Mechanism of the 'Classical' and 'Stereoselective' Pummerer Reaction: A Computational Investigation

Supplemental Information

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Contents

Theoretical Methods

All calculations were performed using the Gaussian09 suite of quantum chemical programs.[1] Density functional theory (DFT) was applied using the B3LYP[2] and M06-2X[3] functionals in combination with the 6-31+G** basis set. Geometry optimizations were carried out in the gas phase for B3LYP (B3LYP-II) and in the solvent phase (PCM, DCM) for B3LYP (B3LYP-I) and M06-2X (M06-2X-S) without any constraints. The calculations were done using the tight convergence criteria and ultrafine grid in the Gaussian 09 suite. Empirical dispersion corrections for the B3LYP functional were included through single-point calculations at the optimized geometries.[4] Harmonic vibrational frequencies were computed at the same level as applied in the optimization. Thermal and entropic corrections were evaluated at 298.15 K and 1 atm as well as at 418.15 K and 1 atm (B3LYP-II level). Zero-point vibrational energies, enthalpies, and Gibbs free energies were determined from these calculations. The number of imaginary modes was used to verify minima (no imaginary frequency) and transition states (one imaginary frequency). Intrinsic reaction coordinate (IRC)[5] calculations were performed to confirm the direct connection between transition states and minima. For visualization the programs Molden[6] and GaussView 3.5[7] were used.

Notation in the following tables for the total energies (all values given in Hartree):

E	total energy
ZPC	zero-point vibrational energy correction
H	enthalpy at the given temperature and pressure
G	Gibbs free energy at the given temperature and pressure
disp	empirical dispersion correction

In the following sections, the notation for the compounds conforms to the definitions in the main paper (see also the plots of the corresponding structures in the last section). For a number of species, results are given for several low-energy conformers; in such cases, the discussion in the main paper always refers to the lowest-energy conformer.

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Total and relative energies of stationary points

Total energies: B3LYP/6-31+G, DCM, 298.15 K, 1 atm (a.u.)**

compound	E	E+ZPC	H	G	E+disp	E+ZPC+disp	H+disp	G+disp
AcO-	-228.637	-228.588	-228.583	-228.616	-228.640	-228.591	-228.586	-228.618
AcOH	-229.113	-229.051	-229.046	-229.078	-229.116	-229.054	-229.049	-229.082
Ac2O	-381.763	-381.665	-381.656	-381.699	-381.771	-381.673	-381.664	-381.707
-OTf	-961.629	-961.603	-961.595	-961.635	-961.635	-961.608	-961.600	-961.641
TMS+	-409.078	-408.968	-408.960	-409.001	-409.086	-408.976	-408.967	-409.009
TfOH	-962.048	-962.010	-962.001	-962.043	-962.054	-962.017	-962.008	-962.050
TMSOTf	-1370.787	-1370.648	-1370.631	-1370.692	-1370.810	-1370.670	-1370.654	-1370.715
TMSOAc	-637.834	-637.672	-637.659	-637.710	-637.854	-637.692	-637.679	-637.730
DMAC/TMS	-697.019	-696.774	-696.758	-696.817	-697.051	-696.807	-696.790	-696.850
DMAC	-287.863	-287.733	-287.725	-287.766	-287.877	-287.748	-287.739	-287.780
DMAC/TMSOTf conformer 1	-1658.661	-1658.661	-1658.389	-1658.363	-1658.450	-1658.707	-1658.435	-1658.409
DMAC/TMSOTf conformer 2	-1658.660	-1658.389	-1658.363	-1658.452	-1658.703	-1658.432	-1658.406	-1658.495
DMAC/TMSOTf conformer 3	-1658.657	-1658.385	-1658.359	-1658.446	-1658.699	-1658.427	-1658.401	-1658.488
DMAC/TMSOAc	-925.670	-925.670	-925.376	-925.353	-925.428	-925.715	-925.421	-925.398
1 conformer 1	-1012.170	-1011.966	-1011.951	-1012.010	-1012.195	-1011.991	-1011.976	-1012.036
1 conformer 2	-1012.170	-1011.966	-1011.951	-1012.011	-1012.195	-1011.992	-1011.976	-1012.036
(1+Ac2O) conformer 1	-1393.934	-1393.631	-1393.606	-1393.697	-1393.971	-1393.668	-1393.643	-1393.734
(1+Ac2O) conformer 2	-1393.932	-1393.630	-1393.604	-1393.695	-1393.971	-1393.668	-1393.643	-1393.734
(1+Ac2O) conformer 3	-1393.933	-1393.631	-1393.605	-1393.698	-1393.970	-1393.668	-1393.642	-1393.735
TS(1-2)	-1393.890	-1393.588	-1393.563	-1393.645	-1393.934	-1393.632	-1393.608	-1393.689
2	-1165.247	-1164.995	-1164.975	-1165.045	-1165.279	-1165.027	-1165.007	-1165.077
(2+AcO-)	-1393.895	-1393.593	-1393.567	-1393.651	-1393.939	-1393.637	-1393.612	-1393.696
3(Sulfurane)	-1393.918	-1393.615	-1393.590	-1393.673	-1393.966	-1393.663	-1393.638	-1393.722
TS(3-4r)	-1393.904	-1393.606	-1393.581	-1393.664	-1393.950	-1393.652	-1393.627	-1393.710
TS(3-4s)	-1393.904	-1393.606	-1393.581	-1393.664	-1393.950	-1393.652	-1393.627	-1393.710
(4r + AcOH)	-1393.926	-1393.625	-1393.598	-1393.689	-1393.965	-1393.664	-1393.637	-1393.728
(4s + AcOH)	-1393.933	-1393.631	-1393.605	-1393.693	-1393.973	-1393.671	-1393.645	-1393.733
4r	-1164.813	-1164.574	-1164.554	-1164.624	-1164.845	-1164.605	-1164.586	-1164.655
TS(4r-4s)	-1164.771	-1164.533	-1164.514	-1164.580	-1164.806	-1164.567	-1164.549	-1164.614
4s	-1164.813	-1164.573	-1164.554	-1164.624	-1164.845	-1164.605	-1164.586	-1164.655
5	-936.139	-935.950	-935.936	-935.992	-936.161	-935.972	-935.958	-936.014
TS(4r-6r)-cyc	-1164.808	-1164.569	-1164.550	-1164.618	-1164.840	-1164.601	-1164.582	-1164.650
TS(4s-6s)-cyc	-1164.806	-1164.568	-1164.548	-1164.617	-1164.839	-1164.600	-1164.582	-1164.650
TS(4r-6r)-slide	-1164.800	-1164.562	-1164.542	-1164.613	-1164.830	-1164.591	-1164.572	-1164.643
TS(4s-6s)-slide	-1164.800	-1164.561	-1164.542	-1164.612	-1164.830	-1164.592	-1164.572	-1164.643
6r	-1164.870	-1164.628	-1164.609	-1164.678	-1164.903	-1164.660	-1164.641	-1164.710
6s	-1164.871	-1164.629	-1164.610	-1164.679	-1164.904	-1164.662	-1164.643	-1164.712
(1r + Ac2O + DMAC + TMS+) conformer 1	-2090.935	-2090.388	-2090.344	-2090.476	-2091.015	-2090.468	-2090.425	-2090.556
(1r + Ac2O + DMAC + TMS+) conformer 2	-2090.933	-2090.385	-2090.342	-2090.473	-2091.013	-2090.466	-2090.422	-2090.554
TS(1r–2r) + DMAC + TMS+	-2091.009	-2090.379	-2090.336	-2090.463	-2091.009	-2090.463	-2090.420	-2090.546
(2r + -OTf + DMAC)	-2414.824	-2414.346	-2414.307	-2414.429	-2414.824	-2414.413	-2414.375	-2414.496
TS(2r-4r) + DMAC + -OTf	-2414.801	-2414.324	-2414.286	-2414.402	-2414.801	-2414.396	-2414.359	-2414.475
(4r + HOTf + DMAC)	-2414.731	-2414.322	-2414.283	-2414.407	-2414.796	-2414.387	-2414.348	-2414.472
TS (4r–6r)-cyc + DMAC	-1452.726	-1452.307	-1452.277	-1452.375	-1452.726	-1452.356	-1452.327	-1452.425
TS (4r–6r)-slide + DMAC	-1452.716	-1452.300	-1452.270	-1452.368	-1452.716	-1452.347	-1452.318	-1452.416

Total energies: B3LYP/6-31+G, DCM, 298.15 K, 1 atm (a.u.)**

compound	E	E+ZPC	H	G	E+disp	E+ZPC+disp	H+disp	G+disp
(1r + Ac2O + TMS+) conformer 1	-1803.067	-1802.651	-1802.618	-1802.722	-1803.128	-1802.712	-1802.678	-1802.783
(1r + Ac2O + TMS+) conformer 2	-1803.065	-1802.648	-1802.615	-1802.719	-1803.127	-1802.710	-1802.677	-1802.780
(1r + Ac2O + TMS+) conformer 3	-1803.064	-1802.647	-1802.614	-1802.718	-1803.122	-1802.705	-1802.672	-1802.776
(2r + -OTf)	-2126.890	-2126.610	-2126.581	-2126.675	-2126.939	-2126.659	-2126.631	-2126.724
(TS(1r–2r) + TMS)	-1803.056	-1802.641	-1802.608	-1802.708	-1803.12	-1802.704	-1802.671	-1802.771
(TS(2r–4r) + $^{-}$OTf)	-2126.863	-2126.588	-2126.560	-2126.653	-2126.911	-2126.637	-2126.608	-2126.701
(4r + HOTf)	-2126.865	-2126.587	-2126.557	-2126.652	-2126.912	-2126.633	-2126.604	-2126.699

Relative energies: B3LYP/6-31+G, DCM, 298.15 K, 1 atm (kcal/mol)**

compound	E	E+ZPC	H	G	E+disp	E+ZPC+disp	H+disp	G+disp
1r + Ac2O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
(1r + Ac2O)	-0.6	0.0	0.6	7.5	-3.1	-2.5	-1.9	5.6
TS(1r–2r)	27.1	27.0	27.6	40.2	20.1	20.1	20.1	33.9
(2r + AcO-)	23.7	23.8	25.1	36.4	16.9	16.9	17.6	29.5
3	9.4	10.0	10.7	22.6	0.0	0.6	1.3	13.2
TS (3–4r)	18.1	15.7	16.3	28.2	10.0	7.5	7.9	20.7
TS (3–4s)	18.1	15.7	16.1	28.4	10.0	7.5	8.2	20.7
4r + AcOH	4.6	4.1	4.4	4.5	3.4	3.1	3.4	3.5
TS(4r-4s)	30.9	29.7	29.4	32.3	27.8	26.8	26.4	29.4
4s + AcOH	4.6	4.4	4.4	4.4	3.4	3.1	3.4	3.5
5 +AcO- + HOAc	27.6	26.1	26.1	14.1	31.1	29.4	29.6	18.1
TS (4r–6r)-cyc + AcOH	7.8	7.1	7.1	8.2	6.1	5.5	5.4	6.6
TS (4s–6s)-cyc + AcOH	8.7	7.5	8.2	8.8	6.9	6.3	5.6	6.9
TS (4r–6r)-slide + AcOH	12.6	11.6	11.8	11.4	12.6	11.7	11.9	11.5
TS (4s–6s)-slide + AcOH	12.9	11.9	11.9	11.9	12.6	11.3	11.9	11.3
6s + AcOH	-32.0	-30.7	-30.7	-30.1	-33.9	-32.6	-32.6	-32.0
6r + AcOH	-31.2	-30.0	-30.0	-29.4	-33.0	-31.6	-31.7	-31.0
1r + Ac2O + TMSOTf	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
(1r + Ac2O + TMS+) + -OTf	14.7	15.6	15.9	27.6	8.1	9.0	9.9	21.6
(TS(1r–2r) + TMS+) + -OTf	21.8	22.0	22.0	36.4	13.2	13.8	14.4	28.9
2r + AcOTMS + -OTf	6.0	6.0	5.6	6.8	4.9	4.7	4.9	6.2
(2r + -OTf) + AcOTMS	-2.3	-1.9	-1.4	10.2	-10.7	-10.9	-9.8	2.5
(TS(2r–4r) + -OTf) +AcOTMS	14.4	11.9	11.9	23.8	6.9	3.1	4.4	16.9
4r + TfOH + AcOTMS	15.9	15.1	15.1	15.1	14.7	12.5	13.5	14.2
TS (4r–6r)-cyc + TfOH + AcOTMS	20.0	18.2	18.8	19.5	18.2	15.7	15.7	17.6
6r + TfOH + AcOTMS	-20.7	-20.1	-20.1	-19.5	-22.6	-23.2	-22.6	-21.3
1r + Ac2O + TMSOTf + DMAC	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
(1r + Ac2O + TMS+ +DMAC) + -OTf	12.0	13.2	15.1	35.1	1.9	3.8	5.0	25.7
(TS(1r–2r) + TMS+ +DMAC) + -OTf	-34.5	18.8	20.1	43.3	5.6	6.9	8.2	32.0
2r + AcOTMS + -OTf +DMAC	6.0	6.0	5.6	6.8	4.9	4.7	4.9	6.2
(2r + -OTf +DMAC) + AcOTMS	-46.8	-3.8	-1.9	17.6	-15.7	-14.4	-13.2	7.5
(TS(2r–4r) + -OTf +DMAC) +AcOTMS	-32.6	10.0	11.3	34.5	-1.3	-3.8	-3.1	20.7
4r + TfOH + AcOTMS +DMAC	15.9	15.1	15.1	15.1	14.7	12.5	13.5	14.2
(TS (4r–6r)-cyc +DMAC) + TfOH + AcOTMS	-15.3	14.4	16.3	24.5	11.9	10.7	11.9	20.7
6r + TfOH + AcOTMS +DMAC	-20.7	-20.1	-20.1	-19.5	-22.6	-23.2	-22.6	-21.3
(1r + Ac2O) conformer 1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
(1r + Ac2O) conformer 2	0.8	0.8	1.2	1.1	0.2	-0.1	0.3	0.2
(1r + Ac2O) conformer 3	0.2	0.0	0.4	-0.4	0.3	-0.1	0.3	-0.5
(1r + Ac2O + TMS+) conformer 1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
(1r + Ac2O + TMS+) conformer 2	1.4	1.7	1.6	2.0	0.7	1.1	0.9	1.4
(1r + Ac2O + TMS+) conformer 3	2.2	2.4	2.4	2.3	3.9	4.1	4.1	4.0
(1r + Ac2O + TMS+ +DMAC) conformer 1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
(1r + Ac2O + TMS+ +DMAC) conformer 2	1.4	1.7	1.3	1.8	1.1	1.5	1.7	1.5

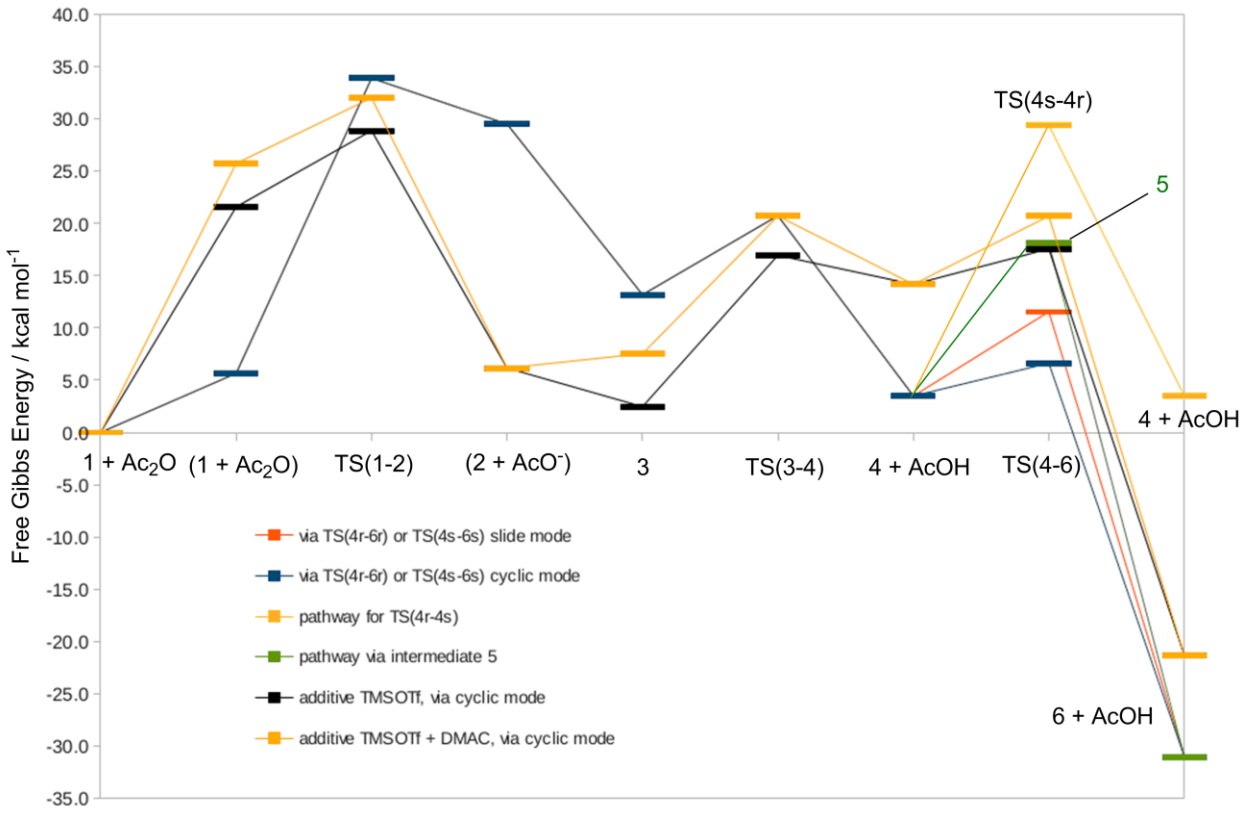

Figure S1: Relative free energy diagram (in kcal/mol) of the classical and stereoselective Pummerer reactions (B3LYP/6-31+G**, DCM, 298.15 K, 1 atm).

Total energies: B3LYP/6-31+G, gas phase, 298.15 K, 1 atm (a.u.)**

compound	E+ZPC	H	G	E+disp	E+ZPC+disp	H+disp	G+disp
AcO-	-228.496	-228.491	-228.522	-228.546	-228.498	-228.494	-228.524
AcOH	-229.044	-229.039	-229.071	-229.109	-229.048	-229.042	-229.075
Ac2O	-381.655	-381.646	-381.689	-381.762	-381.664	-381.655	-381.697
-OTf	-961.527	-961.519	-961.559	-961.559	-961.532	-961.524	-961.565
TMS+	-408.891	-408.882	-408.924	-409.008	-408.899	-408.890	-408.931
TfOH	-962.002	-961.993	-962.035	-962.047	-962.008	-962.000	-962.041
TMSOTf	-1370.640	-1370.624	-1370.684	-1370.803	-1370.663	-1370.646	-1370.707
TMSOAc	-637.662	-637.648	-637.700	-637.844	-637.682	-637.668	-637.720
DMAC	-287.725	-287.716	-287.757	-287.877	-287.747	-287.739	-287.780
1	-1011.952	-1011.937	-1011.997	-1012.182	-1011.978	-1011.963	-1012.023
(1+Ac2O)	-1393.612	-1393.587	-1393.676	-1393.956	-1393.653	-1393.627	-1393.716
TS(1-2)	-1393.565	-1393.541	-1393.621	-1393.914	-1393.611	-1393.587	-1393.668
(2+AcO-)	-1393.565	-1393.540	-1393.624	-1393.916	-1393.613	-1393.588	-1393.671
3(Sulfurane)	-1393.604	-1393.579	-1393.661	-1393.951	-1393.647	-1393.622	-1393.705
TS(3-4)	-1393.588	-1393.564	-1393.646	-1393.934	-1393.635	-1393.610	-1393.693
4	-1164.560	-1164.541	-1164.610	-1164.832	-1164.592	-1164.573	-1164.642
TS(4-6)-cyc	-1164.555	-1164.536	-1164.603	-1164.829	-1164.589	-1164.570	-1164.637
TS(4-6)-slide	-1164.538	-1164.519	-1164.589	-1164.807	-1164.569	-1164.549	-1164.619
6	-1164.609	-1164.591	-1164.658	-1164.887	-1164.645	-1164.626	-1164.694
TS(2-7)	-1393.564	-1393.539	-1393.623	-1393.910	-1393.608	-1393.583	-1393.667
7	-1393.640	-1393.614	-1393.706	-1393.981	-1393.677	-1393.651	-1393.743
(1 + Ac2O + DMAC + TMS+)	-2090.336	-2090.292	-2090.425	-2090.965	-2090.417	-2090.373	-2090.505
TS(1–2) + DMAC + TMS+	-2090.331	-2090.288	-2090.416	-2090.961	-2090.414	-2090.371	-2090.500
(2 + -OTf + DMAC)	-2414.319	-2414.280	-2414.397	-2414.806	-2414.394	-2414.356	-2414.473
TS(2-4) + DMAC + -OTf	-2414.303	-2414.265	-2414.383	-2414.782	-2414.375	-2414.337	-2414.455
TS (4–6)-cyc + DMAC	-1452.288	-1452.260	-1452.353	-1452.715	-1452.345	-1452.316	-1452.409
TS (4–6)-slide + DMAC	-1452.272	-1452.243	-1452.341	-1452.691	-1452.321	-1452.292	-1452.390

Relative energies: B3LYP/6-31+G, gas phase, 298.15 K, 1 atm (kcal/mol)**

compound	E+ZPC	H	G	E+disp	E+ZPC+disp	H+disp	G+disp
1r + Ac2O	0.0	0.0	0.0	0.0	0.0	0.0	0.0
(1r + Ac2O)	-2.7	-1.9	6.4	-7.2	-6.7	-6.0	2.4
TS(1r–2r)	27.1	26.9	40.7	18.7	19.1	18.9	32.7
(2r + AcO-)	26.7	27.1	39.0	17.8	18.3	18.7	30.7
3	2.6	2.9	15.3	-4.6	-3.4	-3.1	9.4
TS (3–4r)	12.3	12.4	24.9	6.5	4.3	4.4	16.9
4r + AcOH	2.2	2.5	2.9	1.5	1.3	1.6	2.0
TS (4r–6r)-cyc + AcOH	5.7	5.6	7.3	3.8	3.4	3.2	5.0
TS (4r–6r)-slide + AcOH	16.1	16.3	16.2	17.2	16.2	16.4	16.2
6r + AcOH	-28.5	-28.6	-27.4	-33.0	-31.6	-31.7	-30.5

Total energies: B3LYP/6-31+G, DCM, 418.15 K, 1 atm (a.u.)**

compound	E+ZPC	H	G	E+disp	E+ZPC+disp	H+disp	G+disp
AcO-	-228.588	-228.581	-228.626	-229.116	-229.068	-229.060	-229.105
AcOH	-229.051	-229.043	-229.089	-229.116	-229.054	-229.046	-229.093
Ac2O	-381.665	-381.651	-381.713	-381.771	-381.673	-381.660	-381.721
1	-1011.966	-1011.941	-1012.030	-1012.195	-1011.991	-1011.967	-1012.056
(1+Ac2O)	-1393.631	-1393.593	-1393.743	-1393.967	-1393.665	-1393.627	-1393.777
TS(1-2)	-1393.588	-1393.549	-1393.673	-1393.934	-1393.632	-1393.594	-1393.717
(2+AcO-)	-1393.593	-1393.553	-1393.680	-1393.939	-1393.637	-1393.597	-1393.724
3(Sulfurane)	-1393.615	-1393.575	-1393.702	-1393.966	-1393.663	-1393.623	-1393.750
TS(3-4)	-1393.606	-1393.567	-1393.692	-1393.950	-1393.652	-1393.613	-1393.738
4	-1164.573	-1164.543	-1164.648	-1164.831	-1164.592	-1164.561	-1164.666
TS(4-6)-cyc	-1164.563	-1164.533	-1164.635	-1164.835	-1164.596	-1164.566	-1164.669
TS(4-6)-slide	-1164.555	-1164.524	-1164.630	-1164.824	-1164.586	-1164.555	-1164.662
6	-1164.629	-1164.599	-1164.703	-1164.904	-1164.662	-1164.632	-1164.736

Relative energies: B3LYP/6-31+G, DCM, 418.15 K, 1 atm (kcal/mol)**

compound	E+ZPC	H	G	E+disp	E+ZPC+disp	H+disp	G+disp
1r + Ac2O	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS(1r–2r)	27.3	27.5	44.2	20.4	20.5	20.7	37.4
(2r + AcO-)	24.2	25.1	39.5	17.1	17.5	18.5	32.8
3	10.1	11.0	25.7	0.4	1.1	2.0	16.7
TS(3–4r)	15.7	16.2	32.1	10.4	8.0	8.5	24.4
4r + AcOH	4.0	4.6	3.9	12.2	11.7	12.3	11.5
TS (4r–6r)-cyc + AcOH	10.8	10.8	11.6	9.7	8.9	8.9	9.7
TS (4r–6r)-slide + AcOH	15.9	16.3	14.7	16.7	15.5	15.8	14.2
6r + AcOH	-30.9	-30.9	-30.9	-33.3	-32.2	-32.2	-32.2
1r + Ac2O + TMSOTf + DMAC	0.0	0.0	0.0	0.0	0.0	0.0	0.0
(1r + Ac2O + TMS+ +DMAC) + -OTf	69.2	70.4	90.1	63.3	64.7	66.0	85.6
(TS(1r–2r) + TMS+ +DMAC) + -OTf	72.6	73.4	95.1	65.8	66.7	67.6	89.3
2r + AcOTMS + -OTf +DMAC	80.0	79.9	80.5	79.6	79.5	79.4	80.1
(2r + -OTf +DMAC) + AcOTMS	-4.5	-3.4	18.8	-16.1	-14.6	-13.5	8.7
(TS(2r–4r) + -OTf +DMAC) +AcOTMS	5.3	6.2	28.1	-1.0	-3.0	-2.0	19.9
4r + TfOH + AcOTMS +DMAC	15.3	15.5	15.8	14.9	14.2	14.5	14.8
(TS (4r–6r)-cyc +DMAC) + TfOH + AcOTMS	13.3	13.9	24.5	11.6	11.2	11.8	22.4
6r + TfOH + AcOTMS +DMAC	-15.4	-15.5	-14.5	-19.6	-18.7	-18.8	-17.8

Total energies: M06-2X/6-31+G, DCM, 298.15 K, 1 atm (a.u.)**

Compound	E+ZPC	H	G
AcO-	-228.483	-228.477	-228.510
AcOH	-228.946	-228.941	-228.974
Ac2O	-381.496	-381.488	-381.530
-OTf	-408.841	-408.833	-408.874
TMS+	-961.775	-961.766	-961.808
TfOH	-1370.303	-1370.286	-1370.346
TMSOTf	-637.456	-637.443	-637.493
TMSOAc	-287.587	-287.578	-287.619
DMAC	-408.841	-408.833	-408.874
1	-1011.653	-1011.638	-1011.697
(1+Ac2O)	-1393.157	-1393.132	-1393.216
TS(1-2)	-1393.117	-1393.094	-1393.172
(2+AcO-)	-1393.121	-1393.097	-1393.177
3(Sulfurane)	-1393.143	-1393.118	-1393.199
TS(3-4)	-1393.134	-1393.110	-1393.191
4	-1164.193	-1164.174	-1164.242
TS(4-6)-cyc	-1164.185	-1164.167	-1164.232
TS(4-6)-slide	-1164.174	-1164.155	-1164.223
6	-1164.263	-1164.245	-1164.311
TS(2-7)	-1393.106	-1393.081	-1393.165
7	-1393.186	-1393.162	-1393.242
(1 + Ac2O + DMAC +TMS+)	-2089.669	-2089.628	-2089.745
TS(1–2) + DMAC + TMS+	-2089.648	-2089.608	-2089.724
(2 + -OTf + DMAC)	-2413.613	-2413.576	-2413.685
TS(2-4) + DMAC + -OTf [8]	-2413.579	-2413.544	-2413.650
TS (4–6)-cyc + DMAC	-1451.787	-1451.759	-1451.848
TS (4–6)-slide + DMAC [8]	-1451.763	-1451.735	-1451.823

Relative energies: M06-2X//6-31+G, DCM, 418.15 K, 1 atm (kcal/mol)**

Compound	E+ZPC	H	G
1r + Ac2O	0.0	0.0	0.0
(1r + Ac2O)	-4.7	-4.2	6.6
TS(1r–2r)	20.2	19.9	34.1
(2r + AcO-)	31.7	31.8	32.1
3	4.4	4.7	17.3
TS(3–4r)	9.8	9.9	22.2
4r + AcOH	6.5	6.8	7.0
TS (4r–6r)-cyc + AcOH	11.4	11.3	13.0
TS (4r–6r)-slide + AcOH	18.6	18.8	18.8
6r + AcOH	-37.5	-37.5	-36.5
1r + Ac2O + TMSOTf + DMAC	0.0	0.0	0.0
(1r + Ac2O + TMS+ +DMAC) + -OTf	0.2	0.4	27.9
(TS(1r–2r) + TMS+ +DMAC) + -OTf	13.4	13.1	41.2
2r + AcOTMS + -OTf +DMAC	-18.5	-18.1	8.8
(2r + -OTf +DMAC) + AcOTMS	2.5	2.4	30.4
(TS(2r–4r) + -OTf +DMAC) +AcOTMS	18.0	18.1	18.7
4r + TfOH + AcOTMS +DMAC	13.8	14.0	27.2
(TS (4r–6r)-cyc +DMAC) + TfOH + AcOTMS	28.9	28.9	42.8
6r + TfOH + AcOTMS +DMAC	-26.0	-26.2	-24.8

Cartesian Coordinates of stationary points

B3LYP/6-31+G**, DCM, in Å

AcO-

6	-3.553598	3.107766	0.566266
6	-4.322316	2.126289	1.474362
8	-4.012508	0.900103	1.407463
8	-5.212525	2.633275	2.2211
1	-3.062145	3.872204	1.178819
1	-2.802424	2.598173	-0.04257
1	-4.256739	3.629703	-0.0929

AcOH

6	-3.553791	3.108922	0.565223
6	-4.256762	2.091912	1.420321
8	-3.791078	0.839176	1.207206
8	-5.143674	2.324201	2.222395
1	-3.673833	2.852298	-0.491502
1	-3.963715	4.099681	0.756559
1	-2.482043	3.099988	0.785569
1	-4.282124	0.230505	1.786828

Ac2O

6	-4.169054	1.930342	1.293896
8	-4.102892	0.75844	1.020705
8	-4.844116	2.405702	2.416534
6	-5.907116	1.717674	2.999032
6	-6.043601	2.100682	4.442636
6	-3.520947	3.065776	0.558879
8	-6.617201	0.968271	2.377379
1	-2.896014	2.675329	-0.243526
1	-4.29649	3.717966	0.144001
1	-2.921349	3.667063	1.24804
1	-6.945475	1.652882	4.858459
1	-5.164736	1.751468	4.994513
1	-6.080889	3.189242	4.541136

1 (conformer 1)

6	-0.397774	-1.505145	-0.037353
6	-0.386923	-0.221308	0.519486
6	0.513477	0.092174	1.541168
6	1.383204	-0.89963	2.004051
6	1.394807	-2.179049	1.448966
6	0.493207	-2.479758	0.423438
16	2.593136	-0.481718	3.303372
6	1.446872	-0.762872	4.740489
6	2.169702	-0.448198	6.033965
8	2.761612	0.596635	6.242398
8	3.608177	-1.621026	3.360194
8	2.06689	-1.451915	6.910311
6	2.705295	-1.265283	8.211366
6	2.459634	-2.520062	9.023744
1	2.10487	-2.915639	1.811638
1	0.491002	-3.472405	-0.016578
1	-1.093944	-1.741866	-0.836227
1	-1.070215	0.538742	0.153301
1	0.535555	1.093855	1.962353
1	3.769611	-1.083361	8.041896
1	2.270418	-0.377642	8.678423
1	2.92924	-2.409419	10.006179
1	1.389296	-2.690842	9.172537
1	2.891855	-3.39737	8.533659
1	1.098402	-1.795999	4.69966
1	0.607323	-0.072042	4.620262

1 (conformer 2)

6	-0.233217	-1.619434	-0.097538
6	-0.607748	-0.437502	0.551302
6	0.132979	0.029002	1.64058
6	1.235046	-0.712391	2.076693
6	1.629151	-1.884677	1.431628
6	0.884129	-2.338625	0.339068
16	2.230514	-0.082128	3.468722
6	1.179083	-0.819967	4.817584
6	1.768809	-0.558054	6.187677
8	1.993313	-1.433608	7.002905
8	3.536772	-0.872855	3.487986
8	1.992712	0.745955	6.389868
6	2.559723	1.135045	7.67831
6	2.725322	2.640788	7.668257
1	2.507777	-2.419789	1.778135
1	1.17938	-3.250205	-0.171603
1	-0.807062	-1.974036	-0.948308
1	-1.468085	0.12689	0.204995
1	-0.146446	0.95556	2.135291
1	1.877288	0.799382	8.463553
1	3.513245	0.614642	7.799504
1	3.150362	2.961527	8.624512
1	3.401467	2.957703	6.868857
1	1.76237	3.142874	7.535503
1	1.109926	-1.894764	4.645418

1+Ac2O (conformer 1)

6	-2.108086	-0.248325	-0.07939
8	0.064751	0.282942	-1.587972
6	-1.908296	-1.749853	-0.028397
8	-2.711017	-2.373669	-0.897863
8	-1.120021	-2.302175	0.718554
6	-2.669082	-3.834977	-0.943234
1	-1.646791	-4.156958	-0.738504
1	-2.926291	-4.06951	-1.977162
6	-3.663627	-4.437731	0.034255
1	-3.655063	-5.52768	-0.071356
1	-3.403004	-4.193423	1.067824
1	-4.677871	-4.082204	-0.170372
6	-1.100823	2.299243	-0.21621
6	-1.329306	2.922889	-1.443216
6	-1.292106	2.971236	0.994283
6	-1.78691	4.243566	-1.45535
1	-1.138859	2.382941	-2.365539
6	-1.7561	4.289388	0.970131
1	-1.079457	2.482546	1.941241
6	-2.003963	4.923479	-0.252117
1	-1.96898	4.740962	-2.403172
1	-1.91103	4.82184	1.903431
1	-2.356183	5.950415	-0.266507
16	-0.456594	0.594791	-0.184475
6	4.070465	-0.118438	-0.78388
8	4.867135	0.750098	-0.529238
6	3.370497	-0.353735	-2.085725
1	2.299792	-0.146376	-1.956562
1	3.789038	0.300801	-2.850127
1	3.470516	-1.400955	-2.384756
8	3.7124	-1.101726	0.14206
6	3.74758	-0.890565	1.515169
8	3.65637	0.203786	2.014177
6	3.851588	-2.201029	2.238842
1	4.814434	-2.668235	2.007701
1	3.76685	-2.035911	3.312375
1	3.06617	-2.881361	1.89779
1	-2.706078	0.061026	-0.937933
1	-2.57993	0.083067	0.850515

1+Ac2O (conformer 2)

6	-2.350758	-0.43649	-0.241139
8	0.264	-0.35674	-0.907568
6	-2.505854	-1.941868	-0.32719
8	-3.099012	-2.301266	-1.470951
8	-2.140069	-2.710106	0.544676
6	-3.362185	-3.723534	-1.689199
1	-2.553135	-4.297333	-1.234385
1	-3.321595	-3.830741	-2.774072
6	-4.721376	-4.116059	-1.135651
1	-4.915717	-5.167238	-1.373268
1	-4.756235	-4.000325	-0.048816
1	-5.515678	-3.511559	-1.583608
6	-0.847747	1.790666	0.300291
6	-0.525324	2.527204	-0.840057
6	-1.282956	2.411376	1.474548
6	-0.667262	3.917445	-0.809747
1	-0.161562	2.01627	-1.726123
6	-1.426627	3.801617	1.491588
1	-1.502916	1.827116	2.364094
6	-1.120496	4.552566	0.351505
1	-0.421012	4.502551	-1.690634
1	-1.765971	4.295789	2.39667
1	-1.226239	5.632957	0.37157
16	-0.622462	-0.01798	0.291926
6	4.180247	-0.65336	-0.198704
8	5.060063	-0.278895	-0.938908
6	3.279347	-1.832624	-0.39351
1	2.257976	-1.470141	-0.569996
1	3.622611	-2.417254	-1.246714
1	3.262306	-2.449493	0.509133
8	3.891525	-0.021141	1.001991
6	4.320068	1.262041	1.34485
8	4.456815	1.484673	2.523599
6	4.488147	2.275311	0.249455
1	3.718962	2.168021	-0.518336
1	4.445961	3.268834	0.696355
1	5.458397	2.132824	-0.232979
1	-2.543945	0.055456	-1.19571
1	-3.02647	-0.049245	0.527675

1+Ac2O (conformer 3)

6	-2.307553	-0.435875	-0.436839
8	0.156757	-0.099272	-1.491412
6	-2.389774	-1.931238	-0.666561
8	-1.761585	-2.613859	0.299884
8	-2.979555	-2.431941	-1.605757
6	-1.759123	-4.073918	0.221814
1	-2.715273	-4.397694	-0.192925
1	-1.688065	-4.389	1.263908
6	-0.5835	-4.575732	-0.59895
1	-0.577075	-5.670771	-0.583287
1	-0.65787	-4.24909	-1.639631
1	0.363982	-4.221352	-0.182596
6	-0.931348	1.903073	-0.035017
6	-0.830587	2.705357	-1.17187
6	-1.257227	2.438983	1.214077
6	-1.08682	4.074703	-1.057346
1	-0.545561	2.261826	-2.12075
6	-1.517832	3.808267	1.315267
1	-1.303498	1.805995	2.096265
6	-1.433602	4.623907	0.181581
1	-1.011347	4.710971	-1.933875
1	-1.774021	4.237022	2.279178
1	-1.62831	5.68868	0.266257
16	-0.555766	0.12409	-0.157007
6	4.236144	0.408048	-1.049358
8	4.849166	1.443218	-1.127327
6	3.484128	-0.285921	-2.141443
1	2.409955	-0.242375	-1.917965
1	3.686606	0.204068	-3.093719
1	3.770544	-1.340334	-2.187426
8	4.185051	-0.344228	0.127663
6	4.315537	0.227298	1.388028
8	4.029241	1.375675	1.620066
6	4.793259	-0.79597	2.376324
1	5.815369	-1.095165	2.121696
1	4.769793	-0.376107	3.38138
1	4.167358	-1.691216	2.324598
1	-2.69728	0.092859	-1.307602
1	-2.873565	-0.163916	0.459504

TS(1-2) 1 imag freq

6	-1.600677	-0.987692	-0.425752
8	0.853798	-0.737917	-1.114788
6	-1.6269	-2.508584	-0.360362
8	-2.550236	-2.980985	-1.197632
8	-0.920434	-3.171732	0.372891
6	-2.775149	-4.430011	-1.226176
1	-1.818781	-4.92742	-1.058073
1	-3.111377	-4.6166	-2.246708
6	-3.820382	-4.83621	-0.202675
1	-4.012389	-5.910205	-0.295859
1	-3.476819	-4.639324	0.816541
1	-4.761431	-4.304515	-0.371384
6	-0.343481	1.409896	0.111321
6	-0.661212	2.036786	-1.098028
6	-0.283156	2.111862	1.317971
6	-0.942219	3.402358	-1.08719
1	-0.667139	1.482884	-2.03078
6	-0.581468	3.477359	1.31318
1	0.012977	1.608296	2.231448
6	-0.909543	4.118613	0.116168
1	-1.183317	3.907315	-2.017051
1	-0.539978	4.037788	2.241436
1	-1.130256	5.181506	0.115715
16	-0.004891	-0.35326	0.209754
6	2.386497	-0.42939	-1.168168
8	2.716107	0.720385	-1.04134
6	2.927862	-1.447294	-2.133645
1	2.59972	-2.454052	-1.882765
1	2.580029	-1.184318	-3.138246
1	4.017344	-1.393021	-2.110836
8	2.890837	-1.456786	0.441349
6	2.944911	-0.843632	1.578631
8	2.25329	0.149504	1.885694
6	3.954089	-1.411528	2.571467
1	4.955399	-1.058356	2.298303
1	3.73046	-1.075798	3.586158
1	3.967949	-2.504008	2.531658
1	-1.76519	-0.617913	-1.438887
1	-2.374568	-0.581816	0.234527

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6	-1.720921	-0.534258	-0.600926
8	0.757365	-0.482852	-1.230638
6	-1.806887	-2.05305	-0.540933
8	-2.876353	-2.469186	-1.219081
8	-1.018302	-2.76109	0.053886
6	-3.165528	-3.907107	-1.232616
1	-2.217081	-4.446397	-1.231548
1	-3.672159	-4.057647	-2.186605
6	-4.045518	-4.292857	-0.057058
1	-4.295245	-5.35636	-0.132411
1	-3.53219	-4.130399	0.894638
1	-4.978184	-3.721197	-0.061684
6	-0.385183	1.798324	0.048961
6	-0.967432	2.455274	-1.04333
6	-0.028837	2.471784	1.222506

6	-1.202052	3.824163	-0.946003
1	-1.214905	1.930483	-1.958924
6	-0.288365	3.843378	1.303937
1	0.445774	1.92334	2.035682
6	-0.867998	4.516025	0.226727
1	-1.643195	4.351985	-1.785245
1	-0.024952	4.382439	2.208269
1	-1.057372	5.582991	0.292981
16	-0.120114	0.025623	0.115402
6	1.885374	0.189624	-1.746433
8	2.045574	1.373465	-1.65707
6	2.747846	-0.812893	-2.453067
1	3.259352	-1.417721	-1.697943
1	2.142896	-1.483117	-3.068231
1	3.480016	-0.287252	-3.06561
8	2.304887	0.097358	1.002804
6	2.359553	-0.013124	2.272511
8	1.4515	0.345604	3.072282
6	3.621085	-0.659409	2.856854
1	3.876408	-0.208802	3.819958
1	3.42289	-1.72429	3.030104
1	4.467168	-0.57874	2.16996
1	-1.846986	-0.170301	-1.621241
1	-2.500873	-0.09818	0.031796
	4		
6	-0.786696	0.188952	0.210703
6	0.044552	1.204272	-0.277152
6	-0.483762	2.245361	-1.041479
6	-1.856024	2.245056	-1.313835
6	-2.704823	1.248683	-0.819101
6	-2.157669	0.212901	-0.056867
16	-2.647921	3.515734	-2.300168
8	-2.448788	5.016093	-0.849015
6	-1.346835	5.73136	-0.809331
6	-1.496628	7.014827	-0.005876
6	-1.715072	3.615825	-3.64444
6	-2.206688	4.434918	-4.761713
8	-3.259912	5.059668	-4.765892
8	-1.344297	4.380076	-5.793366
6	-1.680902	5.127104	-7.000186
6	-1.144496	6.547594	-6.929489
8	-0.288783	5.426455	-1.369431
1	-2.764368	5.107436	-7.130829
1	-1.206583	4.557626	-7.801161
1	-1.356299	7.059304	-7.87439
1	-1.619736	7.110463	-6.121533
1	-0.061595	6.548883	-6.773805
1	0.142421	3.059394	-1.388659
1	-3.769695	1.272112	-1.027798
1	1.106816	1.193715	-0.054193
1	-2.805489	-0.569108	0.32586
1	-0.365533	-0.614941	0.806373
1	-2.058914	7.742436	-0.601202
1	-2.056731	6.83614	0.915371
1	-0.512271	7.426229	0.224276
1	-0.706764	3.223236	-3.666306
	TS(4r-4s)	1 imag freq	
6	-0.854926	0.439491	0.416603
8	1.128808	2.026675	-1.392002
6	-2.244496	0.725023	-0.030638
8	-3.009893	1.047863	1.027109
8	-2.630696	0.730457	-1.19173
6	-4.390223	1.447027	0.774392
1	-4.431167	1.974174	-0.180286
1	-4.61399	2.143599	1.584203
6	-5.32006	0.245254	0.797991
1	-6.353589	0.585974	0.6739
1	-5.089721	-0.449381	-0.014597
1	-5.247342	-0.286654	1.751477
6	1.683485	-0.682339	-0.187711
6	2.020089	-0.554635	1.162906
6	2.636499	-1.040098	-1.15021
6	3.3397	-0.792707	1.548856
1	1.284401	-0.278514	1.906306
6	3.948562	-1.287582	-0.745878
1	2.363371	-1.11351	-2.198041
6	4.300068	-1.161728	0.601233
1	3.613237	-0.692762	2.594198
1	4.693292	-1.565095	-1.484537
1	5.323248	-1.346521	0.913149
16	0.043159	-0.38911	-0.85276
6	1.00322	2.930818	-0.535079
8	0.330986	2.779127	0.562667
6	1.642837	4.290329	-0.741048
1	2.270832	4.540163	0.119775
1	2.242504	4.302804	-1.652471
1	0.861485	5.054627	-0.807991
8	-0.466772	-2.522609	1.253142
6	-0.74672	-2.84868	0.123124
8	-0.584395	-2.020262	-0.967609
6	-1.307391	-4.171855	-0.320423

1	-2.251215	-4.019246	-0.850948
1	-0.611126	-4.654443	-1.012493
1	-1.464089	-4.804467	0.553005
1	-0.240289	1.609979	0.509726
1	-0.797081	-0.05483	1.38211
	TS(3-4)	1 imag freq	
6	-0.854926	0.439491	0.416603
8	1.128808	2.026675	-1.392002
6	-2.244496	0.725023	-0.030638
8	-3.009893	1.047863	1.027109
8	-2.630696	0.730457	-1.19173
6	-4.390223	1.447027	0.774392
1	-4.431167	1.974174	-0.180286
1	-4.61399	2.143599	1.584203
6	-5.32006	0.245254	0.797991
1	-6.353589	0.585974	0.6739
1	-5.089721	-0.449381	-0.014597
1	-5.247342	-0.286654	1.751477
6	1.683485	-0.682339	-0.187711
6	2.020089	-0.554635	1.162906
6	2.636499	-1.040098	-1.15021
6	3.3397	-0.792707	1.548856
1	1.284401	-0.278514	1.906306
6	3.948562	-1.287582	-0.745878
1	2.363371	-1.11351	-2.198041
6	4.300068	-1.161728	0.601233
1	3.613237	-0.692762	2.594198
1	4.693292	-1.565095	-1.484537
1	5.323248	-1.346521	0.913149
16	0.043159	-0.38911	-0.85276
6	1.00322	2.930818	-0.535079
8	0.330986	2.779127	0.562667
6	1.642837	4.290329	-0.741048
1	2.270832	4.540163	0.119775
1	2.242504	4.302804	-1.652471
1	0.861485	5.054627	-0.807991
8	-0.466772	-2.522609	1.253142
6	-0.74672	-2.84868	0.123124
8	-0.584395	-2.020262	-0.967609
6	-1.307391	-4.171855	-0.320423
1	-2.251215	-4.019246	-0.850948
1	-0.611126	-4.654443	-1.012493
1	-1.464089	-4.804467	0.553005
1	-0.240289	1.609979	0.509726
1	-0.797081	-0.05483	1.38211
	3		
6	1.04772	-0.124349	0.48745
8	-0.52863	-2.057625	-0.681871
6	2.381824	-0.451072	-0.158686
8	3.323274	-0.497906	0.786631
8	2.559188	-0.640848	-1.346848
6	4.69823	-0.78965	0.37498
1	4.664661	-1.484114	-0.466064
1	5.126703	-1.28903	1.244938
6	5.444885	0.487543	0.032615
1	6.485341	0.241109	-0.20402
1	5.005611	0.983674	-0.837163
1	5.441152	1.181564	0.878225
6	-1.817366	0.249907	0.011311
6	-1.950766	0.49135	1.3792
6	-2.918693	0.2838	-0.852062
6	-3.22062	0.773424	1.887258
1	-1.098091	0.464535	2.043292
6	-4.181065	0.567219	-0.328019
1	-2.797144	0.093332	-1.913768
6	-4.331911	0.811954	1.040108
1	-3.335953	0.963074	2.949577
1	-5.040559	0.595761	-0.989915
1	-5.314297	1.0324	1.446032
16	-0.254703	-0.125934	-0.808989
6	-0.742525	-2.801177	0.398072
8	-0.664622	-2.395073	1.556035
6	-1.107783	-4.228967	0.046488
1	-1.077901	-4.850665	0.942154
1	-2.119353	-4.246337	-0.372764
1	-0.428694	-4.624631	-0.712914
8	0.159458	2.770763	0.722712
6	0.139559	2.805518	-0.506125
8	0.060803	1.738229	-1.29361
6	0.19627	4.096082	-1.297679
1	0.454159	4.92512	-0.637558
1	0.923405	4.017554	-2.109814
1	-0.784132	4.282871	-1.748409
1	0.773225	-0.873377	1.231965
1	1.061368	0.869404	0.938917
	TS(4-6)-cyc	1 imag freq	
6	-0.860505	0.00232	-1.506254
8	1.056391	1.866684	0.230479

6	-1.586279	-1.03776	-0.726213
8	-2.898992	-0.916085	-0.972682
8	-1.076154	-1.87446	-0.007795
6	-3.80404	-1.840351	-0.2932
1	-3.310971	-2.811232	-0.216479
1	-4.654632	-1.914216	-0.972294
6	-4.214456	-1.30173	1.06716
1	-4.93985	-1.987552	1.517527
1	-3.355281	-1.221118	1.737974
1	-4.68323	-0.31814	0.972204
1	-1.464564	0.68592	-2.094232
6	1.645622	-1.054955	-0.813774
6	2.147998	-0.933372	0.482558
6	1.931413	-2.165034	-1.616824
6	2.927731	-1.973691	0.994958
1	1.921982	-0.04907	1.064815
6	2.71156	-3.194887	-1.086579
1	1.549487	-2.234838	-2.630203
6	3.207365	-3.101164	0.217409
1	3.315825	-1.89816	2.005991
1	2.931308	-4.065658	-1.696258
1	3.815009	-3.90367	0.624204
16	0.742989	0.301851	-1.598084
6	-0.131002	2.270648	0.521073
8	-1.113995	1.495414	0.648451
6	-0.330993	3.774367	0.656257
1	-1.21282	3.993652	1.262791
1	0.552434	4.247832	1.092773
1	-0.481461	4.20466	-0.341438
	TS(4-6)-sld	1 imag freq	
6	-7.0871	5.258438	2.906968
6	-8.261632	4.930234	2.218879
6	-8.407756	3.675898	1.628701
6	-7.358908	2.7569	1.74628
6	-6.165103	3.07734	2.404715
6	-6.041612	4.335677	2.998559
16	-7.395399	1.174104	0.910124
8	-9.348382	1.739213	-0.740047
6	-9.882134	2.18513	-1.822704
6	-8.971533	3.033647	-2.712777
6	-8.673554	0.281222	1.407232
6	-9.698104	0.550347	2.45891
8	-10.664187	-0.366842	2.353837
6	-11.774243	-0.299602	3.306825
6	-12.857905	0.644868	2.815556
8	-9.628731	1.423727	3.301853
8	-11.058574	1.949634	-2.177609
1	-11.373425	0.001756	4.276346
1	-12.126679	-1.330228	3.358768
1	-13.697608	0.615088	3.517725
1	-12.494744	1.674373	2.760157
1	-13.221989	0.342648	1.829788
1	-5.351595	2.361304	2.464382
1	-5.127485	4.591539	3.524326
1	-6.983818	6.238464	3.362278
1	-9.065814	5.654417	2.136182
1	-9.300247	3.412852	1.074103
1	-8.251807	2.378813	-3.217459
1	-9.554997	3.562693	-3.469423
1	-8.400306	3.749533	-2.114464
1	-8.743185	-0.674053	0.894261
	6		
6	1.702809	3.813361	-4.732737
6	1.263036	2.537709	-5.102483
6	1.008226	1.572339	-4.125123
6	1.175064	1.88817	-2.768251
6	1.619642	3.165012	-2.399002
6	1.885213	4.123578	-3.382088
16	0.902571	0.637168	-1.502063
6	-0.93169	0.694257	-1.405237
6	-1.485666	-0.606195	-0.79357
8	-0.845994	-1.632186	-0.683963
8	-2.784719	-0.468384	-0.514912
6	-3.497649	-1.634137	0.007883
6	-3.395731	-1.711337	1.521348
8	-0.85027	1.117097	1.266282
6	-1.323184	1.995584	0.573673
6	-1.84546	3.320696	1.051619
8	-1.443655	1.878882	-0.778441
1	-3.096107	-2.527032	-0.474547
1	-4.525872	-1.473779	-0.319749
1	-3.993634	-2.557914	1.875345
1	-2.36236	-1.863048	1.843324
1	-3.781884	-0.800313	1.987552
1	-1.316459	0.763751	-2.424959
1	0.686695	0.576069	-4.413357
1	1.757168	3.404874	-1.349599
1	1.128897	2.28926	-6.151126
1	2.230506	5.110982	-3.09031
1	1.907571	4.559412	-5.494768
1	-1.255902	4.130431	0.611063

1	-2.881932	3.453614	0.728411
1	-1.783652	3.367355	2.138296

TS(2-7) 1 imag freq

6	0.949881	-0.613368	0.128701
8	-1.583166	-1.747833	0.28899
6	1.698779	0.311089	-0.784791
8	2.261128	-0.36196	-1.796759
8	1.725932	1.520758	-0.643394
6	3.035018	0.399111	-2.773092
1	2.551868	1.367194	-2.918877
1	2.952562	-0.191228	-3.687035
6	4.480885	0.548036	-2.330142
1	5.044174	1.065344	-3.114086
1	4.555084	1.133948	-1.410356
1	4.941097	-0.430265	-2.164013
1	0.657932	-0.232911	1.099174
8	2.869924	-0.840247	1.125887
1	1.055868	-1.679876	-0.009909
6	-1.839307	0.91708	-0.239064
6	-1.721645	1.366867	1.084979
6	-2.569151	1.640351	-1.194454
6	-2.354551	2.553568	1.449222
1	-1.156599	0.80564	1.820879
6	-3.178337	2.838623	-0.81746
1	-2.662467	1.270122	-2.210143
6	-3.074579	3.290767	0.5006
1	-2.275952	2.908628	2.471493
1	-3.740856	3.407779	-1.550212
1	-3.556215	4.218703	0.79256
16	-1.045358	-0.563004	-0.816132
6	2.770807	-0.515099	2.36911
8	1.728618	-0.101848	2.926998
6	4.062491	-0.632756	3.178329
1	3.837938	-0.782647	4.236795
1	4.691208	-1.444846	2.805727
1	4.624882	0.302632	3.075726
6	-2.764118	-2.414698	-0.030205
8	-3.416911	-2.141549	-1.005977
6	-3.048745	-3.459458	1.008192
1	-2.221464	-4.173359	1.052831
1	-3.136256	-2.989753	1.991943
1	-3.975361	-3.972315	0.753219

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6	-3.154911	3.250804	0.024669
6	-2.046715	2.691844	0.670598
6	-1.614833	1.406194	0.336785
6	-2.305554	0.676344	-0.645875
6	-3.417926	1.238157	-1.295029
6	-3.838338	2.526297	-0.958253
16	-1.727009	-0.940675	-1.118692
8	-2.482882	-1.949521	0.093558
6	-3.740792	-2.435026	-0.142067
6	-4.174421	-3.310156	1.007194
8	-4.397842	-2.18124	-1.127939
6	2.346212	-1.020739	0.062746
6	2.979654	0.249613	-0.490923
8	3.754651	0.963263	0.113955
8	2.557971	0.447799	-1.746434
6	3.075644	1.605212	-2.473074
6	4.349745	1.253109	-3.221764
8	2.741311	-1.257009	1.414808
6	2.102974	-0.541387	2.374722
6	2.656465	-0.84317	3.739356
8	1.202277	0.238952	2.127791
1	3.231391	2.417956	-1.761555
1	2.266479	1.868884	-3.155755
1	4.674835	2.120287	-3.806357
1	5.154827	0.986085	-2.531499
1	4.18124	0.419923	-3.9106
1	1.25878	-0.959678	-0.02819
1	2.704484	-1.878879	-0.509543
1	-0.750836	0.971532	0.829634
1	-3.943709	0.664547	-2.050523
1	-1.515441	3.257443	1.430067
1	-4.696877	2.9623	-1.459949
1	-3.484344	4.252446	0.284953
1	3.668451	-0.432241	3.815379
1	2.023006	-0.389711	4.501068
1	2.724869	-1.92282	3.895263
1	-3.44338	-4.10625	1.172128
1	-4.22782	-2.714162	1.923226
1	-5.15237	-3.737776	0.787324

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8	-1.255143	1.274781	-0.682176
16	-0.923341	-0.000144	0.000044
6	0.958557	-0.000005	0.000242
9	1.447331	-1.104445	0.602917
9	1.446811	1.074465	0.655209
9	1.446741	0.030381	-1.257852
8	-1.256247	-0.046874	1.444998
8	-1.255675	-1.228139	-0.76334

TMS+

14	-0.005325	0.008368	0.015166
6	1.818512	-0.242381	-0.004947
1	2.086183	-0.894848	-0.845563
1	2.36565	0.699143	-0.081724
1	2.119486	-0.767465	0.910868
6	-1.126009	-1.451366	0.063835
1	-1.552688	-1.591031	-0.939575
1	-0.597351	-2.364101	0.347168
1	-1.963502	-1.269586	0.745548
6	-0.707915	1.70989	-0.002406
1	-0.161391	2.342788	-0.709312
1	-1.774502	1.711958	-0.237321
1	-0.567635	2.147863	0.996512

TfOH

1	-0.411001	1.042046	0.362998
8	-2.605508	3.134604	-0.891239
16	-2.174052	1.766769	-0.669445
6	-3.518396	0.918548	0.348316
9	-3.076046	-0.270546	0.766663
9	-4.590443	0.749301	-0.427382
9	-3.837972	1.672851	1.399138
8	-1.821023	0.859205	-1.752364
8	-0.990407	1.826217	0.428793

TMSOTf

8	-1.298479	1.875324	0.913799
8	0.443369	0.131432	0.622367
6	-2.037766	-0.571429	0.099612
14	2.079559	-0.207327	-0.018232
6	2.835122	1.444337	-0.460898
1	2.294735	1.926204	-1.281523
1	2.838964	2.120892	0.399939
1	3.873677	1.297555	-0.780108
6	1.878015	-1.35637	-1.479062
1	1.365937	-2.280257	-1.191764
1	1.31477	-0.881526	-2.287923
1	2.867256	-1.6257	-1.867509
6	2.857328	-1.017164	1.474591
1	2.868	-0.336234	2.331546
1	2.3156	-1.925005	1.758651
1	3.892883	-1.296012	1.247949
16	-0.805858	0.848952	0.002189
8	-0.616945	1.14622	-1.416832
9	-2.203551	-0.956154	1.368529
9	-1.602052	-1.609551	-0.622659
9	-3.209805	-0.154102	-0.391811

TMSOAc

8	-2.72713	-1.140466	-0.031159
6	-1.832781	-0.310515	-0.030402
8	-0.554129	-0.713784	-0.063709
6	-2.098256	1.178019	-0.015686
1	-3.164713	1.357085	0.118487
1	-1.541844	1.670215	0.786761
1	-1.777697	1.620472	-0.964108
14	1.017782	-0.002133	0.014934
6	1.261056	0.727056	1.730019
1	0.61727	1.593271	1.914181
1	1.061215	-0.020491	2.505298
1	2.300307	1.058325	1.843134
6	1.211168	1.288198	-1.338375
1	0.926133	0.883321	-2.315641
1	0.618851	2.189113	-1.150996
1	2.263614	1.591049	-1.397524
6	2.138804	-1.474778	-0.276916
1	1.978753	-2.245698	0.48439
1	1.951999	-1.921493	-1.259396
1	3.190913	-1.170209	-0.23675

DMAC

8	-1.077311	-1.478479	-0.019558
6	-0.726916	-0.285993	-0.006831
6	-1.775992	0.815506	-0.006559
1	-1.698979	1.450028	0.881976
1	-1.689288	1.458765	-0.887923
1	-2.756029	0.33899	-0.014423
7	0.587581	0.07651	0.008761
6	1.630524	-0.944904	0.004556
1	2.248884	-0.8511	-0.896228
1	2.276664	-0.825256	0.881982
1	1.168061	-1.929337	0.025376
6	1.077439	1.450929	0.008745
1	1.684311	1.635154	-0.886075
1	0.259198	2.166306	0.023145
1	1.705698	1.625044	0.890363

DMAC/TMSOAc

8	0.970312	-0.995732	-0.15946
6	-0.142853	-1.293449	0.447472
6	-0.231785	-1.234955	1.943237
1	-1.106304	-0.660647	2.249411
1	-0.30179	-2.247954	2.353838
1	0.658806	-0.760079	2.345461
7	-1.123408	-1.786356	-0.275673
6	-1.102095	-1.751447	-1.743501
1	-1.430874	-2.721391	-2.12286
1	-1.794053	-0.96906	-2.069574
1	-0.099286	-1.537007	-2.100915
6	-2.424963	-2.141618	0.306048
1	-2.846156	-2.960825	-0.279024
1	-2.318275	-2.469747	1.337436
1	-3.072005	-1.260307	0.24231
14	2.245717	0.198591	-0.135253
6	1.891875	1.290784	-1.612307
1	0.924873	1.785891	-1.482745
1	2.667781	2.059281	-1.70899
1	1.870484	0.711421	-2.541368
6	3.774633	-0.862062	-0.36506
1	4.665393	-0.227401	-0.439412
1	3.916184	-1.543657	0.480717
1	3.709281	-1.458954	-1.281022
6	2.273717	1.163285	1.469199
1	2.571376	0.554075	2.328699
1	3.010626	1.969718	1.366914
1	1.296381	1.616039	1.65965
8	-0.999401	1.365921	0.488896
8	-2.961957	0.944266	-0.544789
6	-2.4948	3.202273	0.130259
6	-2.128107	1.710715	0.022078
1	-2.120721	3.631586	1.064514
1	-3.574646	3.355715	0.056147
1	-2.017258	3.745527	-0.694901

DMAC/TMSOtf (conformer 1)

8	-2.059165	-0.000334	-0.435554
6	-1.888301	1.06807	0.285397
6	-2.104018	1.043653	1.768479
1	-1.129732	0.97723	2.263514
1	-2.621753	1.938185	2.116612
1	-2.696306	0.173312	2.045111
7	-1.528542	2.160203	-0.350862
6	-1.318577	2.159552	-1.809769
1	-1.542862	3.159975	-2.181604
1	-0.273808	1.90904	-2.015318
1	-1.976652	1.434043	-2.282207
6	-1.199754	3.421535	0.327488
1	-1.987058	4.15686	0.1389
1	-1.074455	3.277084	1.396426
1	-0.258159	3.790177	-0.083709
14	-2.39543	-1.708194	-0.176307
6	-1.968464	-2.417018	-1.851546
1	-0.91093	-2.25883	-2.086481
1	-2.161204	-3.495815	-1.862087
1	-2.571099	-1.95723	-2.641676
6	-4.222699	-1.840846	0.22081
1	-4.500359	-2.89887	0.297214
1	-4.48208	-1.361344	1.170206
1	-4.830892	-1.390841	-0.57095
6	-1.277159	-2.339085	1.186438
1	-1.632404	-2.068993	2.185428
1	-1.237327	-3.433504	1.132627
1	-0.259455	-1.954203	1.066758
8	1.058754	0.534851	1.133709
16	2.20451	0.977656	0.298687
8	1.8854	1.17879	-1.136527
8	3.058472	2.024015	0.908934
6	3.322423	-0.535258	0.279611
9	4.431101	-0.310427	-0.45362
9	3.712368	-0.866916	1.527378
9	2.686566	-1.601421	-0.249995

DMAC/TMSOtf (conformer 2)

8	1.919778	0.257812	0.429862
6	2.005841	0.851724	0.242547
6	2.419839	0.875556	1.681442
1	1.625511	1.296314	2.305047
1	3.313067	1.497746	1.785875
1	2.644938	0.127619	2.034751
7	1.716768	0.385681	1.970514
6	1.368731	1.814309	2.003430
1	2.107866	2.339806	2.613332
1	0.380661	1.927541	2.455984
1	1.364763	2.222482	0.997349
6	1.832582	3.279280	0.284115
1	2.888268	3.531557	0.409593
1	1.330210	3.264823	1.251741
1	1.348805	0.347655	4.022450
14	2.150620	1.981281	0.148352
6	1.764076	2.669157	1.842042
1	0.742400	2.420155	2.147240
1	1.858124	3.760925	1.833105
1	2.456121	2.276379	2.594121
6	3.930777	2.261458	0.357986

1	4.135801	3.338682	0.344251
1	-4.153688	-1.896082	1.364831
1	4.620338	1.780443	0.343160
6	0.901947	2.505676	1.147063
1	1.109888	2.080096	2.133707
1	0.927356	3.597366	1.246128
1	0.113773	2.220439	0.853073
8	-4.937789	2.253901	40.037125
16	-6.333936	2.579665	0.427729
8	-7.305480	1.474431	0.253495
8	-6.462060	3.347116	1.689767
6	-6.856080	3.821870	-0.885242
9	-8.121637	4.239474	-0.683513
9	-6.055597	4.908753	-0.871008
9	-6.791196	3.280780	-2.119565

DMAC/TMSOtf (conformer 3)

8	-1.925413	0.116011	-0.462851
6	-1.829589	1.160927	0.295236
6	-2.096243	1.083790	1.770929
1	-1.151266	1.109008	2.324363
1	-2.715310	1.916917	2.107802
1	-2.606400	0.153789	2.010869
7	-1.479138	2.295468	-0.277999
6	-1.257380	2.392106	-1.730320
1	-1.704643	3.323542	-2.082309
1	-0.182926	2.408155	-1.934261
1	-1.714869	1.546878	-2.236679
6	-1.275376	3.545915	0.469641
1	-2.157200	4.185691	0.372200
1	-1.074294	3.351788	1.519902
1	-0.413272	4.058857	0.040291
14	-2.338998	-1.609989	-0.284253
6	-2.064724	-2.200298	-2.032507
1	-1.024633	-2.055192	-2.342544
1	-2.296606	-3.269054	-2.083121
1	-2.715534	-1.671295	-2.736467
6	-4.131490	-1.673648	0.247557
1	-4.448116	-2.721922	0.221175
1	-4.295253	-1.298350	1.262478
1	-4.766275	-1.105556	-0.440718
6	-1.125220	-2.329468	0.944175
1	-1.269235	-1.951944	1.961069
1	-1.275245	-3.414424	0.963418
1	-0.091817	-2.131133	0.640448
8	-3.106771	-4.974071	-0.240793
16	-3.602728	-6.308280	0.180462
8	-3.323395	-6.662721	1.593046
8	-4.962342	-6.651818	-0.301326
6	-2.498227	-7.489780	-0.781173
9	-2.810991	-8.774198	-0.514339
9	-2.626053	-7.302425	-2.111597
9	-1.198578	-7.308435	-0.464591

DMAC/TMS+

8	0.013732	0.333435	-0.001795
6	1.10041	-0.376013	0.003387
6	1.053767	-1.876182	-0.022711
1	1.353523	-2.245072	-1.009219
1	1.724099	-2.306668	0.723399
1	0.043418	-2.224806	0.178269
7	2.241774	0.279407	0.023505
6	2.282857	1.750911	0.086211
1	3.136509	2.038799	0.701056
1	2.409476	2.156932	-0.921371
1	1.36477	2.13411	0.523468
6	3.555503	-0.378959	-0.042908
1	4.031862	-0.346514	0.94075
1	3.467312	-1.409311	-0.375091
1	4.173098	0.167456	-0.758303
14	-1.736078	0.076058	-0.007465
6	-2.349792	1.834342	-0.138293
1	-2.001664	2.305856	-1.063
1	-3.445521	1.847612	-0.1438
1	-2.008573	2.437598	0.709231
6	-2.176204	-0.731783	1.622875
1	-3.267768	-0.792496	1.706584
1	-1.781147	-1.747501	1.72073
1	-1.809847	-0.135015	2.46468
6	-2.153853	-0.9528	-1.515025
1	-1.784802	-1.98071	-1.450809
1	-3.244428	-0.999543	-1.618443
1	-1.753107	-0.495658	-2.425883

TS(1-2)+TMS++DMAC 1 imag freq

6	-1.413093	1.911387	-0.07987
8	-1.273264	-0.295065	1.394184
6	-0.008544	2.425316	0.19037
8	-0.058995	3.692138	0.598077
8	1.003742	1.7683	0.031485
6	1.205747	4.390276	0.850497
1	1.913426	3.674004	1.270914
1	0.942047	5.13047	1.606562
6	1.730439	5.039578	-0.417711
1	2.635374	5.608174	-0.179371
1	1.987248	4.290962	-1.172192
1	0.99364	5.730574	-0.837415
6	-3.186266	-0.16017	-0.505894
6	-4.158805	-0.029671	0.489279
6	-3.514875	-0.512147	-1.817943
6	-5.496407	-0.241573	0.15068
1	-3.873861	0.215179	1.50731
6	-4.85929	-0.712592	-2.14406
1	-2.742102	-0.632841	-2.571383
6	-5.845515	-0.577624	-1.162674
1	-6.264236	-0.145937	0.911827
1	-5.13052	-0.985067	-3.158916
1	-6.887553	-0.742375	-1.418372
16	-1.437407	0.076313	-0.114695
6	-0.277468	-2.028939	1.747128
8	-0.252463	-2.678812	0.778883
6	-0.725899	-2.141684	3.152907
1	-0.650123	-1.188033	3.667442
1	-1.760024	-2.492769	3.139626
1	-0.088845	-2.885548	3.640385
8	1.306977	-1.055684	2.079045
6	2.233958	-0.874597	1.253741
8	2.14859	-1.350174	0.050351
6	3.431296	-0.078282	1.685521
1	3.427853	0.044351	2.767759
1	4.357597	-0.561424	1.366413
1	3.373501	0.907087	1.212181
1	-2.122408	2.253117	0.676909
1	-1.746667	2.256646	-1.064314
14	3.149356	-1.426844	-1.394776
6	4.440772	-2.741732	-1.06225
1	5.127196	-2.459154	-0.257374
1	3.971207	-3.694902	-0.79804
1	5.038603	-2.900585	-1.967463
6	3.87417	0.266563	-1.737615
1	3.110721	1.046659	-1.654865
1	4.702802	0.515125	-1.068051
1	4.261667	0.279618	-2.763291
6	1.897821	-1.941339	-2.683605
1	1.424789	-2.891616	-2.416059
1	1.114194	-1.184677	-2.793447
1	2.388647	-2.066475	-3.655363

TS(1-2)+TMS+ 1 imag freq

6	0.829284	0.408737	1.5961
8	-1.157405	2.09896	1.008308
6	-0.056314	-0.714577	2.097835
8	0.332761	-1.101579	3.312815
8	-0.968925	-1.213948	1.463962
6	-0.37562	-2.231477	3.91565
1	-0.273368	-3.089569	3.246462
1	-1.433361	-1.966033	3.986693
6	0.245155	-2.484916	5.273541
1	-0.266988	-3.326697	5.749934
1	1.305809	-2.736222	5.181875
1	0.144267	-1.610267	5.922643
6	1.276554	2.590003	-0.033399
6	1.127465	3.869285	0.50223
6	2.361452	2.247816	-0.84629
6	2.104232	4.830457	0.225359
1	0.263407	4.104347	1.114249
6	3.33235	3.217916	-1.106949
1	2.461393	1.244046	-1.248722
6	3.20352	4.505717	-0.57516
1	2.002498	5.830868	0.634291
1	4.184356	2.96763	-1.731266
1	3.957841	5.256678	-0.788819
16	-0.009291	1.344111	0.261484
6	-2.829584	2.421527	-0.082593
8	-2.583052	2.372573	-1.223875
6	-3.408848	3.391054	0.876657
1	-3.31476	3.036311	1.899194
1	-2.880891	4.338078	0.746835
1	-4.464102	3.518498	0.618087
8	-3.61548	0.882574	0.610703
6	-3.602865	-0.2484	0.064282
8	-2.967377	-0.436645	-1.048335
6	-4.328948	-1.374077	0.741506
1	-4.943245	-0.987565	1.553463
1	-4.953396	-1.916972	0.027648
1	-3.585567	-2.066017	1.149032
1	1.102407	1.103705	2.392418
1	1.730526	-0.027735	1.138603
14	-2.707997	-1.756703	-2.185945
6	-2.20897	-3.295585	-1.241542
1	-1.427478	-3.070443	-0.509058
1	-3.049407	-3.766179	-0.722952
1	-1.807203	-4.026603	-1.953353
6	-1.317825	-1.077008	-3.232761
1	-1.604594	-0.131232	-3.703562
1	-0.420614	-0.904438	-2.629634
1	-1.063604	-1.789126	-4.026059
6	-4.31333	-1.946708	-3.132908
1	-5.132808	-2.296304	-2.496568
1	-4.612321	-1.000292	-3.595282
1	-4.177437	-2.684196	-3.93274
8	2.877014	-1.069234	-0.3133
6	3.939802	-1.722479	-0.322781
6	4.828654	-1.741457	0.909565
1	4.343349	-1.144956	1.681583
1	4.976795	-2.757227	1.288657
1	5.814063	-1.312269	0.702522
7	4.332595	-2.427486	-1.415586
6	3.506228	-2.444162	-2.620449
1	3.269496	-3.478483	-2.893676
1	2.585087	-1.896735	-2.433805
1	4.044447	-1.979689	-3.455009
6	5.566689	-3.203128	-1.510547
1	5.33362	-4.259442	-1.687915
1	6.17127	-2.838835	-2.348946
1	6.157266	-3.126308	-0.60151

TS(4-6)cyc+DMAC 1 imag freq

6	-0.777432	4.246963	-1.220485
6	0.560033	4.017558	-0.873859
6	0.98428	2.739713	-0.510735
6	0.04736	1.698866	-0.517093
6	-1.299137	1.909563	-0.838611
6	-1.70176	3.199034	-1.198642
16	0.498025	0.034404	-0.053856
6	1.916814	-0.228659	-0.827244
6	2.555097	-1.559066	-0.697811
8	2.138218	-2.453018	0.022881
8	1.325741	0.768073	2.125604
8	3.631029	-1.638566	-1.485639
6	4.37733	-2.893466	-1.458712
6	5.535471	-2.75596	-2.424893
1	-2.013309	1.089863	-0.822134
1	-2.739364	3.379201	-1.461303
1	-1.099254	5.246281	-1.49731
1	1.271717	4.837204	-0.871533
1	2.005472	2.551187	-0.195634
1	4.711443	-3.063119	-0.431622
1	3.694517	-3.699422	-1.740656
1	6.114531	-3.684647	-2.423654
1	5.179874	-2.574516	-3.443396
1	6.198523	-1.937188	-2.130935
1	2.38871	0.539324	-1.425248
8	-3.452859	-0.635	-0.833162
6	-4.031827	-1.42483	-0.064665
7	-5.308768	-1.208362	0.355695
6	-6.035293	-0.019169	-0.08044
1	-6.986725	-0.311778	-0.538597
1	-6.248462	0.631882	0.776028
1	-5.433398	0.52356	-0.806086
6	-6.039558	-2.065746	1.283792
1	-6.281947	-1.511635	2.198713
1	-6.977994	-2.39748	0.824675
1	-5.460026	-2.944157	1.555542
6	-3.313065	-2.671749	0.424716
1	-3.840957	-3.585539	0.13434
1	-2.320628	-2.680275	-0.024843
1	-3.206133	-2.676127	1.514015
6	2.58983	0.553358	2.095732
8	3.315332	0.831192	1.099914
6	3.211396	-0.117786	3.314342
1	4.282992	0.089065	3.366078
1	2.720497	0.21485	4.232856
1	3.071349	-1.202358	3.234655

TS(4-6)sld+DMAC 1 imag freq

6	-1.386141	4.737079	1.464833
6	-0.379432	4.825709	2.429766
6	0.471242	3.742641	2.649214
6	0.298721	2.569205	1.895043
6	-0.703024	2.470319	0.918705
6	-1.543313	3.563734	0.715943
16	1.476748	1.302942	2.288488
6	1.022114	-0.085932	1.553445
6	1.891625	-1.269362	1.788036
8	2.864321	-1.27282	2.524977
8	4.040992	2.712371	-1.065708
8	1.446028	-2.316746	1.089817
6	2.216236	-3.55339	1.199574
6	1.545226	-4.58952	0.3225
1	-0.840465	1.571766	0.328528
1	-2.321787	3.499732	-0.037567
1	-2.045894	5.581305	1.291083
1	-0.251234	5.733805	3.00942
1	1.258109	3.809526	3.394453
1	3.240198	-3.340046	0.881632
1	2.233351	-3.847513	2.252489
1	2.106675	-5.526902	0.384401

1	0.519873	-4.781382	0.651789
1	1.526983	-4.2684	-0.722878
1	0.143666	-0.182464	0.914398
8	-1.446502	-0.467368	-0.385254
6	-2.342467	-1.310407	-0.591702
7	-2.84865	-1.518375	-1.834301
6	-2.343373	-0.756415	-2.974338
1	-1.968734	-1.441684	-3.742822
1	-3.147802	-0.152273	-3.409703
1	-1.537707	-0.104927	-2.643687
6	-3.902615	-2.476137	-2.157085
1	-4.748724	-1.955794	-2.620294
1	-3.527116	-3.222122	-2.867156
1	-4.259484	-2.991523	-1.269234
6	-2.892656	-2.130182	0.563067
1	-2.756445	-3.203668	0.400872
1	-2.355001	-1.839399	1.465035
1	-3.960722	-1.945136	0.71509
6	3.402257	1.633739	-1.050469
8	2.717927	1.20375	-0.054091
6	3.443554	0.720075	-2.279772
1	4.226597	-0.033322	-2.133031
1	2.495409	0.193043	-2.41501
1	3.685332	1.295098	-3.1769

2+-OTf

6	-1.14705	-3.95869	-1.169562
6	-1.79874	-3.803586	0.053034
6	-1.191314	-3.075626	1.080026
6	0.071289	-2.501394	0.892964
6	0.745327	-2.656653	-0.316797
6	0.123804	-3.387708	-1.337836
16	0.819936	-3.670636	-2.955759
6	2.034609	-2.326369	-3.201251
6	2.625014	-2.46158	-4.597875
8	2.297646	-3.314889	-5.400501
8	1.779545	-5.062406	-2.800751
6	2.837843	-5.204103	-1.893804
8	3.208763	-4.30486	-1.185268
6	3.376716	-6.599166	-1.982245
8	3.533485	-1.513514	-4.789693
6	4.190153	-1.4692	-6.100917
6	5.162791	-0.309534	-6.07987
8	-1.001637	-1.843339	-3.910771
16	-1.04281	-0.353993	-3.989331
6	-2.318398	0.112711	-2.688777
9	-3.512566	-0.444867	-2.966354
8	0.201445	0.295759	-3.50188
8	-1.609626	0.191888	-5.238443
9	-2.482074	1.448384	-2.640452
9	-1.937771	-0.30495	-1.465934
1	-1.622896	-4.499828	-1.980759
1	-2.782185	-4.238734	0.1945
1	-1.70455	-2.948898	2.027942
1	0.537145	-1.93352	1.691304
1	1.727458	-2.222069	-0.445243
1	4.688726	-2.429018	-6.256835
1	3.412662	-1.347132	-6.858554
1	5.668272	-0.251445	-7.048825
1	4.643114	0.63691	-5.906164
1	5.922006	-0.444758	-5.304049
1	2.806571	-2.364826	-2.434311
1	1.462723	-1.39153	-3.123077
1	2.60085	-7.310043	-1.68307
1	3.658192	-6.827545	-3.013595
1	4.240272	-6.687283	-1.323901

2+-OTf+DMAC

6	-0.713698	-3.995481	-1.438408
6	-1.550507	-3.943092	-0.320437
6	-1.24819	-3.098355	0.754331
6	-0.103706	-2.304577	0.725619
6	0.720557	-2.365271	-0.405758
6	0.430188	-3.19836	-1.497044
16	2.205432	-1.401083	-0.62889
8	3.464536	-2.368724	-0.026375
6	3.493188	-2.91765	1.260957
6	4.676476	-3.829024	1.380639
6	2.087622	-0.046747	0.59315
6	3.296641	0.86269	0.423252
8	3.243722	1.843532	1.316624
6	4.320473	2.838765	1.282574
6	4.030777	3.85628	2.365283
8	4.166645	0.700369	-0.411024
8	2.666181	-2.657111	2.096064
8	0.724573	0.309747	-2.226547
16	-0.219149	1.432681	-1.960748
8	-0.346457	1.768227	-0.518637
8	-0.102805	2.581523	-2.881618
6	-1.897067	0.700057	-2.389981
9	-2.874792	1.607454	-2.202628
9	-2.170198	-0.370952	-1.620276
9	-1.933707	0.307393	-3.677992
8	2.70501	-3.394255	-3.844191
6	2.762969	-3.183245	-5.070674
6	2.156496	-4.185539	-6.040217
7	3.360591	-2.072912	-5.579803
6	3.449979	-1.748409	-7.000182
6	3.947121	-1.075233	-4.688309
1	1.083766	-3.225689	-2.366233
1	-0.95278	-4.647143	-2.272232
1	-2.443605	-4.559093	-0.284903
1	-1.900822	-3.059225	1.620093
1	0.129205	-1.666553	1.567708
1	5.265176	2.314179	1.445722
1	4.331416	3.284064	0.28513
1	4.820561	4.613968	2.361955
1	3.074192	4.356404	2.189632
1	4.009203	3.387015	3.353165
1	2.031566	-0.450703	1.602952
1	1.167712	0.500663	0.347814
1	4.541919	-4.684965	0.712249
1	5.587615	-3.308168	1.075589
1	4.758514	-4.169885	2.412195
1	3.441555	-0.111685	-4.817095
1	3.836971	-1.404163	-3.657889
1	5.010266	-0.945354	-4.921379
1	4.500351	-1.626064	-7.289288
1	3.011384	-2.528583	-7.616871
1	2.925855	-0.807177	-7.203949
1	1.355486	-3.737524	-6.636691
1	2.904818	-4.588678	-6.72971
1	1.741866	-5.005181	-5.453821

1+Ac2O+TMS+DMAC (conformer 1)

6	-1.095872	1.562161	-0.412607
8	0.029157	-0.714449	0.544532
6	0.053837	2.473085	-0.036539
8	-0.390673	3.52837	0.651968
8	1.219081	2.278651	-0.340725
6	0.576397	4.554427	1.044591
1	1.523595	4.064411	1.276202
1	0.150101	4.975166	1.95631
6	0.728612	5.604506	-0.04208
1	1.407256	6.388613	0.309858
1	1.148778	5.173352	-0.954849
1	-0.234873	6.06621	-0.277081
6	-2.084679	-0.896074	-1.125815
6	-2.588609	-1.82907	-0.220445
6	-2.747077	-0.60025	-2.32212
6	-3.799001	-2.468209	-0.509231
1	-2.03812	-2.047626	0.688515
6	-3.957122	-1.243295	-2.595388
1	-2.340493	0.12921	-3.01754
6	-4.482215	-2.17581	-1.693061
1	-4.20291	-3.194797	0.189294
1	-4.486862	-1.017813	-3.516008
1	-5.420048	-2.675769	-1.915445
16	-0.464646	-0.129971	-0.786062
6	1.565	-2.177937	3.302437
8	2.183069	-3.172983	3.501734
6	0.18795	-1.771783	3.676328
1	-0.347007	-1.474459	2.767825
1	-0.310506	-2.595989	4.18494
1	0.236816	-0.894718	4.330104
8	2.231802	-1.040926	2.628772
6	2.807875	-1.154438	1.465018
8	2.771372	-2.260575	0.860377
6	3.446727	0.08431	0.953583
1	3.742088	0.722558	1.786367
1	4.305174	-0.147825	0.323475
1	2.698042	0.623105	0.357241
1	-1.841012	1.499794	0.383557
1	-1.55442	1.940837	-1.335996
14	3.386041	-2.99919	-0.670955
6	5.167461	-3.399957	-0.282693
1	5.759754	-2.496898	-0.104016
1	5.246488	-4.05077	0.593522
1	5.610584	-3.925473	-1.136617
6	3.153146	-1.757662	-2.047048
1	2.135001	-1.357113	-2.063844
1	3.858563	-0.923681	-1.993958
1	3.323219	-2.273335	-2.999971
6	2.261896	-4.479709	-0.79502
1	2.350946	-5.117237	0.09002
1	1.216484	-4.173191	-0.90117
1	2.531346	-5.076516	-1.673728
8	-1.552007	2.30828	-3.516767
6	-1.775327	3.160334	-4.399063
7	-1.099605	3.159485	-5.578513
6	-2.826125	4.233322	-4.167059
1	-3.246827	4.077873	-3.173975
1	-2.397578	5.239116	-4.21653
1	-3.63302	4.174909	-4.904316
6	-1.306839	4.11686	-6.661527
1	-0.383384	4.676916	-6.84993
1	-1.580075	3.585727	-7.580514
1	-2.097879	4.8232	-6.424025
6	-0.074406	2.152404	-5.840961
1	0.026265	1.506341	-4.971746
1	-0.352286	1.55095	-6.714282
1	0.884648	2.641015	-6.047454

1+Ac2O+TMS+DMAC (conformer 2)

C	-1.182991	1.55409	-0.502739
O	-0.052865	-0.725337	0.429136
C	-0.020815	2.456105	-0.142688
O	-0.413503	3.411227	0.708503
O	1.107255	2.338149	-0.588312
C	0.562009	4.427992	1.100976
H	1.546957	3.960796	1.149942
H	0.245137	4.718329	2.103743
C	0.536212	5.604717	0.140755
H	1.230056	6.373811	0.496193
H	0.845308	5.303938	-0.864147
H	-0.464139	6.044395	0.088181
C	-2.197997	-0.900758	-1.19493
C	-2.677031	-1.838028	-0.280375
C	-2.892748	-0.598166	-2.370921
C	-3.895818	-2.474298	-0.538717
H	-2.100869	-2.061012	0.611625
C	-4.110482	-1.238893	-2.613722
H	-2.505644	0.134795	-3.073738
C	-4.611329	-2.175289	-1.701645
H	-4.280944	-3.20416	0.166985
H	-4.665368	-1.00832	-3.518123
H	-5.555536	-2.673222	-1.900397
S	-0.567478	-0.141013	-0.893978
C	1.166378	-1.952889	2.884935
O	1.193332	-3.125756	2.676982
C	0.233196	-1.133237	3.700781
H	-0.300633	-0.457618	3.024824
H	-0.466912	-1.789314	4.216061
H	0.793187	-0.526339	4.417271
O	2.195126	-1.071301	2.345571
C	2.866523	-1.279584	1.238163
O	3.724462	-0.381576	1.017215
C	2.636562	-2.447891	0.350316
H	1.567407	-2.526347	0.139711
H	3.197832	-2.337248	-0.57419
H	2.947543	-3.359849	0.867846
H	-1.916205	1.489774	0.303514
H	-1.651262	1.93753	-1.419512
Si	4.94463	0.066158	-0.249091
C	3.961072	0.383074	-1.802257
H	3.566295	-0.533759	-2.24996
H	3.128851	1.066323	-1.605613
H	4.621505	0.853994	-2.540258
C	6.140098	-1.366965	-0.331262
H	6.537637	-1.609439	0.659377
H	5.695721	-2.268313	-0.763204
H	6.984878	-1.077325	-0.967507
C	5.65832	1.600523	0.529705
H	4.890166	2.369092	0.659872
H	6.101171	1.378718	1.505834
H	6.444224	2.010478	-0.114577
O	-1.78732	2.33836	-3.586687
C	-2.074405	3.190821	-4.449762
N	-1.504798	3.175924	-5.683996
C	-3.084033	4.281088	-4.131232
H	-3.410574	4.141405	-3.101066
H	-2.649829	5.280468	-4.23284
H	-3.958085	4.225916	-4.787864
C	-1.802999	4.12402	-6.753842
H	-0.891386	4.657798	-7.046607
H	-2.18471	3.588933	-7.631156
H	-2.546946	4.853488	-6.444683
C	-0.524318	2.150467	-6.03198
H	-0.338963	1.520352	-5.164998
H	-0.89843	1.53488	-6.858417

1+Ac2O+TMS+ (conformer 1)

6	-0.581605	2.526277	-1.084153
6	-1.282466	1.68653	-0.211556
6	-0.591842	0.784988	0.604674
6	0.80407	0.722491	0.558596
6	1.489219	1.574209	-0.30774
6	0.81323	2.46789	-1.143643
16	3.304717	1.47517	-0.420001
6	3.659576	2.856532	0.753132
6	5.153879	3.103748	0.844864
8	5.432863	3.877965	1.894216
6	6.827237	4.271165	2.114596
6	7.154378	5.551105	1.365927
8	3.735468	0.193972	0.302145
8	5.974452	2.664709	0.057115
6	6.049157	-1.511485	-0.429503
8	5.37491	-1.906362	-1.418236
14	5.23456	-1.675272	-3.204014

6	5.697656	0.084732	-3.625297
6	7.120739	-0.484855	-0.474347
8	5.804183	-2.008207	0.751159
6	4.799033	-3.070602	0.97409
8	4.883986	-4.083129	0.357989
6	3.876248	-2.640083	2.053465
6	3.425336	-2.051442	-3.444871
6	6.401948	-2.963089	-3.882804
1	7.469496	3.442447	1.8124
1	6.888175	4.406447	3.195105
1	8.1792	5.853564	1.605334
1	7.085206	5.407895	0.284064
1	6.481136	6.360705	1.662412
1	1.357272	0.02291	1.176489
1	1.358691	3.108069	-1.831798
1	-1.137474	0.128509	1.275487
1	-1.118214	3.218763	-1.72511
1	-2.36659	1.729684	-0.174232
1	3.398907	-1.701764	1.752128
1	3.140693	-3.422029	2.237861
1	4.45387	-2.438733	2.961625
1	7.785459	-0.601032	0.381166
1	7.680181	-0.54796	-1.407747
1	6.644211	0.502627	-0.414758
1	3.23622	2.60322	1.72858
1	3.164002	3.756706	0.375037
1	7.442339	-2.742238	-3.623692
1	6.150564	-3.96101	-3.510333
1	6.324801	-2.979824	-4.976209
1	5.154565	0.810858	-3.012959
1	6.770661	0.276138	-3.536162
1	5.418574	0.260371	-4.671582
1	3.183472	-3.062108	-3.101591
1	2.798258	-1.338313	-2.900327
1	3.172799	-1.983288	-4.509101

1+Ac2O+TMS+ (conformer 2)

6	-1.118465	1.55863	-0.26419
8	0.032843	-0.726339	0.591198
6	0.033701	2.502659	0.026569
8	-0.4084	3.600762	0.64097
8	1.19469	2.285012	-0.275536
6	0.558662	4.65584	0.955622
1	1.509823	4.185126	1.209202
1	0.138699	5.133348	1.841729
6	0.693285	5.630938	-0.200561
1	1.370396	6.440454	0.091406
1	1.107979	5.142504	-1.086664
1	-0.275119	6.070818	-0.456084
6	-2.096419	-0.866065	-1.073755
6	-2.789751	-1.53515	-0.064571
6	-2.58492	-0.805286	-2.381934
6	-4.01468	-2.135128	-0.369369
1	-2.370029	-1.590904	0.934501
6	-3.81418	-1.402875	-2.673663
1	-2.019234	-0.304631	-3.16305
6	-4.527498	-2.06546	-1.669113
1	-4.56534	-2.657817	0.40669
1	-4.206331	-1.359774	-3.684939
1	-5.478325	-2.535124	-1.901415
16	-0.478294	-0.112474	-0.717251
6	1.614085	-2.354877	3.291005
8	2.284633	-3.317351	3.478386
6	0.208021	-2.03887	3.642792
1	-0.320864	-1.730405	2.734853
1	-0.257136	-2.909439	4.103458
1	0.193732	-1.18998	4.334476
8	2.234679	-1.163151	2.664907
6	2.806322	-1.212285	1.495072
8	2.791183	-2.294166	0.846362
6	3.414693	0.059961	1.030911
1	3.691787	0.675315	1.886853
1	4.280525	-0.128649	0.396092
1	2.655853	0.600154	0.44946
1	-1.778781	1.455022	0.600899
1	-1.700177	1.940941	-1.109384
14	3.427555	-2.976048	-0.70217
6	5.209974	-3.368722	-0.309951
1	5.787101	-2.466888	-0.082257
1	5.287546	-4.057373	0.536952
1	5.670918	-3.84879	-1.181011
6	3.191061	-1.695579	-2.041598
1	2.166243	-1.312292	-2.059835
1	3.881577	-0.852161	-1.953431
1	3.382664	-2.179103	-3.007229
6	2.321625	-4.46465	-0.882549
1	2.408562	-5.127365	-0.016004
1	1.273808	-4.167019	-0.990761

1+Ac2O+TMS+ (conformer 3)

6	6.218507	-4.000729	-5.94652
8	4.667956	-4.358633	-3.767631
6	6.448118	-2.507975	-5.80126
8	5.958072	-1.851832	-6.85783
8	7.020516	-1.992804	-4.857917
6	6.164369	-0.404187	-6.924667
1	6.118895	-0.002884	-5.910937
1	5.308014	-0.047429	-7.498527
6	7.478811	-0.073909	-7.610384
1	7.570907	1.013208	-7.704433
1	8.331687	-0.439217	-7.031671
1	7.516684	-0.508356	-8.613652
6	5.887077	-6.499266	-4.881352
6	4.618202	-7.053385	-5.049815
6	7.048439	-7.245361	-5.102115
6	4.511646	-8.381032	-5.474861
1	3.737083	-6.454345	-4.842939
6	6.929562	-8.569637	-5.532172
1	8.030146	-6.808205	-4.940361
6	5.663651	-9.1358	-5.718846
1	3.530142	-8.824644	-5.611595
1	7.823522	-9.159157	-5.710352
1	5.575931	-	-6.045911
		10.167318	
16	6.046653	-4.786357	-4.281419
6	1.75332	-2.236074	2.917064
8	2.578249	-3.079391	3.057505
6	0.38594	-2.09118	3.480252
1	-0.341574	-2.061397	2.662493
1	0.17685	-2.929271	4.143538
1	0.310699	-1.143934	4.022465
8	2.074867	-1.033208	2.122657
6	2.691108	-1.08588	0.966246
8	2.810733	-2.187868	0.379595
6	3.169181	0.224293	0.444957
1	2.881718	1.0309	1.116508
1	4.260292	0.193576	0.354153
1	2.755689	0.396397	-0.551845
1	5.321775	-4.222441	-6.528971
1	7.089486	-4.450094	-6.435194
14	3.570352	-2.918111	-1.141626
6	5.352141	-3.074251	-0.610809
1	5.836547	-2.098972	-0.501926
1	5.428747	-3.613637	0.338539
1	5.898108	-3.638611	-1.372189
6	3.1936	-1.704346	-2.507913
1	2.134757	-1.424669	-2.517474
1	3.803691	-0.798632	-2.447652
1	3.426436	-2.204894	-3.453286
6	2.585543	-4.496832	-1.194271

Cartesian Coordinates from M06-2X/6-31+G**, DCM, in Å

AcO-

6	-3.554047	3.106585	0.566948
6	-4.320475	2.128076	1.472329
8	-4.011895	0.909442	1.404575
8	-5.204682	2.635159	2.213879
1	-3.066264	3.8681	1.182718
1	-2.804809	2.594847	-0.039342
1	-4.260084	3.625305	-0.088569

AcO-

6	-3.554174	3.107655	0.565856
6	-4.25565	2.092495	1.418831
8	-3.791681	0.848474	1.207223
8	-5.138193	2.323992	2.215523
1	-3.677951	2.846879	-0.487632
1	-3.96517	4.096	0.759918
1	-2.484928	3.093323	0.789348
1	-4.27927	0.237865	1.783532

Ac2O

6	-4.18304	1.935942	1.30103
8	-4.137093	0.770288	1.024789
8	-4.84089	2.412266	2.420386
6	-5.890288	1.718433	2.995002
6	-6.041925	2.103977	4.433505
6	-3.523041	3.061831	0.567727
8	-6.581623	0.960742	2.37445
1	-2.927986	2.663258	-0.251317
1	-4.292046	3.736774	0.183401
1	-2.893927	3.630492	1.255862
1	-6.927123	1.625467	4.847283
1	-5.15034	1.791263	4.982954
1	-6.120558	3.190104	4.516613

1

6	-0.448404	-1.528585	0.051387
6	-0.592758	-0.330149	0.753495
6	0.342131	0.027173	1.722879
6	1.403948	-0.837183	1.983132
6	1.570178	-2.028035	1.285754
6	0.630502	-2.372719	0.313596
16	2.634469	-0.374814	3.221423
6	1.657465	-0.942616	4.654078
6	2.431297	-0.66483	5.92448
8	3.272642	0.19855	6.034115
8	3.767409	-1.377357	3.101048
8	2.04939	-1.475218	6.905628
6	2.694665	-1.278809	8.185809
6	2.120722	-2.301951	9.138551
1	2.426467	-2.659163	1.504151
1	0.744462	-3.298742	-0.240528
1	-1.17505	-1.799606	-0.707652
1	-1.426863	0.33026	0.540461
1	0.246945	0.966338	2.262075
1	3.771577	-1.401194	8.046249
1	2.50089	-0.254019	8.51271
1	2.586814	-2.185123	10.11978
1	1.04218	-2.167023	9.248936
1	2.315623	-3.315667	8.780943
1	1.455968	-2.009718	4.532415
1	0.71206	-0.390943	4.677784

1+AcO-

6	-1.984454	-0.561153	-0.252413
8	0.61266	-0.52435	-0.743354
6	-2.138494	-2.066016	-0.259968
8	-3.080723	-2.441807	-1.121024
8	-1.499628	-2.820452	0.438581
6	-3.378719	-3.856722	-1.189399
1	-2.438201	-4.409931	-1.156663
1	-3.842159	-3.983241	-2.167686
6	-4.313323	-4.264684	-0.067904
1	-4.568958	-5.322106	-0.174584
1	-3.838805	-4.121637	0.905434
1	-5.236179	-3.680827	-0.106405
6	-0.569066	1.658747	0.248539
6	-0.062954	2.319332	-0.86335
6	-1.221324	2.336086	1.27654
6	-0.232055	3.700819	-0.955803
1	0.474088	1.756008	-1.62004
6	-1.391226	3.71522	1.169476
1	-1.58539	1.802731	2.151285
6	-0.897624	4.395329	0.05445
1	0.162953	4.234566	-1.814187
1	-1.898311	4.258379	1.960183
1	-1.023587	5.470638	-0.020735
16	-0.329821	-0.124217	0.381271
6	3.165166	0.397378	-1.154976
8	3.044647	1.589786	-1.121119
6	3.115236	-0.481129	-2.364576
1	2.369325	-1.26022	-2.200721
1	2.858995	0.118801	-3.23623
1	4.090968	-0.952855	-2.508306
8	3.499625	-0.349268	-0.035146
6	3.127564	0.02998	1.22948
8	2.275432	0.846785	1.455719
6	3.895628	-0.755753	2.249783
1	4.963727	-0.557872	2.132294
1	3.566318	-0.474898	3.248101
1	3.733283	-1.823303	2.083847
1	-2.089851	-0.143746	-1.256764
1	-2.742643	-0.124217	0.405661

TS(1-2) 1 imag freq

6	-0.830575	4.073542	0.174006
6	-0.805379	3.386657	-1.043002
6	-0.555272	2.018949	-1.066633
6	-0.324743	1.368048	0.14423
6	-0.318731	2.035695	1.364989
6	-0.58871	3.403963	1.37184
16	-0.043476	-0.392018	0.203133
8	0.783699	-0.731924	-1.138675
6	2.264101	-0.481041	-1.127203
6	2.869877	-1.52545	-2.018397
6	-1.633511	-0.945822	-0.459123
6	-1.632214	-2.461812	-0.53948
8	-0.79321	-3.163681	-0.026098
8	-2.677168	-2.883674	-1.236378
6	-2.837314	-4.319708	-1.371656
6	-3.482832	-4.907565	-0.133502
8	2.628719	0.653789	-0.975735
8	2.59043	-1.490837	0.525671
6	2.745477	-0.801257	1.601294
6	3.777292	-1.341302	2.57802
8	2.122393	0.242478	1.858648
1	-1.856245	-4.756121	-1.567885
1	-3.469931	-4.430979	-2.251684
1	-3.646537	-5.977371	-0.286333
1	-2.840237	-4.77967	0.740268
1	-4.448899	-4.434308	0.057465

1	-0.511609	1.477215	-2.006776
1	-0.079248	1.502326	2.278865
1	-0.977229	3.917421	-1.973048
1	-0.590418	3.945179	2.311596
1	-1.027972	5.140437	0.183962
1	2.500103	-2.516766	-1.765534
1	2.607995	-1.280928	-3.052126
1	3.952683	-1.483921	-1.903211
1	3.658691	-2.420662	2.69533
1	4.775187	-1.16167	2.16623
1	3.693893	-0.8443	3.544691
1	-1.802014	-0.491421	-1.437719
1	-2.407003	-0.605671	0.236809
	2+AcO-		
6	-0.96242	4.545345	0.225056
6	-1.051072	3.843584	-0.981372
6	-0.793345	2.478545	-1.013619
6	-0.435948	1.845656	0.177248
6	-0.313554	2.526888	1.384581
6	-0.597239	3.893053	1.400198
16	-0.142785	0.0881	0.247339
8	0.637043	-0.265355	-1.153282
6	1.976386	0.185554	-1.317193
6	2.716284	-0.80002	-2.156152
6	-1.748233	-0.467707	-0.383806
6	-1.757533	-1.983851	-0.467983
8	-0.916857	-2.692898	0.031229
8	-2.817097	-2.392739	-1.150058
6	-2.997597	-3.826919	-1.282674
6	-3.642922	-4.40274	-0.038956
8	2.318371	1.252342	-0.913008
8	2.392362	-1.140612	0.838054
6	2.533734	-0.437402	1.878933
6	3.535279	-0.940931	2.919629
8	1.913506	0.632927	2.114821
1	-2.023848	-4.276794	-1.484497
1	-3.637503	-3.930506	-2.158355
1	-3.822309	-5.470551	-0.187836
1	-2.992868	-4.281445	0.830268
1	-4.601043	-3.91561	0.157023
1	-0.840817	1.929776	-1.949579
1	0.033122	2.002993	2.26885
1	-1.318961	4.361065	-1.896038
1	-0.5116	4.44613	2.329063
1	-1.168362	5.610519	0.241667
1	2.812921	-1.719184	-1.575613
1	2.152401	-1.01084	-3.067651
1	3.696109	-0.393601	-2.400023
1	3.256912	-1.950133	3.236293
1	4.528333	-1.005159	2.46548
1	3.574369	-0.281972	3.787935
1	-1.950814	-0.009088	-1.353286
1	-2.497355	-0.129012	0.33936
	3		
6	-0.939851	0.449604	0.612685
8	0.607818	1.750415	-1.129409
6	-2.316607	0.817575	0.098891
8	-3.095877	1.15327	1.119932
8	-2.648906	0.812039	-1.063771
6	-4.46186	1.523467	0.808004
1	-4.453155	2.152888	-0.083818
1	-4.777863	2.113197	1.66812
6	-5.323048	0.290343	0.622739
1	-6.358441	0.594857	0.449361
1	-4.987249	-0.294042	-0.236689
1	-5.292348	-0.336345	1.517226
6	1.698769	-0.487911	-0.200146
6	2.053576	-0.46447	1.144385
6	2.594984	-0.875869	-1.195044
6	3.346913	-0.843828	1.495004
1	1.346202	-0.160269	1.905096
6	3.885308	-1.252267	-0.828034
1	2.293161	-0.884108	-2.238309
6	4.25902	-1.236027	0.515049
1	3.639118	-0.831271	2.539475
1	4.59243	-1.556199	-1.592183
1	5.264087	-1.529564	0.799917
16	0.077463	-0.030481	-0.815305
6	1.205241	2.594711	-0.299804
8	1.34666	2.398459	0.896988
6	1.698117	3.834701	-1.003593
1	2.069916	4.551201	-0.272644
1	2.500472	3.55615	-1.691758
1	0.891448	4.274461	-1.593277
8	-0.194325	-2.364138	1.416488
6	-0.499931	-2.667066	0.273327
8	-0.544453	-1.813926	-0.739399
6	-0.869857	-4.069385	-0.14306
1	-1.818293	-4.059784	-0.683671
1	-0.103177	-4.451691	-0.821962
1	-0.938785	-4.709563	0.735187
1	-0.467091	1.299422	1.106242
1	-0.992526	-0.394928	1.300536
	TS(3-4)	1 imag freq	
6	1.041745	-0.119018	0.659187
8	-0.382689	-2.089505	-0.635831
6	2.37196	-0.548517	0.156199
8	3.254142	-0.595925	1.156877
8	2.64221	-0.77742	-1.007707
6	4.62638	-0.878633	0.802529
1	4.637188	-1.674865	0.055584
1	5.070903	-1.242973	1.728877
6	5.320677	0.372602	0.301496
1	6.370669	0.149631	0.094113
1	4.854754	0.731248	-0.618995
1	5.276048	1.162509	1.055209
6	-1.715977	0.061381	0.198071
6	-1.758873	0.896288	1.310112
6	-2.871245	-0.411961	-0.42017
6	-3.004795	1.245292	1.825809
1	-0.852088	1.281417	1.762844
6	-4.108215	-0.058172	0.11404
1	-2.813082	-1.050357	-1.296793
6	-4.174652	0.767521	1.235292
1	-3.056374	1.893891	2.693638
1	-5.016015	-0.424808	-0.352517
1	-5.139575	1.043797	1.647082
16	-0.170972	-0.417047	-0.576874
6	-0.660575	-2.84477	0.489952
8	-0.77124	-2.359871	1.581305
6	-0.79378	-4.286508	0.110499
1	-0.987703	-4.872296	1.006732
1	-1.614326	-4.39832	-0.601917
1	0.124028	-4.622779	-0.376141
8	1.175906	2.50018	0.783794
6	0.572652	2.916635	-0.274449
8	-0.056608	2.163151	-1.042924
6	0.658693	4.401554	-0.55131
1	1.70783	4.690439	-0.652942
1	0.113306	4.656735	-1.459222
1	0.246344	4.951998	0.298195
1	0.766586	-0.538933	1.624194
1	1.101889	1.176645	0.752354
	4		
6	0.928168	-0.564663	0.43284
8	-0.817439	-2.369805	-0.920602
6	2.294226	-0.603518	-0.068421
8	3.172111	-0.531545	0.951528
8	2.635723	-0.653868	-1.240239
6	4.566923	-0.456982	0.599557
1	4.762218	-1.150917	-0.220492
1	5.089754	-0.797608	1.49417
6	4.95666	0.96296	0.234051
1	6.028501	1.008328	0.022617
1	4.414019	1.294493	-0.654372
1	4.737304	1.644385	1.060112
6	-1.757229	-0.084648	0.047687
6	-1.723619	0.731377	1.173334
6	-2.954007	-0.380864	-0.603986
6	-2.922927	1.237621	1.671923
1	-0.787792	0.969951	1.665333
6	-4.144152	0.132774	-0.095488
1	-2.960197	-1.010595	-1.487986
6	-4.130065	0.940022	1.041936
1	-2.907251	1.867763	2.554782
1	-5.080414	-0.096785	-0.592815
1	-5.059111	1.339862	1.4345
16	-0.25353	-0.709402	-0.70913
6	-1.096302	-3.12871	0.170952
8	-1.073394	-2.695544	1.298013
6	-1.424195	-4.540074	-0.225913
1	-1.672102	-5.116009	0.663941
1	-2.264371	-4.538658	-0.923791
1	-0.564852	-4.981555	-0.735578
8	1.263676	2.57554	0.385629
6	0.56422	3.008106	-0.673577
8	-0.09958	2.258619	-1.360614
6	0.705843	4.486201	-0.887252
1	1.758374	4.729187	-1.051021
1	0.111858	4.792099	-1.74587
1	0.376996	5.017311	0.008987
1	0.719144	-0.751653	1.477796
1	1.140272	1.605374	0.458412
	TS(4-6)-cyc	1 imag freq	
6	-0.800855	0.044984	-1.719743
8	1.117609	1.683941	0.1174
6	-1.625818	-0.977769	-1.003759
8	-2.895808	-0.590484	-1.017369
8	-1.211738	-2.016423	-0.54853
6	-3.83288	-1.433765	-0.308269
1	-3.620343	-2.475208	-0.558917
1	-4.803291	-1.151196	-0.71572
6	-3.750739	-1.181161	1.184348
1	-4.503374	-1.786947	1.695765
1	-2.765063	-1.450442	1.569769
1	-3.938654	-0.127948	1.403461
1	-1.344999	0.785784	-2.300005
6	1.595721	-1.088331	-0.864926
6	1.379115	-1.258165	0.501901
6	2.514179	-1.858106	-1.575657
6	2.091967	-2.254071	1.159387
1	0.666577	-0.622858	1.016277
6	3.217073	-2.855508	-0.899008
1	2.679461	-1.691382	-2.635759
6	3.005217	-3.051179	0.463428
1	1.936246	-2.407288	2.222046
1	3.931108	-3.468065	-1.438603
1	3.557706	-3.822806	0.989814
16	0.80596	0.214909	-1.791714
6	-0.077416	1.966768	0.447207
8	-0.983791	1.100109	0.563739
6	-0.43399	3.433238	0.625244
1	-0.69539	3.846646	-0.355042
1	-1.294574	3.544702	1.286238
1	0.418676	3.994223	1.011305
	TS(4-6)-sld	1 imag freq	
6	-7.75721	4.859845	2.594926
6	-8.886261	4.162356	2.159931
6	-8.762264	2.88235	1.631291
6	-7.486836	2.318682	1.557942
6	-6.342433	3.007035	1.965811
6	-6.489816	4.286279	2.496449
16	-7.217022	0.71728	0.84501
8	-9.172353	1.237376	-0.893538
6	-9.8303	2.282527	-1.195402
6	-9.130615	3.286036	-2.111448
6	-8.375814	-0.256743	1.396802
6	-9.422186	0.070975	2.433601
8	-10.627844	-0.116697	1.947477
6	-11.748523	0.209717	2.818150
6	-11.944825	1.71085	2.88522
8	-9.121667	0.406234	3.552817
8	-10.963523	2.570503	-0.747783
1	-11.55688	-0.231087	3.798462
1	-12.591144	-0.292358	2.345786
1	-12.866626	1.926425	3.431296
1	-11.115532	2.192453	3.409687
1	-12.026672	2.127208	1.877052
1	-5.359012	2.555014	1.880309
1	-5.613522	4.832705	2.827051
1	-7.865272	5.859987	3.001302
1	-9.869222	4.618609	2.216194
1	-9.632916	2.361377	1.241328
1	-9.841923	3.995438	-2.536579
1	-8.401054	3.841223	-1.509636
1	-8.584117	2.773414	-2.905832
1	-8.365169	-1.265878	0.988595
	6		
6	1.736856	3.719303	-4.866902
6	2.329444	2.456855	-4.857124
6	1.983441	1.52557	-3.879579
6	1.053854	1.863987	-2.891098
6	0.472525	3.136374	-2.886162
6	0.805497	4.051936	-3.883813
16	0.711202	0.642789	-1.634855
6	-1.071015	0.903454	-1.41303
6	-1.758095	-0.401832	-0.984308
8	-1.289927	-1.501726	-1.146819
8	-2.966329	-0.143678	-0.495849
6	-3.724921	-1.277468	-0.012753
6	-3.261551	-1.673485	1.37499
8	-0.731236	0.724274	1.203598
6	-1.151088	1.77601	0.782353
6	-1.47661	2.995279	1.588013
8	-1.389916	1.97778	-0.537745
1	-3.619025	-2.095691	-0.727651
1	-4.756461	-0.925605	-0.011747
1	-3.878901	-2.497547	1.742155
1	-2.2193	-1.999508	1.35803
1	-3.356801	-0.831758	2.065141
1	-1.492229	1.201324	-2.377009
1	2.425443	0.533761	-3.888685
1	-0.229615	3.414927	-2.106638
1	3.05212	2.186714	-5.620515
1	0.343403	5.034145	-3.880685
1	1.999327	4.43918	-5.635207
1	-0.866033	3.832903	1.242703
1	-2.525954	3.260298	1.439719
1	-1.28253	2.796711	2.639982
	TS(2-7)	1 imag freq	
6	-2.680974	3.136196	0.500136

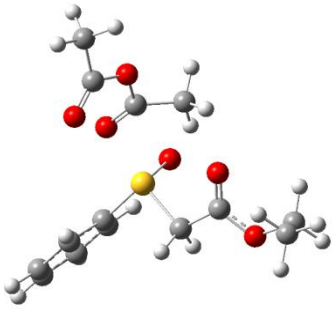
6	-2.126477	2.25983	1.436462
6	-1.621228	1.029754	1.030998
6	-1.704622	0.686378	-0.320877
6	-2.269486	1.542983	-1.266057
6	-2.748972	2.782543	-0.845987
16	-1.039893	-0.838448	-0.92373
8	-1.57815	-1.929443	0.22464
6	-2.895165	-2.350644	0.108891
6	-3.203888	-3.35103	1.17647
8	-3.62177	-1.919199	-0.740695
6	0.926562	-0.902157	-0.011081
6	1.58101	0.205172	-0.784448
8	1.489373	1.374069	-0.484341
8	2.212192	-0.264604	-1.857765
6	2.944105	0.698407	-2.648588
6	4.274211	1.024981	-1.998333
8	2.787822	-1.017652	0.906262
6	2.731765	-0.613147	2.125169
6	4.073847	-0.552321	2.841194
8	1.692707	-0.270777	2.7167
1	2.324332	1.588836	-2.774213
1	3.075131	0.207175	-3.612749
1	4.832213	1.713206	-2.638758
1	4.124735	1.499895	-1.026122
1	4.866817	0.117204	-1.863276
1	0.56946	-0.669163	0.985659
1	1.116318	-1.927611	-0.300008
1	-1.177368	0.353979	1.756042
1	-2.339055	1.244618	-2.307512
1	-2.075295	2.539668	2.482997
1	-3.186989	3.461302	-1.569544
1	-3.063853	4.098038	0.824853
1	4.66119	0.266274	2.414729
1	3.933875	-0.377779	3.908128
1	4.630268	-1.477795	2.678512
1	-2.515903	-4.195111	1.096968
1	-3.060567	-2.888717	2.155698
1	-4.233093	-3.684443	1.062061

7

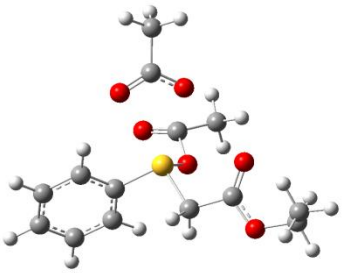
6	-1.604022	3.354366	-0.320248
6	-1.236803	2.253501	0.45112
6	-1.381315	0.957081	-0.043112
6	-1.905686	0.768481	-1.321165
6	-2.29096	1.865098	-2.100494
6	-2.131522	3.15351	-1.597593
16	-2.055623	-0.83219	-2.068076
8	-1.616176	-1.818472	-0.771332
6	-2.573037	-2.106584	0.176721
6	-1.996361	-3.011221	1.223694
8	-3.683194	-1.650405	0.147495
6	1.670392	-1.438738	0.257761
6	1.689615	-0.023434	-0.293806
8	2.037453	0.951688	0.329866
8	1.272876	-0.026617	-1.556267
6	1.223502	1.246025	-2.240503
6	2.594374	1.631512	-2.76054
8	2.177532	-1.460106	1.580384
6	1.356651	-0.991979	2.540586
6	2.045718	-0.923654	3.869242
8	0.207554	-0.676315	2.319766
1	0.817923	1.993881	-1.553576
1	0.513057	1.08199	-3.052117
1	2.519683	2.565578	-3.323686
1	3.295115	1.781122	-1.936102
1	2.984755	0.857602	-3.426122
1	0.648126	-1.82569	0.205393
1	2.32821	-2.070874	-0.33976
1	-1.061141	0.117575	0.565954
1	-2.707119	1.717149	-3.09371
1	-0.818484	2.392197	1.443339
1	-2.426773	4.002247	-2.206294
1	-1.482873	4.360057	0.068161
1	2.791509	-0.125034	3.834164
1	1.316399	-0.711767	4.648394
1	2.566162	-1.861138	4.072346
1	-1.435873	-3.824101	0.759232
1	-1.307966	-2.423044	1.839269
1	-2.80241	-3.400747	1.842817

Figures: Structures of stationary points

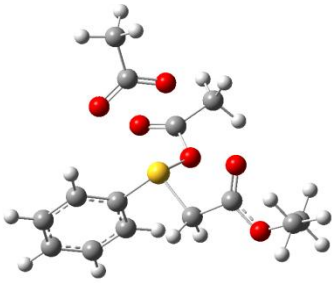
M06-2X/6-31+G, DCM, Å**



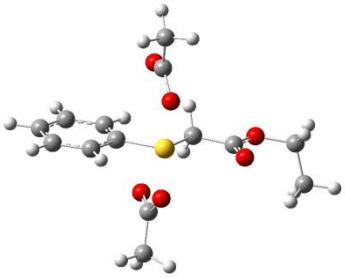
1+AcO-



TS(1-2)



2+AcO-



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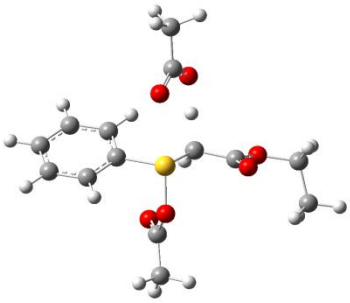
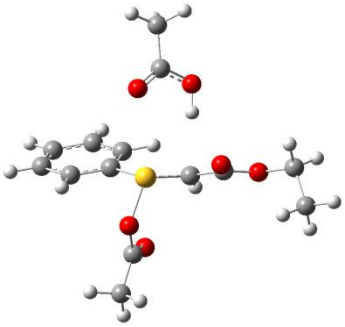


TS(3-4)



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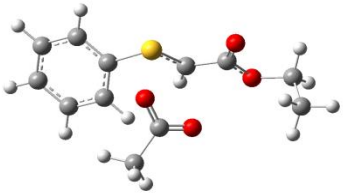
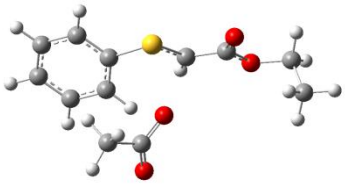
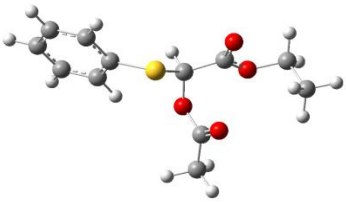


TS(4-6)-cyc

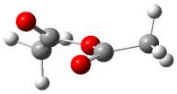


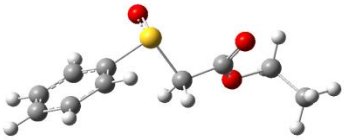
TS(4-6)-sld



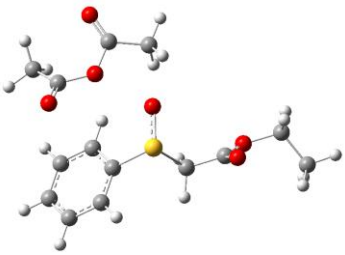
6

B3LYP/6-31+G, DCM, Å**

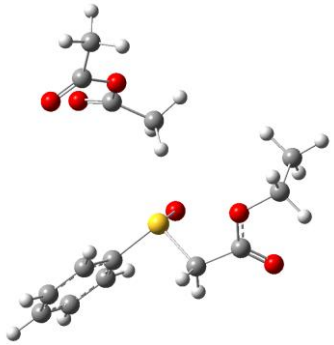




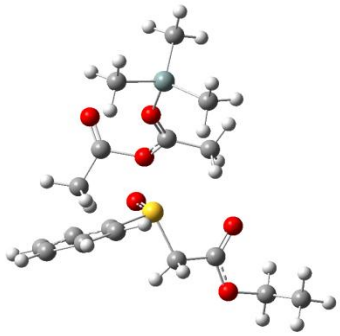
1+Ac2O (conformer 1)



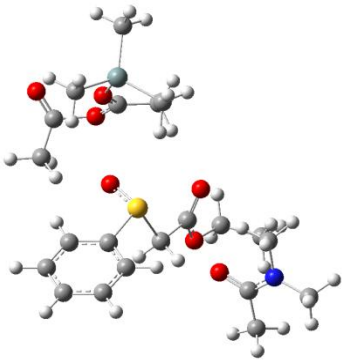
1+Ac2O (conformer 2)



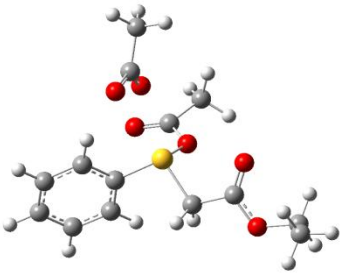
1+Ac2O (conformer 3)



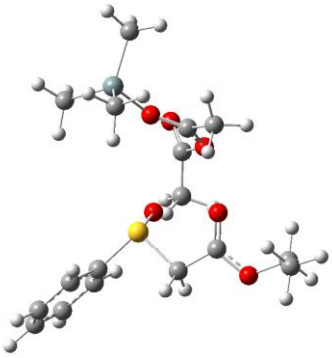
1+Ac2O+TMS+ (conformer 1)



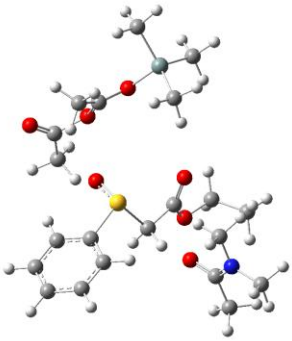
1+Ac2O+TMS++DMAC (conformer 1)



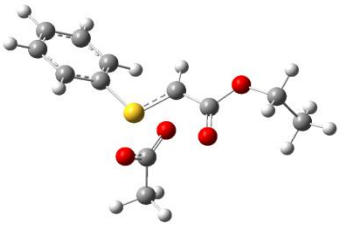
2+Ac2O



1+Ac2O+TMS+ (conformer 2)



1+Ac2O+TMS++DMAC (conformer 2)



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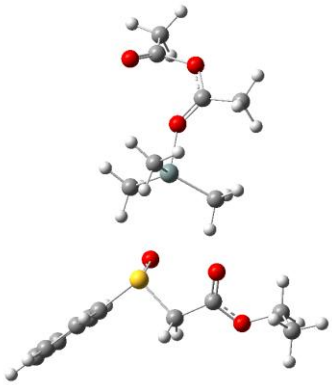
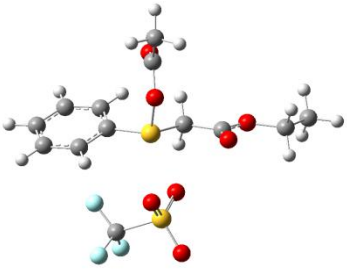
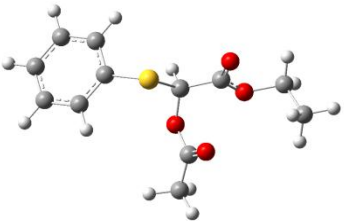


1+Ac2O+TMS+ (conformer 3)



2+Otf-



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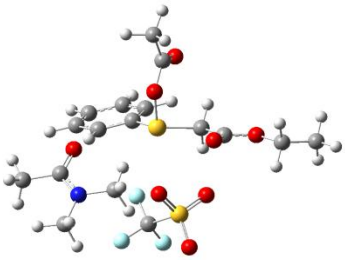
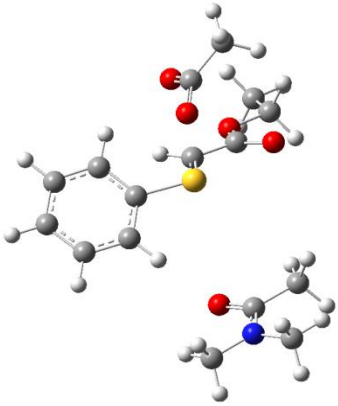
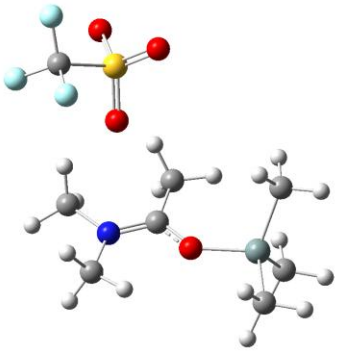


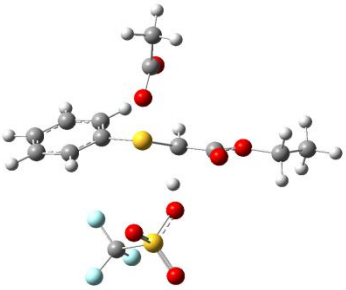
2+Otf-+DMAC



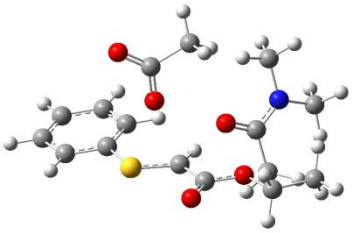
TS(4-6)cyc+DMAC



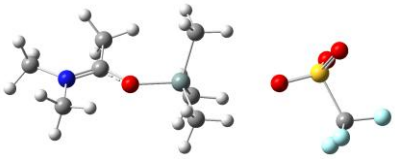
DMAC/TMSOTf (conformer 2)



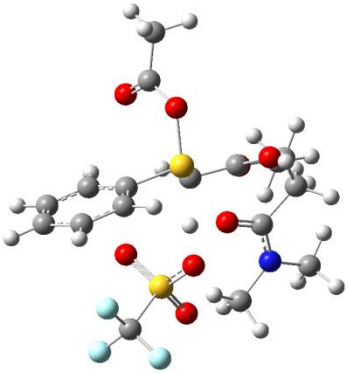
TS(2-4)+OTf-



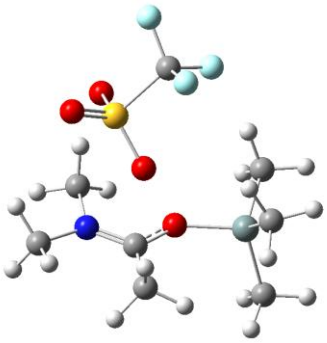
TS(4-6)sld+DMAC



DMAC/TMSOTf (conformer 3)



TS(2-4)+OTF-+DMAC[8]



DMAC/TMSOTf (conformer 1)

(8)gas-phase optimized geometry