6.696016	-0.395339	0.758220
H	-6.344428	-1.703041	2.436630
H	-6.744598	0.922925	-0.947382
H	-7.778502	-0.462795	0.833651
H	-4.264171	1.068854	-1.120000

DMSO

E = -553.080793 a.u.

S	0.000014	0.237593	-0.436490
O	0.000308	1.518143	0.357459
C	-1.352135	-0.810657	0.195796
H	-2.292139	-0.311150	-0.052101
H	-1.314904	-1.789791	-0.293164
H	-1.268905	-0.913011	1.282570
C	1.351875	-0.811150	0.195595
H	1.314209	-1.790275	-0.293349
H	2.292024	-0.311990	-0.052451
H	1.268773	-0.913462	1.282383

4

E = -1627.144756 a.u.

Pd	0.181687	0.060641	-0.539504
S	0.300481	3.009894	0.266001
F	4.889437	0.614872	-0.788975
F	4.544083	-1.202409	0.353807
F	5.014200	0.649358	1.377158
O	2.156712	-0.239033	-0.397841
O	0.456561	2.049877	-0.962649
O	-1.872506	-0.161839	-0.654525
O	2.484775	1.412349	1.125131
O	-0.538458	-1.842999	-0.261122
C	2.845776	0.490885	0.398625
C	4.349630	0.122086	0.343395
C	1.697356	4.138786	0.103364
C	-1.017208	4.114112	-0.300693
C	-1.734159	-1.417647	-0.432485
H	1.553530	4.976235	0.792935
H	2.579461	3.562456	0.385899
H	1.762054	4.484332	-0.931970
H	-1.144897	4.925225	0.423048
H	-0.774299	4.506659	-1.291873
H	-1.930744	3.516800	-0.351283
C	-2.888190	-2.328558	-0.377370
C	-2.685790	-3.690770	-0.124004
C	-4.181350	-1.830970	-0.577541
C	-3.777689	-4.550705	-0.071120
H	-1.675096	-4.057081	0.027717
C	-5.268765	-2.696414	-0.523194
C	-5.067292	-4.054557	-0.270215
H	-3.624917	-5.608457	0.124959
H	-6.274138	-2.314518	-0.678681
H	-5.918770	-4.729159	-0.228636
H	-4.317331	-0.772086	-0.774854

TS2

E = -1627.120660 a.u.

Pd	-0.592885	0.364746	0.164542
S	0.983044	2.956994	-0.502260
F	-5.180809	0.083402	-0.355811
F	-4.794940	-0.871483	1.558086
F	-4.800272	-2.052036	-0.264479
O	-2.575967	0.579142	0.430365
O	-0.363930	2.431637	0.085520
O	1.371969	0.078328	-0.103342
O	-2.183700	-1.476454	-0.301581
O	0.601755	-1.642300	1.045005
C	-2.958033	-0.602280	0.097480
C	-4.463461	-0.871612	0.256592
C	0.586399	4.700893	-0.744585
C	2.102294	3.103444	0.909335
C	1.549885	-1.085902	0.474038
H	1.490465	5.234729	-1.052524
H	-0.163752	4.750544	-1.537049
H	0.177991	5.113940	0.181466
H	3.006283	3.634600	0.595028
H	1.598408	3.626287	1.726996
H	2.350823	2.081118	1.200918
C	2.909372	-1.682296	0.408640
C	3.163083	-2.855741	1.127457
C	3.926219	-1.098254	-0.355044
C	4.427604	-3.434802	1.089546
H	2.356592	-3.297011	1.705122
C	5.189163	-1.682851	-0.394405
C	5.441359	-2.848997	0.329533
H	4.623419	-4.345528	1.649430
H	5.977157	-1.232652	-0.992808
H	6.428196	-3.304231	0.298021
H	3.713605	-0.197851	-0.923443

INT

E = -1627.134720 a.u.

Pd	-0.798891	0.410991	-0.196018
S	1.355609	2.663033	0.430057
F	-5.265672	-0.288368	-0.999841
F	-4.944922	-1.060741	1.005940
F	-4.483643	-2.295895	-0.720884
O	-2.870488	0.752993	-0.028543
O	-0.129651	2.316877	0.069843
O	0.968890	-0.426018	-0.545376
O	-2.051244	-1.242925	-0.436854
O	1.681606	0.096773	1.522538
C	-3.042338	-0.480375	-0.244725
C	-4.465646	-1.050983	-0.246416
C	1.438793	4.354474	-0.203470
C	1.325003	3.024264	2.197284
C	1.809193	-0.503275	0.447577
H	2.394368	4.800289	0.089296
H	1.378196	4.291007	-1.292360
H	0.598204	4.936404	0.183723
H	2.286766	3.461485	2.483574
H	0.498070	3.705007	2.416636
H	1.191309	2.059668	2.688747
C	2.998438	-1.374334	0.179572
C	3.990174	-1.475599	1.161432
C	3.134889	-2.082536	-1.020002
C	5.110193	-2.272729	0.944860
H	3.859950	-0.926059	2.088596
C	4.256822	-2.878934	-1.234271
C	5.245362	-2.974350	-0.253956
H	5.877468	-2.350353	1.711136
H	4.359446	-3.428973	-2.166291
H	6.119707	-3.598295	-0.423007
H	2.356509	-2.003476	-1.771890

TS3

E = -1627.110975 a.u.

Pd	-0.476647	-0.060887	0.140240
S	-3.395476	-1.010835	-0.272772
F	2.760670	-3.337197	-0.330549
F	3.661159	-1.926102	1.056316
F	3.963026	-1.693476	-1.081164
O	0.845347	-1.547421	0.529852
O	-2.116118	-1.283280	0.584767
O	-1.803893	1.344726	-0.302622
O	1.788534	-0.143819	-0.908530
O	-1.931289	3.465554	-0.994735
C	1.819893	-1.162269	-0.209282
C	3.076808	-2.046690	-0.148717
C	-4.253397	-2.590965	-0.102858
C	-4.464677	0.014267	0.760789
C	-1.303120	2.556180	-0.488478
H	-5.240750	-2.513655	-0.568171
H	-3.652692	-3.338062	-0.626477
H	-4.334694	-2.852895	0.955355
H	-5.449439	0.086082	0.288332

H	-4.535598	-0.419652	1.762206
H	-3.990948	0.997079	0.790656
C	0.118666	2.693995	-0.025472
C	0.523164	2.162985	1.216070
C	1.051399	3.359181	-0.829046
C	1.855326	2.284833	1.628530
H	-0.218505	1.763537	1.907630
C	2.373978	3.463688	-0.417000
C	2.778980	2.921599	0.807647
H	2.157734	1.891286	2.595286
H	3.098717	3.967868	-1.050740
H	3.815521	3.009540	1.122142
H	0.722498	3.782598	-1.773366

5

E = -1627.128350 a.u.

Pd	-0.557875	0.865987	0.973478
S	-2.755642	-0.780509	-0.316647
F	2.098056	-2.969376	1.037957
F	3.240771	-1.630966	-0.238880
F	2.000819	-3.178504	-1.118186
O	0.955469	-0.458052	0.807389
O	-1.948474	-0.679858	1.019551
O	-2.006250	2.250202	1.097142
O	0.029685	-1.416887	-1.031921
O	-1.907039	4.333347	0.212874
C	0.879106	-1.306019	-0.154782
C	2.074699	-2.290589	-0.122141
C	-2.858038	-2.557683	-0.597999
C	-4.448189	-0.450512	0.222728
C	-1.396327	3.298454	0.580956
H	-3.552416	-2.746838	-1.422351
H	-1.848497	-2.869955	-0.872217
H	-3.187839	-3.052631	0.319598
H	-5.132698	-0.606678	-0.617054
H	-4.704650	-1.096933	1.066647
H	-4.468409	0.597509	0.532116
C	0.086917	2.992573	0.471543
C	0.794191	2.569973	1.635750
C	0.792466	3.186256	-0.740818
C	2.189957	2.347317	1.557764
H	0.316695	2.629437	2.612602
C	2.149448	2.944546	-0.790013
C	2.849671	2.517886	0.359190
H	2.730977	2.047588	2.450206
H	2.690047	3.089591	-1.721586
H	3.919076	2.337385	0.297438
H	0.247716	3.540167	-1.610897

TS4

E = -1627.098354 a.u.

Pd	-0.558777	0.525626	-0.304302
S	1.404695	2.860843	0.538886
F	2.785546	-2.631048	-0.838584
F	3.511323	-2.231847	1.163698
F	4.109455	-0.946364	-0.483787
O	0.927916	-0.831202	-0.497280
O	0.795852	2.137106	-0.693363
O	-2.268098	1.647260	-0.126939
O	2.049154	0.103358	1.238258
O	-4.210060	0.537884	0.433435
C	1.906217	-0.696286	0.314856
C	3.082395	-1.659804	0.029783
C	3.190676	2.801965	0.274633
C	1.135736	4.606116	0.135720
C	-3.085246	0.753156	0.138508
H	3.678445	3.439092	1.018995
H	3.484328	1.761804	0.423524
H	3.419329	3.134395	-0.741902
H	1.635276	5.233473	0.880616
H	1.510868	4.816779	-0.869778
H	0.057270	4.778019	0.171561
C	-1.984696	-0.899146	-0.031944
C	-2.431277	-1.572664	-1.192516
C	-1.996220	-1.589891	1.202643
C	-2.886205	-2.883863	-1.117643
H	-2.423917	-1.055732	-2.149381
C	-2.449052	-2.900289	1.272811
C	-2.895179	-3.543170	0.113706
H	-3.229973	-3.395823	-2.012489
H	-2.454788	-3.427020	2.223402
H	-3.252499	-4.568433	0.171813
H	-1.650512	-1.085997	2.101951

6

E = -1627.118117 a.u.

Pd	-0.493290	0.329795	-0.136655
S	1.471727	2.786683	0.745001
F	2.993932	-2.455770	-1.382238
F	3.940635	-2.158547	0.543683
F	4.206039	-0.687554	-1.034649
O	1.055423	-0.874242	-0.647267
O	0.598151	2.223909	-0.401460
O	-2.332455	1.592269	0.215658
O	2.313785	0.017036	1.017119
O	-4.461977	1.044492	-0.576020
C	2.115472	-0.715849	0.051508
C	3.319423	-1.538183	-0.467503
C	3.157256	2.840834	0.091542
C	1.125972	4.565404	0.669896
C	-3.397395	1.285409	-0.186402
H	3.789470	3.394292	0.793016
H	3.495989	1.806301	0.026297
H	3.150767	3.315659	-0.893833
H	1.783715	5.095138	1.366135
H	1.264907	4.928305	-0.352559
H	0.084905	4.703114	0.971887
C	-1.588047	-1.281745	0.055243
C	-1.671286	-2.228688	-0.970400
C	-2.338556	-1.455193	1.224793
C	-2.529344	-3.322136	-0.838112
H	-1.057648	-2.121670	-1.860987
C	-3.189296	-2.558125	1.352499
C	-3.290286	-3.487886	0.319781
H	-2.594454	-4.052310	-1.641819
H	-3.765254	-2.689497	2.266000
H	-3.951271	-4.345080	0.420182
H	-2.250573	-0.749726	2.049774

CO_2

E = -188.504221 a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.167941
O	0.000000	0.000000	-1.167941

***cis*-7**

E = -1991.729184 a.u.

Pd	-0.523341	0.659320	-0.165184
S	2.399362	2.193519	0.486044
F	1.690387	-3.456763	-0.126289
F	2.533208	-3.014003	1.818797
F	3.481580	-2.236908	0.023320
O	0.603331	-1.069908	-0.224846
O	1.230319	1.990798	-0.508636
O	1.777711	-0.407330	1.595258
C	1.470843	-1.196260	0.699369
C	2.284538	-2.510165	0.603540
C	3.808470	1.283394	-0.193223
C	2.994879	3.852702	0.047801
H	4.708455	1.584900	0.352121
H	3.629046	0.221393	-0.032531
H	3.900782	1.505222	-1.260297
H	3.916882	4.064066	0.598248
H	3.162623	3.912863	-1.031463
H	2.225258	4.569403	0.343614
C	-2.092539	-0.533420	0.040926
C	-3.026673	-0.681295	-0.988054
C	-2.234789	-1.268573	1.222081
C	-4.102460	-1.561158	-0.829988
H	-2.930060	-0.111058	-1.908877

C	-3.315238	-2.141197	1.373631
C	-4.250698	-2.289121	0.349420
H	-4.824087	-1.672852	-1.636304
H	-3.417509	-2.712827	2.293633
H	-5.088048	-2.972219	0.468640
H	-1.501802	-1.175093	2.020005
S	-1.956622	2.419509	-0.227830
O	-2.687773	2.707353	-1.502285
C	-3.172159	2.346054	1.107381
H	-3.801437	1.475795	0.914307
H	-2.656669	2.227047	2.064338
H	-3.763775	3.265668	1.076074
C	-1.097525	3.935082	0.256109
H	-0.654568	3.807731	1.247669
H	-0.319960	4.104370	-0.489644

***trans*-7**

E = -1991.737226 a.u.

Pd	0.063106	0.131494	-0.529941
S	-0.085389	-2.174562	-0.801632
F	4.274267	1.570315	0.756274
F	4.942860	-0.103851	-0.462068
F	4.850351	-0.299218	1.695604
O	2.191457	0.249340	-0.517502
O	-1.008773	-2.725395	-1.843164
O	2.317059	-1.037322	1.341597
C	1.538711	-2.909965	-1.080375
C	-0.484383	-2.878106	0.809109
C	2.769460	-0.256434	0.507415
C	4.235753	0.223978	0.634867
H	2.175659	-2.711139	-0.217036
H	1.371891	-3.980067	-1.233468
H	1.953736	-2.458010	-1.983290
H	0.249062	-2.500718	1.527499
H	-1.490606	-2.536027	1.061329
H	-0.459391	-3.968994	0.728416
S	0.039100	2.458788	-0.340584
O	-0.122056	3.041730	1.027977
C	1.544494	3.123014	-1.082259
H	2.389660	2.718096	-0.525259
H	1.608132	2.798131	-2.124348
H	1.498748	4.212723	-0.999958
C	-1.189772	3.210026	-1.429824
H	-2.171236	2.907868	-1.060667
H	-1.071972	4.296050	-1.371655
H	-1.045576	2.843393	-2.449823
C	-1.943556	0.170586	-0.445185
C	-2.546341	0.561543	0.757793
C	-2.746613	-0.149906	-1.544548
C	-3.939691	0.631115	0.855927
H	-1.937678	0.834837	1.617727
C	-4.138362	-0.071479	-1.442132
H	-2.298021	-0.492148	-2.473277
C	-4.737208	0.318321	-0.244296
H	-4.396065	0.937733	1.794449
H	-4.753282	-0.327848	-2.301980
H	-5.820184	0.375169	-0.168022

2OS$_{o\text{-OMe}}$

E = -2294.723556 a.u.

Pd	0.617035	-0.207472	-0.470109
S	0.595030	-2.470861	-0.458968
S	0.118113	2.543591	0.695490
F	5.183078	0.754706	-1.076851
F	5.184144	-1.045750	0.143691
F	5.524663	0.892759	1.060020
O	2.653060	-0.272902	-0.547905
O	0.670934	1.865910	-0.597792
O	-1.383811	-0.041559	-0.463979
O	-0.612416	-3.212334	-0.917918
O	2.879730	1.057195	1.281502
O	-1.423185	-1.192578	1.462022
C	2.001425	-3.042747	-1.437778
C	1.069241	-3.034758	1.185787
C	3.299706	0.394881	0.343753
C	4.825767	0.256177	0.118220
C	1.326398	3.840871	1.024292
C	-1.258140	3.537691	0.083694
C	-1.994250	-0.585346	0.550900
H	2.904324	-2.516719	-1.123357
H	2.078155	-4.125438	-1.305012
H	1.772986	-2.808258	-2.480013
H	2.020094	-2.571769	1.462448
H	0.267791	-2.701446	1.846957
H	1.144814	-4.125816	1.159043
H	0.961628	4.467329	1.844136
H	2.241779	3.321619	1.317039
H	1.487686	4.430307	0.117369
H	-1.651733	4.148220	0.902692
H	-0.919231	4.163442	-0.746938
H	-2.014635	2.825358	-0.258561
C	-3.495237	-0.456927	0.564707
C	-4.163077	-1.264344	1.492134
C	-4.268209	0.376748	-0.277101
C	-5.549256	-1.284452	1.594332
H	-3.544648	-1.887659	2.129593
C	-5.665475	0.356039	-0.175215
C	-6.298118	-0.470286	0.750269
H	-6.036656	-1.930675	2.318684
H	-6.269247	0.990405	-0.814575
H	-7.384060	-0.468257	0.806711
O	-3.620794	1.195338	-1.148248
C	-4.381473	1.877360	-2.124572
H	-4.988186	1.181595	-2.717667
H	-5.036457	2.639117	-1.679138
H	-3.655008	2.365250	-2.777339

TS4$_{o\text{-OMe}}$

E = -1741.582094 a.u.

Pd	0.380158	-0.679040	-0.294807
S	-2.437804	-1.982704	0.369740
F	-1.275983	3.616624	-0.640247
F	-1.753848	3.550649	1.473570
F	-3.197049	2.846163	0.007879
O	-0.347365	1.207996	-0.328848
O	-1.532817	-1.513920	-0.800421
O	1.438035	-2.456848	-0.246329
O	-1.903793	0.720729	1.250636
O	3.543599	-2.367166	0.700823
C	-1.335588	1.453563	0.443299
C	-1.883081	2.894845	0.306946
C	-4.017395	-1.148209	0.098956
C	-2.928913	-3.644076	-0.162049
C	2.510422	-2.057318	0.219706
H	-4.762417	-1.572405	0.779415
H	-3.846934	-0.097242	0.337837
H	-4.319096	-1.273153	-0.944947
H	-3.674975	-4.044295	0.531715
H	-3.322494	-3.606048	-1.181801
H	-2.030061	-4.264838	-0.136148
C	2.269171	-0.053157	0.016970
C	3.040085	0.248393	-1.128714
C	2.618508	0.568741	1.249258
C	4.135089	1.099883	-1.062448
H	2.770384	-0.214133	-2.075702
C	3.719242	1.425831	1.316836
C	4.463171	1.679940	0.164433
H	4.725630	1.313455	-1.948345
H	4.000494	1.903523	2.249165
H	5.317988	2.348667	0.232173
O	1.838332	0.258635	2.300158
C	2.125643	0.834828	3.563202
H	2.054743	1.928480	3.523622
H	1.364928	0.447924	4.241793
H	3.120726	0.539614	3.918801

***trans*-7$_{o\text{-OMe}}$**

E = -2106.213995 a.u.

Pd	-0.148788	-0.018959	-0.381108
S	-0.032502	-2.341920	-0.268856

S	-0.221541	2.304501	-0.488497
O	-2.057620	-0.058407	2.002850
O	1.962314	-0.139824	-0.521250
O	2.322173	1.190520	1.277055
O	-1.229571	-3.232010	-0.197943
O	0.867776	2.968265	-1.266547
F	4.373816	-1.175338	0.462917
F	4.597883	0.345404	-1.076094
F	4.951567	0.848665	1.002188
C	-2.150995	-0.111890	-0.348387
C	-2.837689	-0.136769	0.877279
C	-4.232379	-0.226115	0.907111
H	-4.769167	-0.242839	1.850447
C	-4.948400	-0.306517	-0.289792
C	-4.282973	-0.300180	-1.509761
C	-2.886406	-0.203025	-1.528584
H	-2.368101	-0.204945	-2.486263
C	-2.688345	-0.204104	3.260153
H	-3.398515	0.610839	3.456396
H	-1.889149	-0.167005	4.002927
H	-3.212976	-1.165232	3.336270
C	2.676785	0.471176	0.351675
C	4.178392	0.139482	0.180212
C	1.006448	-2.854267	-1.655775
H	1.273507	-3.905806	-1.515760
H	1.883613	-2.203272	-1.688275
H	0.404234	-2.738799	-2.559920
C	1.062419	-2.744815	1.111768
H	0.563982	-2.408530	2.023251
H	2.017485	-2.233173	0.982139
H	1.183610	-3.832045	1.125209
C	-0.246821	2.949820	1.195806
H	0.702916	2.641146	1.637231
H	-1.084105	2.498336	1.734211
H	-0.331352	4.039214	1.140302
C	-1.789999	2.968901	-1.094335
H	-1.697616	4.058606	-1.071366
H	-2.617419	2.613904	-0.477376
H	-1.918360	2.623946	-2.121807
H	-4.836609	-0.375723	-2.442042
H	-6.032290	-0.381127	-0.255579

20S$_{p\text{-OMe}}$

E = -2294.732031 a.u.

Pd	0.360845	-0.240346	-0.500367
S	0.229359	-2.476219	-0.166232
S	0.088539	2.684226	0.283076
F	4.997451	0.398434	-1.049960
F	4.843343	-1.170181	0.449025
F	5.275058	0.870934	1.048416
O	2.389864	-0.409750	-0.439124
O	0.504226	1.788150	-0.926426
O	-1.628177	-0.019396	-0.631634
O	-0.995051	-3.221410	-0.569142
O	2.644869	1.267426	1.074478
O	-1.808293	-0.816986	1.466435
C	1.644246	-3.241900	-0.987071
C	0.606267	-2.809411	1.563946
C	3.049104	0.393623	0.320815
C	4.569789	0.126841	0.194554
C	1.311976	4.008031	0.245573
C	-1.347288	3.580873	-0.350412
C	-2.309015	-0.370330	0.430612
H	2.555692	-2.704669	-0.719682
H	1.672926	-4.293353	-0.688259
H	1.461010	-3.162922	-2.061179
H	1.570844	-2.359209	1.812684
H	-0.200716	-2.340560	2.129603
H	0.619948	-3.894534	1.702470
H	1.017547	4.785059	0.957664
H	2.253785	3.548581	0.551806
H	1.383246	4.407798	-0.769790
H	-1.653471	4.336188	0.380212
H	-1.103461	4.037991	-1.313480
H	-2.138433	2.838250	-0.476811
C	-3.782753	-0.156703	0.306899
C	-4.595091	-0.396213	1.416893
C	-4.379658	0.277113	-0.886996
C	-5.972956	-0.206011	1.356443
H	-4.126615	-0.739842	2.334133
C	-5.749601	0.469523	-0.961593
C	-6.556683	0.230378	0.160854
H	-6.578041	-0.401553	2.235444
H	-6.226220	0.797528	-1.880735
H	-3.755581	0.447777	-1.758599
O	-7.884905	0.448509	-0.012562
C	-8.749164	0.199125	1.076817
H	-9.755515	0.425331	0.719274
H	-8.705735	-0.851078	1.394483
H	-8.516835	0.845277	1.933982

TS4$_{p\text{-OMe}}$

E = -1741.582072 a.u.

Pd	0.318736	-0.658195	-0.334825
S	-2.477935	-1.957998	0.456052
F	-1.434851	3.583053	-0.928486
F	-2.110671	3.588084	1.130379
F	-3.335343	2.669212	-0.413095
O	-0.460240	1.200809	-0.529470
O	-1.586362	-1.571081	-0.752451
O	1.417394	-2.404008	-0.155476
O	-1.893207	0.811551	1.185185
O	3.646914	-2.233346	0.424021
C	-1.413696	1.483313	0.272955
C	-2.064001	2.860970	0.003881
C	-4.057385	-1.131826	0.157579
C	-2.987558	-3.646207	0.039292
C	2.537635	-1.962951	0.122323
H	-4.791481	-1.500706	0.880825
H	-3.878064	-0.067593	0.317641
H	-4.380711	-1.327281	-0.868858
H	-3.725673	-3.996243	0.767744
H	-3.395984	-3.669897	-0.975052
H	-2.092258	-4.270434	0.091407
C	2.179434	0.037234	-0.040247
C	2.932520	0.422725	-1.173056
C	2.523270	0.618584	1.209285
C	3.998815	1.305097	-1.074711
H	2.680798	0.010599	-2.147742
C	3.578770	1.497986	1.320467
C	4.328038	1.844871	0.178830
H	4.562135	1.570602	-1.962631
H	3.854994	1.942415	2.271984
H	1.949499	0.359916	2.095804
O	5.342257	2.701683	0.394371
C	6.134486	3.114705	-0.706975
H	6.877801	3.799181	-0.296009
H	6.642851	2.262186	-1.173829
H	5.530729	3.639906	-1.457089

***trans*-7$_{p\text{-OMe}}$**

E = -2106.210959 a.u.

Pd	-0.114985	-0.069912	-0.369362
S	0.009725	-2.398140	-0.367470
S	-0.188904	2.257286	-0.460255
O	1.999130	-0.172357	-0.515093
O	2.255735	1.101184	1.337417
O	-1.182043	-3.297808	-0.369460
O	0.932211	2.921871	-1.190201
F	4.422559	-1.152241	0.488763
F	4.634373	0.446931	-0.970663
F	4.903368	0.864601	1.139151
C	-2.115354	-0.132932	-0.287312
C	-2.786599	-0.016792	0.930641
C	-4.185774	-0.050542	1.000669
C	-4.933802	-0.208827	-0.168877
C	-4.269227	-0.333811	-1.396942
C	-2.880966	-0.298706	-1.451450
H	-2.395607	-0.407438	-2.419592
C	2.667948	0.431250	0.397415

C	4.185246	0.165784	0.260321
C	1.073963	-2.821395	-1.766048
H	1.348180	-3.876970	-1.681459
H	1.945638	-2.162421	-1.750172
H	0.483413	-2.660857	-2.671025
C	1.090963	-2.878249	1.000123
H	0.575393	-2.619151	1.927411
H	2.038398	-2.342149	0.920738
H	1.232056	-3.961528	0.940369
C	-0.284793	2.906209	1.220822
H	0.627816	2.569067	1.716513
H	-1.173818	2.499511	1.710661
H	-0.326791	3.997666	1.157736
C	-1.731586	2.915673	-1.135181
H	-1.649230	4.006090	-1.106596
H	-2.584323	2.551923	-0.559245
H	-1.805885	2.571479	-2.168519
H	-4.864527	-0.467017	-2.296307
H	-2.229825	0.091006	1.860441
H	-4.669464	0.037313	1.968331
O	-6.292237	-0.254490	-0.222658
C	-7.007028	-0.162611	0.990023
H	-8.063593	-0.225422	0.722954
H	-6.758061	-0.987542	1.671186
H	-6.820849	0.793013	1.499823

20S$_{m\text{-OMe}}$

E = -2294.729951 a.u.

Pd	0.332600	-0.259809	-0.497282
S	0.225440	-2.495969	-0.164668
S	-0.018608	2.672254	0.238137
F	4.966329	0.430325	-1.029956
F	4.819331	-1.141178	0.466767
F	5.216800	0.905506	1.071182
O	2.363790	-0.402181	-0.456190
O	0.453289	1.766094	-0.942520
O	-1.659395	-0.044619	-0.604707
O	-0.988593	-3.252148	-0.577705
O	2.580353	1.245469	1.094878
O	-1.846535	-0.897931	1.470490
C	1.652020	-3.243928	-0.981720
C	0.599678	-2.836497	1.565074
C	3.005099	0.395483	0.325556
C	4.530460	0.152332	0.209973
C	1.217983	3.984064	0.261656
C	-1.412157	3.577561	-0.471440
C	-2.338380	-0.414175	0.449319
H	2.558707	-2.705422	-0.701188
H	1.682862	-4.298063	-0.692652
H	1.478369	-3.155179	-2.056626
H	1.551164	-2.364706	1.824540
H	-0.221782	-2.394557	2.131439
H	0.640243	-3.922251	1.692825
H	0.900007	4.761649	0.962929
H	2.139768	3.512141	0.608075
H	1.340690	4.386810	-0.747567
H	-1.738280	4.348262	0.234031
H	-1.118382	4.016563	-1.428964
H	-2.208951	2.845513	-0.621921
C	-3.817227	-0.172366	0.339288
C	-4.624756	-0.436258	1.453704
C	-4.385439	0.309683	-0.838120
C	-5.991946	-0.210524	1.372290
H	-4.161138	-0.817638	2.357059
C	-5.764835	0.534532	-0.913589
C	-6.573395	0.275053	0.197352
H	-6.627797	-0.413604	2.230569
H	-7.645017	0.440594	0.159878
H	-3.768864	0.497551	-1.710548
O	-6.219300	1.007097	-2.106961
C	-7.606851	1.217927	-2.250823
H	-7.752785	1.575042	-3.272269
H	-8.175535	0.288628	-2.109651
H	-7.978502	1.976612	-1.547989

TS4$_{m\text{-OMe}}$

E = -1741.575810 a.u.

Pd	0.403807	-0.729648	-0.409829
S	-2.382967	-1.817373	0.634137
F	-1.231244	3.461085	-1.479781
F	-1.868536	3.737883	0.572820
F	-3.146264	2.673425	-0.827333
O	-0.327070	1.110063	-0.815088
O	-1.530457	-1.612071	-0.648216
O	1.453115	-2.465109	-0.105285
O	-1.719617	0.988149	0.970416
O	3.729130	-2.316526	-0.440116
C	-1.247010	1.524651	-0.030116
C	-1.862948	2.878144	-0.456433
C	-3.957971	-1.006660	0.278420
C	-2.929611	-3.535840	0.462235
C	2.598150	-2.011734	-0.270635
H	-4.669897	-1.257878	1.070843
H	-3.755692	0.065399	0.284253
H	-4.322538	-1.334357	-0.699256
H	-3.646926	-3.770882	1.254827
H	-3.373316	-3.686911	-0.525905
H	-2.042043	-4.164132	0.568796
C	2.316141	-0.061996	-0.177161
C	2.938397	0.608021	-1.257321
C	2.653360	0.291564	1.142877
C	3.874794	1.593498	-0.999624
H	2.680999	0.346219	-2.279408
C	3.606143	1.285723	1.395148
C	4.216157	1.934601	0.316096
H	4.356931	2.117904	-1.820639
H	4.959482	2.706810	0.484681
H	2.189059	-0.203685	1.991617
O	3.862167	1.544731	2.700733
C	4.793768	2.562387	3.010028
H	4.472681	3.535684	2.615775
H	4.831967	2.611041	4.099457
H	5.794024	2.324650	2.623892

***trans*-7**$_{m\text{-OMe}}$

E = -2106.212781 a.u.

Pd	-0.144875	-0.074948	-0.436348
S	-0.014873	-2.398777	-0.543612
S	-0.214767	2.255952	-0.499861
O	1.981161	-0.177672	-0.421298
O	2.041313	1.053129	1.475903
O	-1.199428	-3.297167	-0.684014
O	0.964168	2.921251	-1.131976
F	4.289870	-1.166278	0.875199
F	4.641611	0.389591	-0.603402
F	4.703757	0.870954	1.508820
C	-2.144049	-0.145357	-0.420798
C	-2.814537	-0.008545	0.793082
C	-4.217883	-0.060914	0.846237
C	-4.952501	-0.244005	-0.328574
C	-4.270763	-0.384832	-1.539264
C	-2.879875	-0.337190	-1.598972
H	-2.378706	-0.461057	-2.555849
C	2.551063	0.405362	0.568334
C	4.074951	0.143416	0.585803
C	1.148288	-2.745578	-1.882951
H	1.415251	-3.805447	-1.838156
H	2.015942	-2.091921	-1.766463
H	0.624450	-2.531523	-2.817481
C	0.965060	-2.949746	0.872116
H	0.374585	-2.752315	1.769535
H	1.906315	-2.397374	0.898555
H	1.129183	-4.025637	0.760287
C	-0.459228	2.913652	1.162338
H	0.405230	2.581272	1.740017
H	-1.387330	2.509264	1.575388
H	-0.495323	4.004575	1.088067
C	-1.695971	2.904625	-1.308478
H	-1.630317	3.995604	-1.265840
H	-2.592590	2.526942	-0.813453

H	-1.671951	2.567267	-2.346509
H	-4.842743	-0.539268	-2.451728
H	-6.036107	-0.288110	-0.313726
H	-2.281915	0.119313	1.733358
O	-4.761128	0.083351	2.084442
C	-6.165264	-0.009919	2.208080
H	-6.381736	0.105831	3.271763
H	-6.675505	0.785554	1.647965
H	-6.535758	-0.985794	1.867366

20S$_{o\text{-NO2}}$

E = -2384.668854 a.u.

Pd	0.552167	-0.229009	-0.290700
S	0.578825	-2.453071	0.157853
S	0.171694	2.858524	0.133915
F	5.086765	0.585420	-1.250229
F	5.128730	-1.089583	0.137666
F	5.552015	0.920782	0.840689
O	2.573923	-0.322180	-0.491265
O	0.600566	1.758344	-0.891860
O	-1.454787	-0.134747	-0.233775
O	-0.638671	-3.278497	-0.083062
O	2.925244	1.141484	1.207471
O	-1.489527	-1.019495	1.846657
C	1.933271	-3.195799	-0.777217
C	1.153008	-2.688691	1.850083
C	3.283522	0.401367	0.303451
C	4.791448	0.212520	0.004951
C	1.647500	3.887058	0.299014
C	-0.827651	3.971815	-0.874552
C	-2.034724	-0.573640	0.842039
H	2.849907	-2.626752	-0.616685
H	2.021771	-4.236139	-0.452306
H	1.645023	-3.154773	-1.830107
H	2.097118	-2.154715	1.985999
H	0.372748	-2.263914	2.483618
H	1.269471	-3.763012	2.020696
H	1.401412	4.753776	0.920590
H	2.397373	3.264431	0.792575
H	1.993320	4.198226	-0.690855
H	-0.992930	4.895686	-0.311749
H	-0.301319	4.169971	-1.812416
H	-1.786547	3.484049	-1.055321
C	-3.540583	-0.603227	0.720973
C	-4.189663	-1.806140	1.005848
C	-4.324649	0.454467	0.250991
C	-5.562870	-1.942174	0.812021
H	-3.591951	-2.637445	1.365613
C	-5.693748	0.334372	0.033590
C	-6.316381	-0.875605	0.321338
H	-6.045477	-2.888969	1.038578
H	-6.249753	1.188427	-0.337756
H	-7.386545	-0.980801	0.168807
N	-3.724840	1.765568	0.028122
O	-4.143731	2.439537	-0.906832
O	-2.855299	2.127186	0.813746

TS4$_{o\text{-NO2}}$

E = -1831.516431 a.u.

Pd	0.288197	-0.724429	-0.288794
S	-2.491697	-1.899390	0.442344
F	-0.605996	3.805090	0.523255
F	-2.732137	3.444641	0.760553
F	-1.831677	3.328461	-1.208441
O	-0.303140	1.194498	-0.342688
O	-1.620410	-1.469265	-0.778777
O	1.244504	-2.534148	-0.270617
O	-2.101872	0.886234	1.009329
O	3.435084	-2.518391	0.449512
C	-1.354009	1.551205	0.302754
C	-1.639217	3.059951	0.095237
C	-4.116204	-1.198158	0.089663
C	-2.852753	-3.632406	0.062599
C	2.360499	-2.150258	0.115335
H	-4.840222	-1.612831	0.797767
H	-4.015059	-0.122406	0.240753
H	-4.394120	-1.429735	-0.942334
H	-3.570586	-4.020431	0.792052
H	-3.242226	-3.718223	-0.955681
H	-1.909978	-4.178196	0.147229
C	2.264197	-0.205488	0.052664
C	2.893391	0.268605	-1.115774
C	2.615464	0.427735	1.262897
C	3.815488	1.313973	-1.072939
H	2.650487	-0.193853	-2.069276
C	3.526806	1.466184	1.328312
C	4.130133	1.908005	0.146959
H	4.282858	1.665931	-1.988251
H	3.755421	1.918789	2.286445
H	4.848617	2.721668	0.188975
N	2.019453	-0.031385	2.531397
O	1.425929	-1.104030	2.526613
O	2.169578	0.678661	3.514191

***trans*-7$_{o\text{-NO2}}$**

E = -2196.160247 a.u.

Pd	-0.109223	0.032253	-0.329356
S	-0.020480	-2.304213	-0.408814
S	-0.103865	2.367818	-0.345695
O	1.977622	-0.130624	-0.450452
O	2.457896	1.199291	1.322021
O	-1.249969	-3.151368	-0.470187
O	0.985070	3.015004	-1.136069
F	4.334727	-1.312505	0.416646
F	4.628161	0.255805	-1.061532
F	5.048151	0.645884	1.029271
C	-2.108131	-0.056047	-0.392985
C	-2.944888	-0.206233	0.721123
C	-4.337004	-0.298855	0.621825
H	-4.922480	-0.411647	1.527222
C	-4.931382	-0.258513	-0.630441
C	-4.129517	-0.123284	-1.766026
C	-2.744555	-0.019259	-1.643094
H	-2.143685	0.083849	-2.544200
C	2.745811	0.445973	0.404313
C	4.219398	0.022206	0.194292
C	1.074768	-2.747588	-1.774218
H	1.313961	-3.811697	-1.690915
H	1.964273	-2.115850	-1.719850
H	0.520892	-2.559007	-2.696723
C	0.980239	-2.824188	1.000725
H	0.442294	-2.518517	1.900534
H	1.955565	-2.336846	0.949704
H	1.068309	-3.913661	0.954928
C	-0.066813	2.968179	1.355228
H	0.872407	2.601230	1.773324
H	-0.917023	2.553765	1.903399
H	-0.097442	4.061408	1.326250
C	-1.663510	3.106400	-0.887710
H	-1.531671	4.190820	-0.833228
H	-2.487761	2.769460	-0.255761
H	-1.834189	2.801831	-1.921652
H	-4.584315	-0.101519	-2.753522
H	-6.010283	-0.341154	-0.721945
N	-2.383296	-0.289597	2.073086
O	-1.162321	-0.417307	2.198710
O	-3.153087	-0.227979	3.021716

20S$_{p\text{-NO2}}$

E = -2384.674588 a.u.

Pd	0.327893	-0.210074	-0.478618
S	0.181871	-2.442131	-0.124989
S	0.132438	2.750898	0.265902
F	4.975080	0.347466	-1.021982
F	4.779995	-1.202745	0.491517
F	5.248898	0.835542	1.073551
O	2.348996	-0.403282	-0.418836
O	0.487624	1.810265	-0.929999
O	-1.666968	0.007248	-0.620986
O	-1.058522	-3.167311	-0.514553

O	2.626586	1.282756	1.079277
O	-1.888676	-0.752956	1.489951
C	1.581773	-3.233853	-0.944929
C	0.559646	-2.760629	1.607507
C	3.020455	0.394976	0.337166
C	4.536109	0.097005	0.222381
C	1.406743	4.023724	0.183864
C	-1.271037	3.694506	-0.372511
C	-2.356923	-0.336722	0.429766
H	2.501547	-2.707948	-0.683482
H	1.595823	-4.282991	-0.637090
H	1.396435	-3.160885	-2.019089
H	1.532896	-2.324727	1.847645
H	-0.236450	-2.273541	2.173254
H	0.554908	-3.844067	1.758987
H	1.146067	4.829915	0.876431
H	2.333118	3.538883	0.497193
H	1.484187	4.393028	-0.842470
H	-1.540138	4.474456	0.346650
H	-1.017298	4.124752	-1.345269
H	-2.094270	2.984901	-0.481160
C	-3.843530	-0.160525	0.264491
C	-4.668372	-0.383542	1.372725
C	-4.406828	0.217177	-0.960466
C	-6.044397	-0.224115	1.268871
H	-4.208843	-0.685356	2.308178
C	-5.782558	0.378182	-1.079416
C	-6.578956	0.157826	0.041041
H	-6.705536	-0.389059	2.111637
H	-6.246154	0.665900	-2.015866
H	-3.758339	0.371940	-1.816183
N	-8.031437	0.334527	-0.075876
O	-8.475156	0.681737	-1.163746
O	-8.710143	0.126840	0.922464

TS4$_{p\text{-}NO2}$

E = -1831.515168 a.u.

Pd	0.396432	-0.769974	-0.301161
S	-2.451432	-1.907617	0.445653
F	-1.071098	3.567747	-0.900231
F	-1.883156	3.580282	1.109103
F	-3.034716	2.719952	-0.522023
O	-0.263395	1.120426	-0.517058
O	-1.525540	-1.546881	-0.753586
O	1.366440	-2.557951	-0.104961
O	-1.730485	0.817419	1.182981
O	3.613484	-2.464879	0.398331
C	-1.211389	1.461420	0.274274
C	-1.788845	2.865721	-0.019923
C	-3.985699	-1.011588	0.123648
C	-3.013926	-3.570741	0.005706
C	2.507324	-2.132185	0.140180
H	-4.745438	-1.350112	0.834979
H	-3.763094	0.043481	0.289435
H	-4.301551	-1.190670	-0.907883
H	-3.778350	-3.894976	0.718687
H	-3.404254	-3.572045	-1.015855
H	-2.144545	-4.229255	0.071454
C	2.337391	-0.178447	0.041622
C	3.029547	0.306235	-1.091195
C	2.596400	0.405785	1.302564
C	3.950167	1.339060	-0.974542
H	2.843451	-0.133431	-2.067605
C	3.513982	1.438897	1.432185
C	4.174508	1.881986	0.288041
H	4.488969	1.730886	-1.829388
H	3.725040	1.906219	2.387061
H	2.073212	0.043538	2.183460
N	5.153813	2.975354	0.419784
O	5.334115	3.436570	1.538397
O	5.721125	3.347379	-0.598202

***trans*-7$_{p\text{-}NO2}$**

E = -2196.156297 a.u.

Pd	-0.081478	-0.046132	-0.468328
S	0.003570	-2.370545	-0.580148
S	-0.072048	2.290373	-0.530522
O	2.027082	-0.192105	-0.460827
O	2.080340	1.022233	1.444623
O	-1.213589	-3.222815	-0.721364
O	1.145529	2.907816	-1.133450
F	4.318763	-1.215216	0.811427
F	4.695091	0.387178	-0.611140
F	4.738508	0.797189	1.517016
C	-2.080182	-0.080471	-0.453379
C	-2.770088	0.037309	0.763406
C	-4.162709	0.005315	0.804231
C	-4.863449	-0.146162	-0.388353
C	-4.210179	-0.278274	-1.610626
C	-2.818598	-0.245074	-1.634850
H	-2.310417	-0.356452	-2.589777
C	2.596742	0.378045	0.538756
C	4.117696	0.104494	0.563685
C	1.153108	-2.744506	-1.923150
H	1.386783	-3.812391	-1.884069
H	2.041515	-2.119409	-1.804796
H	0.635765	-2.509947	-2.856313
C	0.966596	-2.952567	0.834094
H	0.382966	-2.741576	1.732844
H	1.923611	-2.427910	0.861213
H	1.099681	-4.032320	0.718979
C	-0.339801	2.960252	1.123555
H	0.499234	2.606154	1.725181
H	-1.290022	2.584784	1.513027
H	-0.343439	4.051393	1.045273
C	-1.507919	2.984506	-1.381746
H	-1.404282	4.072862	-1.348519
H	-2.431291	2.650558	-0.904731
H	-1.472010	2.638026	-2.416634
H	-4.792889	-0.406913	-2.516030
H	-2.222794	0.141730	1.698236
H	-4.708559	0.092603	1.737234
N	-6.327064	-0.168382	-0.356090
O	-6.872824	-0.047495	0.734684
O	-6.916454	-0.301685	-1.422131

2OS$_{m\text{-}NO2}$

E = -2384.674712 a.u.

Pd	0.333182	-0.198751	-0.493910
S	0.194632	-2.432878	-0.146135
S	0.119368	2.744051	0.286044
F	4.985750	0.386126	-1.004442
F	4.781183	-1.191736	0.478700
F	5.244358	0.835383	1.101958
O	2.354352	-0.385689	-0.423024
O	0.486365	1.825896	-0.924123
O	-1.663516	0.007108	-0.644023
O	-1.040349	-3.164102	-0.542049
O	2.623930	1.292893	1.085292
O	-1.868843	-0.736552	1.473829
C	1.601648	-3.216796	-0.961526
C	0.567052	-2.749820	1.587807
C	3.021455	0.408668	0.340891
C	4.538042	0.112475	0.232134
C	1.383518	4.028180	0.230995
C	-1.290925	3.684579	-0.341724
C	-2.346505	-0.336049	0.412191
H	2.518527	-2.688938	-0.693751
H	1.617157	-4.266995	-0.657482
H	1.421732	-3.140273	-2.036368
H	1.527623	-2.290157	1.834407
H	-0.243216	-2.282862	2.150731
H	0.587635	-3.833326	1.737291
H	1.111134	4.822356	0.932858
H	2.311083	3.545774	0.544527
H	1.466401	4.412607	-0.789328
H	-1.570943	4.448975	0.389817
H	-1.039013	4.134024	-1.306262
H	-2.105531	2.967400	-0.464975
C	-3.834421	-0.180802	0.250034

C	-4.645311	-0.381302	1.367952
C	-4.414922	0.151944	-0.979447
C	-6.019354	-0.234585	1.231532
H	-4.203162	-0.648568	2.320290
C	-5.798422	0.286687	-1.093521
C	-6.615483	0.096497	0.016601
H	-6.243603	0.537781	-2.052110
H	-7.693399	0.195196	-0.039034
H	-3.770804	0.292186	-1.841537
N	-6.875974	-0.434437	2.407248
O	-6.330961	-0.721427	3.464906
O	-8.084652	-0.298375	2.256314

TS4$_{m\text{-}NO2}$
E = -1831.516544 a.u.

Pd	0.384002	-0.711217	-0.296041
S	-2.437904	-1.947087	0.374066
F	-1.208457	3.599733	-0.726999
F	-1.893814	3.542429	1.328613
F	-3.141075	2.729410	-0.255843
O	-0.318827	1.172378	-0.427751
O	-1.518941	-1.499540	-0.800583
O	1.388267	-2.490517	-0.144679
O	-1.761142	0.761122	1.270682
O	3.514243	-2.366091	0.740558
C	-1.265092	1.456687	0.387232
C	-1.867629	2.864874	0.172009
C	-3.986793	-1.057896	0.107149
C	-2.974625	-3.589474	-0.164777
C	2.469424	-2.053318	0.281633
H	-4.740631	-1.451160	0.796298
H	-3.781371	-0.011250	0.336715
H	-4.300387	-1.179212	-0.933482
H	-3.732909	-3.968203	0.527564
H	-3.366150	-3.534648	-1.184376
H	-2.094782	-4.236782	-0.139485
C	2.309761	-0.101307	0.061578
C	3.024700	0.271613	-1.094630
C	2.561135	0.587933	1.270919
C	3.954620	1.298153	-1.011916
H	2.868170	-0.226353	-2.046053
C	3.493344	1.616943	1.325944
C	4.200841	1.977721	0.178680
H	3.674832	2.145116	2.257427
H	4.938331	2.772511	0.189745
H	2.015877	0.306266	2.167992
N	4.702743	1.684824	-2.217478
O	5.508951	2.599176	-2.109662
O	4.470623	1.065674	-3.246527

***trans*-7$_{m\text{-}NO2}$**
E = -2196.156628 a.u.

Pd	-0.093551	-0.045765	-0.475289
S	0.014510	-2.366082	-0.643211
S	-0.113008	2.289893	-0.475855
O	2.016576	-0.170724	-0.478510
O	2.096165	0.999553	1.454401
O	-1.193348	-3.219489	-0.849108
O	1.083109	2.932211	-1.096187
F	4.302137	-1.241518	0.784763
F	4.686052	0.353376	-0.643653
F	4.756280	0.766274	1.483105
C	-2.094440	-0.108242	-0.449235
C	-2.769779	0.046851	0.764433
C	-4.163162	-0.016761	0.787487
C	-4.918568	-0.239271	-0.358393
C	-4.242404	-0.401538	-1.564119
C	-2.847454	-0.337237	-1.610170
H	-2.347018	-0.478679	-2.565374
C	2.597990	0.372160	0.529494
C	4.116098	0.080920	0.537531
C	1.213512	-2.716044	-1.948664
H	1.450023	-3.783450	-1.915037
H	2.093405	-2.088216	-1.790722
H	0.728437	-2.471116	-2.896412
C	0.924434	-2.969924	0.796287
H	0.309230	-2.771564	1.676732
H	1.880309	-2.446562	0.865731
H	1.062539	-4.047892	0.670331
C	-0.344354	2.927514	1.195854
H	0.511601	2.567463	1.769409
H	-1.281672	2.544302	1.608188
H	-0.353318	4.019787	1.135311
C	-1.575405	2.983794	-1.281865
H	-1.488638	4.072432	-1.221312
H	-2.484702	2.622193	-0.798044
H	-1.551497	2.665154	-2.326064
H	-4.805154	-0.585383	-2.475538
H	-5.999119	-0.284608	-0.291079
H	-2.245435	0.204078	1.701781
N	-4.854924	0.167081	2.069855
O	-4.169141	0.421338	3.053971
O	-6.074732	0.063392	2.077010

20S$_{o\text{-}Me}$
E = -2219.552031 a.u.

Pd	-0.602846	-0.074433	0.423359
S	-0.552213	-2.327903	0.616432
S	-0.285189	2.578936	-1.035638
F	-5.202808	0.864178	0.957632
F	-5.137605	-1.030321	-0.109322
F	-5.545818	0.811205	-1.183276
O	-2.636190	-0.172483	0.470344
O	-0.653133	2.002085	0.368520
O	1.400323	0.067086	0.447378
O	0.669976	-2.990406	1.152754
O	-2.912318	1.139467	-1.365737
O	1.432206	-1.088451	-1.478450
C	-1.960669	-2.840856	1.622860
C	-0.980640	-3.044457	-0.980202
C	-3.306375	0.464150	-0.425841
C	-4.826823	0.280481	-0.192823
C	-1.462305	3.928724	-1.243021
C	1.212318	3.533567	-0.698557
C	2.010045	-0.507494	-0.556108
H	-2.864661	-2.348631	1.259892
H	-2.026655	-3.931206	1.573017
H	-1.744371	-2.524637	2.645954
H	-1.941178	-2.638388	-1.308384
H	-0.179469	-2.742765	-1.657551
H	-1.021962	-4.131197	-0.861329
H	-1.182121	4.511516	-2.125835
H	-2.433940	3.454306	-1.393017
H	-1.464568	4.549798	-0.342963
H	1.503197	4.080865	-1.600694
H	1.038271	4.215042	0.138782
H	1.984343	2.806855	-0.435504
C	3.506551	-0.361560	-0.551578
C	4.124402	-0.412267	-1.808386
C	4.286264	-0.193012	0.613947
C	5.500228	-0.268131	-1.942426
H	3.493137	-0.576535	-2.676523
C	5.672264	-0.067973	0.453668
C	6.278229	-0.092598	-0.799956
H	5.960810	-0.302341	-2.926403
H	6.289877	0.046556	1.342136
H	7.357528	0.013610	-0.880616
C	3.713054	-0.179195	2.007781
H	3.141296	0.734769	2.198740
H	3.023326	-1.013223	2.167187
H	4.518139	-0.244752	2.747523

TS4$_{o\text{-}Me}$
E = -1666.404258 a.u.

Pd	0.358871	-0.685552	-0.308807
S	-2.469604	-1.947141	0.327054
F	-1.242166	3.649279	-0.641560
F	-2.100520	3.510818	1.343123
F	-3.175071	2.698765	-0.363090
O	-0.360502	1.205355	-0.401174

O	-1.567683	-1.473402	-0.844193
O	1.380479	-2.473787	-0.200727
O	-1.805107	0.771192	1.290794
O	3.378955	-2.378702	0.950685
C	-1.314539	1.472191	0.405969
C	-1.947512	2.865068	0.178104
C	-4.027432	-1.060178	0.102554
C	-3.014395	-3.581996	-0.230819
C	2.407621	-2.060764	0.355523
H	-4.768455	-1.466881	0.797830
H	-3.820846	-0.016903	0.346147
H	-4.358853	-1.163447	-0.934538
H	-3.762665	-3.974202	0.465020
H	-3.419776	-3.511258	-1.244149
H	-2.133411	-4.228342	-0.228964
C	2.256499	-0.081736	0.066676
C	3.027724	0.128023	-1.099757
C	2.578712	0.619133	1.263643
C	4.107935	1.003633	-1.096189
H	2.773491	-0.412740	-2.008962
C	3.664554	1.490753	1.241363
C	4.419441	1.683126	0.080102
H	4.697586	1.156477	-1.995788
H	3.928639	2.035026	2.145351
H	5.261081	2.371378	0.100311
C	1.796951	0.402765	2.529049
H	2.134794	1.076099	3.322844
H	0.723919	0.556999	2.373937
H	1.927101	-0.626786	2.887543

***trans*-7$_{o\text{-Me}}$**

E = -2031.035508 a.u.

Pd	-0.088360	0.079081	-0.324943
S	-0.236853	2.387424	-0.061987
S	-0.024690	-2.221473	-0.744201
O	-2.214675	0.160988	-0.337017
O	-2.274945	-1.318920	1.372063
O	0.945014	3.293689	0.050463
O	-1.211240	-2.772174	-1.466143
F	-4.575758	0.915552	1.006289
F	-4.858200	-0.468957	-0.647219
F	-4.938265	-1.191370	1.394688
C	1.917236	0.167785	-0.333797
C	2.661988	0.059322	0.853659
C	4.062044	0.090736	0.767176
C	4.715645	0.255760	-0.451101
C	3.969461	0.399824	-1.619191
C	2.576093	0.352973	-1.554903
H	2.000650	0.461623	-2.473091
C	-2.786917	-0.563862	0.551678
C	-4.317554	-0.345483	0.572526
C	-1.282372	2.935186	-1.431018
H	-1.561302	3.978281	-1.254894
H	-2.153618	2.277218	-1.485202
H	-0.680582	2.857654	-2.339448
C	-1.346903	2.724332	1.325423
H	-0.844010	2.382540	2.232614
H	-2.287006	2.189508	1.180354
H	-1.496954	3.807275	1.365431
C	0.211317	-3.127410	0.798863
H	-0.639632	-2.863382	1.429530
H	1.154257	-2.817853	1.257264
H	0.213732	-4.195038	0.559842
C	1.447843	-2.769695	-1.639181
H	1.364264	-3.854768	-1.749437
H	2.351590	-2.479645	-1.100255
H	1.429581	-2.292024	-2.620566
H	4.464614	0.546406	-2.576327
H	5.801870	0.280482	-0.486019
H	4.646223	-0.004041	1.681480
C	2.007912	-0.023171	2.211880
H	2.610967	-0.607254	2.917019
H	1.895980	0.981641	2.641754
H	1.006503	-0.466208	2.165483

2OS$_{p\text{-Me}}$

E = -2219.556767 a.u.

Pd	-0.588097	-0.255164	0.426170
S	-0.641399	-2.518497	0.400389
S	-0.154463	2.505522	-0.773188
F	-5.122678	0.823417	1.123226
F	-5.176170	-0.941369	-0.147187
F	-5.495161	1.027632	-1.003524
O	-2.623343	-0.265527	0.498958
O	-0.554976	1.817479	0.570386
O	1.416632	-0.180849	0.420656
O	0.548658	-3.296672	0.841801
O	-2.850265	1.201273	-1.223023
O	1.414843	-1.262936	-1.554096
C	-2.056435	-3.051955	1.387672
C	-1.143192	-3.049820	-1.246532
C	-3.269066	0.475715	-0.332504
C	-4.794192	0.352024	-0.091327
C	-1.278134	3.912796	-0.859433
C	1.376783	3.366261	-0.347368
C	2.004332	-0.721717	-0.615686
H	-2.941087	-2.484820	1.093386
H	-2.178385	-4.128343	1.238724
H	-1.804670	-2.844371	2.430277
H	-2.087977	-2.565216	-1.506525
H	-0.341382	-2.723475	-1.911086
H	-1.239115	-4.139544	-1.233567
H	-0.974616	4.560034	-1.687985
H	-2.266701	3.490282	-1.049391
H	-1.258804	4.451771	0.091859
H	1.688714	3.988510	-1.192084
H	1.225513	3.968320	0.552931
H	2.120924	2.589058	-0.158574
C	3.498392	-0.606766	-0.598159
C	4.221507	-1.045283	-1.712263
C	4.190582	-0.078219	0.497010
C	5.608149	-0.949679	-1.731796
H	3.675255	-1.465930	-2.551000
C	5.579163	0.011680	0.470697
C	6.311334	-0.416755	-0.643407
H	6.158372	-1.298744	-2.603550
H	3.632617	0.242884	1.371158
H	6.106889	0.414493	1.333156
C	7.811655	-0.290428	-0.679699
H	8.116977	0.660543	-1.136885
H	8.241720	-0.320398	0.326978
H	8.267974	-1.093674	-1.268150

TS4$_{p\text{-Me}}$

E = -1666.404197 a.u.

Pd	0.356494	-0.695482	-0.311452
S	-2.477196	-1.911483	0.432762
F	-1.291496	3.571995	-0.982098
F	-1.916933	3.639599	1.091937
F	-3.212369	2.741880	-0.405779
O	-0.360713	1.184032	-0.524983
O	-1.561806	-1.540889	-0.764880
O	1.384336	-2.465408	-0.100577
O	-1.833830	0.840702	1.164718
O	3.585003	-2.344388	0.578802
C	-1.320894	1.496057	0.258784
C	-1.925561	2.891873	-0.022424
C	-4.032393	-1.048371	0.114127
C	-3.016505	-3.586967	0.003859
C	2.500674	-2.035096	0.222592
H	-4.784291	-1.400960	0.827072
H	-3.829831	0.011211	0.277742
H	-4.346211	-1.235623	-0.916729
H	-3.770705	-3.923366	0.722175
H	-3.412849	-3.598695	-1.015438
H	-2.135102	-4.229835	0.065022
C	2.251736	-0.062348	0.018155
C	3.012253	0.305811	-1.116429
C	2.552435	0.561512	1.252604
C	4.038633	1.233943	-1.013229

H	2.794150	-0.149101	-2.080111
C	3.577992	1.488083	1.345783
C	4.340843	1.834550	0.217645
H	4.614866	1.504798	-1.895255
H	3.796320	1.959911	2.301456
H	1.973466	0.307108	2.137141
C	5.475900	2.812043	0.336194
H	6.400531	2.294174	0.625202
H	5.669538	3.321654	-0.612915
H	5.275009	3.569102	1.101196

***trans*-7$_{p\text{-Me}}$**
E = -2031.037606 a.u.

Pd	-0.097341	0.111551	-0.381041
S	-0.250646	2.430739	-0.232483
S	-0.011784	-2.198748	-0.706578
O	-2.222361	0.187347	-0.329813
O	-2.223380	-1.249110	1.417071
O	0.924460	3.350288	-0.293531
O	-1.200807	-2.802374	-1.380136
F	-4.524389	0.989491	1.078939
F	-4.878700	-0.439441	-0.522472
F	-4.883394	-1.103369	1.540745
C	1.902303	0.194805	-0.378194
C	2.608936	-0.062589	0.801357
C	4.006386	-0.021997	0.817576
C	4.736299	0.280425	-0.335649
C	4.020966	0.543907	-1.510074
C	2.626610	0.505392	-1.534507
H	2.109572	0.722684	-2.467250
C	-2.763136	-0.512888	0.598205
C	-4.290542	-0.284826	0.671654
C	-1.439745	2.908734	-1.507421
H	-1.711485	3.955944	-1.345788
H	-2.302112	2.240340	-1.446761
H	-0.931991	2.799157	-2.468497
C	-1.212188	2.817288	1.249167
H	-0.606898	2.529512	2.111571
H	-2.149156	2.257296	1.229377
H	-1.385665	3.897453	1.256758
C	0.280128	-3.034448	0.866078
H	-0.574358	-2.781681	1.496538
H	1.212955	-2.663439	1.299156
H	0.328858	-4.109550	0.669629
C	1.453606	-2.740371	-1.616905
H	1.395021	-3.829814	-1.696058
H	2.360273	-2.414086	-1.104154
H	1.402872	-2.289333	-2.609935
H	4.562395	0.789021	-2.422545
H	2.077739	-0.288222	1.725062
H	4.534409	-0.225068	1.748059
C	6.241086	0.355881	-0.310934
H	6.679760	-0.038491	-1.234444
H	6.583016	1.394203	-0.208088
H	6.658276	-0.209526	0.529013

2OS$_{m\text{-Me}}$
E = -2219.556271 a.u.

Pd	-0.557566	-0.204602	0.416906
S	-0.576011	-2.467901	0.447956
S	-0.182578	2.530585	-0.859194
F	-5.100535	0.823436	1.158579
F	-5.141341	-0.977044	-0.061184
F	-5.503928	0.961655	-0.967876
O	-2.590611	-0.238945	0.531790
O	-0.551736	1.871623	0.507844
O	1.445200	-0.100822	0.375906
O	0.630501	-3.214045	0.899890
O	-2.867040	1.166540	-1.233444
O	1.439739	-1.232954	-1.570287
C	-1.975286	-3.001604	1.457452
C	-1.080287	-3.049749	-1.181120
C	-3.260781	0.464301	-0.313216
C	-4.780143	0.323531	-0.046603
C	-1.335955	3.911788	-0.969757
C	1.336410	3.432759	-0.477867
C	2.029568	-0.656569	-0.653737
H	-2.872610	-2.460027	1.153543
H	-2.076504	-4.083712	1.337030
H	-1.722751	-2.761654	2.492873
H	-2.032649	-2.584153	-1.448367
H	-0.286876	-2.731547	-1.859595
H	-1.162432	-4.139809	-1.137928
H	-1.056108	4.541714	-1.819717
H	-2.317702	3.463813	-1.135354
H	-1.316474	4.477417	-0.034087
H	1.624268	4.037920	-1.343287
H	1.185247	4.055952	0.407947
H	2.098819	2.676014	-0.278951
C	3.523760	-0.513654	-0.659115
C	4.234203	-0.962314	-1.775798
C	4.210963	0.059741	0.417108
C	5.619064	-0.828277	-1.810215
H	3.684751	-1.409604	-2.598021
C	5.601366	0.193073	0.397461
C	6.294785	-0.254147	-0.734720
H	6.176779	-1.171764	-2.678130
H	7.378222	-0.154133	-0.771026
H	3.643409	0.390764	1.282375
C	6.341977	0.778570	1.572544
H	5.668522	1.332519	2.234505
H	6.816645	-0.008421	2.173128
H	7.136480	1.460767	1.248446

TS4$_{m\text{-Me}}$
E = -1666.402919 a.u.

Pd	0.369606	-0.714909	-0.307929
S	-2.475343	-1.918114	0.402169
F	-1.267801	3.563021	-0.919514
F	-1.828002	3.622988	1.173673
F	-3.182835	2.758968	-0.291057
O	-0.330592	1.174660	-0.479247
O	-1.553791	-1.530729	-0.786242
O	1.377125	-2.494764	-0.127584
O	-1.812830	0.808593	1.197453
O	3.521030	-2.391500	0.715077
C	-1.291983	1.478000	0.306463
C	-1.883133	2.885080	0.053693
C	-4.022434	-1.036047	0.096036
C	-3.026531	-3.580141	-0.061776
C	2.471063	-2.070124	0.275068
H	-4.779526	-1.397373	0.799004
H	-3.812396	0.018326	0.282164
H	-4.333947	-1.199921	-0.939462
H	-3.785360	-3.924558	0.647818
H	-3.420264	-3.568340	-1.082072
H	-2.150501	-4.231178	-0.010937
C	2.277685	-0.105538	0.035015
C	3.043065	0.212451	-1.108405
C	2.558560	0.556609	1.253118
C	4.065142	1.151798	-1.020881
H	2.838109	-0.284888	-2.053488
C	3.575370	1.500852	1.351363
C	4.323885	1.782356	0.194787
H	4.660522	1.397551	-1.896365
H	5.127391	2.514565	0.252785
H	1.966290	0.317178	2.133938
C	3.875647	2.206440	2.647347
H	4.891307	1.980670	2.994877
H	3.804965	3.294586	2.532219
H	3.177883	1.907235	3.435026

***trans*-7$_{m\text{-Me}}$**
E = -2031.037705 a.u.

Pd	-0.100170	0.104648	-0.375433
S	-0.248216	2.424092	-0.213550
S	-0.021870	-2.203759	-0.712888
O	-2.227622	0.188240	-0.332141
O	-2.248081	-1.252208	1.411268
O	0.929720	3.341311	-0.249104

O	-1.206634	-2.797552	-1.402544
F	-4.537736	0.987542	1.082430
F	-4.882117	-0.406141	-0.551691
F	-4.911387	-1.112746	1.497000
C	1.899865	0.185847	-0.371654
C	2.596042	-0.064824	0.814631
C	3.999067	-0.018284	0.866007
C	4.696012	0.286500	-0.306424
C	4.011597	0.546980	-1.493104
C	2.617851	0.499364	-1.531459
H	2.099514	0.717789	-2.462810
C	-2.778336	-0.512503	0.589334
C	-4.305581	-0.279330	0.651278
C	-1.413613	2.909834	-1.507250
H	-1.686149	3.957044	-1.346846
H	-2.278178	2.243080	-1.463388
H	-0.889445	2.802230	-2.459682
C	-1.234808	2.806999	1.252434
H	-0.647260	2.511016	2.124257
H	-2.174294	2.252576	1.212372
H	-1.401903	3.888147	1.262653
C	0.246374	-3.046187	0.860425
H	-0.612486	-2.788293	1.482853
H	1.177151	-2.682562	1.304116
H	0.289383	-4.121203	0.661943
C	1.450877	-2.751768	-1.606885
H	1.388296	-3.840848	-1.687114
H	2.353043	-2.429414	-1.083749
H	1.413790	-2.300154	-2.600241
H	4.567271	0.798162	-2.394047
H	5.782892	0.331524	-0.287869
H	2.049273	-0.284831	1.732147
C	4.725968	-0.302629	2.155820
H	4.716393	-1.374557	2.394271
H	5.773095	0.011550	2.101232
H	4.261682	0.220064	2.999979

2OS$_{o\text{-}CN}$

E = -2272.452610 a.u.

Pd	0.301929	-0.199670	-0.484603
S	0.191839	-2.409846	0.003821
S	-0.226952	2.864281	-0.252765
F	4.916406	0.439646	-1.033269
F	4.789769	-1.254296	0.326277
F	5.211623	0.732442	1.094364
O	2.324875	-0.372075	-0.530837
O	0.514141	1.771108	-1.086668
O	-1.699186	0.010866	-0.562932
O	-1.045692	-3.180077	-0.303334
O	2.567925	0.979527	1.278252
O	-1.884690	-0.782029	1.538950
C	1.569971	-3.231765	-0.824203
C	0.636724	-2.633401	1.735858
C	2.982235	0.285391	0.362678
C	4.504121	0.059984	0.185628
C	1.111363	3.782023	0.540033
C	-0.710201	4.056085	-1.514413
C	-2.365510	-0.352346	0.490316
H	2.500413	-2.705611	-0.606411
H	1.584428	-4.270171	-0.481938
H	1.358510	-3.192639	-1.895263
H	1.593165	-2.140709	1.928529
H	-0.163904	-2.156181	2.303089
H	0.687657	-3.707619	1.936524
H	0.679412	4.592141	1.135988
H	1.633898	3.065075	1.179379
H	1.794300	4.172655	-0.219458
H	-1.065553	4.965493	-1.019597
H	0.153240	4.265877	-2.151991
H	-1.522510	3.597958	-2.085812
C	-3.861976	-0.244429	0.340738
C	-4.644615	-1.013457	1.203768
C	-4.508926	0.566234	-0.614063
C	-6.033495	-1.006070	1.117026
H	-4.129517	-1.620112	1.941087
C	-5.911513	0.581899	-0.689731
C	-6.669364	-0.208141	0.166366
H	-6.620352	-1.623092	1.792124
H	-6.393142	1.219859	-1.424509
H	-7.753235	-0.195640	0.093221
C	-3.812289	1.447645	-1.503721
N	-3.369349	2.232332	-2.240040

TS4$_{o\text{-}CN}$

E = -1719.294781 a.u.

Pd	0.340310	-0.744514	-0.295757
S	-2.486571	-1.829907	0.509562
F	-0.894902	3.644269	-1.000722
F	-2.003423	3.691833	0.860603
F	-2.921564	2.866711	-0.927968
O	-0.276237	1.154846	-0.552303
O	-1.580128	-1.519545	-0.720927
O	1.299506	-2.544333	-0.124540
O	-1.922881	0.945444	0.993814
O	3.575468	-2.483038	0.235883
C	-1.285240	1.546030	0.134872
C	-1.764035	2.968883	-0.241305
C	-4.059308	-1.035861	0.116272
C	-2.967444	-3.548098	0.203467
C	2.457217	-2.136262	0.061633
H	-4.806690	-1.354943	0.849283
H	-3.883526	0.037430	0.203085
H	-4.359527	-1.307697	-0.899573
H	-3.715750	-3.850972	0.942498
H	-3.355791	-3.651233	-0.813645
H	-2.067129	-4.155982	0.320842
C	2.289550	-0.180869	0.043668
C	2.955452	0.361905	-1.074014
C	2.597478	0.353655	1.327398
C	3.882254	1.389513	-0.932320
H	2.736258	-0.033023	-2.062848
C	3.533917	1.379959	1.468392
C	4.169606	1.892894	0.337457
H	4.378889	1.801302	-1.806368
H	3.758251	1.774015	2.454863
H	4.895439	2.693321	0.451987
C	1.962547	-0.177035	2.497323
N	1.474134	-0.615176	3.458388

***trans*-7$_{o\text{-}CN}$**

E = -2083.937878 a.u.

Pd	-0.067161	0.022233	-0.366362
S	-0.214091	2.324117	-0.002702
S	0.025247	-2.292638	-0.662285
O	-2.165741	0.134028	-0.393609
O	-2.586545	-1.444165	1.179613
O	0.987148	3.210881	0.015875
O	-1.036117	-2.879325	-1.533345
F	-4.516622	1.138522	0.668354
F	-4.825943	-0.220413	-1.001703
F	-5.189860	-0.896140	1.025895
C	1.926859	0.176058	-0.470695
C	2.736493	0.151744	0.683403
C	4.132213	0.301427	0.600597
C	4.733152	0.482507	-0.638135
C	3.943716	0.521348	-1.788763
C	2.558505	0.368811	-1.703755
H	1.964771	0.409638	-2.614885
C	-2.905588	-0.574405	0.383287
C	-4.389891	-0.152269	0.264761
C	-1.412254	2.975829	-1.186118
H	-1.662178	3.997851	-0.887116
H	-2.284002	2.317885	-1.194055
H	-0.920173	2.980990	-2.161524
C	-1.123754	2.533936	1.543793
H	-0.516849	2.092895	2.338124
H	-2.088406	2.028725	1.467225
H	-1.243263	3.609115	1.707591
C	0.008162	-3.088424	0.956485
H	-0.955794	-2.828757	1.398323

H	0.824457	-2.689521	1.565124
H	0.105101	-4.166928	0.799656
C	1.615306	-2.893940	-1.277817
H	1.530210	-3.982006	-1.349759
H	2.422563	-2.595852	-0.605721
H	1.773065	-2.463136	-2.267967
H	4.407955	0.675518	-2.759999
H	5.810546	0.602078	-0.706617
H	4.725944	0.281507	1.510196
C	2.121862	-0.013332	1.966636
N	1.611304	-0.150991	3.005195

20S$_{p\text{-CN}}$

E = -2272.453522 a.u.

Pd	0.326815	-0.206240	-0.484640
S	0.182445	-2.442279	-0.155751
S	0.125887	2.741766	0.299639
F	4.975801	0.359000	-1.012374
F	4.777454	-1.206197	0.485198
F	5.245827	0.826001	1.088437
O	2.348291	-0.397856	-0.420669
O	0.484743	1.820098	-0.909812
O	-1.667185	0.010688	-0.630161
O	-1.055327	-3.166050	-0.556175
O	2.623908	1.275261	1.092447
O	-1.890615	-0.769869	1.472943
C	1.586036	-3.223116	-0.979980
C	0.556018	-2.777940	1.574430
C	3.018467	0.393643	0.343345
C	4.534283	0.096280	0.228617
C	1.392228	4.023331	0.232104
C	-1.285107	3.685076	-0.322503
C	-2.359187	-0.343329	0.416668
H	2.503995	-2.697383	-0.711875
H	1.602105	-4.275054	-0.681962
H	1.402556	-3.140658	-2.053778
H	1.528420	-2.343973	1.821470
H	-0.241896	-2.296672	2.142603
H	0.551445	-3.862841	1.715113
H	1.128427	4.818514	0.936110
H	2.322206	3.539817	0.536689
H	1.465180	4.406967	-0.789294
H	-1.557935	4.452825	0.408299
H	-1.036417	4.130830	-1.289572
H	-2.103618	2.971314	-0.439442
C	-3.844210	-0.164514	0.251863
C	-4.671138	-0.396598	1.355998
C	-4.407577	0.224774	-0.968732
C	-6.045785	-0.234240	1.251403
H	-4.212771	-0.707639	2.289203
C	-5.782423	0.387118	-1.085709
C	-6.607675	0.161598	0.027073
H	-6.691665	-0.411535	2.105874
H	-6.226259	0.684151	-2.031006
H	-3.758649	0.387235	-1.822896
C	-8.024048	0.336805	-0.086778
N	-9.174690	0.483682	-0.178558

TS4$_{p\text{-CN}}$

E = -1719.295070 a.u.

Pd	0.386245	-0.753866	-0.298057
S	-2.463794	-1.888677	0.440667
F	-1.093119	3.572711	-0.946689
F	-1.861797	3.615619	1.079279
F	-3.054279	2.745197	-0.516751
O	-0.273414	1.136595	-0.529862
O	-1.539519	-1.525952	-0.758339
O	1.351200	-2.544187	-0.072273
O	-1.744320	0.843650	1.168747
O	3.560383	-2.450340	0.578531
C	-1.223030	1.481826	0.256913
C	-1.797097	2.886351	-0.043073
C	-3.999252	-0.992499	0.124182
C	-3.028225	-3.551212	-0.000133
C	2.477147	-2.119720	0.235139
H	-4.759064	-1.337039	0.832601
H	-3.778619	0.061839	0.297167
H	-4.314328	-1.165205	-0.908725
H	-3.791420	-3.876181	0.713816
H	-3.420508	-3.551209	-1.020961
H	-2.158905	-4.210084	0.063087
C	2.321758	-0.166594	0.045170
C	3.042346	0.240005	-1.100679
C	2.583956	0.476467	1.276796
C	3.993791	1.246441	-1.023269
H	2.854092	-0.243187	-2.056137
C	3.531181	1.483810	1.364412
C	4.240110	1.868000	0.212042
H	4.546305	1.561285	-1.903007
H	3.730940	1.981653	2.308175
H	2.038163	0.176664	2.167480
C	5.225234	2.902699	0.299553
N	6.028077	3.741516	0.371168

***trans*-7$_{p\text{-CN}}$**

E = -2083.934682 a.u.

Pd	-0.085923	0.102446	-0.379351
S	-0.239339	2.421480	-0.233745
S	-0.026148	-2.211131	-0.706445
O	-2.199037	0.182132	-0.336513
O	-2.191377	-1.240164	1.420125
O	0.949062	3.322640	-0.294830
O	-1.231042	-2.794206	-1.366766
F	-4.499010	0.988267	1.071438
F	-4.852590	-0.451593	-0.520620
F	-4.853172	-1.102699	1.546948
C	1.911870	0.191995	-0.372956
C	2.616076	-0.048666	0.815860
C	4.007604	0.012851	0.849556
C	4.721733	0.320051	-0.317704
C	4.025887	0.575738	-1.509216
C	2.635789	0.511886	-1.530016
H	2.117062	0.721335	-2.462720
C	-2.738068	-0.513144	0.598427
C	-4.265448	-0.288245	0.671967
C	-1.419520	2.904661	-1.513978
H	-1.683751	3.954164	-1.355107
H	-2.287300	2.243261	-1.454834
H	-0.909490	2.789687	-2.473205
C	-1.198460	2.815893	1.246541
H	-0.595896	2.525982	2.110120
H	-2.139320	2.262387	1.226852
H	-1.364739	3.897176	1.252019
C	0.279381	-3.057079	0.857979
H	-0.563259	-2.799910	1.502298
H	1.222196	-2.699538	1.280798
H	0.314498	-4.131490	0.655173
C	1.420634	-2.759033	-1.641894
H	1.351866	-3.847119	-1.729809
H	2.338672	-2.449586	-1.138772
H	1.360773	-2.300552	-2.631115
H	4.578728	0.826169	-2.410122
H	4.545093	-0.172834	1.775186
H	2.080555	-0.275273	1.735947
C	6.151490	0.371153	-0.293575
N	7.314564	0.404575	-0.275114

20S$_{m\text{-CN}}$

E = -2272.453696 a.u.

Pd	0.331899	-0.219831	-0.475642
S	0.201057	-2.455338	-0.143680
S	0.067059	2.749614	0.233089
F	4.979622	0.386174	-0.969375
F	4.785621	-1.177079	0.530773
F	5.216226	0.863933	1.132938
O	2.355761	-0.393062	-0.421695
O	0.483718	1.799824	-0.934414
O	-1.662389	-0.000393	-0.605462
O	-1.030386	-3.188532	-0.546163
O	2.586676	1.253145	1.127468

O	-1.895636	-0.848590	1.470581
C	1.607927	-3.222670	-0.975100
C	0.581871	-2.799748	1.583590
C	3.005008	0.393867	0.365238
C	4.526364	0.120998	0.266542
C	1.361125	4.005155	0.228192
C	-1.282520	3.708772	-0.491165
C	-2.357761	-0.384014	0.428176
H	2.525009	-2.698289	-0.701774
H	1.625856	-4.277607	-0.687949
H	1.425030	-3.129511	-2.048118
H	1.545402	-2.348837	1.835240
H	-0.225524	-2.341104	2.156958
H	0.599628	-3.885854	1.713597
H	1.074739	4.811903	0.909903
H	2.261588	3.504007	0.588636
H	1.500834	4.378158	-0.790165
H	-1.574189	4.503912	0.202092
H	-0.968295	4.120280	-1.454320
H	-2.112972	3.014095	-0.634536
C	-3.841495	-0.191896	0.264813
C	-4.681917	-0.505297	1.337865
C	-4.387477	0.291391	-0.924533
C	-6.059708	-0.333111	1.228060
H	-4.230627	-0.886365	2.248561
C	-5.773434	0.468440	-1.032847
C	-6.612409	0.155111	0.048305
H	-6.707642	-0.580402	2.064337
H	-7.684937	0.294606	-0.047514
H	-3.737037	0.518676	-1.762065
C	-6.334378	0.977677	-2.248370
N	-6.789991	1.400136	-3.232157

TS4$_{m\text{-}CN}$

E = -1719.295146 a.u.

Pd	0.392740	-0.772700	-0.343773
S	-2.440423	-1.797028	0.615614
F	-1.111593	3.429093	-1.519302
F	-1.821542	3.743617	0.504184
F	-3.063954	2.683034	-0.930493
O	-0.278751	1.071208	-0.797133
O	-1.533677	-1.613887	-0.637256
O	1.398864	-2.522939	0.002328
O	-1.730709	0.996501	0.940878
O	3.666922	-2.391894	-0.393737
C	-1.218689	1.514789	-0.048066
C	-1.793482	2.873283	-0.513573
C	-3.984208	-0.964085	0.186377
C	-3.000018	-3.508673	0.431928
C	2.544178	-2.076345	-0.188639
H	-4.733452	-1.198295	0.948946
H	-3.766038	0.104824	0.193289
H	-4.310509	-1.294318	-0.803721
H	-3.751626	-3.728286	1.196582
H	-3.405648	-3.660465	-0.572232
H	-2.125954	-4.147520	0.579218
C	2.324614	-0.140698	-0.046811
C	2.957998	0.570750	-1.091191
C	2.610949	0.210545	1.287075
C	3.847214	1.598801	-0.810140
H	2.743353	0.308087	-2.123546
C	3.516040	1.241916	1.568690
C	4.131533	1.934216	0.513937
H	4.324210	2.147228	-1.617257
H	4.831879	2.732774	0.739928
H	2.138581	-0.321653	2.108181
C	3.813492	1.588771	2.925941
N	4.057606	1.867062	4.028526

***trans*-7$_{m\text{-}CN}$**

E = -2083.934729 a.u.

Pd	-0.095178	0.088472	-0.383118
S	-0.242026	2.408407	-0.252955
S	-0.037599	-2.225043	-0.697791
O	-2.209665	0.173519	-0.345927
O	-2.221463	-1.241430	1.417108
O	0.947436	3.306376	-0.341054
O	-1.238238	-2.805751	-1.368110
F	-4.500444	1.001848	1.083506
F	-4.866800	-0.400971	-0.538027
F	-4.886061	-1.093187	1.515936
C	1.905230	0.180975	-0.361386
C	2.590715	-0.081831	0.827158
C	3.994961	-0.001861	0.875244
C	4.722831	0.346489	-0.270488
C	4.038345	0.617134	-1.450731
C	2.644779	0.536483	-1.497852
H	2.136431	0.763925	-2.432217
C	-2.757759	-0.512843	0.590514
C	-4.282689	-0.269970	0.660227
C	-1.440485	2.890336	-1.516244
H	-1.702410	3.939861	-1.353934
H	-2.306458	2.228266	-1.444665
H	-0.943328	2.774830	-2.482204
C	-1.173913	2.811882	1.241730
H	-0.557357	2.523898	2.096098
H	-2.116384	2.260514	1.240474
H	-1.337996	3.893545	1.245717
C	0.252355	-3.072147	0.868296
H	-0.590285	-2.805348	1.508602
H	1.197170	-2.728088	1.297630
H	0.275043	-4.147050	0.666162
C	1.414694	-2.774692	-1.624176
H	1.350150	-3.863503	-1.705088
H	2.330110	-2.458339	-1.120500
H	1.355237	-2.323034	-2.616624
H	4.592752	0.899488	-2.342083
H	5.805635	0.407355	-0.225370
H	2.055389	-0.338820	1.738388
C	4.675523	-0.288292	2.102187
N	5.219753	-0.534061	3.101029

TS5

E = -1627.098219 a.u.

Pd	-0.337241	0.399982	0.849277
S	-1.951012	-2.043487	0.213575
F	-3.312755	3.372948	-1.180210
F	-3.190171	4.063786	0.877992
F	-4.873030	2.854250	0.234480
O	-1.502872	1.929499	0.344356
O	-1.190050	-0.850155	-0.492744
O	0.842878	-1.011289	1.590181
O	-3.371386	0.757578	0.859059
O	1.783537	-2.530566	0.229122
C	-2.776069	1.756469	0.481084
C	-3.557583	3.035527	0.096211
C	-3.530786	-2.040274	-0.651191
C	-1.154089	-3.486089	-0.507698
C	1.849283	-1.484484	0.864851
H	-4.096668	-2.925538	-0.344800
H	-4.041929	-1.128261	-0.334657
H	-3.357002	-2.038281	-1.730548
H	-1.632909	-4.385208	-0.106903
H	-1.231947	-3.447648	-1.597633
H	-0.103683	-3.422809	-0.193560
C	3.116154	-0.683684	0.897653
C	4.164344	-1.036677	0.038749
C	3.274705	0.403142	1.766888
C	5.344009	-0.300313	0.033902
H	4.029148	-1.889882	-0.618826
C	4.459413	1.136633	1.765675
C	5.492655	0.788579	0.896217
H	6.151110	-0.573183	-0.641214
H	4.578534	1.975403	2.446645
H	6.416435	1.361793	0.893136
H	2.475692	0.649473	2.460226

TS6

E = -1627.089573 a.u.

Pd	-0.463093	-1.124493	0.819947

S	-3.327652	-0.209885	1.709015
F	-0.352435	3.498674	2.471629
F	1.653456	2.752928	2.099808
F	0.791656	2.589818	4.081431
O	0.396524	0.587501	1.412700
O	1.025722	-2.365535	0.899977
O	-2.285404	-0.209550	0.535870
O	-1.085811	0.804133	3.117735
O	1.788901	-3.307561	-0.973498
C	-4.815222	-0.786684	0.856812
C	-3.779517	1.526446	1.901111
C	-0.133770	1.159313	2.432650
C	0.526526	2.519804	2.772243
C	1.893824	-2.441631	-0.122302
H	-5.670013	-0.707592	1.535542
H	-4.977288	-0.196036	-0.048975
H	-4.651444	-1.834583	0.594267
H	-4.644726	1.588341	2.568341
H	-2.920587	2.019353	2.357995
H	-4.005331	1.951571	0.919381
C	3.024788	-1.465343	-0.114488
C	3.341910	-0.706956	1.017412
C	3.807928	-1.348625	-1.269759
C	4.427369	0.165542	0.990273
H	2.739439	-0.812980	1.912861
C	4.885229	-0.470086	-1.297702
C	5.196062	0.288312	-0.166676
H	4.671945	0.751841	1.872136
H	5.487189	-0.377344	-2.198167
H	6.040450	0.973135	-0.187494
H	3.556238	-1.960649	-2.130741

8

E = -1627.118934 a.u.

Pd	0.504225	-0.584467	-0.060692
S	-0.027835	2.525054	-0.379019
F	-4.254474	0.699265	0.350049
F	-4.025320	-1.451637	0.545494
F	-4.417495	-0.581090	-1.399897
O	-1.492510	-0.886488	0.251022
O	0.748113	-2.514064	-0.476910
O	0.333734	1.371591	0.613170
O	-1.942222	0.647884	-1.350745
O	2.597547	-3.737960	-0.011573
C	1.072493	3.841914	0.199160
C	-1.575955	3.216184	0.245775
C	-2.251012	-0.192295	-0.504908
C	-3.760842	-0.412631	-0.246592
C	2.012820	-2.688185	-0.159779
H	0.837582	4.767872	-0.334814
H	0.956737	3.972465	1.278629
H	2.093428	3.529797	-0.027875
H	-1.756821	4.167450	-0.264578
H	-2.365928	2.507914	-0.002601
H	-1.495972	3.357961	1.327122
C	2.661977	-1.326917	0.020053
C	3.418518	-1.011640	1.175204
C	2.594347	-0.394881	-1.051181
C	4.080648	0.195322	1.255541
H	3.483480	-1.746983	1.971686
C	3.307657	0.823965	-0.955618
C	4.029927	1.113875	0.185035
H	4.665893	0.434591	2.139389
H	3.311780	1.504819	-1.803164
H	4.592850	2.041677	0.252443
H	2.190824	-0.703721	-2.013827

TS7

E = -1627.093483 a.u.

Pd	0.245555	-0.751982	0.185698
S	-0.109529	2.310022	-0.149435
F	-4.553397	0.602507	0.295343
F	-4.366634	-1.558848	0.392560
F	-4.602825	-0.581688	-1.527434
O	-1.799800	-1.072861	0.251591
O	0.769362	-2.644601	-0.365246
O	-0.003410	1.161392	0.909404
O	-2.130327	0.640357	-1.191339
O	2.990699	-3.175891	-0.036658
C	1.103375	3.493714	0.488320
C	-1.612686	3.193988	0.315652
C	-2.499818	-0.279908	-0.455929
C	-4.027681	-0.481774	-0.320331
C	1.987226	-2.559050	-0.148232
H	1.050925	4.415884	-0.099070
H	0.909645	3.692373	1.546073
H	2.087523	3.034466	0.369626
H	-1.654414	4.131117	-0.248246
H	-2.444521	2.548247	0.031264
H	-1.602356	3.380867	1.393002
C	2.297049	-0.608057	0.031706
C	3.044972	-0.293168	1.187470
C	2.756191	-0.143087	-1.220277
C	4.205553	0.464214	1.093624
H	2.708933	-0.651771	2.157322
C	3.922377	0.614073	-1.313589
C	4.644654	0.914706	-0.157048
H	4.776393	0.702575	1.987579
H	4.272420	0.962030	-2.282137
H	5.560386	1.496771	-0.228651
H	2.196280	-0.385656	-2.121283

9

E = -1627.114227 a.u.

Pd	0.347261	-0.495236	0.022540
S	-0.280763	2.507248	-0.118720
F	-4.594515	0.262799	0.517307
F	-4.192329	-1.858751	0.291123
F	-4.646836	-0.655066	-1.452759
O	-1.690148	-1.095430	0.074714
O	0.829667	-2.525379	-0.750208
O	-0.041149	1.330506	0.890436
O	-2.289958	0.766073	-1.064006
O	2.637253	-3.897644	-0.196650
C	0.908017	3.737885	0.474635
C	-1.796408	3.275387	0.485786
C	-2.512849	-0.288217	-0.455977
C	-4.003686	-0.661061	-0.273944
C	1.752643	-3.196111	-0.459848
H	0.770656	4.668980	-0.084423
H	0.773282	3.902235	1.547285
H	1.904182	3.332238	0.282888
H	-1.936445	4.227593	-0.035302
H	-2.600329	2.582704	0.231220
H	-1.719775	3.423339	1.566517
C	2.263456	-0.036890	-0.016220
C	2.954855	0.292611	1.156627
C	2.958538	-0.065596	-1.233253
C	4.324571	0.564852	1.114366
H	2.424063	0.340449	2.105000
C	4.328344	0.214724	-1.272011
C	5.013380	0.526532	-0.098718
H	4.853335	0.809435	2.033320
H	4.856223	0.189365	-2.223003
H	6.078734	0.740954	-0.129059
H	2.436037	-0.297576	-2.160696

TS8

E = -2180.226482 a.u.

Pd	0.417694	-0.428983	0.317583
S	0.067367	-2.323012	-0.831915
S	0.331555	2.964762	-0.666158
F	4.895763	0.368906	0.954554
F	4.211151	0.157470	3.005202
F	4.037580	2.072202	1.992263
O	2.457453	-0.662729	0.573101
O	0.999127	1.679817	-1.142151
O	-1.494564	0.085360	0.291803
O	-1.111531	-2.495894	-1.721806
O	1.560549	1.001364	1.725553

O	-2.029879	-1.845051	1.315680
C	1.563670	-2.529655	-1.824602
C	0.194779	-3.729166	0.289442
C	2.551110	0.350610	1.344111
C	3.955443	0.745150	1.825920
C	1.674027	4.103749	-0.220986
C	-0.214685	3.825354	-2.170822
C	-2.336832	-0.744399	0.855890
H	2.444913	-2.420371	-1.188466
H	1.520148	-3.513238	-2.301097
H	1.547833	-1.740817	-2.580139
H	1.120309	-3.639479	0.864673
H	-0.676399	-3.656596	0.942145
H	0.177519	-4.643017	-0.312148
H	1.253844	5.077435	0.050781
H	2.178560	3.664683	0.642432
H	2.376142	4.198633	-1.055226
H	-0.624039	4.806291	-1.908759
H	0.623854	3.923723	-2.867014
H	-0.995367	3.207174	-2.620920
C	-3.748037	-0.242518	0.905816
C	-4.718779	-1.051869	1.505205
C	-4.113806	0.998727	0.373956
C	-6.041643	-0.625062	1.572751
H	-4.413242	-2.011861	1.909297
C	-5.438209	1.423454	0.441701
C	-6.403347	0.613283	1.040904
H	-6.792285	-1.258245	2.039136
H	-5.719675	2.388174	0.026604
H	-7.437055	0.946781	1.092834
H	-3.354562	1.619347	-0.090329

INT′

E = -1627.136511 a.u.

Pd	-0.613065	0.166878	-0.179012
S	-0.028229	2.338371	-0.264480
F	-4.720206	-1.618163	-1.028165
F	-4.965457	-0.813712	0.976198
F	-4.114699	-2.792806	0.697430
O	-2.675576	0.330870	0.095414
O	1.232924	-0.455620	-0.501698
O	1.188061	2.800862	-0.979580
O	-1.766336	-1.671008	-0.033832
O	1.910205	0.674975	1.317652
C	-1.463982	3.162199	-0.992543
C	-0.061948	3.001093	1.411322
C	-2.776551	-0.939944	0.093927
C	-4.176624	-1.560315	0.197458
C	2.133469	-0.093040	0.380055
H	-2.373943	2.850259	-0.474266
H	-1.304425	4.241802	-0.919982
H	-1.504262	2.860111	-2.041587
H	-1.015204	2.739132	1.878919
H	0.770448	2.522638	1.929040
H	0.069200	4.085116	1.343316
C	3.481452	-0.700878	0.157747
C	4.515585	-0.361746	1.036850
C	3.725551	-1.593010	-0.892617
C	5.783483	-0.908935	0.866794
H	4.303703	0.331765	1.844513
C	4.995282	-2.139205	-1.059259
C	6.024752	-1.798425	-0.181241
H	6.584869	-0.642586	1.551284
H	5.182498	-2.832371	-1.875388
H	7.015503	-2.226430	-0.313555
H	2.917772	-1.851427	-1.569430

TS3′

E = -1627.118586 a.u.

Pd	-0.728743	-0.382510	-0.035724
S	-1.203649	-2.589903	-0.071464
F	3.416566	0.866606	-1.655574
F	3.910635	-0.383735	0.053285
F	3.636112	1.754199	0.314003
O	1.233827	-0.659076	-0.553235
O	-2.597939	-0.095424	0.586301
O	-1.765884	-3.168847	-1.324600
O	1.006695	1.285672	0.492970
O	-3.987557	1.604861	0.981617
C	0.287606	-3.500764	0.370856
C	-2.300501	-2.967804	1.304477
C	1.698738	0.448107	-0.092782
C	3.197654	0.682256	-0.343880
C	-3.010043	1.155615	0.419586
H	0.640515	-3.166162	1.349648
H	0.042779	-4.566820	0.369018
H	1.036400	-3.271649	-0.390001
H	-1.805160	-2.708389	2.243658
H	-3.187983	-2.345011	1.174842
H	-2.543711	-4.032663	1.250343
C	-2.146419	1.968622	-0.502086
C	-1.710193	1.444698	-1.735764
C	-1.785590	3.271895	-0.137506
C	-0.899814	2.217270	-2.574953
H	-2.085171	0.483470	-2.085579
C	-0.970690	4.026423	-0.971613
C	-0.521251	3.498282	-2.186763
H	-0.583997	1.817773	-3.534912
H	-0.680112	5.031512	-0.677996
H	0.113099	4.096711	-2.835321
H	-2.149372	3.672211	0.804027

5′

E = -1627.127487 a.u.

Pd	-0.774130	-0.176772	-0.334903
S	-0.880565	-2.471378	-0.179449
F	3.562130	1.373997	-0.090963
F	3.914957	-0.616449	-0.893306
F	4.188079	-0.233723	1.223986
O	1.229903	-0.066540	-0.633214
O	-2.749378	-0.109142	0.016338
O	-1.787349	-3.155652	-1.144566
O	1.596585	-0.756251	1.491705
O	-3.891418	1.584407	0.981886
C	0.725093	-3.288475	-0.227536
C	-1.410616	-2.813848	1.507733
C	1.948406	-0.300015	0.410631
C	3.433700	0.060045	0.164099
C	-2.914967	1.135516	0.425510
H	1.344579	-2.913233	0.589035
H	0.534440	-4.362083	-0.143139
H	1.175914	-3.059437	-1.195396
H	-0.685576	-2.369790	2.195401
H	-2.390291	-2.343345	1.620103
H	-1.485715	-3.898096	1.632977
C	-1.666282	1.944775	0.131307
C	-1.158743	1.987799	-1.196112
C	-1.028736	2.695153	1.143430
C	-0.027433	2.776399	-1.485413
H	-1.734107	1.549608	-2.010390
C	0.089390	3.449302	0.838644
C	0.593873	3.487609	-0.475120
H	0.344631	2.823219	-2.504394
H	0.582803	4.022193	1.619121
H	1.471569	4.088388	-0.695091
H	-1.440675	2.675668	2.147931

TS4′

E = -1627.095998 a.u.

Pd	-0.291523	-0.778105	-0.120190
S	1.613905	-2.192378	-0.244920
F	2.818571	3.196684	1.133270
F	1.325777	3.546766	-0.397851
F	3.155322	2.476975	-0.887514
O	0.721662	0.939304	-0.486490
O	-1.648064	-2.282983	0.231678
O	1.413282	-3.477834	-0.988159
O	1.936279	0.694141	1.409439
O	-3.814832	-1.667692	0.740983
C	3.087270	-1.378466	-0.900177

C	2.179206	-2.556432	1.431060
C	1.568105	1.301462	0.409648
C	2.218661	2.663599	0.066546
C	-2.679760	-1.628809	0.425108
H	3.363569	-0.547862	-0.248611
H	3.877348	-2.133337	-0.947856
H	2.846509	-1.019954	-1.903008
H	2.350100	-1.606727	1.944027
H	1.381122	-3.122495	1.917536
H	3.084867	-3.166800	1.367434
C	-2.064224	0.256910	-0.017746
C	-2.670132	0.579286	-1.251430
C	-2.291288	1.091460	1.098615
C	-3.498255	1.691665	-1.358185
H	-2.498063	-0.051827	-2.120556
C	-3.118326	2.201228	0.986382
C	-3.721740	2.497395	-0.240084
H	-3.968233	1.933403	-2.307711
H	-3.294433	2.840159	1.847667
H	-4.370309	3.365840	-0.323784
H	-1.822155	0.859215	2.051812

6′

E = -1627.113643 a.u.

Pd	0.400791	0.611943	-0.109482
S	-1.263288	2.414987	-0.059046
F	-3.257150	-2.936276	0.893363
F	-2.395860	-3.010333	-1.093190
F	-3.811421	-1.439488	-0.580123
O	-1.017713	-0.750061	-0.638757
O	2.062913	2.033929	0.365337
O	-0.826738	3.840819	-0.248370
O	-1.528121	-1.007520	1.555341
O	4.350635	1.698907	0.694147
C	-2.575458	2.052682	-1.250568
C	-2.215907	2.297054	1.474471
C	-1.657766	-1.247161	0.363043
C	-2.787582	-2.193954	-0.109201
C	3.212917	1.835891	0.525518
H	-2.944211	1.035672	-1.101280
H	-3.368157	2.795956	-1.126706
H	-2.131774	2.141371	-2.245054
H	-2.513021	1.257120	1.634205
H	-1.549359	2.612805	2.280777
H	-3.074192	2.972296	1.412971
C	1.733170	-0.849375	-0.135012
C	2.496111	-1.066653	-1.285348
C	1.950896	-1.612930	1.014814
C	3.504109	-2.035695	-1.272111
H	2.304850	-0.500067	-2.194747
C	2.962127	-2.578209	1.016934
C	3.738679	-2.788105	-0.122161
H	4.098314	-2.204239	-2.167340
H	3.132917	-3.172387	1.911744
H	4.519758	-3.544010	-0.116816
H	1.328789	-1.472646	1.895340

***cis*-7′**

E = -1991.731355 a.u.

Pd	0.476172	-0.231459	0.087852
S	-0.177122	-2.600396	0.212929
F	-4.452889	1.067393	-1.106698
F	-3.779038	1.617650	0.878101
F	-4.244627	-0.458717	0.425292
O	-1.503754	0.150026	0.531575
O	0.751112	-3.714448	-0.203353
O	-1.936866	0.385904	-1.680243
C	-0.642697	-2.850420	1.940731
C	-1.776865	-2.904366	-0.573981
C	-2.239086	0.401407	-0.495553
C	-3.702084	0.680394	-0.075141
H	-1.338257	-2.058456	2.232016
H	-1.090131	-3.842856	2.047909
H	0.275948	-2.785927	2.528828
H	-2.548132	-2.286201	-0.111898
H	-1.677921	-2.652691	-1.631636
H	-1.992292	-3.969856	-0.451582
C	0.827739	1.737407	0.182608
C	1.414984	2.280212	1.329129
C	0.439921	2.571481	-0.868818
C	1.623447	3.660300	1.416499
H	1.714602	1.639493	2.156000
C	0.655640	3.949721	-0.773402
C	1.249359	4.495229	0.364197
H	2.078201	4.078071	2.312006
H	0.348108	4.596602	-1.592156
H	1.412377	5.567754	0.434331
H	-0.051377	2.156569	-1.744619
S	2.716071	-0.588407	-0.215469
C	2.944492	-1.837835	-1.497514
H	2.430281	-2.743583	-1.158765
H	2.505356	-1.476593	-2.432378
H	4.019031	-2.013625	-1.603972
C	3.592494	0.787946	-0.988580
H	3.581050	1.620114	-0.283352
H	4.616478	0.453878	-1.179373
H	3.080931	1.077324	-1.909899
O	3.481171	-1.002158	1.003632

10$_{o\text{-OMe}}$

E = -1862.647428 a.u.

C	3.875728	-0.794524	-0.246818
C	2.773439	-1.552381	0.178234
C	2.849262	-2.203799	1.418757
C	3.986117	-2.102879	2.214853
C	5.073065	-1.345115	1.780860
C	5.011732	-0.692148	0.548428
C	1.561913	-1.747759	-0.637420
C	1.326663	-1.301660	-1.936342
Pd	0.049930	-0.128250	-0.693712
O	-1.450698	-1.755016	-0.981918
S	-2.259257	-2.435523	0.148375
C	-3.982343	-1.943582	-0.104370
C	1.356575	1.351907	-0.629136
C	1.756246	2.024719	-1.777793
C	2.629038	3.118942	-1.701848
C	3.090274	3.537357	-0.460312
C	2.683653	2.881863	0.704823
C	1.811725	1.792206	0.625720
O	-1.367933	1.342337	-0.272325
C	-2.176341	1.082322	0.675220
O	-2.242758	0.087508	1.400277
C	-3.268452	2.161153	0.874800
F	-4.426288	1.706367	0.332364
F	-2.984228	3.331126	0.296432
F	-3.496127	2.385309	2.176426
C	-2.423032	-4.134770	-0.471301
H	2.052819	-0.686434	-2.460038
H	3.045724	3.229771	1.667228
H	1.376899	1.711571	-2.748284
H	0.596986	-1.817101	-2.556581
H	0.914005	-2.544270	-0.272141
H	3.766214	4.385522	-0.383322
H	2.930656	3.636873	-2.608776
H	-1.426401	-4.582860	-0.460992
H	-3.085643	-4.702421	0.189662
H	-2.810833	-4.121838	-1.494049
H	-4.617183	-2.552160	0.547420
H	-4.059866	-0.895781	0.184094
H	-4.248596	-2.083259	-1.156096
H	2.000711	-2.792744	1.761037
H	4.023874	-2.616753	3.172013
H	5.965046	-1.265446	2.397126
H	5.854475	-0.098345	0.204391
H	3.842384	-0.272068	-1.197713
O	1.351903	1.100938	1.705746
C	1.730489	1.540700	2.991812
H	1.407082	2.574289	3.175137
H	1.224527	0.876531	3.694548
H	2.816220	1.467141	3.140487

TS8$_{o\text{-}OMe}$

E = -1862.628367 a.u.

C	-3.069448	-1.214494	1.365438
C	-3.125776	-0.847721	0.009605
C	-4.178295	-0.020032	-0.413727
C	-5.152198	0.415917	0.480364
C	-5.089503	0.038614	1.821339
C	-4.042469	-0.775312	2.257437
C	-2.136626	-1.303088	-0.987878
C	-1.338143	-2.482013	-0.859615
Pd	-0.272503	-0.466298	-0.591943
O	-1.070052	1.503744	-0.972299
S	-0.264661	2.696381	-0.390066
C	0.814197	3.259292	-1.727971
C	0.630803	-2.310947	-0.436085
C	1.462462	-2.648377	-1.511505
C	2.615970	-3.406407	-1.322626
C	2.933356	-3.855875	-0.042606
C	2.100075	-3.565930	1.036962
C	0.940484	-2.809212	0.846944
O	1.555549	0.566140	-0.277671
C	2.165624	0.556028	0.852481
O	1.878201	0.004012	1.903505
C	3.429105	1.455788	0.809712
F	4.215189	1.283547	1.874988
F	3.057338	2.764073	0.787898
F	4.171094	1.242842	-0.291454
C	-1.490528	4.025751	-0.459255
H	-2.359138	-0.985598	-2.008778
H	-1.127603	-3.021397	-1.777429
H	2.360566	-3.926749	2.026541
H	1.209448	-2.290611	-2.507368
H	-1.504280	-3.120087	0.004139
H	3.831343	-4.445380	0.123775
H	3.260036	-3.638622	-2.166347
H	1.276814	4.208193	-1.440106
H	1.578775	2.487920	-1.834650
H	0.230649	3.364414	-2.647270
H	-1.017934	4.969657	-0.170454
H	-1.911942	4.089238	-1.466381
H	-2.276093	3.770179	0.255634
H	-4.230121	0.278203	-1.458527
H	-5.963070	1.049096	0.128162
H	-5.849021	0.376358	2.521915
H	-3.982097	-1.068131	3.302897
H	-2.245605	-1.826765	1.720010
O	0.049458	-2.540240	1.834308
C	0.486445	-2.659735	3.178200
H	0.649887	-3.709093	3.458443
H	1.395325	-2.071452	3.334816
H	-0.319970	-2.250570	3.789597

11$_{o\text{-}OMe}$

E = -1862.647351 a.u.

C	3.955125	-0.985782	0.206256
C	2.723421	-1.659578	0.239129
C	2.381896	-2.380657	1.395941
C	3.235782	-2.415637	2.493790
C	4.454321	-1.737851	2.448717
C	4.811669	-1.027379	1.301246
C	1.794396	-1.690109	-0.898489
C	1.869422	-0.980198	-2.081950
Pd	0.255474	0.027495	-0.953486
C	1.518200	1.577868	-0.838206
C	1.579899	2.449670	-1.942161
C	2.366401	3.604029	-1.885414
C	3.104079	3.886082	-0.732538
C	3.065421	3.025505	0.357976
C	2.269633	1.872366	0.295918
O	-1.251896	-1.468666	-0.966286
C	-1.435536	-2.259856	-1.961828
O	-0.731561	-2.464636	-2.940594
C	-2.781118	-3.017753	-1.827455
F	-3.812905	-2.144530	-1.908940
F	-2.875976	-3.639696	-0.636663
F	-2.947083	-3.932013	-2.783685
H	2.675244	-0.279847	-2.278413
H	3.643656	3.239929	1.253247
H	1.258269	-1.306344	-2.921183
H	1.055222	-2.488350	-0.856804
H	2.241963	1.198473	1.149809
H	3.711737	4.786980	-0.698915
H	2.410078	4.285226	-2.729347
H	1.435230	-2.916057	1.425104
H	2.955401	-2.978241	3.380372
H	5.127975	-1.769985	3.301138
H	5.764226	-0.505966	1.258410
H	4.246609	-0.433772	-0.681834
S	-1.439461	1.520794	-0.218775
O	-1.807018	2.695729	-1.069484
C	-1.030568	2.127744	1.434027
C	-2.947582	0.609617	0.176797
H	-0.856803	1.279532	2.102528
H	-0.121211	2.724055	1.337835
H	-1.862372	2.746945	1.782645
H	-3.315500	0.155346	-0.743064
H	-2.718917	-0.181831	0.893654
H	-3.665621	1.333153	0.573626
O	0.848178	2.076328	-3.028782
C	0.686206	3.006011	-4.081765
H	-0.002777	2.539354	-4.787438
H	0.253094	3.945411	-3.716779
H	1.638228	3.211526	-4.589984

TS9$_{o\text{-}OMe}$

E = -1862.633367 a.u.

Pd	0.179726	-0.262039	-0.070074
S	0.963060	-1.934681	1.457153
F	-3.322055	-1.325646	2.948804
F	-4.285387	-1.645904	1.025810
F	-4.735734	0.132143	2.180973
O	-1.688533	-0.807304	0.746786
O	2.414245	-2.282028	1.612150
O	-2.601675	1.252263	1.058506
C	0.292540	-1.572187	3.097937
C	0.035070	-3.444876	1.095707
C	-2.577767	0.031179	1.137224
C	-3.758346	-0.702296	1.825603
H	-0.788410	-1.442295	3.025806
H	0.559783	-2.400009	3.761404
H	0.767536	-0.649827	3.439311
H	-1.024098	-3.186523	1.020899
H	0.406528	-3.823287	0.140477
H	0.226417	-4.174991	1.887633
C	2.406750	-0.820238	-1.925346
C	3.097416	0.523173	-0.035171
C	3.729518	-1.187237	-2.163628
H	1.619378	-1.197537	-2.574241
C	4.426182	0.174341	-0.286129
C	4.735241	-0.680370	-1.343874
H	3.970757	-1.857047	-2.984432
H	5.224001	0.546777	0.347552
H	5.773087	-0.949903	-1.520853
O	2.706555	1.340539	0.980398
C	3.698150	1.841287	1.858566
H	4.217730	1.025528	2.375842
H	4.429907	2.463515	1.326832
H	3.166816	2.455357	2.587580
C	2.064830	0.026290	-0.860745
C	-1.355346	0.780264	-2.480215
C	0.836856	1.559163	-1.414611
C	-0.790442	0.303322	-3.675842
C	-2.756791	0.803448	-2.370299
H	1.234109	2.281944	-0.708080
H	1.321942	1.567460	-2.384778
C	-1.597762	-0.142481	-4.717471
H	0.289048	0.284768	-3.801306
C	-3.562438	0.360021	-3.414036
H	-3.204302	1.173412	-1.451635

C	-2.987335	-0.118176	-4.591386
H	-1.140384	-0.505453	-5.634624
H	-4.643768	0.388078	-3.307061
H	-3.616094	-0.465111	-5.407257
C	-0.555708	1.282869	-1.347385
H	-1.129172	1.791222	-0.571056

$10_{o\text{-}NO2}$
E = -1952.595528 a.u.

C	3.911426	-0.923470	-0.563849
C	2.805618	-1.574558	0.004527
C	2.949100	-2.139595	1.281376
C	4.150056	-2.042761	1.977489
C	5.238001	-1.386329	1.403438
C	5.113825	-0.829845	0.129909
C	1.517995	-1.735215	-0.699368
C	1.153410	-1.167978	-1.924778
Pd	-0.015110	-0.164353	-0.449789
O	-1.460440	-1.779388	-0.765212
S	-2.372684	-2.320116	0.370636
C	-4.062449	-2.062359	-0.219183
C	1.267373	1.304306	-0.242441
C	1.643064	2.121458	-1.312591
C	2.507335	3.199580	-1.122892
C	3.018047	3.488981	0.145087
C	2.647584	2.703651	1.226525
C	1.775358	1.632338	1.020525
O	-1.458868	1.382226	-0.448760
C	-2.508829	1.235673	0.254696
O	-2.814649	0.333009	1.035042
C	-3.575020	2.334299	0.019921
F	-4.552453	1.818540	-0.764290
F	-3.099773	3.425517	-0.589429
F	-4.141209	2.716132	1.172442
C	-2.301378	-4.111383	0.085352
H	1.817850	-0.484819	-2.447607
H	3.006424	2.901561	2.230442
H	1.236853	1.929148	-2.301696
H	0.385674	-1.641470	-2.531768
H	0.930170	-2.588250	-0.362853
H	3.689849	4.329848	0.290243
H	2.777371	3.823614	-1.971625
H	-1.290448	-4.442236	0.335559
H	-3.019561	-4.611298	0.742965
H	-2.515177	-4.332391	-0.964320
H	-4.749691	-2.583295	0.454837
H	-4.243701	-0.988610	-0.171661
H	-4.152030	-2.438025	-1.242466
H	2.100111	-2.644231	1.736456
H	4.235172	-2.478484	2.969340
H	6.178398	-1.311450	1.943098
H	5.959895	-0.324169	-0.328346
H	3.836751	-0.494640	-1.558915
N	1.378576	0.856529	2.190413
O	1.925760	1.086703	3.258575
O	0.494089	0.003479	2.052039

$TS8_{o\text{-}NO2}$
E = -1952.566547 a.u.

C	-3.334629	-0.942618	1.348240
C	-3.177416	-0.785768	-0.039649
C	-4.119825	-0.006471	-0.732607
C	-5.188240	0.588305	-0.068619
C	-5.334203	0.421848	1.308375
C	-4.401479	-0.343578	2.010429
C	-2.086165	-1.403941	-0.818315
C	-1.323797	-2.559185	-0.413146
Pd	-0.262437	-0.507580	-0.409282
O	-1.071007	1.423461	-0.871718
S	-0.356732	2.641630	-0.219104
C	0.697370	3.335663	-1.513617
C	0.603271	-2.377749	-0.249029
C	1.259334	-2.743071	-1.442801
C	2.447773	-3.462515	-1.437480
C	2.999877	-3.894401	-0.229118
C	2.362277	-3.582856	0.963708
C	1.190274	-2.829532	0.948561
O	1.531850	0.601558	-0.182890
C	2.379688	0.509065	0.778453
O	2.433735	-0.268189	1.716733
C	3.454132	1.624949	0.675639
F	4.486951	1.418784	1.492395
F	2.906483	2.824575	1.002937
F	3.935727	1.748234	-0.578693
C	-1.672795	3.882461	-0.256267
H	-2.219109	-1.293854	-1.897489
H	-1.197689	-3.316806	-1.180586
H	2.766363	-3.887137	1.921766
H	0.817259	-2.450020	-2.392289
H	-1.529047	-2.965892	0.572378
H	3.920847	-4.469524	-0.216314
H	2.937437	-3.698756	-2.378704
H	1.083797	4.303110	-1.178773
H	1.518377	2.628966	-1.641346
H	0.118578	3.437793	-2.436171
H	-1.275548	4.840807	0.092346
H	-2.073021	3.968779	-1.270270
H	-2.454992	3.535003	0.422561
H	-4.008011	0.128892	-1.806017
H	-5.909509	1.179205	-0.627974
H	-6.168966	0.882265	1.830793
H	-4.503552	-0.475962	3.084557
H	-2.610034	-1.515175	1.916935
N	0.601221	-2.512057	2.249926
O	-0.382474	-1.774468	2.277590
O	1.097631	-3.021229	3.243320

$11_{o\text{-}NO2}$
E = -1952.600327 a.u.

C	4.069262	-0.974995	-0.034071
C	2.800183	-1.495292	0.267180
C	2.559143	-1.964792	1.569716
C	3.545300	-1.894788	2.548211
C	4.799365	-1.367972	2.236161
C	5.058870	-0.914665	0.941904
C	1.734836	-1.622404	-0.735508
C	1.697159	-1.077078	-2.012494
Pd	0.221663	0.096539	-0.910560
C	1.486585	1.627406	-0.930363
C	1.462720	2.556497	-1.981111
C	2.306610	3.668943	-2.035941
C	3.198267	3.886046	-0.996436
C	3.232610	2.992121	0.076351
C	2.392568	1.878234	0.104059
O	-1.339608	-1.325118	-0.772366
C	-1.564871	-2.301545	-1.580254
O	-0.870037	-2.755090	-2.474755
C	-2.952465	-2.929132	-1.291023
F	-3.930200	-2.019740	-1.513269
F	-3.047452	-3.307502	0.000132
F	-3.200233	-3.991561	-2.053708
H	2.500895	-0.441579	-2.375458
H	3.918915	3.162782	0.902242
H	1.033682	-1.529222	-2.747110
H	0.995928	-2.391814	-0.516253
H	2.444905	1.197984	0.948947
H	3.854211	4.751283	-1.015876
H	2.236253	4.342558	-2.882802
H	1.584687	-2.385719	1.808250
H	3.340116	-2.259570	3.551107
H	5.575393	-1.321133	2.995617
H	6.038979	-0.518262	0.690209
H	4.287722	-0.631950	-1.040837
S	-1.394488	1.419996	0.291438
O	-1.104792	2.809733	0.768341
C	-1.976592	0.429528	1.687884
C	-2.895624	1.441658	-0.712755
H	-2.213569	-0.572839	1.324690
H	-1.161963	0.398444	2.415046
H	-2.847403	0.928641	2.122918

H	-2.664915	2.008859	-1.616760
H	-3.162760	0.414020	-0.967100
H	-3.680242	1.940255	-0.136184
N	0.500668	2.402474	-3.065639
O	0.593395	3.124602	-4.045179
O	-0.389487	1.547239	-2.939705

TS9$_{o\text{-}NO2}$

E = -1952.574011 a.u.

Pd	-0.226145	-0.035740	-0.045160
S	-0.910786	-1.987845	1.174990
F	3.324381	-3.048208	0.281732
F	4.364578	-1.250793	0.927242
F	4.686474	-2.033328	-1.069694
O	1.671180	-0.881031	0.267344
O	-2.352954	-2.222488	1.521009
O	2.632367	-0.487291	-1.755920
C	-0.292526	-3.430510	0.278687
C	0.083734	-2.119453	2.679283
C	2.581959	-0.970288	-0.633449
C	3.765654	-1.833940	-0.127173
H	0.789840	-3.344156	0.165070
H	-0.572292	-4.323974	0.845027
H	-0.782308	-3.429882	-0.697123
H	1.130987	-1.961468	2.411051
H	-0.261628	-1.336430	3.358233
H	-0.083413	-3.103721	3.126279
C	-2.385380	1.596438	0.993732
C	-3.241623	0.060290	-0.630151
C	-3.647433	1.683777	1.571053
H	-1.567328	2.180042	1.407383
C	-4.520632	0.177559	-0.090891
C	-4.724867	0.987063	1.018746
H	-3.794714	2.309511	2.447473
H	-5.328083	-0.392745	-0.535523
H	-5.715654	1.065602	1.455824
C	-2.133696	0.770786	-0.122765
C	1.085092	2.675737	-0.504986
C	-1.059359	1.648341	-1.470443
C	0.451388	3.743575	0.156394
C	2.491743	2.629842	-0.495363
H	-1.393462	1.116222	-2.355947
H	-1.583214	2.584978	-1.303129
C	1.194576	4.714811	0.818627
H	-0.631707	3.833999	0.141147
C	3.232348	3.603978	0.164261
H	2.992139	1.816325	-1.013658
C	2.588186	4.647894	0.829591
H	0.684338	5.534509	1.318843
H	4.317505	3.549271	0.157397
H	3.166915	5.410789	1.344382
C	0.357111	1.624153	-1.234572
H	0.966314	1.044468	-1.929777
N	-3.083158	-0.873086	-1.743847
O	-4.091377	-1.264598	-2.314276
O	-1.940106	-1.220971	-2.052277

styrene

E = -309.522460 a.u.

C	-3.022030	-1.319234	1.414617
C	-3.061670	-0.885374	0.078647
C	-4.056287	0.036075	-0.284259
C	-4.977940	0.509122	0.646597
C	-4.924022	0.068251	1.967071
C	-3.940635	-0.848654	2.345391
C	-2.116748	-1.349067	-0.946541
C	-1.109047	-2.217222	-0.796759
H	-2.277940	-0.919947	-1.936164
H	-0.874734	-2.693707	0.151813
H	-0.474234	-2.483252	-1.636842
H	-4.103707	0.384344	-1.314251
H	-5.738387	1.222655	0.339091
H	-5.640931	0.434307	2.697486
H	-3.890772	-1.198398	3.373687
H	-2.264741	-2.032264	1.729054

Cartesian coordinates for all the species calculated at the B3LYP level in this study

10S

E = -1510.775420 a.u.

Pd	0.045926	-0.242385	-0.517241
S	-0.025825	-2.513896	-0.174170
S	-0.336800	2.706114	0.246586
F	4.693757	0.488747	-1.000476
F	4.521880	-1.124647	0.458538
F	4.933394	0.908676	1.120218
F	-4.937047	-0.558169	1.133271
F	-4.635223	-0.443607	-1.015665
F	-4.291227	1.315065	0.229363
O	2.077392	-0.367994	-0.441915
O	0.138141	1.788690	-0.956340
O	-1.968510	-0.047627	-0.648947
O	-1.223784	-3.289591	-0.651420
O	2.292197	1.297865	1.096959
O	-2.308349	-0.946209	1.411717
C	1.469558	-3.260406	-0.912623
C	0.249435	-2.842973	1.598724
C	2.719789	0.436655	0.340012
C	4.246514	0.182200	0.232370
C	0.907073	4.037244	0.226245
C	-1.760536	3.589249	-0.478113
C	-2.673728	-0.418602	0.370584
C	-4.164677	-0.042005	0.174269
H	2.350538	-2.706558	-0.586395
H	1.489331	-4.309808	-0.608610
H	1.346565	-3.179465	-1.994445
H	1.183033	-2.365173	1.906578
H	-0.607670	-2.399497	2.106297
H	0.283973	-3.927592	1.731706
H	0.587892	4.828104	0.911385
H	1.831493	3.572513	0.572223
H	1.008263	4.408891	-0.796420
H	-2.058868	4.396837	0.197513
H	-1.477334	3.972842	-1.461283
H	-2.560778	2.852442	-0.566275

100

E = -1510.779955 a.u.

Pd	-0.000070	-0.000018	0.687707
S	-0.190013	-2.754608	-0.575699
S	0.189970	2.754606	-0.575614
F	-4.709225	0.093178	1.138407
F	-4.328149	-1.300406	-0.496784
F	-4.995480	0.727978	-0.920105
O	-2.022465	-0.231914	0.657232
O	-0.114577	2.041082	0.809711
O	2.022325	0.231887	0.657414
O	0.114441	-2.041121	0.809667
O	-2.401807	1.310812	-0.980625
O	2.401795	-1.310726	-0.980523
C	-1.707913	-3.693428	-0.187245
C	1.029166	-4.107683	-0.573513
C	-2.732525	0.445093	-0.176424
C	-4.218588	-0.000325	-0.109970
C	-1.029098	4.107782	-0.573415
C	1.707937	3.693284	-0.187078
C	2.732442	-0.445041	-0.176257
H	-1.933712	-4.368544	-1.018652

H	-1.560024	-4.243065	0.745541
H	-2.499560	-2.950761	-0.071389
H	0.798926	-4.792276	-1.395160
H	1.993538	-3.622266	-0.728209
H	0.988886	-4.614404	0.393824
H	-0.798779	4.792388	-1.395029
H	-1.993505	3.622449	-0.728156
H	-0.988802	4.614459	0.393944
H	1.933796	4.368439	-1.018437
H	1.560081	4.242868	0.745744
H	2.499527	2.950547	-0.071267
C	4.218491	0.000400	-0.109678
F	4.995450	-0.727842	-0.919804
F	4.328041	1.300508	-0.496411
F	4.709050	-0.093162	1.138724

1SS

E = -1510.761132 a.u.

Pd	0.012916	0.070283	-0.309936
S	-0.061492	-2.289518	-0.483526
F	4.766063	0.148930	-0.847571
F	4.229218	-1.559849	0.401145
F	5.060901	0.238383	1.305543
F	-4.916262	-0.521820	1.366171
F	-4.658211	-0.682512	-0.788595
F	-4.426079	1.248214	0.196834
O	2.039412	-0.119237	-0.428998
O	-2.001273	0.230983	-0.414381
O	-1.282420	-2.917450	-1.102611
O	2.528620	1.102504	1.424929
O	-2.291690	-1.064032	1.425522
C	1.407791	-2.900418	-1.383176
C	0.225006	-2.995187	1.176196
C	2.806720	0.347256	0.509437
C	4.248240	-0.201929	0.345230
C	-2.693535	-0.361478	0.513318
C	-4.205541	-0.078849	0.326440
H	2.314480	-2.515885	-0.916860
H	1.353817	-3.991760	-1.363131
H	1.318429	-2.533812	-2.407481
H	1.163521	-2.598769	1.572982
H	-0.625297	-2.671120	1.777249
H	0.256969	-4.083013	1.071277
S	-0.120015	2.428812	-0.137349
O	-0.633154	3.010475	1.152101
C	1.425211	3.282386	-0.602064
H	2.130609	3.078464	0.203512
H	1.786665	2.881815	-1.552935
H	1.199951	4.349614	-0.671320
C	-1.225139	2.960753	-1.490914
H	-2.180867	2.467785	-1.309670
H	-1.317704	4.047998	-1.427747
H	-0.804060	2.643350	-2.448999