Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supporting Information

Comparison of nitrate formation mechanisms from free amino acids and amines during ozonation: a computational study

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Text S1

Calculation details of estimations of pK_a values for the nitroalkanes

Based on the results from our previous work,[1] the linear equation of the bond dissociation energies (BDEs) of C−H bonds and their experimental pK_a values is displayed in eq. (1).

$$pK_a = 0.504 \times BDEs - 70.788 \quad (1)$$

Based on the above equation, the calculated pK_a and BDEs of 9 nitroalkanes (O_2N-CHR) formed from amines were calculated at the M06-2X/6-311G(d) level with the SMD solvent model and are listed in Table S1.

Table S1

Table S1 The pK_a values and BDEs of nine nitroalkanes.

Nitroalkanes	BDEs (kcal/mol)	pK_a
O_2N-CH_3	170.3	15.0
O_2N-CH_2CH_3	169.0	14.4
O_2N-$CH(CH_3)$-C_6H_5	164.4	12.1
O_2N-CH_2CH_2OH	165.2	12.5
O_2N-CH_2-C_6H_5-CH_3	163.0	11.4
O_2N-CH_2-C_6H_5	162.5	11.1
O_2N-CH_2-C_6H_5-Cl	161.5	10.6
O_2N-CH_2-C_6H_5-NO_2	157.5	8.6
O_2N-CH_2-COOH	168.7	14.2

Reference：

1 Y. Han, Y. Zhou, Y. D. Liu and R. Zhong, Reaction Mechanisms of Histidine and Carnosine with Hypochlorous Acid Along with Chlorination Reactivity of N-Chlorinated Intermediates: A Computational Study, *Chem. Res. Toxicol*., 2022, **35**, 750-759.

Table S2

Table S2 Activation free energies (at 298 K and 1 atm, in kcal/mol) calculated with different methods and basis sets for reactions of glycine with ozone.

basis set	M05		M06		LC-ωPBE	
	SMD	CPCM	SMD	CPCM	SMD	CPCM
6-31G(d)	7.2	11.0	2.5	4.2	9.4	8.0
6-311G(d)	9.2	10.3	2.0	5.6	6.7	7.8
6-31+G(d)	2.9	8.7	4.7	0.8	8.7	7.9
6-311+G(d)	3.3	9.7	0.4	3.8	6.9	6.2

Table S3

Table S3 Activation free energies (at 298 K and 1 atm, in kcal/mol) calculated with different methods and basis sets for reactions of serine with ozone.

basis set	M05		M06		LC-ωPBE	
	SMD	CPCM	SMD	CPCM	SMD	CPCM
6-31G(d)	6.2	10.8	3.7	5.0	9.1	6.7
6-311G(d)	7.2	10.6	2.4	5.2	7.2	7.0
6-31+G(d)	3.3	7.3	1.5	3.1	8.2	7.6
6-311+G(d)	5.4	8.0	3.8	3.9	8.1	6.7

Table S4

Table S4 Activation free energies (at 298 K and 1 atm, in kcal/mol) calculated with different methods and basis sets for reactions of alanine with ozone.

basis set	M05		M06		LC-ωPBE	
	SMD	CPCM	SMD	CPCM	SMD	CPCM
6-31G(d)	7.4	10.9	1.5	4.9	7.0	9.6
6-311G(d)	6.5	10.5	1.9	4.5	7.3	9.4
6-31+G(d)	2.8	8.7	4.8	3.6	7.7	9.2
6-311+G(d)	3.8	8.3	2.3	3.2	6.8	9.5

Table S5

Table S5. Activation free energies (at 298 K and 1 atm, in kcal/mol) calculated with different methods along with 6-311++G(d,p) basis set for ozonation of TMA/TEA, DMA/DEA and MA/EA.

Calculation models		$TMA+O_3$	$TEA+O_3$	$DMA+O_3$	$DEA+O_3$	$MA+O_3$	$EA+O_3$
M05	cpcm	13.9	14.3	13.7	13.0	12.9	13.7
	smd	9.0	11.9	8.4	7.4	6.5	6.3
LC-ωPBE	cpcm	8.4	9.6	8.9	9.4	10.1	10.4
	smd	10.4	12.8	4.7	5.9	5.3	5.1

Table S6

Table S6 The $\Delta G^{\neq}$ values (at 298 K and 1 atm, in kcal/mol) calculated with different functionals and CPCM solvent model.

Step	M05-2X	M06-2X	ωB97X-D	BMK	LC-ωPBE
G-e	7.8 (10.8)	7.8 (10.6)	8.3 (10.6)	7.3 (10.3)	12.7 (10.4)
G-e'	9.0 (8.3)	10.0 (8.2)	7.0 (6.9)	7.5 (7.4)	12.4 (11.7)
G-g	15.8 (19.0)	14.8 (18.2)	16.0 (18.5)	14.1 (18.9)	20.9 (18.6)

values in ( ) were obtained with the singlet point calculation at the CCSD(T)/6-311+G(d) level.

Table S7

Table S7 Activation free energies ($\Delta G^{\neq}$, at 298 K and 1 atm, in kcal/mol) of step M-h for nitro-compounds in the neutral and anionic forms.

Nitro-compounds	$\Delta G^{\neq}$ of neutral form	$\Delta G^{\neq}$ of anionic form	pK_a
Nitromethane (NM)	44.4	14.9	15.0
Nitroethane (NE)	41.6	11.2	14.4
Nitromethylbenzene (NMB)	29.7	4.3	11.1

Table S8

Table S8 $\Delta G^{\neq}$ values (kcal/mol) of steps M-a, M-c, M-d, and M-h for nitrate formation in the ozonation of primary amines and the values in bracket are activation free energies of rate-limiting step ($\Delta G_{rls}^{\neq}$).

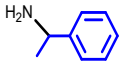
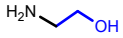
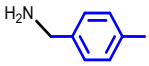
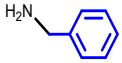
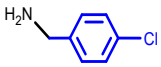
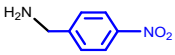
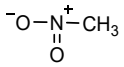
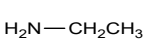
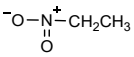
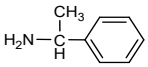
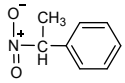
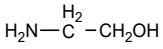
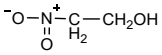
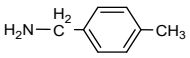
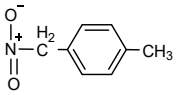
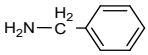
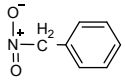
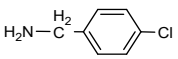
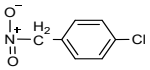
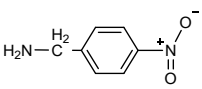
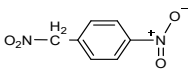
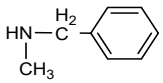
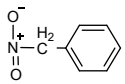
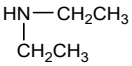
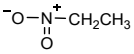
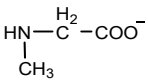
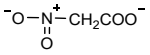
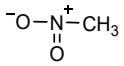
Compounds	Structure formula	Step M-a	Step M-c	Step M-d	Step M-h	Yield(%)
Methylamine (MA)		10.4	10.4	9.5	(28.5)	--
Ethylamine (EA)		10.1	10.1	9.3	(20.8)	8.5±1.6
α-Methylbenzylamine		11.3	12.0	9.4	(12.6)	19.0±0.8
Ethanolamine		12.0	(13.5)	12.4	11.7	22.0±1.4
4-Methylbenzylamine		11.1	(12.9)	9.1	11.3	23.0±5.4
Benzylamine(BA)		10.6	(12.0)	9.0	9.8	33.0±0.6
4-Chlorobenzylamine		13.1	(13.6)	8.9	9.3	41.7±1.2
4-Nitrobenzylamine		14.4	(15.5)	9.1	3.3	71.7±0.7

Table S9

Table S9 $\Delta G_{nycs}^{\neq}$ values (at 298 K and 1 atm, in kcal/mol) of nitrate formation from primary and secondary amines during ozonation and BDEs(C_{α}–H) (in kcal/mol) for nitroalkanes.

Amine	Structure formula	Nitroalkane	$\Delta G_{nycs}^{\neq}$	BDEs
Methylamine (MA)			25.8	170.3
Ethylamine (EA)			21.3	169.0
α-Methylbenzylamine			12.6	164.4
Ethanolamine			11.7	165.2
4-Methylbenzylamine			11.3	163
Benzylamine(BA)			9.8	162.5
4-Chlorobenzylamine			9.3	161.5
4-Nitrobenzylamine			3.3	157.5
N-methylbenzylamine			9.8	162.5
Diethylamine (DEA)			21.3	169.0
Sarcosine			23.2	168.7
Dimethylamine (DMA)			25.8	170.3

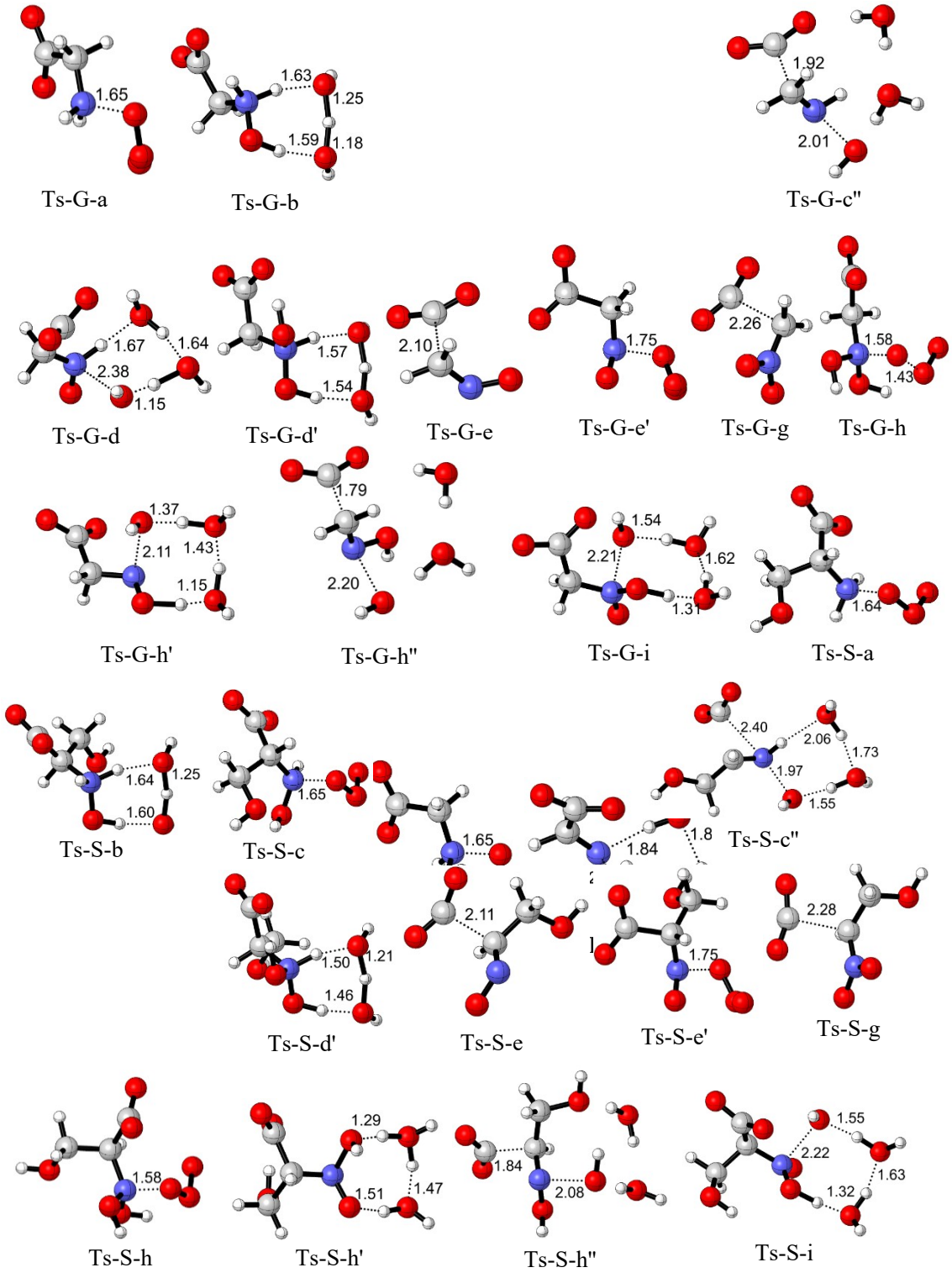


Figure S1

Fig. S1 Structures of transition states and important geometric parameters calculated at the M05/6-311+G(d) and M05-2X/6-311+G(d) levels involved in each elementary step of oxime (FAO/HAO) formation from Gly and Ser during ozonati lor represent nitrogen atom; atoms

in red represent oxygen atom, atoms in white represent hydrogen atom; atoms in grey color represent carbon atom).

Figure S2

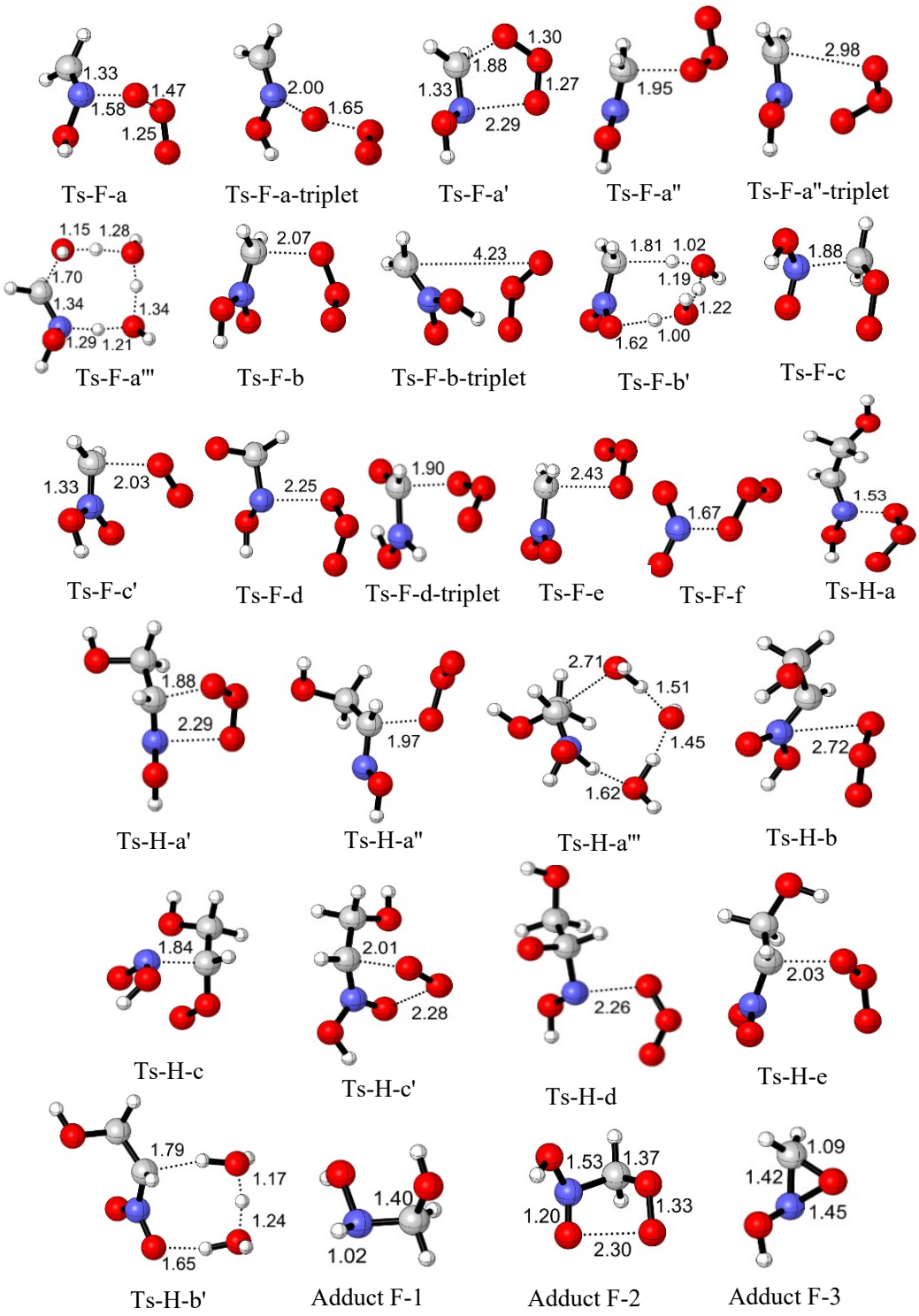


Fig. S2 Structures of transition states and important geometric parameters calculated at the M05/6-311G(d) levels involved in each elementary step of nitrate formation from FAO/HAO during ozonation (atoms in blue color represent nitrogen atom; atoms in red represent oxygen atom, atoms

in white represent hydrogen atom; atoms in grey color represent carbon atom).

Figure S3

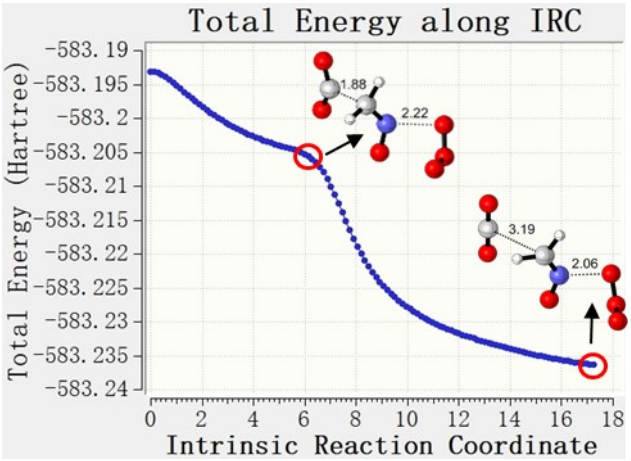


Fig. S3 IRC calculation results for the reactant formation in the ozonation of nitroso-Gly

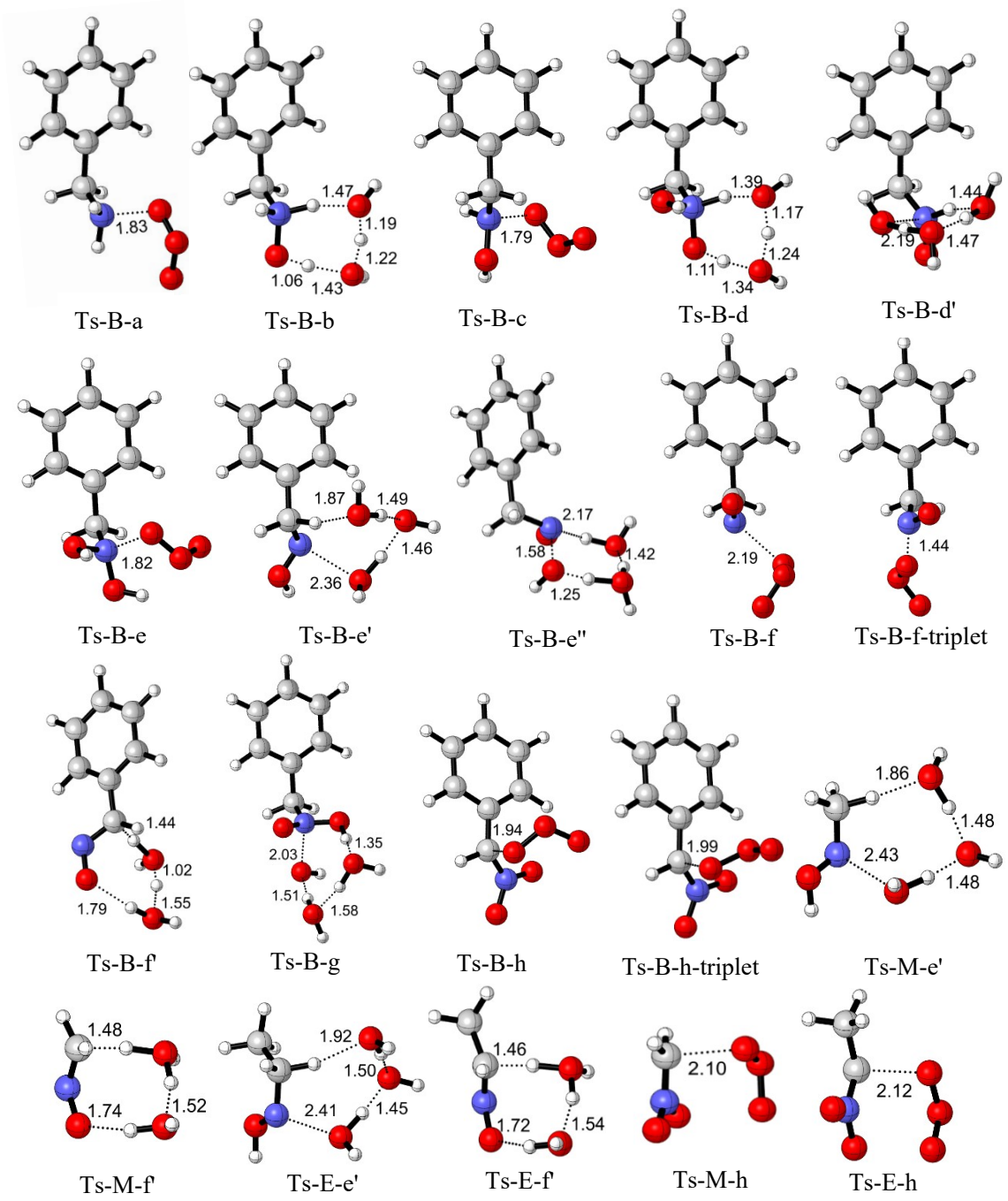
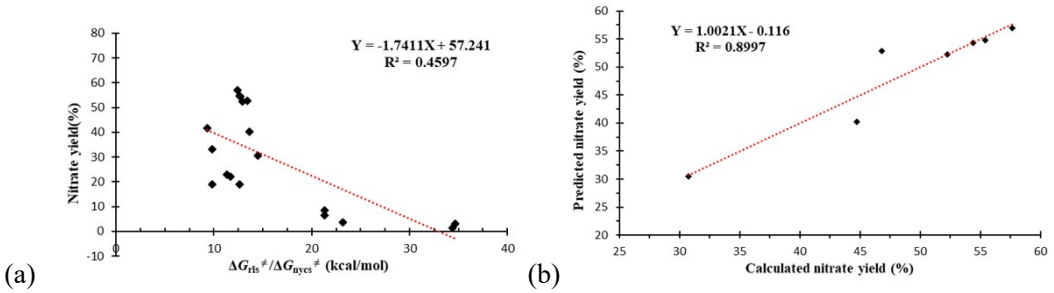


Figure S4

Fig. S4 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/EA/BA 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 S5



(a) (b)

Fig. S5 (a) Correlation between nitrate yields and $\Delta G_{rls}^{\neq}/\Delta G_{nycs}^{\neq}$ for AAs and amines; (b) correlation between nitrate yields and $\Delta G_{rls}^{\neq}$ along with the ratio of k_{est}(G-e)/k_{est}(G-e') for 7 AAs.

Standard orientation of Ts-G-a

Cartesian coordinates of all the transition states optimized at the M05/6-311G(d) level:

Standard orientation of transition state of Ts-G-a

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -503.47 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.307930	-0.522992	0.574912
2	6	0	0.919263	-0.947619	-0.065027
3	8	0	-2.614130	-0.071001	0.091247
4	8	0	-1.661713	-0.911114	-0.292996
5	8	0	-2.364479	1.185120	-0.337453
6	1	0	-0.474441	-0.884329	1.505023
7	1	0	0.685703	-1.164581	-1.111425
8	1	0	-0.347406	0.503564	0.549785
9	1	0	1.297852	-1.855435	0.399079
10	6	0	1.961513	0.218972	-0.030119
11	8	0	1.493270	1.330022	0.291199
12	8	0	3.110696	-0.103826	-0.351493

Standard orientation of Ts-G-b

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-G-b

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -586.63 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.216304	-0.420153	0.447535
2	1	0	0.740179	0.527699	0.433406
3	1	0	-0.299294	-0.487482	1.330539
4	6	0	-0.794129	-0.472008	-0.618917
5	1	0	-0.437162	0.078403	-1.487386
6	1	0	-0.927750	-1.518618	-0.892144
7	8	0	1.144111	-1.451806	0.383950
8	8	0	1.798311	1.658385	0.292048
9	1	0	2.595937	0.847312	-0.143595
10	1	0	1.604508	2.351403	-0.342276
11	8	0	3.169126	-0.171642	-0.427623
12	1	0	2.009973	-1.035225	0.006523
13	1	0	3.365916	-0.207376	-1.365923
14	6	0	-2.125312	0.090734	-0.092021
15	8	0	-2.203774	0.215207	1.151598
16	8	0	-2.988997	0.333929	-0.950756

Standard orientation of Ts-G-c

Cartesian coordinates of all the transition states optimized at the M05/6-311G(d) level:

Standard orientation of transition state of Ts-G-c

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -443.33 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.748225	-0.782216	0.184648
2	6	0	0.426337	-0.834960	-0.660278
3	8	0	-1.288704	1.517519	0.266489
4	8	0	-1.755148	0.478541	-0.246048
5	8	0	-0.232986	1.987022	-0.281625
6	1	0	0.238676	-0.316776	-1.602443
7	1	0	-0.442704	-0.690816	1.151528
8	1	0	0.659395	-1.882899	-0.888590
9	6	0	1.647705	-0.213639	0.076058
10	8	0	1.514888	-0.055655	1.308608
11	8	0	2.630143	0.022321	-0.644285
12	8	0	-1.562909	-1.896177	0.123721
13	1	0	-2.104310	-1.770978	-0.662585

Standard orientation of Ts-G-c'

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-G-c'

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -267.98 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.080696	-0.943588	1.141774
2	6	0	1.245664	-0.709396	0.963969
3	1	0	1.958520	-1.557553	1.019317
4	1	0	1.469712	-0.006183	1.791729
5	8	0	-0.735918	-1.296268	-0.877489
6	1	0	-0.285078	-0.465781	-1.115679
7	1	0	-0.960817	0.675854	1.068191
8	8	0	-3.203043	-0.097850	-0.429073
9	1	0	-3.693448	-0.490842	0.294463
10	1	0	-1.664062	-1.044166	-0.711888
11	8	0	-1.357284	1.524342	0.749396
12	1	0	-0.716535	1.769322	0.070476
13	1	0	-2.690517	0.639234	-0.036962
14	6	0	1.788431	0.257178	-0.248020
15	8	0	0.911494	0.888131	-0.876828
16	8	0	3.002567	0.206461	-0.399474

Standard orientation of Ts-G-c''

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-G-c''

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -484.26 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.038025	-0.996069	-0.749872
2	6	0	-0.466014	-0.936319	0.481770
3	1	0	-0.032195	-0.270492	1.236766
4	1	0	-0.871641	-1.866346	0.878962
5	8	0	1.991123	-1.484745	-0.653556
6	1	0	1.805846	-2.333691	-0.246636
7	1	0	0.432001	-0.090917	-0.993477
8	8	0	2.518363	0.419597	1.061933
9	1	0	3.446373	0.650803	1.018932
10	1	0	2.383855	-0.372577	0.458269
11	8	0	1.019232	1.981715	-0.655401
12	1	0	0.114241	1.939761	-0.329194
13	1	0	1.573925	1.543040	0.017366
14	6	0	-2.081826	0.129969	0.132725
15	8	0	-1.744154	1.263305	-0.082385
16	8	0	-3.013507	-0.603496	0.269553

Standard orientation of Ts-G-d

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-G-d

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -670.10 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.049926	1.184448	-0.352330
2	6	0	1.433287	0.896996	0.025817
3	1	0	1.609465	1.351650	0.997326
4	1	0	2.045261	1.417199	-0.717252
5	8	0	-0.837538	0.249643	1.449993
6	1	0	-0.273229	-0.336160	1.963016
7	1	0	-0.574728	0.418887	-0.830313
8	8	0	-0.356828	2.295411	-0.320262
9	8	0	-2.777506	-0.966869	0.680931
10	1	0	-3.609070	-0.522014	0.856536
11	1	0	-1.821142	-0.343497	1.149493
12	8	0	-1.516946	-0.568870	-1.510620
13	1	0	-0.843776	-1.260633	-1.562364
14	1	0	-2.140848	-0.802976	-0.749768
15	6	0	1.750810	-0.604913	-0.028218
16	8	0	1.113867	-1.270151	-0.873402
17	8	0	2.644200	-0.984924	0.745114

Standard orientation of Ts-G-d'

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-G-d'

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -665.45 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.290014	-0.483110	0.070542
2	1	0	0.685584	0.544662	0.000758
3	6	0	-0.957824	-0.656774	-0.697963
4	1	0	-0.732022	-0.379430	-1.725017
5	1	0	-1.207170	-1.717675	-0.657961
6	8	0	1.230710	-1.339045	-0.409176
7	8	0	1.565824	1.745931	-0.002543
8	1	0	2.547637	1.040397	-0.123699
9	1	0	1.453274	2.333446	-0.752786
10	8	0	3.276353	0.078320	-0.165777
11	1	0	2.157018	-0.846246	-0.314625
12	1	0	3.846117	0.107758	-0.937348
13	6	0	-2.125955	0.183463	-0.154791
14	8	0	-2.025867	0.598152	1.032741
15	8	0	-3.068311	0.347336	-0.934570
16	8	0	0.078980	-0.762436	1.420159
17	1	0	-0.739361	-0.207348	1.606743

Standard orientation of Ts-G-e

Cartesian coordinates of all the transition states optimized at the M05-2X/6-311+G(d) level:
Standard orientation of transition state of Ts-G-e

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -527.85 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.336226	-0.469881	-0.424100
2	8	0	2.023364	0.551262	-0.152182
3	6	0	0.536621	-0.930854	0.528966
4	1	0	0.667892	-0.568376	1.550696
5	1	0	0.127465	-1.920056	0.364223
6	6	0	-1.166580	0.204750	0.000652
7	8	0	-0.854634	1.325571	0.210361
8	8	0	-1.964878	-0.610055	-0.323670

Standard orientation of Ts-G-e'

Cartesian coordinates of all the transition states optimized at the M05-2X/6-311G(d) level:
Standard orientation of transition state of Ts-G-e'

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -282.31 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.248068	0.234486	-0.492454
2	6	0	0.697138	-0.596689	0.221353
3	6	0	2.164671	-0.055811	0.044974
4	8	0	-0.643497	1.194895	0.100011
5	8	0	-2.559317	-0.029779	-0.217378
6	8	0	-1.742392	-0.777273	-0.846891
7	8	0	-2.433162	-0.053873	1.040794
8	1	0	0.446458	-0.600622	1.261567
9	8	0	2.282996	1.149507	-0.215757
10	8	0	3.029920	-0.924706	0.232346
11	1	0	0.642762	-1.595949	-0.157357

Standard orientation of Ts-G-g

Cartesian coordinates of all the transition states optimized at the M05-2X/6-311+G(d) level:
Standard orientation of transition state of Ts-G-g

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -426.43 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.309310	-0.155844	-0.025756
2	8	0	-1.768486	0.010339	1.098655
3	8	0	-1.767649	0.365634	-1.015933
4	6	0	-0.078466	-0.947184	-0.146399
5	1	0	-0.092044	-1.414602	-1.126918
6	1	0	-0.088670	-1.691500	0.643870
7	6	0	1.425316	0.118644	0.012190
8	8	0	1.238128	1.332440	0.129349
9	8	0	2.456105	-0.562382	-0.028496

Standard orientation of Ts-G-h

Cartesian coordinates of all the transition states optimized at the M05/6-311G(d) level:

Standard orientation of transition state of Ts-G-h

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -623.80 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.255889	1.063519	-0.075934
2	6	0	0.888657	0.495629	-0.793866
3	1	0	0.508226	0.102754	-1.736852
4	1	0	1.607390	1.296302	-1.013937
5	8	0	-0.743676	2.102571	-0.841280
6	1	0	-1.705444	2.119444	-0.648933
7	6	0	1.596907	-0.633712	-0.008767
8	8	0	1.367564	-0.704292	1.227936
9	8	0	2.346382	-1.353888	-0.683114
10	8	0	0.255188	1.678513	1.107751
11	8	0	-1.260221	-1.190539	-0.278621
12	8	0	-2.167823	-2.081457	0.074823
13	8	0	-1.506444	-0.045406	0.330021
14	1	0	0.139906	2.621348	1.246931

Standard orientation of Ts-G-h'

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-G-h'

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -966.87 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.145838	-0.501735	-0.099953
2	8	0	0.958108	-1.488829	0.261875
3	1	0	2.261659	-1.086690	-0.345068
4	6	0	-2.293530	0.147901	-0.255974
5	8	0	-2.021545	1.018865	-1.108217
6	8	0	-3.378449	0.013025	0.358910
7	8	0	0.271172	0.573738	1.005129
8	1	0	0.457182	0.058181	1.807334
9	6	0	-1.242951	-0.925511	0.053977
10	1	0	-1.396050	-1.340256	1.055632
11	1	0	-1.372108	-1.740290	-0.662590
12	8	0	3.084589	-0.578231	-0.729186
13	1	0	1.321190	1.201385	0.608461
14	1	0	3.888853	-0.958935	-0.368212
15	8	0	2.267529	1.610283	0.126825
16	1	0	2.759522	0.776611	-0.263667
17	1	0	2.826551	2.076999	0.757081

Standard orientation of Ts-G-h''

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-G-h''

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -304.83 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.118638	-1.269917	0.410670
2	6	0	0.575490	-0.846505	-0.768823
3	1	0	0.088431	-0.026262	-1.307286
4	1	0	1.002741	-1.615368	-1.409343
5	8	0	-1.824050	-1.783390	0.276380
6	1	0	-1.685894	-2.596038	-0.217592
7	8	0	-2.599855	0.488824	-0.842475
8	1	0	-3.535608	0.629192	-0.688893
9	1	0	-2.373468	-0.411887	-0.480703
10	8	0	-0.918896	2.520307	0.108208
11	1	0	-0.048329	2.120482	0.220988
12	1	0	-1.511811	1.821636	-0.224281
13	6	0	2.083810	0.152456	-0.137398
14	8	0	1.680848	1.148284	0.410517
15	8	0	3.073166	-0.427838	-0.481690
16	8	0	-0.413298	-0.235889	1.115958
17	1	0	-0.705642	-0.550436	1.974559

Standard orientation of Ts-G-i

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-G-i

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -606.17 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.008701	-0.740430	-0.373397
2	8	0	0.297918	-0.773731	0.874694
3	1	0	1.663321	-0.799205	1.056125
4	8	0	0.415512	0.985623	-0.888217
5	1	0	-0.190014	1.478775	-0.304962
6	8	0	2.735521	-0.649304	1.146258
7	1	0	1.852050	1.198671	-0.664993
8	1	0	2.980861	-0.451562	2.056974
9	8	0	2.876088	1.190711	-0.454196
10	1	0	2.943998	0.183596	0.498695
11	1	0	3.154621	2.059742	-0.154627
12	8	0	0.633459	-1.425314	-1.165874
13	6	0	-1.478650	-0.653824	-0.614918
14	1	0	-1.590302	-0.421342	-1.670977
15	6	0	-2.295464	0.332218	0.241697
16	8	0	-3.457569	-0.058533	0.464309
17	8	0	-1.785560	1.422005	0.581608
18	1	0	-1.831883	-1.667693	-0.431794

Standard orientation of Ts-S-a

Cartesian coordinates of all the transition states optimized at the M05/6-311G(d) level:

Standard orientation of transition state of Ts-S-a

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -513.09 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.443043	0.409829	0.331420
2	6	0	-0.840831	0.136933	-0.297031
3	8	0	2.792395	0.504139	-0.154095
4	8	0	1.627988	0.533727	-0.794565
5	8	0	3.082148	-0.733319	0.300792
6	1	0	0.489179	1.286844	0.838414
7	1	0	-0.720921	0.317697	-1.369783
8	1	0	0.749302	-0.417568	0.855842
9	6	0	-1.231657	-1.355312	-0.056988
10	8	0	-0.454262	-1.996321	0.679131
11	8	0	-2.279000	-1.713114	-0.613169
12	6	0	-1.889039	1.084737	0.250749
13	1	0	-2.810715	0.935857	-0.318094
14	1	0	-2.092886	0.844132	1.302336
15	8	0	-1.393999	2.401822	0.125668
16	1	0	-1.948261	2.990628	0.640871

Standard orientation of Ts-S-b

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-S-b

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -622.95 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.144106	-0.833054	-0.243346
2	1	0	0.752298	-0.705020	0.639117
3	1	0	-0.419566	-1.685082	-0.117004
4	6	0	-0.857379	0.241062	-0.423790
5	8	0	0.979450	-1.016635	-1.337806
6	8	0	1.960123	-0.637377	1.650941
7	1	0	2.688482	-0.369548	0.716796
8	1	0	1.948288	0.068294	2.300718
9	8	0	3.176599	-0.220574	-0.378479
10	1	0	1.909076	-0.661293	-1.049950
11	1	0	3.283371	0.720492	-0.535494
12	6	0	-2.231941	-0.296598	0.053885
13	8	0	-2.274365	-1.525358	0.292309
14	8	0	-3.148518	0.535832	0.124998
15	1	0	-0.918001	0.411584	-1.500696
16	6	0	-0.454022	1.518822	0.266905
17	1	0	-1.264285	2.239896	0.143413
18	1	0	-0.313278	1.343328	1.339620
19	8	0	0.746210	1.982394	-0.324718
20	1	0	1.068920	2.742752	0.166936

Standard orientation of Ts-S-c

Cartesian coordinates of all the transition states optimized at the M05/6-311G(d) level:

Standard orientation of transition state of Ts-S-c

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -420.35 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.449230	0.155021	0.269446
2	6	0	-0.874042	0.037650	-0.376201
3	8	0	2.759385	0.180437	-0.313089
4	8	0	1.584671	0.367969	-0.911600
5	8	0	2.921745	-1.122770	0.029094
6	1	0	0.743828	-0.770127	0.613822
7	6	0	-1.464413	-1.376739	-0.027276
8	8	0	-0.686345	-2.136366	0.580261
9	8	0	-2.624825	-1.554469	-0.413342
10	8	0	0.624644	1.049601	1.254215
11	1	0	0.266300	1.889642	0.894148
12	1	0	-0.676713	0.077985	-1.450531
13	6	0	-1.790686	1.168855	0.015114
14	1	0	-2.703091	1.080120	-0.574813
15	1	0	-2.057410	1.098548	1.075108
16	8	0	-1.113919	2.394921	-0.245415
17	1	0	-1.665531	3.125492	0.045332

Standard orientation of Ts-S-c'

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-S-c'

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -377.03 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.267807	-1.127604	0.197273
2	6	0	0.952192	-0.447568	-0.286983
3	1	0	1.076753	-0.742549	-1.329303
4	8	0	-1.563320	-0.365358	-1.466552
5	1	0	-1.261442	0.539185	-1.290702
6	1	0	-1.222805	-0.400305	0.921966
7	8	0	-3.741979	-0.384844	-0.214170
8	1	0	-3.989926	-1.294437	-0.043673
9	1	0	-2.518007	-0.419985	-1.025781
10	8	0	-2.091971	0.248124	1.588621
11	1	0	-1.736453	1.100536	1.315194
12	1	0	-3.081222	-0.066671	0.657316
13	6	0	0.935323	1.097152	-0.144907
14	8	0	-0.189737	1.651529	-0.113602
15	8	0	2.059621	1.602243	-0.113263
16	6	0	2.102094	-1.081409	0.517736
17	1	0	1.984087	-2.144795	0.531336
18	1	0	2.084201	-0.707718	1.520200
19	8	0	3.351480	-0.748235	-0.092944
20	1	0	4.009061	-1.406751	0.142733

Standard orientation of Ts-S-c''

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-S-c''

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -363.74 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.341132	0.068994	1.311642
2	1	0	1.866519	1.780469	-1.792636
3	6	0	-0.697909	0.202511	-0.033039
4	1	0	0.234372	0.505695	-0.584993
5	8	0	1.993089	-0.207560	1.492742
6	8	0	1.587761	0.861691	-1.796041
7	1	0	2.281169	0.617901	1.890649
8	1	0	2.353235	0.320199	-1.360372
9	8	0	-0.511372	-1.095506	1.724556
10	1	0	-0.208784	-1.130166	2.655785
11	8	0	3.287232	-0.556625	-0.595042
12	1	0	2.595649	-0.349209	0.632108
13	1	0	4.202060	-0.270215	-0.573552
14	6	0	-1.322772	-1.067378	-0.640104
15	8	0	-0.799219	-2.135687	-0.953422
16	8	0	-2.658470	-0.938100	-0.841620
17	6	0	-1.585331	1.458492	-0.114237
18	1	0	-1.871962	1.627549	-1.131175
19	1	0	-2.460859	1.315885	0.484106
20	8	0	-0.856201	2.589413	0.369797
21	1	0	-1.309943	3.396163	0.115096

Standard orientation of Ts-S-d

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-S-d

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -611.81 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.157299	-0.882471	-0.203066
2	6	0	1.110622	0.203730	-0.400283
3	1	0	1.385909	0.201105	-1.453037
4	8	0	-1.479858	0.005187	-1.411939
5	1	0	-1.371335	0.931277	-1.648091
6	1	0	-0.607624	-0.807067	0.582110
7	8	0	0.324574	-1.931502	-0.730922
8	8	0	-3.492909	-0.303927	-0.114682
9	1	0	-4.046524	-1.020168	-0.432078
10	1	0	-2.520973	-0.135421	-0.839614
11	8	0	-1.685244	-0.708952	1.654374
12	1	0	-1.413277	0.173829	1.941636
13	1	0	-2.514449	-0.596946	1.086780
14	6	0	0.484157	1.539654	0.058747
15	8	0	-0.038549	1.514444	1.194098
16	8	0	0.602542	2.493294	-0.725010
17	6	0	2.346919	-0.091324	0.465290
18	1	0	2.054695	-0.192005	1.512849
19	1	0	2.992280	0.784097	0.379416
20	8	0	3.077154	-1.203406	0.015223
21	1	0	2.828325	-1.994863	0.499825

Standard orientation of Ts-S-d'

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-S-d'

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -652.85 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.434667	-0.243524	-0.531825
2	1	0	0.862492	-0.627616	0.408724
3	6	0	-0.924839	0.331111	-0.330863
4	8	0	1.270111	0.701718	-1.031322
5	8	0	1.799314	-1.091682	1.480386
6	1	0	2.719138	-0.499469	0.954494
7	1	0	1.622704	-0.769991	2.366885
8	8	0	3.391128	0.110859	0.157567
9	1	0	2.217627	0.514394	-0.614706
10	1	0	3.838332	0.849896	0.575478
11	6	0	-1.921873	-0.763979	0.147744
12	8	0	-1.554041	-1.963207	0.018773
13	8	0	-3.001708	-0.354044	0.577770
14	8	0	0.390965	-1.305264	-1.434333
15	1	0	-0.311210	-1.883085	-1.008056
16	1	0	-1.248347	0.666975	-1.318835
17	6	0	-0.856818	1.522120	0.605189
18	1	0	-1.757810	1.516648	1.219581
19	1	0	0.012768	1.433761	1.266327
20	8	0	-0.788722	2.714271	-0.156409
21	1	0	-0.833573	3.466439	0.441005

Standard orientation of Ts-S-e

Cartesian coordinates of all the transition states optimized at the M05-2X/6-311+G(d) level:
Standard orientation of transition state of Ts-S-e

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -322.02 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.110213	1.237906	-0.553408
2	8	0	-0.513233	2.235693	-0.116607
3	6	0	0.388336	0.262135	0.311743
4	1	0	0.262815	0.484320	1.375023
5	6	0	-1.444871	-0.777389	0.049205
6	8	0	-2.265926	-0.028455	0.451606
7	8	0	-1.126807	-1.830690	-0.394306
8	6	0	1.442935	-0.708737	-0.089246
9	1	0	1.296546	-1.664248	0.421876
10	1	0	1.380648	-0.885701	-1.167628
11	8	0	2.727882	-0.177121	0.250101
12	1	0	3.394773	-0.851187	0.088014

Standard orientation of Ts-S-e'

Cartesian coordinates of all the transition states optimized at the M05-2X/6-311G(d) level:
Standard orientation of transition state of Ts-S-e'

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -289.77 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.474894	-0.415159	-0.521606
2	6	0	-0.519303	-0.074887	0.473168
3	6	0	-1.905955	-0.735304	0.129143
4	8	0	1.045320	-1.451936	-0.349930
5	8	0	2.740735	0.089573	-0.207627
6	8	0	1.781144	0.878997	-0.487620
7	8	0	2.709987	-0.381616	0.965629
8	1	0	-0.200540	-0.451412	1.448352
9	8	0	-1.874314	-1.756361	-0.571723
10	8	0	-2.867149	-0.149929	0.650858
11	6	0	-0.667664	1.457747	0.498149
12	1	0	-1.245301	1.746304	1.351360
13	1	0	0.300928	1.908979	0.554003
14	8	0	-1.327918	1.892215	-0.693573
15	1	0	-1.284258	2.849357	-0.753343

Standard orientation of Ts-S-g

Cartesian coordinates of all the transition states optimized at the M05-2X/6-311+G(d) level:
Standard orientation of transition state of Ts-S-g

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -379.14 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.492620	1.157458	-0.089675
2	8	0	-0.907027	1.436201	1.052288
3	8	0	-0.155136	2.065953	-0.875321
4	6	0	-0.303898	-0.156726	-0.468133
5	1	0	-0.183451	-0.241799	-1.542749
6	6	0	1.831528	-0.539317	0.054301
7	8	0	1.917138	-1.692630	-0.193170
8	8	0	2.253666	0.503761	0.411372
9	6	0	-1.064594	-1.214709	0.235580
10	1	0	-0.611341	-2.181940	-0.003630
11	1	0	-1.013980	-1.071019	1.319296
12	8	0	-2.436830	-1.215081	-0.187744
13	1	0	-2.895595	-1.928554	0.264911

Standard orientation of Ts-S-h

Cartesian coordinates of all the transition states optimized at the M05/6-311G(d) level:

Standard orientation of transition state of Ts-S-h

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -654.60 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.625918	-0.457824	0.586104
2	6	0	-0.586999	-0.094892	-0.221140
3	1	0	-0.207902	-0.095932	-1.238654
4	8	0	1.190618	-1.614559	0.183478
5	1	0	2.031281	-1.325333	-0.265310
6	6	0	-1.302766	1.254956	0.096148
7	8	0	-0.880841	1.971568	1.008471
8	8	0	-2.261389	1.406002	-0.681107
9	8	0	0.322815	-0.513139	1.889929
10	8	0	2.663475	0.224247	-0.564612
11	8	0	2.259143	0.517943	-1.801097
12	8	0	1.742931	0.653556	0.438543
13	1	0	1.136380	-0.795656	2.338851
14	6	0	-1.550071	-1.278908	-0.015713
15	1	0	-1.948700	-1.246378	0.976727
16	1	0	-1.020771	-2.197945	-0.157528
17	8	0	-2.618989	-1.193578	-0.961775
18	1	0	-3.074807	-2.037239	-1.007234

Standard orientation of Ts-S-h'

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-S-h'

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1001.73 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.377811	0.159335	-0.289323
2	8	0	1.086106	0.907812	-1.118749
3	1	0	2.332817	1.162700	-0.295619
4	6	0	-1.857474	-0.850465	0.118138
5	8	0	-2.507307	-1.686337	-0.534765
6	8	0	-1.839923	-0.729855	1.373714
7	8	0	0.829255	-1.316953	-0.562001
8	1	0	1.050070	-1.296510	-1.507520
9	6	0	-1.044636	0.192929	-0.667351
10	1	0	-1.126765	-0.004027	-1.742365
11	8	0	3.134633	1.096013	0.356037
12	1	0	1.823844	-1.418872	0.092362
13	1	0	3.927527	1.393618	-0.096535
14	8	0	2.742390	-1.328656	0.763995
15	1	0	3.065913	-0.340965	0.684062
16	1	0	3.444282	-1.945387	0.531344
17	6	0	-1.591193	1.586069	-0.383082
18	1	0	-0.994451	2.326415	-0.916846
19	1	0	-2.616430	1.632808	-0.773415
20	8	0	-1.562423	1.902154	0.993727
21	1	0	-1.653507	1.050259	1.467895

Standard orientation of Ts-S-h''

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-S-h''

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -363.74 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.341132	0.068994	1.311642
2	1	0	1.866519	1.780469	-1.792636
3	6	0	-0.697909	0.202511	-0.033039
4	1	0	0.234372	0.505695	-0.584993
5	8	0	1.993089	-0.207560	1.492742
6	8	0	1.587761	0.861691	-1.796041
7	1	0	2.281169	0.617901	1.890649
8	1	0	2.353235	0.320199	-1.360372
9	8	0	-0.511372	-1.095506	1.724556
10	1	0	-0.208784	-1.130166	2.655785
11	8	0	3.287232	-0.556625	-0.595042
12	1	0	2.595649	-0.349209	0.632108
13	1	0	4.202060	-0.270215	-0.573552
14	6	0	-1.322772	-1.067378	-0.640104
15	8	0	-0.799219	-2.135687	-0.953422
16	8	0	-2.658470	-0.938100	-0.841620
17	6	0	-1.585331	1.458492	-0.114237
18	1	0	-1.871962	1.627549	-1.131175
19	1	0	-2.460859	1.315885	0.484106
20	8	0	-0.856201	2.589413	0.369797
21	1	0	-1.309943	3.396163	0.115096

Standard orientation of Ts-S-i

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-S-i

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -631.38 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.492620	1.157458	-0.089675
2	8	0	-0.907027	1.436201	1.052288
3	8	0	-0.155136	2.065953	-0.875321
4	6	0	-0.303898	-0.156726	-0.468133
5	1	0	-0.183451	-0.241799	-1.542749
6	6	0	1.831528	-0.539317	0.054301
7	8	0	1.917138	-1.692630	-0.193170
8	8	0	2.253666	0.503761	0.411372
9	6	0	-1.064594	-1.214709	0.235580
10	1	0	-0.611341	-2.181940	-0.003630
11	1	0	-1.013980	-1.071019	1.319296
12	8	0	-2.436830	-1.215081	-0.187744
13	1	0	-2.895595	-1.928554	0.264911

Standard orientation of Ts-F-a

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-F-a

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -546.78 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.478652	0.328029	0.547583
2	8	0	-1.649593	-0.535628	0.333123
3	8	0	-2.412697	0.446530	0.114679
4	8	0	-0.652012	-0.659622	-0.520750
5	8	0	2.472553	-0.342244	-0.062311
6	1	0	3.009974	-0.705297	0.652492
7	6	0	0.631684	0.802864	-0.340084
8	1	0	0.866889	0.797301	-1.400234
9	1	0	-0.083547	1.522322	0.037238

Standard orientation of Ts-F-a'

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-F-a'

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -483.44 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.085921	-0.031875	0.580010
2	8	0	-1.581866	-0.195216	0.127720
3	8	0	-1.076815	0.750501	-0.605920
4	8	0	-0.830887	-1.215101	0.154316
5	8	0	1.772708	-0.431619	-0.503182
6	1	0	2.218147	-1.244353	-0.234447
7	6	0	0.498066	1.137610	0.338425
8	1	0	0.043919	1.593173	1.207667
9	1	0	0.882975	1.780120	-0.447321

Standard orientation of Ts-F-a''

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-F-a''

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -772.47 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.049418	0.005718	0.358865
2	8	0	0.952391	1.277877	-0.093193
3	1	0	0.869701	1.824574	0.698704
4	6	0	1.629092	-0.815134	-0.514533
5	1	0	1.620435	-1.865141	-0.268879
6	8	0	-1.342271	-0.597740	-0.199239
7	8	0	-1.961438	0.465564	-0.398857
8	8	0	-0.356944	-0.481735	0.887751
9	1	0	2.055486	-0.420384	-1.426375

Standard orientation of Ts-F-a'''

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-F-a'''

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1232.75 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.937519	2.322529	0.537764
2	1	0	0.061804	1.182947	-0.359540
3	8	0	-0.187288	-1.671196	0.276966
4	8	0	-0.994528	1.754482	-0.231275
5	1	0	0.190829	-1.646805	1.161655
6	1	0	-1.750996	0.686036	0.050334
7	8	0	-2.186139	-0.304714	0.267238
8	1	0	-1.165158	-1.074210	0.286204
9	1	0	-2.793156	-0.548814	-0.432960
10	7	0	1.107215	0.429083	-0.454698
11	6	0	0.917106	-0.863384	-0.739075
12	1	0	0.381784	-1.017117	-1.671668
13	8	0	1.910017	0.562278	0.712722
14	1	0	2.665230	1.082025	0.424126
15	1	0	1.757551	-1.536667	-0.583782

Standard orientation of Ts-F-b

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-F-b

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -348.11 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.164281	0.119357	0.122193
2	8	0	1.570955	-0.700654	-0.899685
3	1	0	1.750731	-1.551300	-0.470460
4	6	0	0.665738	1.286768	-0.269553
5	1	0	0.577217	2.026713	0.506353
6	8	0	1.198852	-0.309099	1.265000
7	8	0	-1.673671	-0.111260	0.412215
8	8	0	-1.624764	-1.175754	-0.277222
9	8	0	-1.375578	0.975799	-0.245509
10	1	0	0.761292	1.536227	-1.312311

Standard orientation of Ts-F-b'

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-F-b'

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -304.80 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.231555	-0.087217	-0.069161
2	6	0	0.727686	0.906261	-0.861438
3	1	0	1.379928	1.765756	-0.942528
4	1	0	0.218208	0.543611	-1.746561
5	8	0	0.687922	-1.239264	-0.083355
6	1	0	-0.933591	-1.290355	-0.077762
7	8	0	2.166726	0.120629	0.706408
8	8	0	-1.912290	-1.101136	0.044303
9	1	0	-2.388174	-1.379628	-0.742827
10	1	0	-1.962566	0.103577	0.212549
11	8	0	-1.775626	1.279055	0.304352
12	1	0	-1.816800	1.588056	1.214599
13	1	0	-0.817858	1.367659	-0.038388

Standard orientation of Ts-F-c

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-F-c

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -325.77 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.959521	-0.009552	0.452541
2	8	0	1.581093	0.811024	-0.374253
3	8	0	1.221994	-0.475557	-0.437526
4	8	0	-0.739037	1.156543	0.442073
5	8	0	-1.661947	-0.499823	-0.617194
6	1	0	-1.836261	0.251363	-1.213650
7	6	0	0.667270	-0.941887	0.633109
8	1	0	0.929852	-0.481606	1.578922
9	1	0	0.402612	-1.989068	0.563475

Standard orientation of Ts-F-c'

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-F-c'

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -266.71 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.767721	-0.020490	0.278672
2	8	0	-1.701731	-0.616521	-0.204591
3	8	0	-1.403188	0.558396	-0.480710
4	8	0	0.389970	-1.120703	0.634297
5	6	0	0.188376	1.118865	0.641032
6	1	0	-0.327315	1.092814	1.585723
7	8	0	1.652650	0.072682	-0.762497
8	1	0	1.775258	-0.841588	-1.061454
9	1	0	0.546149	2.028178	0.186843

Standard orientation of Ts-F-d

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-F-d

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -705.29 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.632912	0.304756	-0.232273
2	8	0	-2.654113	-0.345094	-0.615032
3	8	0	-0.718033	1.405407	0.461534
4	1	0	-0.163648	2.063726	0.013161
5	6	0	-1.658721	-0.622658	0.249088
6	1	0	-1.241258	-1.635511	0.171828
7	1	0	-1.951364	-0.417676	1.291405
8	8	0	2.035945	-0.629859	-0.237821
9	8	0	1.126265	-0.782510	0.642074
10	8	0	2.427308	0.551071	-0.418881

Standard orientation of Ts-F-e

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-F-e

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -460.56 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.223023	0.045296	0.102241
2	8	0	-1.825543	0.088124	-0.990564
3	8	0	-1.015726	1.063328	0.794924
4	6	0	-0.674346	-1.144601	0.519359
5	8	0	1.796286	0.015778	0.252727
6	8	0	1.534471	1.127973	-0.399135
7	8	0	1.249760	-1.075493	-0.326659
8	1	0	-0.337219	-1.179760	1.541953
9	1	0	-0.969528	-2.027373	-0.024138

Standard orientation of Ts-F-f

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-F-f

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -288.49 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.010404	-0.069963	0.000272
2	8	0	-0.882692	-1.229356	-0.212679
3	8	0	-1.949023	0.561607	0.371157
4	8	0	2.006582	-0.224177	0.667256
5	8	0	1.380165	0.079694	-0.505373
6	8	0	0.329071	0.873450	-0.320599

Standard orientation of Ts-H-a

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-H-a

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -561.11 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.284596	0.647956	0.166134
2	8	0	-0.953519	1.749269	-0.253405
3	1	0	-1.837506	1.644085	0.125228
4	6	0	1.046902	0.821778	0.200298
5	8	0	-1.636463	-1.285377	-0.076332
6	8	0	-2.499898	-0.551193	0.467383
7	8	0	-0.636003	-0.515242	-0.758913
8	1	0	1.434330	1.797005	-0.069613
9	6	0	1.939707	-0.283629	0.612951
10	1	0	2.462459	0.025103	1.529774
11	1	0	1.348331	-1.174516	0.852114
12	8	0	2.860788	-0.524292	-0.429670
13	1	0	3.585677	-1.041580	-0.072427

Standard orientation of Ts-H-a'

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-H-a'

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -447.63 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.093277	1.070326	-0.373516
2	8	0	-1.345555	-1.323537	-0.198920
3	8	0	-0.856460	-0.991758	0.961624
4	8	0	-1.860611	-0.325784	-0.785891
5	8	0	-0.793223	1.991100	0.303263
6	1	0	-1.142948	2.589338	-0.368495
7	6	0	0.492729	0.224247	0.479982
8	1	0	0.625960	0.557332	1.506515
9	6	0	1.524257	-0.688483	-0.111857
10	1	0	1.657271	-1.548009	0.551758
11	1	0	1.166619	-1.050517	-1.084107
12	8	0	2.710325	0.059880	-0.239614
13	1	0	3.408308	-0.534224	-0.523509

Standard orientation of Ts-H-a''

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-H-a''

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -514.71 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.227086	-1.156269	-0.329348
2	8	0	2.028427	0.512902	-0.318348
3	8	0	2.512477	0.237555	0.815910
4	8	0	1.176599	-0.389765	-0.784368
5	8	0	-0.938625	-2.241620	0.400622
6	1	0	-1.440023	-2.962637	-0.001169
7	6	0	-0.554982	-0.106234	0.114759
8	1	0	-0.100398	-0.158537	1.104216
9	6	0	-0.965510	1.233217	-0.425432
10	1	0	-0.094974	1.893681	-0.481667
11	1	0	-1.365033	1.105370	-1.431654
12	8	0	-1.989438	1.793795	0.362973
13	1	0	-1.602527	2.151162	1.165433

Standard orientation of Ts-H-a'''

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-H-a'''

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -139.31 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.188041	1.072960	-1.952408
2	1	0	-0.286857	0.987108	-0.873241
3	8	0	-0.527596	-0.594053	1.969746
4	8	0	-1.524910	0.412916	-1.750752
5	1	0	-0.820322	0.190823	2.436166
6	1	0	-1.907821	-0.220237	-1.000468
7	8	0	-2.236054	-1.048060	0.144875
8	1	0	-1.262380	-0.812162	1.272494
9	1	0	-2.247382	-1.972387	-0.102527
10	7	0	0.448335	1.158268	-0.130176
11	6	0	1.005345	0.191348	0.508192
12	8	0	0.420098	2.389710	0.458078
13	1	0	0.677040	3.019697	-0.227638
14	1	0	1.632889	0.455800	1.348931
15	6	0	1.093702	-1.171489	-0.123128
16	1	0	1.200860	-1.909733	0.672519
17	1	0	0.171701	-1.381189	-0.662054
18	8	0	2.157897	-1.202598	-1.040459
19	1	0	2.982201	-1.321031	-0.562841

Standard orientation of Ts-H-b

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-H-b

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -313.63 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.309736	-1.173267	0.002484
2	8	0	-0.529305	-2.122398	-0.513656
3	1	0	-0.860930	-2.598883	0.263328
4	6	0	0.730278	-0.257872	-0.868128
5	8	0	0.552745	-1.206314	1.207527
6	8	0	-1.420482	1.276308	0.235143
7	8	0	-2.359408	0.466515	0.497582
8	8	0	-0.860247	1.101404	-0.928612
9	1	0	0.536762	-0.495488	-1.902559
10	6	0	1.851495	0.651205	-0.464891
11	1	0	1.963532	1.398420	-1.249472
12	1	0	2.775343	0.051748	-0.450032
13	8	0	1.658194	1.335826	0.736586
14	1	0	1.594535	0.686347	1.442897

Standard orientation of Ts-H-b'

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-H-b'

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -357.41 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.250084	-0.928785	0.160652
2	6	0	0.527547	0.343436	-0.287363
3	1	0	0.142655	0.503474	-1.290053
4	8	0	-0.730284	-1.560621	-0.343029
5	1	0	-2.151677	-0.757386	-0.574950
6	8	0	0.889876	-1.450410	1.074270
7	8	0	-2.917498	-0.118836	-0.511686
8	1	0	-3.224640	0.093944	-1.397020
9	1	0	-2.429452	0.861775	0.070155
10	8	0	-1.751357	1.669665	0.583919
11	1	0	-1.911936	1.731913	1.530885
12	1	0	-0.808990	1.298479	0.420345
13	6	0	1.829835	0.950358	0.074580
14	1	0	1.772898	2.031936	-0.106368
15	1	0	2.024573	0.798464	1.141627
16	8	0	2.882586	0.383406	-0.705753
17	1	0	3.705096	0.790496	-0.424258

Standard orientation of Ts-H-c

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-H-c

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -278.43 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.961839	-0.725672	-0.049540
2	8	0	-0.296962	1.651295	-0.814199
3	8	0	0.055788	1.394653	0.447088
4	8	0	0.910811	-0.489523	-1.210285
5	8	0	2.193156	-0.550699	0.553536
6	1	0	2.802661	-0.243969	-0.141448
7	6	0	-0.280416	0.223631	0.926078
8	1	0	0.102344	0.140290	1.938808
9	6	0	-1.597413	-0.456828	0.698708
10	1	0	-1.620106	-1.297085	1.401616
11	1	0	-2.342996	0.278747	1.044374
12	8	0	-1.837955	-0.874588	-0.608256
13	1	0	-2.606503	-1.448197	-0.588357

Standard orientation of Ts-H-c'

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-H-c'

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -276.31 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.775430	-0.622995	0.216690
2	8	0	-0.323477	1.895297	0.193020
3	8	0	-0.184934	1.346354	-0.921527
4	8	0	-0.691987	-0.070490	1.293774
5	6	0	0.166554	-0.624914	-0.734811
6	8	0	-2.026647	-0.990495	-0.233816
7	1	0	-2.639032	-0.561785	0.383798
8	1	0	-0.190229	-0.994480	-1.685938
9	6	0	1.626364	-0.739862	-0.482654
10	1	0	2.111433	-0.326328	-1.376906
11	1	0	1.851009	-1.819402	-0.473155
12	8	0	2.045983	-0.114260	0.688085
13	1	0	2.985812	-0.279637	0.783871

Standard orientation of Ts-H-d

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-H-d

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1066.05 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.232783	-0.811666	-0.207759
2	8	0	1.691782	-1.230030	-1.055134
3	8	0	-0.202374	-1.277215	1.008336
4	1	0	-0.980281	-1.848376	1.109651
5	6	0	1.059356	-0.172948	-0.527599
6	1	0	0.822576	0.619847	-1.253910
7	8	0	-2.577259	0.737765	-0.489543
8	8	0	-1.433187	1.102365	-0.063221
9	8	0	-3.174258	-0.119715	0.209072
10	6	0	1.819470	0.478778	0.649532
11	1	0	1.129354	1.165429	1.143778
12	1	0	2.118214	-0.298606	1.357220
13	8	0	2.902342	1.233198	0.193934
14	1	0	3.610291	0.637434	-0.061582

Standard orientation of Ts-H-e

Cartesian coordinates of all the transition states optimized at the M05/6-311+G(d) level:
Standard orientation of transition state of Ts-H-e

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -166.47 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.306147	-0.677783	-0.059391
2	8	0	0.769574	1.773310	0.267814
3	8	0	0.814299	0.989674	-0.816628
4	8	0	-0.337709	2.430502	0.387143
5	8	0	-2.181210	-0.472698	-0.913171
6	6	0	0.007872	-0.845996	-0.478984
7	1	0	0.101083	-1.078254	-1.529380
8	8	0	-1.553554	-0.728900	1.157556
9	6	0	1.033055	-1.318268	0.489606
10	1	0	0.934751	-0.741701	1.418254
11	1	0	0.869778	-2.371045	0.746899
12	8	0	2.318344	-1.212486	-0.065619
13	1	0	2.353892	-0.314155	-0.420519

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-B-e'

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1134.96 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.503413	-0.168415	-0.367801
2	6	0	-1.285805	0.713177	0.607489
3	1	0	-0.834372	0.360743	1.538458
4	8	0	-0.866614	-1.253089	-0.322806
5	1	0	0.799940	-1.264416	0.171065
6	8	0	1.736589	-0.947372	0.180927
7	1	0	2.114560	-1.175071	1.035791
8	1	0	1.511490	0.527691	-0.111516
9	8	0	1.068092	1.443883	-0.256058
10	1	0	1.151845	1.709470	-1.181776
11	1	0	-0.033048	1.244517	0.023309
12	1	0	-1.976222	1.549539	0.637840

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) = -159.82 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.074869	-1.509253	-0.391407
2	1	0	-1.032278	-1.305401	-0.037053
3	1	0	-0.138914	-1.463726	-1.349335
4	8	0	-2.339603	-0.865405	0.487872
5	1	0	-3.087120	-1.313185	0.087488
6	1	0	-2.113096	0.509483	-0.007207
7	8	0	-1.807694	1.439027	-0.356991
8	1	0	-2.209320	2.097140	0.214896
9	1	0	0.037468	1.318987	-0.156822
10	8	0	2.424670	-0.439455	-0.090456
11	1	0	2.599364	-1.311451	0.323168
12	7	0	1.495401	0.103047	0.533668
13	6	0	1.149335	1.345301	0.004200
14	1	0	1.720816	1.633818	-0.875640
15	1	0	1.239231	2.041887	0.847486

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 = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -559.44 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.146387	-0.033486	0.141143
2	8	0	1.870743	-0.155523	-0.878359
3	8	0	0.715381	-1.048524	0.763807
4	6	0	0.670257	1.177682	0.521433
5	8	0	-1.736639	0.013317	0.190609
6	8	0	-1.307658	-1.138779	-0.364332
7	8	0	-1.210461	1.066505	-0.414881
8	1	0	0.241326	1.235103	1.509037
9	1	0	1.061492	2.037230	-0.000384

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) = -1235.47 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.681467	-0.998574	-0.515721
2	6	0	-1.074240	-0.091322	0.376586
3	1	0	-0.580161	-0.121551	1.354203
4	8	0	0.416084	-1.589553	-0.311371
5	1	0	1.780475	-0.757472	0.337085
6	8	0	2.439635	-0.021578	0.401468
7	1	0	2.739149	0.025286	1.314282
8	1	0	1.536482	1.111617	-0.107525
9	8	0	0.713742	1.641044	-0.409538
10	1	0	0.780531	1.837953	-1.353411
11	1	0	-0.172679	0.901667	-0.187815
12	6	0	-2.480875	0.432594	0.291154
13	1	0	-2.537959	1.468258	0.631491
14	1	0	-2.836807	0.392824	-0.739486
15	1	0	-3.163758	-0.155492	0.910314

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) = -154.93 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.381318	-0.420359	-0.730034
2	1	0	-2.333691	1.336908	-1.503248
3	6	0	1.047177	0.904017	-0.418799
4	1	0	1.455829	1.449540	-1.284889
5	1	0	-0.048783	0.970779	-0.638419
6	8	0	-0.530404	-1.768033	-0.154418
7	8	0	-1.907356	1.460969	-0.652251
8	1	0	-0.824907	-2.105977	-1.003799
9	1	0	-2.214745	0.677502	-0.054438
10	8	0	2.030074	-0.977271	0.176535
11	1	0	2.212811	-1.897794	-0.103220
12	8	0	-2.428840	-0.497145	0.851296
13	1	0	-1.361717	-1.284483	0.268566
14	1	0	-3.292723	-0.911193	0.812252
15	6	0	1.431492	1.453866	0.927190
16	1	0	1.095197	2.488022	0.985648
17	1	0	0.952810	0.891964	1.730368
18	1	0	2.510875	1.431786	1.081778

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 = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -535.19 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.614742	0.846782	0.162224
2	8	0	-1.176588	1.342624	-0.848727
3	8	0	0.344499	1.446965	0.739152
4	6	0	-0.909886	-0.410037	0.584960
5	8	0	1.769038	-0.793593	0.184481
6	8	0	2.038150	0.385424	-0.410953
7	8	0	0.720930	-1.384419	-0.366806
8	1	0	-0.508319	-0.647077	1.559239
9	6	0	-2.045467	-1.138727	-0.013619
10	1	0	-1.950335	-1.171725	-1.099686
11	1	0	-2.083553	-2.153286	0.380464
12	1	0	-2.990727	-0.638805	0.219200

Standard orientation of Ts-B-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-B-a

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -172.77 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.193517	-0.615344	0.103969
2	6	0	-0.102401	-0.524177	1.105523
3	1	0	-0.129404	-1.490864	1.614462
4	6	0	1.244611	-0.195044	0.543849
5	6	0	2.127645	-1.208655	0.193661
6	6	0	1.618452	1.130089	0.354143
7	6	0	3.368566	-0.902253	-0.341732
8	1	0	1.844642	-2.245866	0.344166
9	6	0	2.857826	1.437734	-0.182435
10	1	0	0.935710	1.927534	0.631090
11	6	0	3.734476	0.421330	-0.531207
12	1	0	4.053061	-1.700096	-0.608461
13	1	0	3.142123	2.474637	-0.324757
14	1	0	4.706541	0.661801	-0.948119
15	8	0	-0.939489	-0.480670	-1.040447
16	8	0	-3.575699	0.611282	-0.418505
17	8	0	-2.900375	0.620951	0.686174
18	8	0	-4.438214	-0.313209	-0.490561
19	1	0	-0.462900	0.219276	1.819746

Standard orientation of Ts-B-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-B-b

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -896.61 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.278637	-0.786333	-0.305315
2	1	0	-1.462980	0.288874	-0.531800
3	1	0	-0.890397	-1.231375	-1.137640
4	6	0	-0.331553	-0.936350	0.823492
5	1	0	-0.760811	-0.392521	1.664097
6	1	0	-0.294676	-1.997293	1.070051
7	8	0	-2.490351	-1.403747	-0.028379
8	8	0	-2.052793	1.609901	-0.788430
9	1	0	-3.093596	1.234159	-0.351891
10	1	0	-1.707164	2.341914	-0.272851
11	8	0	-4.026520	0.544616	0.029512
12	1	0	-3.201818	-0.625810	0.050559
13	1	0	-4.319689	0.822234	0.900102
14	6	0	1.021045	-0.403020	0.442653
15	6	0	1.372448	0.909067	0.736733
16	6	0	1.928330	-1.216466	-0.226975
17	6	0	2.611768	1.402771	0.362628
18	1	0	0.674720	1.547275	1.269786
19	6	0	3.166660	-0.723040	-0.604210
20	1	0	1.669186	-2.247955	-0.446941
21	6	0	3.509190	0.587824	-0.310039
22	1	0	2.878764	2.426599	0.600671
23	1	0	3.868695	-1.366327	-1.123220
24	1	0	4.480225	0.973679	-0.601043

Standard orientation of Ts-B-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-B-c

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -261.62 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.244899	-1.008790	-0.274982
2	6	0	0.363079	-0.872125	0.889603
3	8	0	2.820912	0.885783	-0.540392
4	8	0	1.663320	0.586769	-0.980966
5	8	0	2.786463	1.502227	0.664345
6	1	0	0.867906	-0.197821	1.577361
7	1	0	0.804742	-1.474987	-1.070006
8	1	0	0.273741	-1.863124	1.341455
9	8	0	2.417924	-1.572226	0.070650
10	1	0	2.952532	-1.653207	-0.734309
11	6	0	-0.978181	-0.347664	0.460559
12	6	0	-1.235634	1.017706	0.464951
13	6	0	-1.972720	-1.230120	0.056209
14	6	0	-2.473160	1.494933	0.066614
15	1	0	-0.460097	1.706593	0.781032
16	6	0	-3.209604	-0.752527	-0.347401
17	1	0	-1.783123	-2.299455	0.064045
18	6	0	-3.460369	0.610477	-0.341948
19	1	0	-2.668607	2.561640	0.076786
20	1	0	-3.981080	-1.447785	-0.659454
21	1	0	-4.429727	0.985165	-0.652645

Standard orientation of Ts-B-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-B-d

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -814.48 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.403743	-1.137864	0.317166
2	6	0	-0.127525	-1.780494	-0.058955
3	1	0	-0.285548	-2.232093	-1.036709
4	1	0	-0.011616	-2.581448	0.676892
5	8	0	-1.571187	0.148702	-1.446050
6	1	0	-0.746297	0.388011	-1.877843
7	1	0	-1.451492	-0.137729	0.839364
8	8	0	-2.396132	-1.784685	0.284456
9	8	0	-2.537781	2.182756	-0.605409
10	1	0	-3.478706	2.250640	-0.780640
11	1	0	-2.095349	1.196487	-1.097014
12	8	0	-1.811227	1.082727	1.507487
13	1	0	-1.091755	1.554065	1.936970
14	1	0	-2.164116	1.664087	0.723739
15	6	0	1.028850	-0.829052	-0.019969
16	6	0	1.472943	-0.315400	1.193213
17	6	0	1.682329	-0.470675	-1.191885
18	6	0	2.538688	0.568777	1.229125
19	1	0	0.992375	-0.614576	2.120234
20	6	0	2.754846	0.405763	-1.155401
21	1	0	1.355860	-0.886047	-2.140440
22	6	0	3.179864	0.931514	0.054548
23	1	0	2.875896	0.967675	2.179448
24	1	0	3.259831	0.677855	-2.075659
25	1	0	4.017762	1.619528	0.083571

Standard orientation of Ts-B-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-B-d'

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1120.48 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.266754	-0.617518	0.080527
2	1	0	-1.367096	0.474364	-0.260384
3	6	0	-0.166624	-0.855037	1.043898
4	1	0	-0.479517	-0.350666	1.956218
5	1	0	-0.147164	-1.930959	1.220019
6	8	0	-2.445608	-1.008212	0.637675
7	8	0	-1.863763	1.639930	-0.823616
8	1	0	-2.959329	1.379269	-0.497658
9	1	0	-1.557380	2.458777	-0.426723
10	8	0	-3.958275	0.741952	-0.126704
11	1	0	-3.202747	-0.260491	0.334038
12	1	0	-4.422103	1.197757	0.579558
13	8	0	-0.979999	-1.377673	-1.054018
14	1	0	-1.441168	-0.942029	-1.784702
15	6	0	1.149603	-0.331179	0.546559
16	6	0	2.027019	-1.159375	-0.142701
17	6	0	1.507041	0.990789	0.783472
18	6	0	3.240748	-0.670661	-0.596869
19	1	0	1.756021	-2.194049	-0.324682
20	6	0	2.719269	1.482737	0.326160
21	1	0	0.836334	1.640975	1.337089
22	6	0	3.587114	0.652188	-0.365283
23	1	0	3.920168	-1.325464	-1.131584
24	1	0	2.989161	2.515686	0.516904
25	1	0	4.538229	1.034704	-0.719896

Standard orientation of Ts-B-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-B-e

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -172.77 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.193517	-0.615344	0.103969
2	6	0	-0.102401	-0.524177	1.105523
3	1	0	-0.129404	-1.490864	1.614462
4	6	0	1.244611	-0.195044	0.543849
5	6	0	2.127645	-1.208655	0.193661
6	6	0	1.618452	1.130089	0.354143
7	6	0	3.368566	-0.902253	-0.341732
8	1	0	1.844642	-2.245866	0.344166
9	6	0	2.857826	1.437734	-0.182435
10	1	0	0.935710	1.927534	0.631090
11	6	0	3.734476	0.421330	-0.531207
12	1	0	4.053061	-1.700096	-0.608461
13	1	0	3.142123	2.474637	-0.324757
14	1	0	4.706541	0.661801	-0.948119
15	8	0	-0.939489	-0.480670	-1.040447
16	8	0	-3.575699	0.611282	-0.418505
17	8	0	-2.900375	0.620951	0.686174
18	8	0	-4.438214	-0.313209	-0.490561
19	1	0	-0.462900	0.219276	1.819746

Standard orientation of Ts-B-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-B-e'

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1234.23 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.226060	1.309764	-0.326559
2	6	0	0.602731	0.131814	-0.495461
3	1	0	1.030216	-0.543459	-1.243463
4	8	0	2.410858	1.392154	-0.718813
5	1	0	3.582134	0.045273	-0.536957
6	8	0	4.020291	-0.670781	-0.025184
7	1	0	4.315056	-1.337308	-0.653176
8	1	0	2.858250	-1.046286	0.934622
9	8	0	1.937222	-1.109942	1.366652
10	1	0	1.960938	-0.708568	2.245542
11	1	0	1.245057	-0.498727	0.628839
12	6	0	-0.856275	0.054395	-0.257699
13	6	0	-1.590883	-0.963295	-0.860200
14	6	0	-1.521263	0.951480	0.577306
15	6	0	-2.955539	-1.078669	-0.643862
16	1	0	-1.087506	-1.671518	-1.511620
17	6	0	-2.885009	0.839223	0.787074
18	1	0	-0.960559	1.742461	1.062774
19	6	0	-3.610249	-0.176423	0.179133
20	1	0	-3.509453	-1.878071	-1.125006
21	1	0	-3.386597	1.549075	1.436793
22	1	0	-4.678005	-0.263828	0.348574

Standard orientation of Ts-B-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-B-f

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -250.70 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.291351	-0.901937	0.026895
2	6	0	-0.270192	-0.764058	1.085496
3	1	0	-0.708185	-0.069530	1.798263
4	1	0	-0.176579	-1.751310	1.544502
5	8	0	-2.509114	-1.141220	0.530000
6	8	0	-0.910584	-1.835840	-0.872723
7	8	0	-2.584211	1.148821	-0.556518
8	8	0	-2.350162	1.971096	0.475741
9	8	0	-1.528828	0.587250	-0.998282
10	1	0	-1.417273	-1.658329	-1.682050
11	6	0	1.042674	-0.268081	0.554377
12	6	0	2.049952	-1.163407	0.220215
13	6	0	1.267207	1.097336	0.425767
14	6	0	3.269372	-0.699418	-0.246923
15	1	0	1.880891	-2.229917	0.328565
16	6	0	2.485360	1.561230	-0.041748
17	1	0	0.476762	1.793140	0.687003
18	6	0	3.487116	0.663096	-0.379150
19	1	0	4.052693	-1.404015	-0.503823
20	1	0	2.655412	2.627929	-0.139255
21	1	0	4.442447	1.027131	-0.741937
22	1	0	-3.092449	-0.422576	0.186537

Standard orientation of Ts-B-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-B-f'

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -777.43 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.063134	-0.425604	0.051075
2	8	0	1.208771	0.102366	-1.141810
3	1	0	2.053555	1.235055	-0.931980
4	8	0	2.286935	-1.410694	0.253192
5	1	0	2.449728	-1.766142	-0.636529
6	8	0	2.808284	1.928039	-0.663369
7	1	0	2.394933	2.702076	-0.271934
8	1	0	3.181388	-0.600255	0.560995
9	8	0	3.880886	0.289586	0.829180
10	1	0	3.523587	1.092983	0.238926
11	1	0	4.803784	0.106655	0.621033
12	6	0	-0.060984	-1.377852	0.056020
13	1	0	0.044067	-1.993189	0.949086
14	1	0	-0.004036	-2.011199	-0.835640
15	6	0	-1.357117	-0.616553	0.089554
16	6	0	-2.174197	-0.550097	-1.030569
17	6	0	-1.753012	0.036371	1.252366
18	6	0	-3.368122	0.155448	-0.992807
19	1	0	-1.873478	-1.056276	-1.942414
20	6	0	-2.941333	0.746680	1.292072
21	1	0	-1.122861	-0.014923	2.135074
22	6	0	-3.753122	0.806648	0.168075
23	1	0	-3.998829	0.196356	-1.874581
24	1	0	-3.239129	1.250922	2.205325
25	1	0	-4.686332	1.358910	0.199314

Standard orientation of Ts-B-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-B-f''

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -158.64 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.078795	0.289590	-0.644529
2	1	0	-2.782253	-0.712634	-0.695032
3	1	0	-3.622840	0.358029	0.145513
4	8	0	-2.236478	-2.067862	-0.634322
5	1	0	-2.897010	-2.746663	-0.785576
6	1	0	-1.899644	-1.832343	0.802992
7	8	0	-1.656861	-1.472889	1.741608
8	1	0	-0.953047	-2.031427	2.080138
9	1	0	-0.980290	0.132997	1.063693
10	8	0	-1.536365	2.536362	-0.322716
11	1	0	-1.995812	2.776395	-1.155506
12	7	0	-1.007896	1.420501	-0.486886
13	6	0	-0.341796	0.973301	0.675419
14	1	0	-0.286344	1.755708	1.434248
15	6	0	0.986349	0.377699	0.267422
16	6	0	1.027611	-0.838774	-0.402290
17	6	0	2.160384	1.051396	0.567995
18	6	0	2.249556	-1.377341	-0.768530
19	1	0	0.100475	-1.359464	-0.630225
20	6	0	3.382283	0.501807	0.208735
21	1	0	2.124313	2.003822	1.086948
22	6	0	3.427026	-0.709968	-0.461036
23	1	0	2.284401	-2.326947	-1.291442
24	1	0	4.300179	1.026181	0.450660
25	1	0	4.382663	-1.137476	-0.744822

Standard orientation of Ts-B-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-B-g

State = 1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -370.48 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.825833	-0.227136	0.050231
2	8	0	-1.077557	0.972358	0.476388
3	1	0	-1.909174	1.391528	-0.106389
4	8	0	-2.339992	-1.250292	0.944866
5	1	0	-2.423917	-0.974578	1.863377
6	8	0	-3.017139	1.810143	-0.748838
7	1	0	-3.552260	-0.799185	0.170544
8	1	0	-3.429909	2.583593	-0.350941
9	8	0	-4.288317	-0.392980	-0.430486
10	1	0	-3.659608	1.032144	-0.668256
11	1	0	-5.119437	-0.444578	0.047758
12	8	0	-1.020843	-0.523470	-1.088909
13	6	0	0.241442	-0.919285	0.841067
14	1	0	0.088138	-1.975192	0.643698
15	1	0	0.039370	-0.694456	1.883434
16	6	0	1.586271	-0.425025	0.388258
17	6	0	2.235070	-1.045495	-0.672137
18	6	0	2.188911	0.651389	1.027157
19	6	0	3.472999	-0.589438	-1.094248
20	1	0	1.771072	-1.892588	-1.167053
21	6	0	3.427589	1.106514	0.606020
22	1	0	1.687203	1.133615	1.859981
23	6	0	4.069244	0.487337	-0.455847
24	1	0	3.975965	-1.079684	-1.920490
25	1	0	3.894788	1.944852	1.110919
26	1	0	5.040220	0.842428	-0.783980

Standard orientation of Ts-B-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-B-h

State = 1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -151.19 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.684685	-1.181836	0.304730
2	8	0	-0.988262	2.007476	-0.557438
3	8	0	-1.442057	0.939223	-1.233676
4	8	0	-1.714770	2.318044	0.455889
5	8	0	-2.728232	-1.675764	-0.179387
6	6	0	-0.728931	-0.738952	-0.585451
7	1	0	-0.887782	-1.164418	-1.566043
8	6	0	0.651021	-0.447348	-0.201319
9	6	0	1.634773	-0.730773	-1.151536
10	6	0	1.032476	0.133417	1.008489
11	6	0	2.967186	-0.465879	-0.894082
12	1	0	1.347889	-1.171147	-2.101198
13	6	0	2.368231	0.399267	1.260759
14	1	0	0.281022	0.371369	1.747639
15	6	0	3.338668	0.098641	0.317437
16	1	0	3.717739	-0.701352	-1.640667
17	1	0	2.652735	0.849330	2.205851
18	8	0	-1.536960	-1.052575	1.536069
19	1	0	4.382897	0.307600	0.523862