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Supporting Information

Degradation mechanisms of simple aliphatic amines under ozonation: a DFT study

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Text SI-1

Calculation details of validation of calculation method on the decomposition of the simple amines during ozonation

Regarding there is less information on the ozone-reactivity of nitrogenous compounds, computed thermokinetic methods have been developed based on the current kinetic/mechanistic knowledge to predict the reactivities of molecules toward ozone in cases where no experimental data were available. Therefore, the first and most important thing is to obtain a relatively accurate calculation method. To obtain a suitable method for this research work, the basis set 6-311++G (d, p), three DFT methods M05, LC-ωPBE and WB97XD along with implicit CPCM and SMD solvent models have been tested for TMA/TEA and DEA/DMA with ozone, and the calculated results are listed in Table SI-1.

Previous studies have been reported that the experimental rate constants k of TEA/TMA and DEA/DMA with ozone are in the range of 10^5~10^7 M^{-1} s^{-1}. As shown in Table SI-1 that the activation free energies ($\Delta G^{\neq}$) calculated with LC-ωPBE functional method along with CPCM solvent model are 8~10 kcal/mol whereas those with SMD model are 4~13 kcal/mol, and the estimated $\Delta G^{\neq}$ based on the experimental rate constant are also around 8~10 kcal/mol. It is clear that the results calculated with CPCM model are significantly better than those from SMD model. However, the results calculated with WB97XD and M05 functional method, no matter which solvent model, are both not well suitable for the reactions, considering the experimental rate constants. As discussed above, it can be concluded that the activation free energies obtained with

LC-ωPBE along with 6-311++G (d, p) basis set and the CPCM solvent model are in great agreement with the experimental results.

Table SI-1. Activation free energies (at 298 K and 1 atm, in kcal/mol) calculated with different methods for reactions of TMA and DMA with ozone. (basis set is 6-311++G**)

parents	M05		LC-ωPBE		WB97XD	
	cpcm	smd	cpcm	smd	cpcm	smd
TMA+O_3	13.9	9.0	8.4	10.4	8.0	5.7
DMA+O_3	13.7	8.4	8.9	4.7	8.8	4.4
TEA+O_3	14.3	11.9	9.6	12.8	9.3	9.5
DEA+O_3	13.0	7.4	9.4	5.9	8.2	4.8

Table SI-2 Activation Free Energies and Reaction Energies (at 298 K and 1 atm, in kcal/mol) Calculated at the LC-ωPBE(CPCM)/6-311++G(d,p) Level for Elementary Steps of TMA/TEA Degradation Pathways during Ozonation.

Reaction step	$\Delta G^{\neq}$(TMA/TEA)	ΔH(TMA/TEA)	ΔG(TMA/TEA)
T-a	8.4/9.6	-9.0/-8.8	-9.2/-9.8
T-a'		15.4/14.9	3.2/3.6
T-b	--	-38.3/-38.2	-46.1/-45.6
T-b'	34.4/39.5	-10.3/-17.5	-10.6/-18.2
T-c	5.6/5.1	-64.6/-61.0	-72.2/-69.6
T-d	18.5/24.3	-7.5/-16.7	-7.5/-17.4
T-e	25.1/33.8	-8.7/-0.6	3.2/11.5
T-f	9.2/8.3	16.1/7.8	3.8/-5.0

Table SI-3 Activation Free Energies and Reaction Energies (at 298 K and 1 atm, in kcal/mol) Calculated at the LC-ωPBE (CPCM)/6-311++G(d,p) Level for Elementary Steps of DMA and Some Key Steps of DEA Degradation Pathways during Ozonation (D-k was calculated at 6-311+G(d)).

Reaction step	$\Delta G^{\neq}$(DMA/DEA)	ΔH(DMA/DEA)	ΔG(DMA/DEA)
D-a	8.9/9.3	-9.3/-17.9	-9.7/-16.0
D-b	--/--	-38.6/-29.8	-46.2/-40.2
D-b'	34.1/36.9	-12.1/-18.9	-11.0/-17.6
D-c	5.4/5.2	-8.5/-7.7	-9.7/-7.9
D-d	8.4/11.0	-48.6/-49.5	-47.6/-48.2
D-d'	12.6/10.6	-29.6/-36.4	-30.0/-37.4
D-e	18.9/16.5	-24.6/-30.4	-35.5/-42.3
D-f	8.4/12.8	-10.4/-12.5	2.4/1.7
D-g	5.4/7.4	-44.0/-46.8	-69.5/-72.7
D-h	8.9/9.3	-77.6/-78.0	-75.6/-77.1
D-i	5.4	-66.6	-74.7
D-j	10.5	13.4	2.0
D-j'	15.6	-37.4	-35.2
D-j"	23.6	8.3	-2.1
D-k	3.7	-0.6	-13.7
D-l	14.6/12.4	-11.9/-20.7	-11.2/-21.3
D-m	21.4/27.3	-10.9/-4.5	0.1/7.3
D-n	6.9	-2.3	8.0
D-n'	18.7	-27.8	-15.2
D-n"	23.2	-50.9	-49.8
D-o	5.5	-104.9	-114.0
D-p	56.5	-81.6	-92.9
D-p'	10.8	-23.1	-34.6

Table SI-4 Activation Free Energies and Reaction Energies (at 298 K and 1 atm, in kcal/mol) Calculated at the LC-ωPBE (CPCM)/6-311++G(d,p) Level for Elementary Steps of MA and Some Key Steps of EA Degradation Pathways during Ozonation (M-m was calculated at 6-311+G(d)).

Reaction step	$\Delta G^{\neq}$(MA/EA)	ΔH(MA/EA)	ΔG(MA/EA)
M-a	10.4/10.1	-8.4/-8.7	-7.8/-8.2
M-b	--	-37.7/-37.1	-45.5/-45.4
M-b'	35.3/38.0	-26.9/-32.0	-36.5/-42.0
M-c	5.7/6.0	-9.8/-9.5	-10.2/-9.9
M-d	10.4/10.1	-46.3/-46.9	-45.4/-45.9
M-e	11.6/10.2	-20.8/-20.2	-32.1/-31.9
M-e'	9.5/9.3	-9.3/-8.1	-9.2/-8.0
M-f	8.9/9.3	-77.6/-78.0	-75.6/-77.1
M-g	11.1/9.8	-47.1/-48.8	-45.9/-47.9
M-g'	24.1/24.1	-11.5/-12.1	-23.0/-23.9
M-h	8.6/8.6	-42.0/-41.2	-52.6/-53.1
M-i	24.1	-13.1	-2.7
M-j	4.4/5.4	-17.1/-27.1	-18.0/-27.7
M-k	21.6/29.3	-14.4/-7.9	-3.8/3.5
M-l	12.1	11.6	0.5
M-l'	18.0	-34.1	-32.6
M-l''	28.0	13.1	2.7
M-m	4.4	-2.2	-14.7
M-n	9.9	-13.0	-7.9
M-n'	19.2	-24.8	-12.4
M-o	2.6	-112.0	-121.9
M-p	52.7	-87.7	-99.6
M-p'	12.2	-22.9	-34.5
M-q	9.8	-7.2	-7.5

Figure SI-1

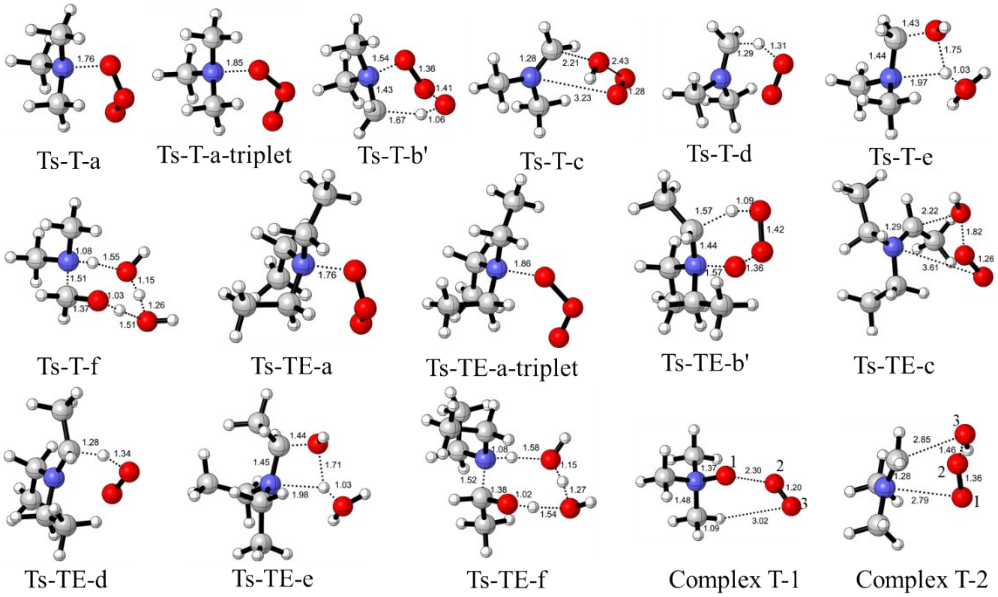

Fig. SI-1 Structures of transition states and important geometric parameters calculated at the LC-ωPBE/6-311++G(d,p) levels involved in each elementary step of TMA/TEA degradation pathways during Ozonation (atoms in blue color represent nitrogen atom; atoms in red represent oxygen atom, atoms in white represent hydrogen atom; atoms in grey color represent carbon atom).

Figure SI-2

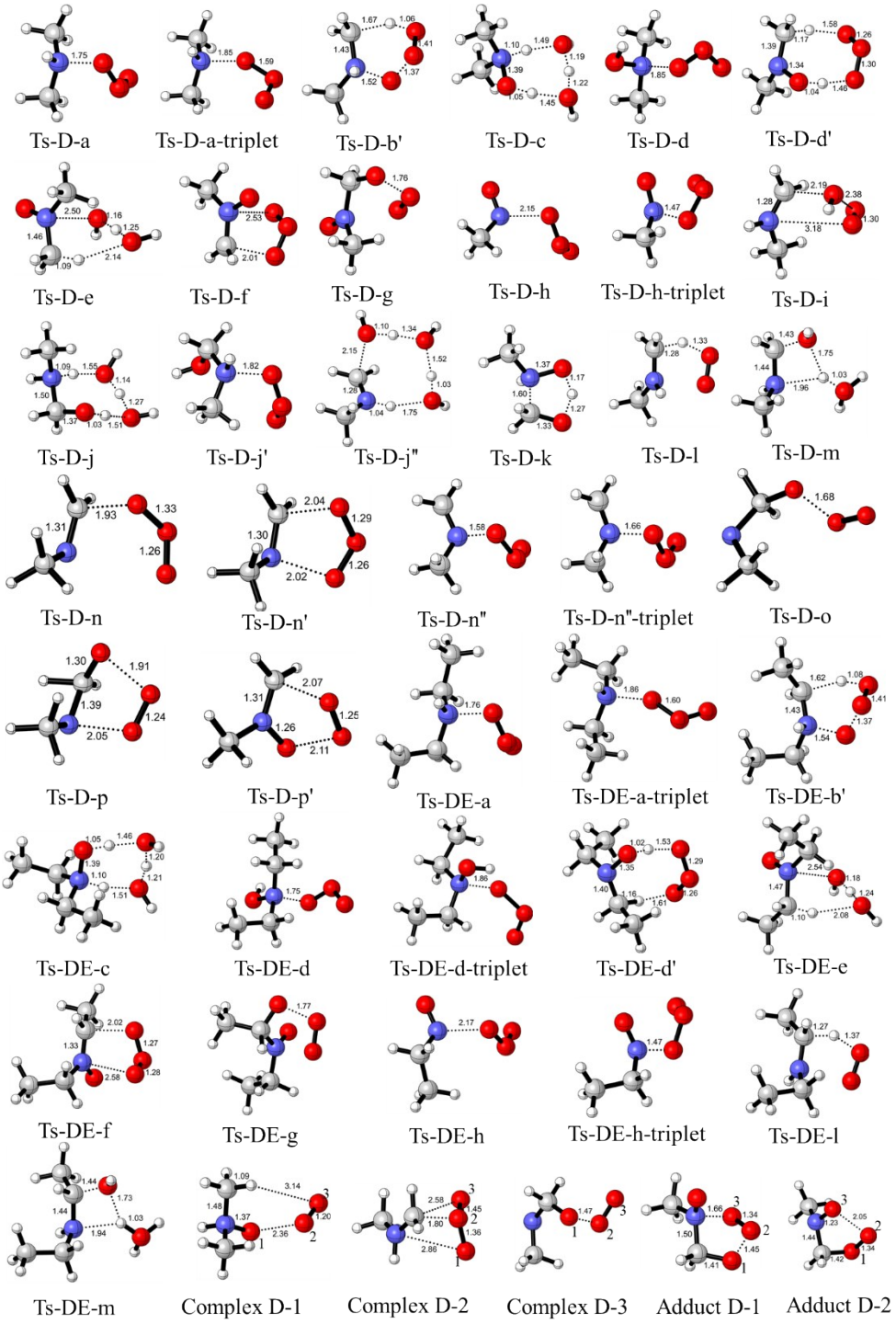

Fig. SI-2 Structures of transition states and important geometric parameters calculated at the LC-ωPBE/6-311++G(d,p) levels involved in each elementary step of DMA and some key steps of DEA degradation pathways during Ozonation (Ts-D-k was calculated at 6-311+G(d), atoms in blue color represent nitrogen atom; atoms in red represent oxygen atom, atoms in white represent hydrogen atom; atoms in grey color represent carbon atom).

Figure SI-3

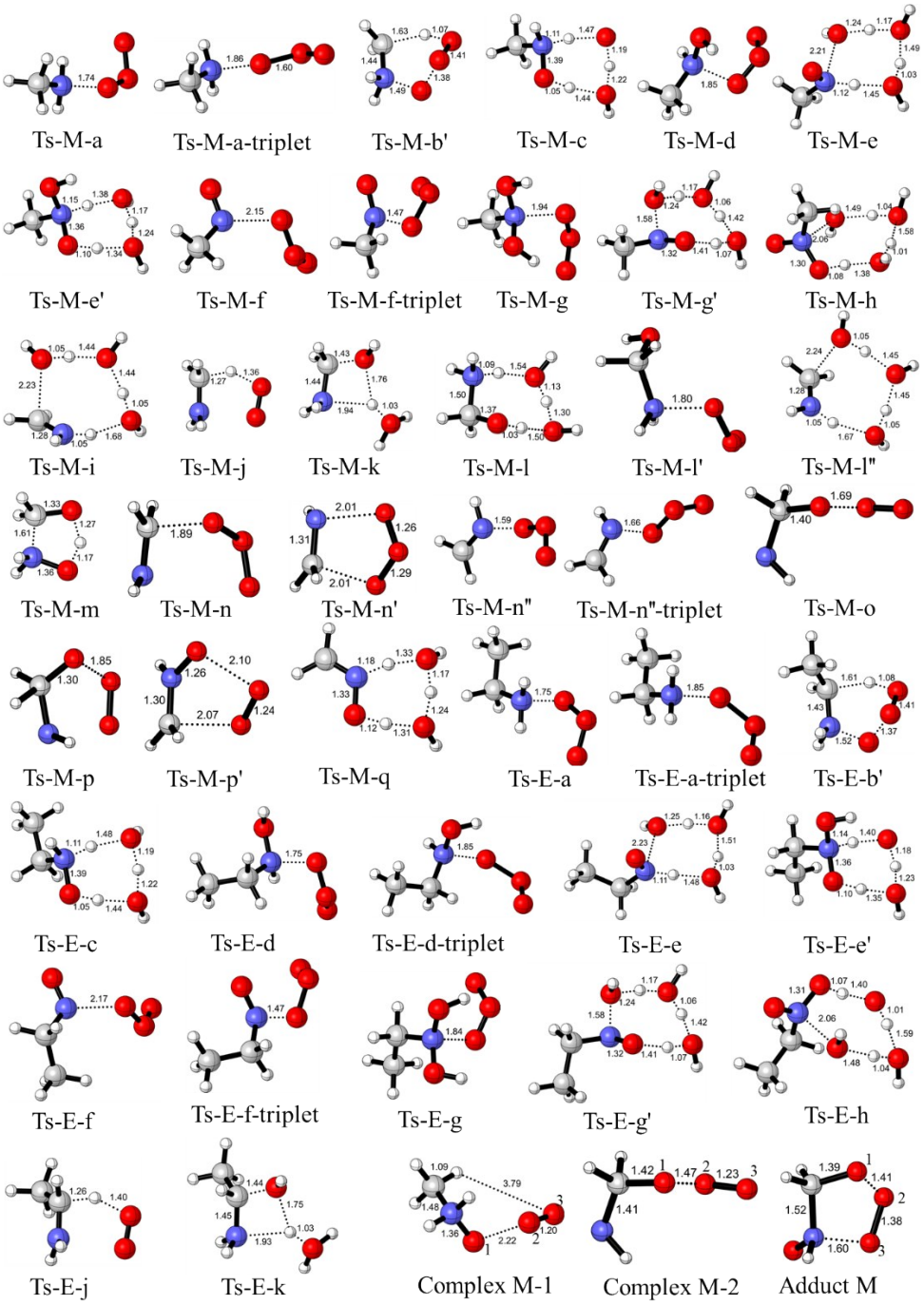

Fig. SI-3 Structures of transition states and important geometric parameters calculated at the LC-ωPBE/6-311++G(d,p) levels involved in each elementary step of MA and some key steps of EA degradation pathways during Ozonation (Ts-M-m was calculated at 6-311+G(d), atoms in blue color represent nitrogen atom; atoms in red represent oxygen atom, atoms in white represent hydrogen atom; atoms in grey color represent carbon atom).

Standard orientation of Ts-T-a

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-T-a

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -935.64 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.802344	0.074208	0.055072
2	6	0	0.816659	1.455841	-0.419656
3	1	0	0.771896	1.450413	-1.507051
4	1	0	1.741991	1.936737	-0.092874
5	8	0	-1.622711	-0.658687	0.032807
6	8	0	-0.578437	-0.689106	-0.724918
7	8	0	-2.290010	0.520709	-0.041693
8	6	0	0.590747	-0.077228	1.484368
9	1	0	-0.307458	0.465117	1.771177
10	1	0	0.477295	-1.134167	1.718720
11	6	0	1.887121	-0.734263	-0.486507
12	1	0	2.844517	-0.312753	-0.173879
13	1	0	1.791317	-1.754436	-0.122207
14	1	0	1.822943	-0.722024	-1.573648
15	1	0	-0.050450	1.974658	-0.021664
16	1	0	1.453642	0.327584	2.017115

Standard orientation of Ts-T-b'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-T-b'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -529.65 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.707354	-0.090845	0.084879
2	8	0	-1.460060	0.737979	-0.134509
3	8	0	-0.362515	0.446681	-0.891114
4	8	0	-2.207898	-0.453722	-0.006193
5	6	0	1.637420	-0.688331	-0.891282
6	1	0	1.162674	-1.569363	-1.315203
7	6	0	0.135644	-1.004735	1.028858
8	1	0	-1.467611	-0.935596	0.571975
9	6	0	1.262082	1.133415	0.697072
10	1	0	2.115628	0.844381	1.306409
11	1	0	0.313993	-0.656295	2.041399
12	1	0	1.561180	1.822846	-0.089011
13	1	0	2.543656	-0.963410	-0.356509
14	1	0	1.859152	0.039175	-1.669950
15	1	0	0.505354	-2.009641	0.843431
16	1	0	0.487403	1.574214	1.319957

Standard orientation of Ts-T-c

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-T-c

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -529.65 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.707354	-0.090845	0.084879
2	8	0	-1.460060	0.737979	-0.134509
3	8	0	-0.362515	0.446681	-0.891114
4	8	0	-2.207898	-0.453722	-0.006193
5	6	0	1.637420	-0.688331	-0.891282
6	1	0	1.162674	-1.569363	-1.315203
7	6	0	0.135644	-1.004735	1.028858
8	1	0	-1.467611	-0.935596	0.571975
9	6	0	1.262082	1.133415	0.697072
10	1	0	2.115628	0.844381	1.306409
11	1	0	0.313993	-0.656295	2.041399
12	1	0	1.561180	1.822846	-0.089011
13	1	0	2.543656	-0.963410	-0.356509
14	1	0	1.859152	0.039175	-1.669950
15	1	0	0.505354	-2.009641	0.843431
16	1	0	0.487403	1.574214	1.319957

Standard orientation of Ts-T-d

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-T-d

State=1-A
Charge = 1 Multiplicity = 2
Lowest Harmonic Vibrational Frequency (LHVF) = -2055.63 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.689552	0.000001	0.189850
2	6	0	1.177008	1.240515	-0.401418
3	1	0	2.231407	1.349082	-0.139240
4	1	0	1.075368	1.187470	-1.482888
5	1	0	0.613425	2.083310	-0.008552
6	8	0	-1.322048	-0.000012	-0.909249
7	8	0	-2.006019	-0.000002	0.084480
8	6	0	1.177017	-1.240520	-0.401392
9	1	0	0.613534	-2.083324	-0.008405
10	1	0	1.075248	-1.187553	-1.482854
11	1	0	2.231455	-1.349001	-0.139332
12	6	0	0.109566	0.000015	1.395817
13	1	0	0.156631	0.932624	1.951876
14	1	0	-1.137579	0.000007	1.068652
15	1	0	0.156637	-0.932578	1.951902

Standard orientation of Ts-T-e

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-T-e

State=1-A
Charge = 1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -579.13 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.631705	0.128754	-0.018150
2	6	0	0.242926	-1.209399	-0.382048
3	1	0	0.797451	-1.985513	0.156430
4	1	0	0.380028	-1.345907	-1.454293
5	8	0	-1.152406	-1.333402	-0.110168
6	1	0	-1.305045	-1.874016	0.670452
7	6	0	1.032262	0.238489	1.379590
8	1	0	1.982354	-0.277023	1.572260
9	1	0	1.144721	1.289832	1.646777
10	1	0	0.264915	-0.191594	2.025500
11	6	0	1.615929	0.720739	-0.913746
12	1	0	1.760124	1.768044	-0.645834
13	1	0	2.588533	0.214804	-0.856444
14	1	0	1.256033	0.677317	-1.942305
15	1	0	-2.810175	0.997703	-0.418688
16	8	0	-1.966392	1.201197	0.019454
17	1	0	-1.553507	1.982047	-0.386077
18	1	0	-1.323687	0.401701	-0.017794

Standard orientation of Ts-T-f

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-T-f

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -550.33 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.966106	0.125392	-0.004108
2	6	0	-0.340774	-1.092219	-0.632472
3	1	0	1.495492	-1.076146	0.038878
4	1	0	-1.146834	-1.815743	-0.780789
5	8	0	0.635544	-1.623170	0.162516
6	8	0	2.612247	-0.084474	-0.214429
7	1	0	1.904851	0.937822	0.012072
8	1	0	3.336786	-0.149793	0.410645
9	8	0	1.095083	1.748426	0.138292
10	1	0	-0.163634	0.841509	0.123698
11	1	0	1.250095	2.230647	0.953412
12	6	0	-1.538717	-0.179310	1.318329
13	1	0	-0.767480	-0.630228	1.937324
14	1	0	-1.888824	0.745321	1.773783
15	6	0	-1.961973	0.724635	-0.908988
16	1	0	-1.482298	0.978174	-1.852858
17	1	0	-2.772680	0.017396	-1.085011
18	1	0	-2.358960	1.628340	-0.450814
19	1	0	0.034583	-0.757614	-1.605445
20	1	0	-2.372572	-0.872321	1.201612

Standard orientation of Ts-TE-a

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-TE-a

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -926.47 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.455832	0.039356	-0.040797
2	6	0	-0.431933	0.377983	1.391653
3	1	0	-0.483107	-0.571893	1.923339
4	1	0	-1.356527	0.923948	1.606150
5	8	0	1.731074	-1.001401	-0.894611
6	8	0	0.659879	-1.311795	-0.235287
7	8	0	2.734823	-0.553372	-0.096628
8	6	0	0.024661	1.067373	-0.968502
9	1	0	1.039937	1.319535	-0.667733
10	1	0	0.083149	0.595813	-1.950428
11	6	0	-1.719060	-0.584926	-0.480041
12	1	0	-2.485270	0.194391	-0.470824
13	1	0	-1.560081	-0.888849	-1.514866
14	6	0	-0.855972	2.304157	-1.015352
15	1	0	-0.380914	3.035623	-1.669625
16	1	0	-1.845092	2.091190	-1.420399
17	1	0	-0.970607	2.761972	-0.031821
18	6	0	-2.167633	-1.764034	0.358564
19	1	0	-2.473570	-1.468254	1.361975
20	1	0	-3.035260	-2.209939	-0.128972
21	1	0	-1.393613	-2.527184	0.430695
22	6	0	0.782360	1.158429	1.836607
23	1	0	0.778263	2.183272	1.463256
24	1	0	0.777478	1.204286	2.926280
25	1	0	1.695299	0.659256	1.503184

Standard orientation of Ts-TE-b'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-TE-b'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -912.87 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.338364	-0.040598	0.226237
2	8	0	-1.447930	0.733704	-1.116436
3	8	0	-0.148541	0.334294	-1.220290
4	8	0	-2.248631	-0.433672	-1.083690
5	6	0	1.500939	-0.908588	-0.134749
6	1	0	1.071840	-1.764422	-0.649982
7	6	0	-0.705763	-0.690916	0.965245
8	1	0	-1.865670	-0.686014	-0.097082
9	6	0	0.803005	1.253929	0.812497
10	1	0	1.357610	0.967557	1.708352
11	6	0	-0.266189	2.272390	1.138966
12	1	0	-0.783138	2.615854	0.245486
13	1	0	-1.001552	1.910481	1.855458
14	1	0	0.240167	3.128748	1.587921
15	6	0	-0.576768	-2.178713	1.213516
16	1	0	-1.425115	-2.467963	1.837380
17	1	0	-0.652444	-2.778730	0.301617
18	1	0	0.328689	-2.493306	1.746288
19	6	0	2.580998	-0.269138	-0.982507
20	1	0	2.179483	0.185004	-1.887298
21	1	0	3.165681	0.470664	-0.436811
22	1	0	3.265383	-1.063568	-1.283680
23	1	0	-0.912041	-0.118089	1.862147
24	1	0	1.499216	1.682327	0.095392
25	1	0	1.906817	-1.252746	0.816672

Standard orientation of Ts-TE-c

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-TE-c

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -912.87 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.338364	-0.040598	0.226237
2	8	0	-1.447930	0.733704	-1.116436
3	8	0	-0.148541	0.334294	-1.220290
4	8	0	-2.248631	-0.433672	-1.083690
5	6	0	1.500939	-0.908588	-0.134749
6	1	0	1.071840	-1.764422	-0.649982
7	6	0	-0.705763	-0.690916	0.965245
8	1	0	-1.865670	-0.686014	-0.097082
9	6	0	0.803005	1.253929	0.812497
10	1	0	1.357610	0.967557	1.708352
11	6	0	-0.266189	2.272390	1.138966
12	1	0	-0.783138	2.615854	0.245486
13	1	0	-1.001552	1.910481	1.855458
14	1	0	0.240167	3.128748	1.587921
15	6	0	-0.576768	-2.178713	1.213516
16	1	0	-1.425115	-2.467963	1.837380
17	1	0	-0.652444	-2.778730	0.301617
18	1	0	0.328689	-2.493306	1.746288
19	6	0	2.580998	-0.269138	-0.982507
20	1	0	2.179483	0.185004	-1.887298
21	1	0	3.165681	0.470664	-0.436811
22	1	0	3.265383	-1.063568	-1.283680
23	1	0	-0.912041	-0.118089	1.862147
24	1	0	1.499216	1.682327	0.095392
25	1	0	1.906817	-1.252746	0.816672

Standard orientation of Ts-TE-d

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-TE-d

State=1-A
Charge = 1 Multiplicity = 2
Lowest Harmonic Vibrational Frequency (LHVF) = -2110.06 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.190093	-0.028572	-0.442604
2	6	0	-0.617641	1.366052	-0.632690
3	1	0	-1.240523	1.361569	-1.532902
4	1	0	-1.265362	1.613670	0.207039
5	8	0	0.238489	0.202820	1.889328
6	8	0	1.410498	-0.071339	1.791598
7	6	0	-1.253598	-1.037915	-0.332152
8	1	0	-0.840242	-1.891093	0.202938
9	1	0	-1.458732	-1.367106	-1.356758
10	6	0	1.081344	-0.416069	-0.683956
11	1	0	1.678077	0.353832	-1.169030
12	1	0	1.580352	-0.297403	0.483803
13	6	0	0.493647	2.381179	-0.755338
14	1	0	1.070364	2.269264	-1.673939
15	1	0	0.031026	3.367582	-0.782207
16	1	0	1.170062	2.361394	0.100688
17	6	0	1.400393	-1.836401	-1.071966
18	1	0	2.474442	-1.916447	-1.228196
19	1	0	1.111776	-2.566213	-0.316665
20	1	0	0.895813	-2.085193	-2.008138
21	6	0	-2.521758	-0.563927	0.340614
22	1	0	-3.037530	0.208663	-0.228439
23	1	0	-3.192585	-1.420045	0.413954
24	1	0	-2.332511	-0.201839	1.351602

Standard orientation of Ts-TE-e

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-TE-e

State=1-A
Charge = 1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -584.09 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.130575	-0.103411	-0.136553
2	6	0	0.409035	1.241972	-0.177812
3	1	0	0.260194	1.612783	-1.193354
4	8	0	1.833844	1.106167	-0.029771
5	1	0	2.108104	1.356991	0.858944
6	6	0	-0.464157	-0.583087	1.206845
7	1	0	-1.329295	-0.048039	1.618457
8	1	0	0.384621	-0.350384	1.855632
9	6	0	-1.125990	-0.394864	-1.170712
10	1	0	-1.224897	-1.479916	-1.239171
11	1	0	-0.703173	-0.071333	-2.125282
12	1	0	3.209838	-1.083587	-1.042584
13	8	0	2.341406	-1.372516	-0.714718
14	1	0	1.887401	-1.900886	-1.392010
15	1	0	1.773345	-0.558172	-0.432945
16	6	0	-0.124060	2.254839	0.813910
17	1	0	0.321355	3.229545	0.611501
18	1	0	-1.206109	2.347204	0.722173
19	1	0	0.107319	1.975315	1.843840
20	6	0	-0.720498	-2.077040	1.264929
21	1	0	-0.829299	-2.383309	2.306607
22	1	0	-1.636995	-2.359822	0.744657
23	1	0	0.108871	-2.641066	0.833312
24	6	0	-2.499005	0.232406	-0.977256
25	1	0	-2.451830	1.323117	-0.994180
26	1	0	-3.160893	-0.081496	-1.786737
27	1	0	-2.958483	-0.077628	-0.036509

Standard orientation of Ts-TE-f

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-TE-f

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -507.83 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.493328	0.049904	0.047917
2	6	0	-0.382090	-0.916306	0.837210
3	1	0	-2.021156	-0.881508	-0.275219
4	1	0	0.299337	-1.677688	1.225462
5	8	0	-1.267651	-1.525793	-0.020266
6	8	0	-3.035258	0.203695	-0.678765
7	1	0	-2.170907	1.118541	-0.813421
8	1	0	-3.464586	0.024151	-1.517817
9	8	0	-1.275630	1.843010	-0.794217
10	1	0	-0.169049	0.814642	-0.320481
11	1	0	-1.151651	2.216251	-1.669711
12	6	0	1.075479	-0.596121	-1.161784
13	1	0	0.233032	-0.991189	-1.724898
14	1	0	1.522245	0.200778	-1.755240
15	6	0	1.502188	0.722474	0.910783
16	1	0	0.945732	1.304894	1.642285
17	6	0	2.081670	-1.688223	-0.868874
18	1	0	2.466916	-2.063018	-1.817880
19	1	0	2.932865	-1.329089	-0.288228
20	1	0	1.630963	-2.530894	-0.343391
21	6	0	-1.070922	-0.200436	1.983914
22	1	0	-1.790817	-0.896174	2.414531
23	1	0	-0.377455	0.088310	2.772549
24	1	0	-1.610845	0.680259	1.632016
25	1	0	2.057525	-0.047024	1.450905
26	6	0	2.431139	1.642538	0.146900
27	1	0	3.021408	2.210079	0.866973
28	1	0	3.126323	1.102766	-0.496287
29	1	0	1.870345	2.355731	-0.460485

Standard orientation of Ts-D-a

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-a

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -971.87 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.011383	0.092123	-0.376734
2	6	0	-1.474746	-1.116555	0.289234
3	1	0	-1.307347	-1.964937	-0.371267
4	1	0	-2.541598	-1.026937	0.505267
5	8	0	1.482428	0.320888	-0.259710
6	8	0	0.590665	-0.230079	-1.011331
7	8	0	1.758346	-0.418807	0.840696
8	6	0	-0.947787	1.308518	0.410798
9	1	0	-0.384880	1.112740	1.320178
10	1	0	-0.452747	2.083182	-0.172469
11	1	0	-1.480564	0.241707	-1.265678
12	1	0	-0.908171	-1.248392	1.207239
13	1	0	-1.961320	1.629974	0.656442

Standard orientation of Ts-D-b'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-b'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -490.54 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.824629	0.069785	-0.367473
2	8	0	-1.390771	-0.563802	-0.436451
3	8	0	-0.177014	-0.993533	0.039529
4	8	0	-1.932300	0.306161	0.530845
5	6	0	0.350880	1.402211	-0.139433
6	1	0	-1.187254	1.044914	0.392356
7	1	0	0.926632	-0.123626	-1.363948
8	1	0	0.926162	1.864119	0.658897
9	6	0	2.027068	-0.372633	0.357445
10	1	0	1.879806	-0.156061	1.412668
11	1	0	2.175608	-1.438520	0.197440
12	1	0	0.370670	1.958924	-1.071384
13	1	0	2.868963	0.193678	-0.033179

Standard orientation of Ts-D-c

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-c

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -863.22 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.756733	-0.003123	0.002075
2	1	0	-0.061995	0.735372	0.036811
3	6	0	1.380982	-0.087947	1.330116
4	1	0	2.156935	-0.851478	1.307073
5	1	0	1.808377	0.881830	1.580966
6	8	0	0.197325	-1.234881	-0.331818
7	8	0	-1.349898	1.483544	-0.014664
8	1	0	-1.935509	0.442417	-0.027609
9	1	0	-1.565935	1.989780	0.771547
10	8	0	-2.238048	-0.729340	-0.146383
11	1	0	-0.842412	-1.116670	-0.235432
12	1	0	-2.676559	-1.046397	0.646154
13	6	0	1.708452	0.382064	-1.047998
14	1	0	1.167954	0.449472	-1.988977
15	1	0	2.140231	1.348466	-0.792816
16	1	0	2.487864	-0.375764	-1.114017
17	1	0	0.612279	-0.354456	2.051980

Standard orientation of Ts-D-d

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-d

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -220.12 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.833133	0.040225	0.037971
2	8	0	1.672227	-0.572811	0.000079
3	8	0	0.690287	-0.594213	-0.795488
4	8	0	2.271264	0.620227	0.068827
5	6	0	-1.117990	1.356130	-0.502865
6	1	0	-0.358063	2.042960	-0.140616
7	1	0	-1.076820	1.293154	-1.588278
8	1	0	-2.112470	1.674947	-0.182265
9	8	0	-1.782941	-0.837959	-0.417473
10	1	0	-1.355456	-1.707499	-0.434315
11	6	0	-0.615464	-0.061671	1.467621
12	1	0	-0.150580	-1.024630	1.686054
13	1	0	0.053695	0.738177	1.774941
14	1	0	-1.574350	0.012616	1.982587

Standard orientation of Ts-D-d'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-d'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -425.60 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.164392	-0.465765	1.275348
2	8	0	-2.084877	-0.747510	0.055376
3	8	0	-1.660068	-0.664519	-1.127157
4	8	0	-1.307881	-1.390101	0.856452
5	8	0	0.502470	0.282843	1.466828
6	7	0	1.071503	0.689088	0.315690
7	6	0	0.203973	1.249185	-0.635280
8	1	0	0.799340	1.620232	-1.471055
9	1	0	-0.453345	0.407579	-1.091654
10	6	0	2.200009	-0.118289	-0.112826
11	1	0	2.708095	0.444944	-0.897239
12	1	0	2.878823	-0.183166	0.739212
13	6	0	-0.754081	2.287416	-0.096227
14	1	0	-1.346067	2.692433	-0.916979
15	1	0	-1.436714	1.866887	0.643022
16	1	0	-0.203702	3.103762	0.374463
17	6	0	1.829419	-1.511351	-0.604016
18	1	0	1.171142	-1.466954	-1.472981
19	1	0	2.738864	-2.041534	-0.891046
20	1	0	1.334363	-2.089502	0.177185

Standard orientation of Ts-D-e

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-e

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -584.69 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.039447	0.124537	0.009889
2	1	0	-3.160506	0.459861	0.399585
3	6	0	0.570051	0.764344	-1.219281
4	1	0	0.823691	0.114930	-2.050936
5	1	0	-0.500039	0.944385	-1.114499
6	1	0	1.116625	1.709279	-1.282473
7	8	0	-0.931791	-1.415540	0.041424
8	8	0	-2.321470	0.543881	-0.056146
9	1	0	-1.038341	-1.949455	-0.748808
10	1	0	-1.683505	-0.533014	-0.011443
11	6	0	0.543008	0.642392	1.281289
12	1	0	0.806396	-0.068387	2.057370
13	1	0	1.056366	1.596135	1.428271
14	1	0	-0.532719	0.798147	1.170300
15	8	0	1.897955	-0.676347	-0.021357

Standard orientation of Ts-D-f

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-f

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -336.70 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.922581	0.301889	0.132192
2	8	0	-1.457664	-0.389256	0.363426
3	8	0	-1.565910	0.692531	-0.293664
4	8	0	-0.953973	-1.322850	-0.340734
5	6	0	1.865231	-0.674125	-0.434781
6	1	0	1.725809	-1.615323	0.086162
7	1	0	1.674572	-0.787335	-1.498498
8	1	0	2.871765	-0.291906	-0.267836
9	8	0	0.660981	0.244527	1.356173
10	6	0	0.341169	1.241638	-0.596129
11	1	0	0.055383	2.144936	-0.077857
12	1	0	0.508539	1.231706	-1.663458

Standard orientation of Ts-D-g

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-g

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -202.90 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.932531	0.088235	-0.063749
2	8	0	1.684378	-0.615045	0.090077
3	8	0	1.176914	1.037550	0.432117
4	8	0	0.826195	-1.094909	-0.712225
5	6	0	-1.015002	-0.467592	1.284677
6	1	0	-1.714967	-1.296550	1.256744
7	1	0	-0.017158	-0.755726	1.605255
8	1	0	-1.382559	0.340135	1.921621
9	8	0	-1.794038	-0.101243	-0.854476
10	6	0	0.118927	1.157964	-0.352757
11	1	0	0.276987	1.044428	-1.432220
12	1	0	-0.405724	2.097009	-0.140623

Standard orientation of Ts-D-h

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-h

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -212.06 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.620678	0.329981	0.342321
2	8	0	-0.772888	-0.575567	0.731242
3	8	0	-2.240556	0.034124	-0.720715
4	6	0	1.607499	1.167150	0.057651
5	1	0	0.839076	1.697257	0.616904
6	1	0	2.541032	1.085767	0.612713
7	1	0	1.761193	1.678535	-0.894607
8	7	0	1.089468	-0.162223	-0.270488
9	8	0	1.832551	-1.079650	-0.201286

Standard orientation of Ts-D-i

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-i

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -266.75 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.576595	0.418081	-0.078117
2	8	0	-1.436314	-0.480650	-0.525934
3	8	0	-1.457585	-1.041192	0.652112
4	8	0	-1.221735	1.121324	-0.312892
5	6	0	1.728744	-1.018348	-0.260464
6	1	0	0.900190	-1.514284	0.243100
7	1	0	1.698760	-1.247227	-1.324402
8	6	0	0.714017	0.955718	0.703684
9	1	0	0.711129	2.030078	0.826278
10	1	0	-1.055934	1.387496	-1.228072
11	1	0	0.135822	0.314218	1.358572
12	1	0	2.684542	-1.339108	0.152680
13	1	0	2.157833	1.022185	-0.646944

Standard orientation of Ts-D-j

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-j

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -505.72 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.128708	0.404369	0.467046
2	6	0	0.708946	-1.024165	0.673498
3	1	0	-0.946138	-1.151644	-0.363836
4	1	0	1.620892	-1.605638	0.824214
5	8	0	0.021179	-1.494114	-0.411083
6	8	0	-2.281095	-0.467807	-0.158290
7	1	0	-1.791167	0.695889	0.014483
8	1	0	-2.849546	-0.495017	-0.930322
9	8	0	-1.180468	1.633923	0.253992
10	1	0	0.227345	0.998473	0.358257
11	1	0	-1.301119	2.278966	-0.446295
12	6	0	2.007317	0.597015	-0.699677
13	1	0	1.485141	0.246814	-1.586233
14	1	0	2.237524	1.655669	-0.799279
15	1	0	0.115802	-1.026389	1.593605
16	1	0	2.926754	0.029047	-0.564412
17	1	0	1.599043	0.730135	1.310619

Standard orientation of Ts-D-j'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-j'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -256.11 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.607324	0.760335	-0.364510
2	6	0	-1.675083	-0.228874	-0.565189
3	8	0	1.865377	0.109851	-0.177138
4	8	0	0.929865	0.061765	-1.034838
5	8	0	1.907681	-0.965155	0.630764
6	6	0	-0.361868	1.299682	0.952852
7	1	0	-0.989497	2.174721	1.129098
8	1	0	-0.539423	0.534534	1.703128
9	1	0	0.687604	1.604240	1.002631
10	1	0	-2.630350	0.305034	-0.580197
11	8	0	-1.651175	-1.226292	0.392548
12	1	0	-2.283172	-1.031743	1.089575
13	1	0	-1.495698	-0.670046	-1.546978
14	1	0	-0.690477	1.494717	-1.062363

Standard orientation of Ts-D-j''

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-j''

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -293.80 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.427655	-2.439413	-0.833119
2	1	0	-0.499789	-1.149143	-0.238626
3	8	0	0.411464	1.864783	0.275329
4	8	0	1.038365	-1.978545	-0.086709
5	1	0	0.707207	2.672551	-0.153941
6	1	0	1.600594	-1.132416	0.079473
7	1	0	-1.551856	1.486679	-1.046519
8	8	0	2.209203	0.218600	0.399749
9	1	0	1.269658	1.176553	0.325532
10	1	0	2.983020	0.440914	-0.121408
11	6	0	-0.864361	0.655824	-0.960068
12	1	0	-0.039754	0.565465	-1.652934
13	7	0	-1.187496	-0.371660	-0.263806
14	6	0	-2.313199	-0.416848	0.649854
15	1	0	-1.954803	-0.388963	1.679230
16	1	0	-2.965815	0.435816	0.471471
17	1	0	-2.870547	-1.338986	0.491814

Standard orientation of Ts-D-k

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311+G(d) level:
Standard orientation of transition state of Ts-D-k

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1069.40 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.479351	0.070916	0.392373
2	1	0	0.609461	0.103418	1.402098
3	8	0	0.114365	1.316361	-0.036352
4	6	0	-0.779244	-0.862809	0.075957
5	1	0	-0.446437	-1.487973	-0.764017
6	1	0	-0.912060	-1.473914	0.975713
7	8	0	-1.766712	-0.010608	-0.201816
8	1	0	-0.994248	0.999583	-0.241418
9	6	0	1.712415	-0.396647	-0.245606
10	1	0	1.916932	-1.411101	0.095374
11	1	0	1.561087	-0.380956	-1.321965
12	1	0	2.529557	0.265251	0.030846

Standard orientation of Ts-D-l

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-l

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1820.47 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.799748	0.184364	0.447947
2	8	0	1.194705	-0.870753	0.240388
3	8	0	1.765855	0.042136	-0.289830
4	6	0	-1.623544	-0.756328	-0.290277
5	1	0	-1.396421	-0.683776	-1.351858
6	1	0	-1.432543	-1.763157	0.072666
7	1	0	-2.670972	-0.499342	-0.121248
8	6	0	-0.345914	1.336119	-0.055100
9	1	0	-0.146049	2.125204	0.665238
10	1	0	0.856811	1.015764	-0.351704
11	1	0	-0.725587	1.612983	-1.035530
12	1	0	-0.754732	0.051964	1.454616

Standard orientation of Ts-D-m

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-m

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -580.84 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.721810	-0.342159	0.536906
2	6	0	0.682984	1.078047	0.333378
3	1	0	1.529683	1.451830	-0.249164
4	1	0	0.650373	1.587586	1.295495
5	8	0	-0.537997	1.381099	-0.350293
6	1	0	-0.366013	1.619659	-1.265974
7	6	0	1.500198	-1.097972	-0.438412
8	1	0	2.558608	-0.816319	-0.439205
9	1	0	1.420411	-2.162387	-0.219035
10	1	0	1.097350	-0.933585	-1.439365
11	1	0	-2.802139	-0.319766	0.053182
12	8	0	-1.980728	-0.833548	-0.027229
13	1	0	-1.920803	-1.495194	0.682210
14	1	0	-1.157409	-0.220997	-0.009783
15	1	0	0.987973	-0.576578	1.483673

Standard orientation of Ts-D-n

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-n

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -739.23 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.700500	0.118648	-0.109345
2	8	0	0.827086	0.707155	0.698945
3	8	0	1.534579	-1.128622	-0.190289
4	7	0	-1.182716	-0.054885	-0.646672
5	6	0	-0.756784	1.136223	-0.320100
6	1	0	-1.168291	1.674221	0.537183
7	1	0	-0.261269	1.727458	-1.085202
8	6	0	-1.959236	-0.752541	0.342106
9	1	0	-2.899050	-1.071560	-0.115415
10	1	0	-1.425317	-1.664022	0.623916
11	1	0	-2.168273	-0.161439	1.239696

Standard orientation of Ts-D-n'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-n'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -435.90 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.955378	0.076734	-0.599072
2	8	0	1.526845	-0.326246	-0.150561
3	8	0	1.236651	0.598172	0.701654
4	8	0	0.593113	-1.166274	-0.235415
5	6	0	-1.846747	-0.425960	0.426612
6	1	0	-1.854229	-1.515024	0.392741
7	1	0	-1.569154	-0.096008	1.431401
8	1	0	-2.856560	-0.079377	0.196605
9	6	0	-0.383812	1.221646	-0.367776
10	1	0	0.220749	1.669417	-1.150935
11	1	0	-0.722678	1.864526	0.445258

Standard orientation of Ts-D-n''

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-n''

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -695.69 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.504408	0.449005	-0.225965
2	8	0	0.382224	-0.121890	-0.850084
3	8	0	2.026507	-0.343779	0.599729
4	6	0	-1.403524	1.181188	0.201298
5	1	0	-2.110901	1.225526	1.028440
6	1	0	-0.639183	1.941030	0.356144
7	1	0	-1.921926	1.364420	-0.741919
8	7	0	-0.779097	-0.130149	0.223491
9	6	0	-1.521992	-1.212480	0.067699
10	1	0	-2.595835	-1.122778	-0.057584
11	1	0	-1.030491	-2.176090	0.047058

Standard orientation of Ts-D-o

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-o

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -649.66 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.373310	0.090637	-0.470472
2	8	0	-0.363965	-0.744947	0.588560
3	8	0	-2.330809	0.502512	0.113037
4	7	0	1.860575	-0.152216	-0.148154
5	6	0	0.771410	-1.073787	-0.153318
6	1	0	1.113858	-2.036230	0.245695
7	1	0	0.486922	-1.261019	-1.202433
8	6	0	1.510660	1.212126	0.101714
9	1	0	2.412428	1.814583	0.202756
10	1	0	0.928139	1.606780	-0.742605
11	1	0	0.886878	1.325752	0.994291

Standard orientation of Ts-D-p

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-p

State=1-A
Charge = 0 Multiplicity = 3
Lowest Harmonic Vibrational Frequency (LHVF) = -959.41 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.903650	0.058058	-0.669444
2	8	0	1.527774	-0.518093	0.102568
3	8	0	0.682597	1.104808	0.667414
4	8	0	0.594363	-1.264633	-0.225282
5	6	0	-1.670634	-0.446602	0.449187
6	1	0	-1.813790	-1.513235	0.282456
7	1	0	-1.209777	-0.266891	1.419531
8	1	0	-2.661275	0.010882	0.389860
9	6	0	0.014403	1.070065	-0.442717
10	1	0	0.508519	1.402022	-1.362389
11	1	0	-0.998612	1.643383	-0.439779

Standard orientation of Ts-D-p'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-D-p'

State=1-A
Charge = 0 Multiplicity = 3
Lowest Harmonic Vibrational Frequency (LHVF) = -152.21 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.734950	0.016130	-0.334389
2	8	0	1.600246	-0.645308	0.259943
3	8	0	1.417863	0.552516	0.550426
4	8	0	-0.199726	-1.034046	-0.772208
5	6	0	-1.721842	-0.136425	0.736323
6	1	0	-2.507937	-0.793072	0.371592
7	1	0	-1.219364	-0.592642	1.588128
8	1	0	-2.129641	0.834876	1.001790
9	6	0	-0.182998	1.167123	-0.617325
10	1	0	0.464195	1.206928	-1.480211
11	1	0	-0.580627	2.061513	-0.159848

Standard orientation of Ts-DE-a

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-DE-a

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -938.85 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.505362	0.156629	-0.287171
2	6	0	0.586783	1.297474	0.629840
3	1	0	1.584321	1.280865	1.079746
4	8	0	-1.751649	-0.931758	-0.408681
5	8	0	-1.147699	0.104019	-0.881049
6	8	0	-2.177157	-0.742156	0.863648
7	6	0	0.882933	-1.151034	0.230726
8	1	0	0.673493	-1.152179	1.299920
9	1	0	0.211684	-1.881044	-0.231943
10	6	0	2.332037	-1.481054	-0.072230
11	1	0	2.563750	-2.469772	0.324379
12	1	0	2.516486	-1.498498	-1.148150
13	1	0	3.012362	-0.763565	0.389039
14	1	0	0.960114	0.351668	-1.176985
15	6	0	0.340728	2.607730	-0.083240
16	1	0	0.412467	3.425313	0.634131
17	1	0	1.085458	2.781529	-0.863043
18	1	0	-0.652013	2.632456	-0.531870
19	1	0	-0.148508	1.117294	1.413055

Standard orientation of Ts-DE-b'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-DE-b'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -763.86 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.380009	-0.176472	-0.259935
2	8	0	-1.883562	-0.589818	-0.556800
3	8	0	-0.703627	-1.265040	-0.393386
4	8	0	-2.345225	-0.247398	0.734715
5	6	0	-0.050529	0.955735	0.490904
6	1	0	-1.528562	0.434426	0.899697
7	1	0	0.528861	0.052059	-1.245229
8	1	0	0.531488	1.002569	1.409710
9	6	0	1.521647	-0.969390	0.252323
10	1	0	1.304528	-1.165780	1.301812
11	6	0	-0.077868	2.234223	-0.316867
12	1	0	-0.760597	2.158787	-1.168006
13	1	0	-0.455483	3.043931	0.310170
14	1	0	0.902335	2.551695	-0.697062
15	1	0	1.525311	-1.914306	-0.291133
16	6	0	2.820151	-0.218358	0.065822
17	1	0	2.816392	0.726989	0.608691
18	1	0	3.635869	-0.830327	0.450669
19	1	0	3.018706	-0.019948	-0.989095

Standard orientation of Ts-DE-c

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-DE-c

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -838.08 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.385625	-0.004707	0.115298
2	1	0	0.477822	-0.204173	0.761775
3	6	0	-0.728005	1.434690	0.176652
4	1	0	-1.504645	1.611225	-0.567237
5	1	0	-1.146361	1.613165	1.168822
6	8	0	-0.025089	-0.346831	-1.185332
7	8	0	1.750514	-0.712987	1.403581
8	1	0	2.220444	-0.842336	0.300994
9	1	0	2.255840	-0.086663	1.926021
10	8	0	2.379124	-0.975498	-0.885823
11	1	0	0.989438	-0.596345	-1.150784
12	1	0	3.017718	-0.335330	-1.207412
13	6	0	-1.473581	-0.899734	0.580515
14	1	0	-1.065061	-1.907673	0.510709
15	1	0	-1.627411	-0.669191	1.636362
16	6	0	-2.753228	-0.773065	-0.213902
17	1	0	-3.442551	-1.553046	0.110763
18	1	0	-3.244808	0.187483	-0.056773
19	1	0	-2.565654	-0.908266	-1.279227
20	6	0	0.481347	2.304755	-0.076498
21	1	0	0.901416	2.112789	-1.063872
22	1	0	0.182000	3.352219	-0.032038
23	1	0	1.255590	2.141732	0.674808

Standard orientation of Ts-DE-d

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-DE-d

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -982.69 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.434043	0.132859	0.235602
2	6	0	-0.397224	1.153323	-0.825629
3	1	0	-1.434093	1.319308	-1.129070
4	8	0	1.758455	-1.103811	0.375257
5	8	0	1.169725	-0.073163	0.888208
6	8	0	2.335793	-0.826337	-0.823225
7	6	0	-0.880122	-1.207964	-0.166170
8	1	0	-0.217892	-1.510487	-0.976655
9	1	0	-0.684132	-1.862292	0.685846
10	6	0	-2.339027	-1.248726	-0.572273
11	1	0	-2.607419	-2.287053	-0.767035
12	1	0	-2.982725	-0.874350	0.223621
13	1	0	-2.525872	-0.679520	-1.482665
14	6	0	0.248866	2.446555	-0.385955
15	1	0	0.221724	3.140029	-1.227005
16	1	0	-0.290936	2.899501	0.444655
17	1	0	1.287071	2.292491	-0.098362
18	1	0	0.147955	0.689107	-1.645503
19	8	0	-1.108057	0.633434	1.306182
20	1	0	-0.917660	0.043143	2.051733

Standard orientation of Ts-DE-d'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-DE-d'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -425.60 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.164392	-0.465765	1.275348
2	8	0	-2.084877	-0.747510	0.055376
3	8	0	-1.660068	-0.664519	-1.127157
4	8	0	-1.307881	-1.390101	0.856452
5	8	0	0.502470	0.282843	1.466828
6	7	0	1.071503	0.689088	0.315690
7	6	0	0.203973	1.249185	-0.635280
8	1	0	0.799340	1.620232	-1.471055
9	1	0	-0.453345	0.407579	-1.091654
10	6	0	2.200009	-0.118289	-0.112826
11	1	0	2.708095	0.444944	-0.897239
12	1	0	2.878823	-0.183166	0.739212
13	6	0	-0.754081	2.287416	-0.096227
14	1	0	-1.346067	2.692433	-0.916979
15	1	0	-1.436714	1.866887	0.643022
16	1	0	-0.203702	3.103762	0.374463
17	6	0	1.829419	-1.511351	-0.604016
18	1	0	1.171142	-1.466954	-1.472981
19	1	0	2.738864	-2.041534	-0.891046
20	1	0	1.334363	-2.089502	0.177185

Standard orientation of Ts-DE-e

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-DE-e

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -674.62 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.601185	0.359938	0.243998
2	1	0	2.951801	-1.663935	-0.963839
3	6	0	0.181722	0.944498	-0.850966
4	1	0	0.980530	0.214366	-1.041667
5	1	0	-0.504960	0.906008	-1.704581
6	8	0	1.463914	-0.628406	1.341251
7	8	0	2.011097	-1.578743	-0.799476
8	1	0	2.125082	0.009977	1.617034
9	1	0	1.820953	-1.110513	0.327516
10	6	0	-1.041759	-1.044762	0.116262
11	1	0	-1.031809	-1.436437	1.130139
12	1	0	-0.286626	-1.544727	-0.488319
13	8	0	-0.983736	1.014415	1.141642
14	6	0	-2.430103	-1.080190	-0.501620
15	1	0	-2.438027	-0.678993	-1.515058
16	1	0	-2.741533	-2.123184	-0.548847
17	1	0	-3.148711	-0.535450	0.110911
18	6	0	0.655333	2.335601	-0.541548
19	1	0	1.303596	2.337000	0.335480
20	1	0	1.230117	2.694605	-1.394816
21	1	0	-0.173469	3.022702	-0.372032

Standard orientation of Ts-DE-f

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-DE-f

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -311.04 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.510174	0.104410	0.186635
2	8	0	-1.750778	-0.925201	0.306977
3	8	0	-1.932957	0.103914	-0.414766
4	8	0	-1.109010	-1.837338	-0.313166
5	6	0	1.579340	-0.765078	-0.353718
6	1	0	1.487792	-1.714687	0.166623
7	1	0	1.374767	-0.918879	-1.412120
8	8	0	0.208040	0.000841	1.398945
9	6	0	-0.128024	0.993471	-0.572697
10	1	0	0.116985	0.934767	-1.626861
11	6	0	-0.628046	2.277520	-0.014029
12	1	0	-1.454251	2.648242	-0.618891
13	1	0	-0.952460	2.162258	1.016559
14	1	0	0.183457	3.009250	-0.061094
15	6	0	2.930479	-0.120230	-0.123726
16	1	0	3.710355	-0.780916	-0.503828
17	1	0	3.008472	0.834935	-0.645750
18	1	0	3.108804	0.042326	0.940017

Standard orientation of Ts-DE-g

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-DE-g

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -191.97 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.378224	-0.212184	0.225437
2	8	0	-2.068963	-0.946182	0.126244
3	8	0	-1.717439	0.781580	0.308812
4	8	0	-1.256206	-1.393878	-0.725757
5	6	0	1.514566	-0.732054	-0.564952
6	1	0	1.369654	-0.381763	-1.585516
7	8	0	0.271977	-0.489738	1.372444
8	6	0	-0.575756	0.858281	-0.355949
9	1	0	-0.642768	0.542495	-1.406430
10	6	0	0.090985	2.214148	-0.219431
11	1	0	-0.582042	2.957200	-0.644493
12	1	0	0.262077	2.447042	0.831205
13	1	0	1.031591	2.248614	-0.768786
14	1	0	1.417330	-1.815959	-0.543293
15	6	0	2.830130	-0.274931	0.034639
16	1	0	3.638910	-0.697103	-0.561059
17	1	0	2.928238	0.810535	0.022007
18	1	0	2.934935	-0.632689	1.058516

Standard orientation of Ts-DE-h

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-DE-h

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -207.21 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.777675	-0.689361	-0.143288
2	8	0	-1.051473	0.045713	-0.930536
3	8	0	-2.522617	-0.029632	0.637693
4	6	0	1.838455	-0.094129	-0.266419
5	1	0	1.748171	-0.115984	-1.356161
6	1	0	2.744490	0.455900	-0.004718
7	7	0	0.683276	0.707621	0.185520
8	8	0	0.812453	1.883212	0.225031
9	6	0	1.780850	-1.482835	0.324230
10	1	0	2.618574	-2.070669	-0.051106
11	1	0	1.847424	-1.450975	1.412361
12	1	0	0.857071	-1.989299	0.042923

Standard orientation of Ts-DE-l

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-DE-l

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1780.75 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.355459	0.099024	-0.327111
2	8	0	1.299824	-1.564114	-0.434209
3	8	0	2.018909	-1.027026	0.360499
4	6	0	0.397853	0.909432	0.436705
5	1	0	0.028948	1.008826	1.459386
6	1	0	1.371647	0.133016	0.678347
7	6	0	1.040774	2.109087	-0.205124
8	1	0	1.829068	2.498561	0.435945
9	1	0	1.469146	1.857988	-1.175927
10	1	0	0.287720	2.886885	-0.342196
11	6	0	-1.446970	-0.727538	0.178023
12	1	0	-1.425764	-1.668664	-0.370473
13	1	0	-1.245079	-0.932962	1.229220
14	6	0	-2.779500	-0.020913	-0.003583
15	1	0	-2.976072	0.184326	-1.056659
16	1	0	-3.571431	-0.669669	0.371131
17	1	0	-2.808766	0.916624	0.552301
18	1	0	-0.294010	0.200622	-1.337743

Standard orientation of Ts-DE-m

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-DE-m

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -609.49 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.303213	-0.191903	-0.476368
2	6	0	0.142410	0.951454	0.279985
3	1	0	-0.579540	1.230979	1.052823
4	8	0	1.355384	0.534698	0.939063
5	1	0	1.224169	0.473844	1.889887
6	6	0	-1.355471	-1.005804	0.134356
7	1	0	-1.368808	-1.971406	-0.376068
8	1	0	-1.060772	-1.208125	1.167843
9	1	0	2.957930	-1.539280	-0.196245
10	8	0	2.007830	-1.729737	-0.272365
11	1	0	1.791602	-2.015192	-1.175779
12	1	0	1.439383	-0.909586	-0.014657
13	1	0	-0.540337	0.056123	-1.429148
14	6	0	0.455635	2.127904	-0.610407
15	1	0	-0.451570	2.484371	-1.100806
16	1	0	0.877833	2.941145	-0.021203
17	1	0	1.180584	1.837240	-1.374034
18	6	0	-2.737589	-0.376399	0.088056
19	1	0	-3.470385	-1.032238	0.562152
20	1	0	-2.761643	0.583103	0.609436
21	1	0	-3.051582	-0.210278	-0.945148

Standard orientation of Ts-M-a

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-a

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1044.35 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.920064	0.213625	0.517714
2	6	0	2.116510	0.136989	-0.295689
3	1	0	2.888001	0.786611	0.120054
4	8	0	-1.424909	-0.439624	0.210759
5	8	0	-0.272128	-0.793033	-0.257206
6	8	0	-1.779229	0.779861	-0.242201
7	1	0	1.005335	-0.157075	1.458943
8	1	0	1.873034	0.459376	-1.305727
9	1	0	0.430471	1.106944	0.495389
10	1	0	2.473782	-0.890803	-0.309342

Standard orientation of Ts-M-b'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-b'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -529.82 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.168044	-0.440206	0.014613
2	8	0	1.068441	-0.378280	0.461397
3	8	0	0.149963	-1.052260	-0.316782
4	8	0	1.419707	0.791410	-0.237354
5	6	0	-1.159412	0.997556	0.061087
6	1	0	0.442401	1.225142	-0.153065
7	1	0	-1.417413	-0.873149	0.904628
8	1	0	-1.719771	1.390854	-0.782415
9	1	0	-1.536181	1.325300	1.024803
10	1	0	-1.741142	-0.858997	-0.720857

Standard orientation of Ts-M-c

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-c

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -880.71 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.954181	0.029624	-0.455112
2	1	0	0.118010	0.755271	-0.372711
3	1	0	1.339079	0.084404	-1.397763
4	6	0	1.998378	0.330814	0.530074
5	1	0	1.549300	0.316194	1.520478
6	1	0	2.784105	-0.418411	0.459754
7	8	0	0.456078	-1.256901	-0.284444
8	8	0	-1.177020	1.446251	-0.229072
9	1	0	-1.682398	0.415791	0.073529
10	1	0	-1.235706	2.079361	0.489961
11	8	0	-1.926794	-0.772428	0.238669
12	1	0	-0.559086	-1.140103	-0.026115
13	1	0	-2.199882	-0.940757	1.143073
14	1	0	2.398934	1.320627	0.313915

Standard orientation of Ts-M-d

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-d

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -238.73 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.858993	0.116956	0.373226
2	8	0	-1.464809	-0.100615	-0.518839
3	8	0	-0.506283	-0.904592	-0.341365
4	8	0	-2.163595	0.126884	0.598530
5	6	0	2.089813	-0.599551	0.109713
6	1	0	2.021822	-1.561234	0.614983
7	1	0	2.183941	-0.760411	-0.963737
8	1	0	2.943315	-0.035731	0.488200
9	8	0	0.734012	1.339227	-0.191208
10	1	0	0.886554	1.231704	-1.142554
11	1	0	0.617932	0.217049	1.355314

Standard orientation of Ts-M-e

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-e

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -763.25 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.129448	0.273937	-0.135242
2	6	0	-1.931272	-0.263714	0.958081
3	1	0	-2.458835	-1.146527	0.606833
4	1	0	-1.277763	-0.478114	1.797353
5	1	0	-2.644312	0.521012	1.220380
6	8	0	0.321734	-1.392662	-0.181815
7	1	0	0.168361	-2.070905	0.481672
8	1	0	-0.182865	0.837107	0.074262
9	8	0	-1.584312	0.322468	-1.228349
10	8	0	2.514294	-0.439622	0.061914
11	1	0	3.055244	-0.565806	-0.720432
12	1	0	1.483967	-0.986662	-0.071509
13	8	0	1.049245	1.585306	0.182493
14	1	0	1.162806	2.093687	0.990441
15	1	0	1.779483	0.857014	0.145260

Standard orientation of Ts-M-e'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-e'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1113.10 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.739414	-0.011561	0.006599
2	1	0	0.089652	0.781451	-0.074051
3	6	0	-1.812490	0.181801	-0.970888
4	1	0	-1.367112	0.116868	-1.959998
5	1	0	-2.549101	-0.606672	-0.828211
6	1	0	-2.252985	1.162642	-0.809595
7	8	0	-0.177607	-1.242958	-0.147405
8	8	0	1.282380	1.476723	-0.010559
9	1	0	1.897807	0.478407	-0.036508
10	1	0	1.468531	2.026278	-0.775760
11	8	0	2.197363	-0.723566	0.037368
12	1	0	0.914135	-1.102494	-0.071206
13	1	0	2.721531	-1.001348	-0.717414
14	8	0	-1.335530	0.107762	1.265379
15	1	0	-0.604464	0.191293	1.893613

Standard orientation of Ts-M-f

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-f

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -212.06 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.620678	0.329981	0.342321
2	8	0	-0.772888	-0.575567	0.731242
3	8	0	-2.240556	0.034124	-0.720715
4	6	0	1.607499	1.167150	0.057651
5	1	0	0.839076	1.697257	0.616904
6	1	0	2.541032	1.085767	0.612713
7	1	0	1.761193	1.678535	-0.894607
8	7	0	1.089468	-0.162223	-0.270488
9	8	0	1.832551	-1.079650	-0.201286

Standard orientation of Ts-M-g

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-g

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -219.61 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.786074	0.043351	0.003016
2	8	0	1.680405	-0.564809	0.292091
3	8	0	0.824142	-1.136103	-0.401003
4	8	0	1.920053	0.662882	-0.117929
5	8	0	-0.624144	0.588270	1.248657
6	1	0	0.254240	1.001718	1.244103
7	8	0	-0.760025	0.983234	-0.987316
8	1	0	0.187361	1.065775	-1.203872
9	6	0	-2.042301	-0.679021	-0.033607
10	1	0	-2.101438	-1.185429	-0.993466
11	1	0	-2.036111	-1.401853	0.777715
12	1	0	-2.871167	0.022663	0.080046

Standard orientation of Ts-M-g'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-g'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -797.91 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.902909	0.164028	-0.323861
2	6	0	2.360574	0.097087	-0.331625
3	1	0	2.708072	1.008348	-0.817726
4	1	0	2.759145	0.056143	0.687037
5	1	0	2.679303	-0.768000	-0.909609
6	8	0	0.496206	1.074634	0.534150
7	1	0	-0.860923	1.299564	0.210409
8	8	0	0.534283	-1.239792	0.308908
9	1	0	0.671115	-1.111367	1.262475
10	8	0	-1.899237	1.251711	-0.023355
11	1	0	-2.067411	1.780423	-0.807714
12	1	0	-0.676669	-1.302723	0.056462
13	8	0	-1.796202	-1.194732	-0.262661
14	1	0	-1.985676	-0.153168	-0.204911
15	1	0	-2.391164	-1.674502	0.324017

Standard orientation of Ts-M-h

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-h

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -335.29 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.286127	0.085639	-0.031564
2	8	0	-0.081774	-1.416921	-0.338905
3	1	0	0.116410	-1.639313	-1.254130
4	8	0	0.722896	1.034650	-0.723877
5	1	0	-0.280739	1.233277	-0.389092
6	6	0	0.996519	0.049985	1.420575
7	1	0	1.324366	-0.917652	1.779833
8	1	0	1.579769	0.862862	1.853570
9	1	0	-0.065950	0.195005	1.574937
10	8	0	2.317580	-0.345493	-0.435770
11	8	0	-1.608957	1.503636	-0.138651
12	1	0	-1.820060	2.107349	0.579815
13	1	0	-1.539639	-1.203439	-0.139563
14	8	0	-2.517140	-0.888360	-0.001876
15	1	0	-2.840521	-1.278803	0.813597
16	1	0	-2.116471	0.641229	-0.008838

Standard orientation of Ts-M-i

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-i

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -155.93cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.685087	1.474478	-0.335517
2	6	0	-1.395620	0.795527	0.482426
3	1	0	-2.472341	0.777231	0.385793
4	1	0	-0.928328	0.409702	1.377835
5	8	0	1.918451	0.892331	-0.020945
6	1	0	0.358326	1.465328	-0.234446
7	1	0	2.425384	1.112028	0.763648
8	8	0	-1.336424	-1.318743	-0.236737
9	1	0	-1.765874	-1.957094	0.339367
10	1	0	-0.296970	-1.455154	-0.125484
11	1	0	-1.108429	1.893986	-1.152897
12	8	0	1.130086	-1.465003	0.078472
13	1	0	1.591538	-2.078818	-0.495940
14	1	0	1.669121	-0.130396	0.029861

Standard orientation of Ts-M-j

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-j

State=1-A
Charge = 1 Multiplicity = 2
Lowest Harmonic Vibrational Frequency (LHVF) = -1503.05 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.054308	0.678174	-0.000139
2	8	0	-1.207291	0.591665	0.000203
3	8	0	-1.282553	-0.598512	-0.000091
4	6	0	1.208713	-0.649386	0.000039
5	1	0	1.548602	-1.089564	0.933945
6	1	0	0.001865	-1.042398	0.000656
7	1	0	1.547615	-1.089988	-0.934025
8	1	0	1.095148	1.213197	0.861492
9	1	0	1.093092	1.212623	-0.862220

Standard orientation of Ts-M-k

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-k

State=1-A
Charge = 1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -591.31 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.604132	1.131154	-0.071796
2	6	0	-1.336439	-0.091851	0.114342
3	1	0	-2.120432	-0.234175	-0.629968
4	1	0	-1.773996	-0.122499	1.111117
5	8	0	-0.393952	-1.167207	0.027569
6	1	0	-0.556945	-1.695785	-0.759195
7	1	0	2.386234	-0.646734	0.476833
8	8	0	1.974994	0.049554	-0.062774
9	1	0	2.239177	0.928774	0.256508
10	1	0	0.952515	-0.033435	-0.056387
11	1	0	-0.753684	1.806222	0.665596
12	1	0	-0.773645	1.571884	-0.966343

Standard orientation of Ts-M-l

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-l

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -406.77 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.189981	1.052679	-0.149922
2	1	0	1.694062	1.758282	0.385023
3	1	0	1.518764	1.091444	-1.113045
4	6	0	1.413719	-0.324599	0.404292
5	1	0	1.008036	-0.306847	1.420612
6	1	0	-0.192310	-1.269959	-0.203063
7	1	0	2.490897	-0.488672	0.444217
8	8	0	0.819562	-1.256417	-0.401277
9	8	0	-1.631809	-1.071553	0.172925
10	1	0	-1.620788	0.221493	0.093113
11	1	0	-2.243639	-1.457996	-0.456518
12	8	0	-1.398981	1.329133	0.078586
13	1	0	0.125434	1.278426	-0.123050
14	1	0	-1.902811	1.743358	-0.625466

Standard orientation of Ts-M-l'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-l'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -415.89cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.498586	-0.623786	0.623149
2	6	0	1.775726	-0.397205	-0.048060
3	8	0	-1.881280	-0.309465	-0.110503
4	8	0	-0.763646	-0.548272	-0.658810
5	8	0	-2.001921	0.971989	0.264610
6	1	0	2.575103	-0.825594	0.562521
7	8	0	1.961524	0.955383	-0.293909
8	1	0	2.402274	1.366273	0.455632
9	1	0	1.736352	-0.921661	-1.004482
10	1	0	0.392561	-1.545596	1.036930
11	1	0	0.231839	0.119228	1.264613

Standard orientation of Ts-M-l''

Cartesian coordinates of all the transition states optimized at the LC-ωPBE /6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-l''

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -152.46 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.472157	-1.022540	0.734117
2	1	0	-0.413601	-1.448775	-0.219423
3	8	0	1.392382	1.263457	-0.273516
4	8	0	-1.958047	-0.823883	-0.051516
5	1	0	1.851909	1.908888	0.270560
6	1	0	-1.670429	0.188179	-0.001913
7	1	0	2.432112	-0.861784	0.438520
8	8	0	-1.081308	1.507095	-0.048427
9	1	0	0.361291	1.442971	-0.160778
10	1	0	-1.388380	2.093303	0.645575
11	6	0	1.353862	-0.831497	0.513607
12	1	0	0.885211	-0.396097	1.385202
13	7	0	0.630729	-1.503234	-0.298832
14	1	0	1.051557	-1.965877	-1.094002

Standard orientation of Ts-M-m

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311+G(d) level:
Standard orientation of transition state of Ts-M-m

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1042.85 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.761209	0.605357	0.000028
2	1	0	-1.122781	1.077281	0.825619
3	8	0	-1.138200	-0.705565	-0.000027
4	6	0	0.851386	0.598782	-0.000031
5	1	0	1.130203	1.157372	-0.900627
6	1	0	1.130275	1.157470	0.900480
7	8	0	1.168152	-0.694737	0.000028
8	1	0	-0.034322	-1.097259	-0.000003
9	1	0	-1.122842	1.077363	-0.825488

Standard orientation of Ts-M-n

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-n

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -802.76 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.169907	-0.344115	0.338201
2	8	0	0.235972	-0.904928	-0.427293
3	8	0	1.525657	0.789473	-0.077571
4	7	0	-1.396627	0.930907	0.041891
5	6	0	-1.458990	-0.371020	0.209579
6	1	0	-1.950962	-1.024111	-0.511321
7	1	0	-1.359341	-0.753884	1.222327
8	1	0	-1.611661	1.164332	-0.928406

Standard orientation of Ts-M-n'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-n'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -464.19 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.207582	0.753737	0.041450
2	8	0	1.151972	-0.088904	0.331103
3	8	0	0.610468	-1.050138	-0.335428
4	8	0	0.777946	1.027744	-0.108904
5	6	0	-1.271410	-0.545641	0.166808
6	1	0	-1.210430	-0.971445	1.164505
7	1	0	-1.684327	-1.172110	-0.621796
8	1	0	-1.346798	1.031633	-0.927871

Standard orientation of Ts-M-n''

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-n''

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -707.32 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.361117	-0.407789	0.094895
2	8	0	-0.120705	-0.665702	-0.512743
3	8	0	-1.643840	0.816196	0.072224
4	7	0	1.000823	-0.148225	0.490579
5	6	0	1.994163	0.449527	-0.143171
6	1	0	3.009057	0.080843	-0.046262
7	1	0	1.768639	1.303916	-0.768973
8	1	0	1.256854	-0.985979	1.005195

Standard orientation of Ts-M-o

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-o

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -656.58 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.106117	-0.213633	0.417830
2	8	0	0.053312	0.656198	-0.444794
3	8	0	-2.148534	-0.201020	-0.163772
4	7	0	1.971705	-0.728469	-0.087247
5	6	0	1.241740	0.438963	0.255720
6	1	0	1.866360	1.325059	0.066534
7	1	0	1.049752	0.439661	1.339702
8	1	0	1.442231	-1.231580	-0.803946

Standard orientation of Ts-M-p

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-p

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1167.96 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.624456	1.153816	-0.005994
2	8	0	1.132595	-0.600521	0.212262
3	8	0	-0.548165	-1.101512	-0.380948
4	8	0	1.213423	0.612789	-0.076415
5	6	0	-1.046208	-0.122617	0.309332
6	1	0	-1.314515	-0.277495	1.356803
7	1	0	-1.959965	0.446492	-0.193693
8	1	0	-0.459897	1.203944	-1.016341

Standard orientation of Ts-M-p'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-p'

State=1-A
Charge = 0 Multiplicity = 3
Lowest Harmonic Vibrational Frequency (LHVF) = -180.77 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.065849	-0.121751	-0.285778
2	8	0	-1.371908	-0.506482	0.071326
3	8	0	-1.168264	0.690530	-0.201681
4	8	0	0.605566	-1.195030	0.179847
5	6	0	0.819547	1.022708	0.289552
6	1	0	0.554969	1.014424	1.336381
7	1	0	1.138024	1.922514	-0.218412
8	1	0	1.405628	-0.133074	-1.250762

Standard orientation of Ts-M-q

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-M-q

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1301.06 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.097678	0.861425	-0.016346
2	8	0	0.507956	-1.199855	-0.010242
3	8	0	-1.078166	1.471669	-0.100954
4	1	0	-1.638933	0.442924	-0.043868
5	1	0	-1.285164	2.022776	0.658370
6	8	0	-1.874646	-0.777538	-0.074195
7	1	0	-0.611446	-1.111382	-0.017647
8	1	0	-2.362253	-1.062652	0.702179
9	7	0	0.960286	0.051175	-0.000581
10	6	0	2.201578	0.289296	0.023152
11	1	0	2.914972	-0.526993	0.037705
12	1	0	2.512528	1.325695	0.027885

Standard orientation of Ts-E-a

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-E-a

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1034.22 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.346092	-0.549340	0.506612
2	6	0	-1.568089	-0.667027	-0.275820
3	1	0	-2.052909	-1.606555	0.001894
4	8	0	1.812144	0.578408	0.231861
5	8	0	0.603857	0.730320	-0.205508
6	8	0	2.383899	-0.522277	-0.296930
7	1	0	-0.470883	-0.278799	1.478301
8	6	0	-2.486448	0.513220	-0.049122
9	1	0	-3.385476	0.393834	-0.653483
10	1	0	-2.791272	0.579867	0.997223
11	1	0	-2.004250	1.448694	-0.334071
12	1	0	-1.263445	-0.745854	-1.320374
13	1	0	0.318904	-1.314572	0.398506

Standard orientation of Ts-E-b'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-E-b'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -793.14 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.347729	1.119829	0.158429
2	8	0	1.276436	-0.295749	-0.650181
3	8	0	1.141822	0.956571	-0.101894
4	8	0	1.311869	-1.211948	0.422945
5	6	0	-1.014462	-0.068944	0.589127
6	1	0	0.278496	-1.023200	0.686265
7	1	0	-0.683489	1.496576	-0.730750
8	1	0	-1.385910	0.097351	1.597989
9	6	0	-2.044548	-0.555437	-0.404533
10	1	0	-1.587377	-0.815123	-1.363287
11	1	0	-2.503897	-1.468581	-0.022165
12	1	0	-2.857460	0.156714	-0.598460
13	1	0	-0.313210	1.872752	0.846890

Standard orientation of Ts-E-c

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-E-c

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -875.69 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.429410	-0.433774	-0.517799
2	1	0	-0.115266	0.530574	-0.472572
3	1	0	0.815235	-0.549105	-1.455404
4	6	0	1.518400	-0.457198	0.478807
5	1	0	1.051358	-0.281374	1.447823
6	1	0	1.939229	-1.462566	0.472183
7	8	0	-0.472651	-1.470018	-0.313615
8	8	0	-1.118364	1.613274	-0.331180
9	1	0	-1.902847	0.822332	0.092282
10	1	0	-0.923172	2.287028	0.323904
11	8	0	-2.501242	-0.201710	0.373982
12	1	0	-1.360148	-1.015151	0.022077
13	1	0	-2.714670	-0.222169	1.309368
14	6	0	2.556999	0.593999	0.154912
15	1	0	3.338786	0.568745	0.913644
16	1	0	3.025960	0.408803	-0.813525
17	1	0	2.125336	1.596135	0.149000

Standard orientation of Ts-E-d

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-E-d

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -934.75 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.344703	0.401460	0.198930
2	8	0	-1.832175	-0.482172	-0.467009
3	8	0	-1.192953	0.635232	-0.611183
4	8	0	-2.173356	-0.667592	0.829669
5	6	0	1.154680	-0.543080	-0.559910
6	1	0	0.491874	-1.385966	-0.764557
7	1	0	1.397728	-0.062400	-1.509553
8	6	0	2.391811	-0.970478	0.202890
9	1	0	2.950793	-1.682576	-0.404123
10	1	0	3.038217	-0.118485	0.413950
11	1	0	2.128110	-1.458098	1.142414
12	8	0	0.852968	1.631473	0.404553
13	1	0	1.092510	1.990119	-0.463952
14	1	0	-0.026969	0.053008	1.087190

Standard orientation of Ts-E-e

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-E-e

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -687.85 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.629100	-0.603522	0.205296
2	6	0	-1.601167	-0.203082	-0.818730
3	1	0	-1.030897	0.306798	-1.591217
4	1	0	-1.940185	-1.161826	-1.228194
5	8	0	0.490432	1.325782	0.295238
6	1	0	0.180984	2.025120	-0.286432
7	1	0	0.383352	-0.944566	-0.100214
8	8	0	-0.972008	-0.791067	1.322362
9	8	0	2.809329	0.831053	-0.112864
10	1	0	3.353824	1.010992	0.656404
11	1	0	1.713259	1.153279	0.101271
12	8	0	1.752245	-1.441836	-0.333895
13	1	0	1.915460	-1.856107	-1.185797
14	1	0	2.327211	-0.594585	-0.269831
15	6	0	-2.740856	0.610007	-0.263078
16	1	0	-3.408125	0.879220	-1.081283
17	1	0	-3.312334	0.048537	0.474760
18	1	0	-2.366707	1.524772	0.197578

Standard orientation of Ts-E-e'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-E-e'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1086.97 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.430819	0.505754	-0.025723
2	1	0	-0.304300	0.131521	0.764360
3	6	0	1.793740	-0.042679	0.130910
4	1	0	2.395214	0.410094	-0.658419
5	1	0	2.147273	0.311988	1.098349
6	8	0	-0.066883	0.213928	-1.258177
7	8	0	-1.471704	-0.174974	1.471255
8	1	0	-2.040934	-0.425883	0.470618
9	1	0	-1.419627	-0.936359	2.053787
10	8	0	-2.347201	-0.477139	-0.724487
11	1	0	-1.105700	-0.109959	-1.111079
12	1	0	-2.558443	-1.375157	-0.990163
13	8	0	0.552655	1.887411	0.142020
14	1	0	-0.345510	2.210340	0.302024
15	6	0	1.786484	-1.550314	0.052167
16	1	0	1.428950	-1.891652	-0.918388
17	1	0	2.805594	-1.911561	0.190908
18	1	0	1.165465	-1.989495	0.834720

Standard orientation of Ts-E-f

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-E-f

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -207.21 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.777675	-0.689361	-0.143288
2	8	0	-1.051473	0.045713	-0.930536
3	8	0	-2.522617	-0.029632	0.637693
4	6	0	1.838455	-0.094129	-0.266419
5	1	0	1.748171	-0.115984	-1.356161
6	1	0	2.744490	0.455900	-0.004718
7	7	0	0.683276	0.707621	0.185520
8	8	0	0.812453	1.883212	0.225031
9	6	0	1.780850	-1.482835	0.324230
10	1	0	2.618574	-2.070669	-0.051106
11	1	0	1.847424	-1.450975	1.412361
12	1	0	0.857071	-1.989299	0.042923

Standard orientation of Ts-E-g

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-E-g

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -210.00 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.376931	0.008342	-0.018272
2	8	0	2.121867	-0.509066	0.328397
3	8	0	1.305480	-1.134824	-0.362631
4	8	0	2.322875	0.710477	-0.108249
5	8	0	-0.272859	0.594459	1.217400
6	1	0	0.593841	1.029059	1.230955
7	8	0	-0.367757	0.927846	-1.030941
8	1	0	0.577151	1.021285	-1.248047
9	6	0	-1.596164	-0.794312	-0.066908
10	1	0	-1.543762	-1.335705	-1.011054
11	1	0	-1.503913	-1.512438	0.747101
12	6	0	-2.867366	0.024154	0.042203
13	1	0	-3.722071	-0.651275	-0.004833
14	1	0	-2.909067	0.563615	0.988353
15	1	0	-2.949326	0.736870	-0.778150

Standard orientation of Ts-E-g'

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-E-g'

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -805.42 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.515127	-0.124539	-0.120838
2	6	0	1.918537	-0.534469	0.013367
3	1	0	2.125328	-0.772422	1.063866
4	1	0	2.050020	-1.431506	-0.591395
5	8	0	0.203707	0.750743	0.809949
6	1	0	-1.003888	1.328299	0.375689
7	8	0	-0.233151	-1.464213	0.264645
8	1	0	-0.196580	-1.483078	1.235470
9	8	0	-1.986082	1.558107	0.025353
10	1	0	-1.921896	2.190373	-0.695152
11	1	0	-1.383045	-1.207377	-0.113903
12	8	0	-2.399763	-0.802380	-0.527583
13	1	0	-2.357748	0.242865	-0.350519
14	1	0	-3.157817	-1.186829	-0.073852
15	6	0	2.817098	0.581178	-0.476691
16	1	0	2.702178	1.473884	0.138166
17	1	0	3.859017	0.260934	-0.428835
18	1	0	2.587040	0.838317	-1.512639

Standard orientation of Ts-E-h

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-E-h

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -315.42 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.956108	-0.607215	-0.235177
2	8	0	0.221380	0.800462	-1.176107
3	1	0	0.201731	0.444642	-2.069973
4	8	0	-0.099381	-1.592881	-0.215418
5	1	0	0.800239	-1.319305	0.286560
6	6	0	-1.027014	0.226383	1.009481
7	1	0	-1.359867	-0.489839	1.764863
8	1	0	-0.009244	0.534915	1.225662
9	8	0	-1.908603	-0.732121	-0.931780
10	8	0	2.077794	-1.070611	0.813636
11	1	0	2.186282	-1.110832	1.768449
12	1	0	1.608286	1.099829	-0.739360
13	8	0	2.565123	1.171225	-0.346582
14	1	0	2.628138	2.005593	0.124338
15	1	0	2.408341	-0.178670	0.484593
16	6	0	-1.975081	1.380444	0.851660
17	1	0	-2.993694	1.039651	0.671152
18	1	0	-1.964356	1.953742	1.779327
19	1	0	-1.651036	2.021216	0.033791

Standard orientation of Ts-E-j

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-E-j

State=1-A
Charge = 1 Multiplicity = 2
Lowest Harmonic Vibrational Frequency (LHVF) = -1403.65 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.284173	1.208207	-0.029597
2	8	0	-1.806551	0.139344	-0.325528
3	8	0	-1.451452	-0.876033	0.187233
4	6	0	0.864118	0.119809	0.504860
5	1	0	1.025483	0.201267	1.581129
6	1	0	-0.122252	-0.660027	0.551741
7	6	0	1.884852	-0.625095	-0.310395
8	1	0	2.061851	-1.608166	0.120964
9	1	0	1.560043	-0.744448	-1.344282
10	1	0	2.822329	-0.066468	-0.296840
11	1	0	0.366825	1.419729	-1.018848
12	1	0	-0.133289	1.925888	0.552875

Standard orientation of Ts-E-k

Cartesian coordinates of all the transition states optimized at the LC-ωPBE/6-311++G(d,p) level:
Standard orientation of transition state of Ts-E-k

State=1-A
Charge = 1 Multiplicity = 2
Lowest Harmonic Vibrational Frequency (LHVF) = -599.58 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.079744	1.179591	-0.350099
2	6	0	-0.903435	-0.005190	-0.428005
3	1	0	-1.432255	-0.062156	-1.381728
4	8	0	0.008394	-1.117758	-0.355934
5	1	0	0.042887	-1.578738	-1.199347
6	1	0	2.573841	-0.766893	0.873301
7	8	0	2.343411	-0.023333	0.291211
8	1	0	2.533786	0.822924	0.729544
9	1	0	1.353529	-0.057918	0.015378
10	1	0	-0.414734	1.854637	0.325173
11	1	0	0.037760	1.641316	-1.242963
12	6	0	-1.868095	-0.097454	0.727789
13	1	0	-2.586733	0.722560	0.688857
14	1	0	-2.411147	-1.040992	0.687836
15	1	0	-1.323982	-0.047291	1.673728