Supporting Information

The formation mechanism of chloropicrin from methylamine during chlorination: a DFT study

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Scheme S1: TCNM formation pathways from NCNMHA, NCCMHA and NDCMNDHA during chlorination

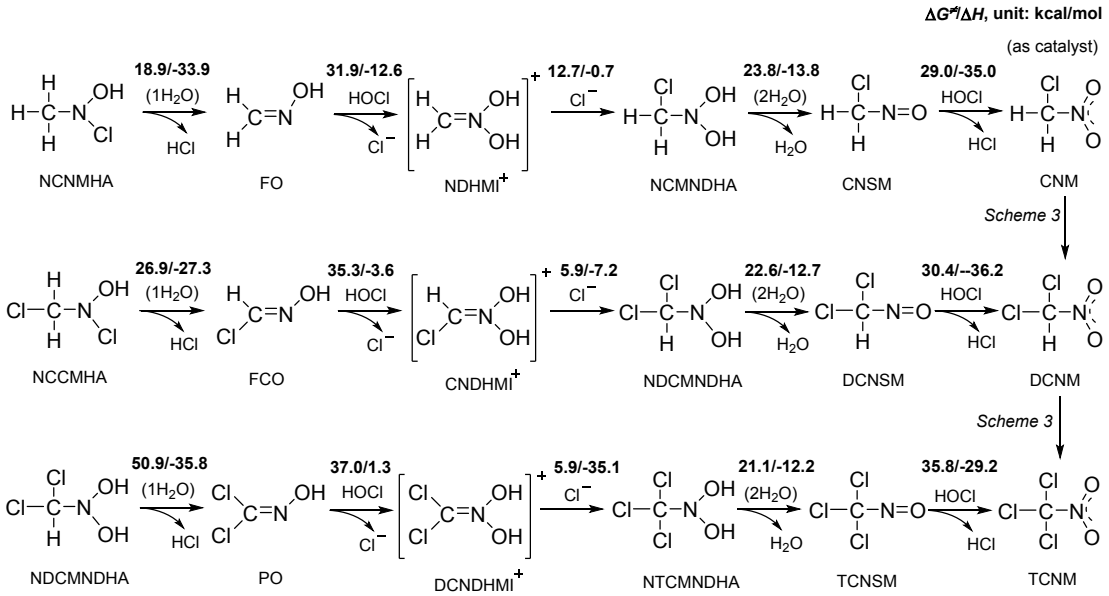

Table S1. Activation free energies and reaction energies (at 298 K and 1 atm, in kcal/mol) calculated at the CCSD(T)/6-311++G(2d,p)//M06-2X/6-311+G(d,p) level for elementary steps of TCNM formation from NCNMHA, NCCMHA and NDCMNDHA during chlorination

Reactions	Name of transition states	$\Delta G^{\neq}$	ΔH	ΔG
NCNMHA + H_2O → FO + HCl + H_2O	(TS-NCNMHA)	18.9	-33.9	-32.5
FO + HOCl → $NDHMI^+$ + Cl^-	(TS-FO)	31.9	-12.6	-9.8
$NDHMI^+$ + Cl^- → NCMNDHA	($TS\text{-}NDHMI^+$)	12.7	-0.7	0.4
NCMNDHA + $2H_2O$ → CNSM + $3H_2O$	(TS-NCMNDHA)	23.8	-13.8	-17.3
CNSM + HOCl → CNM + HCl	(TS-CNSM)	29.0	-35.0	-35.0
NCCMHA+ H_2O → FCO + HCl + H_2O	(TS-NCCMHA)	26.9	-27.3	-26.2
FCO + HOCl → $CNDHMI^+$ + Cl^-	(TS- FCO)	35.3	-3.6	-1.5
$CNDHMI^+$ + Cl^- → NDCMNDHA	($TS\text{-}CNDHMI^+$)	5.9	-7.2	-6.0
NDCMNDHA + $2H_2O$ → DCNSM + $3H_2O$	(TS-NDCMNDHA)	22.6	-12.7	-16.7
DCNSM → DCNM + HCl	(TS-DNSM)	30.4	-36.2	-34.4
NDCMNDHA + H_2O → PO + $2H_2O$	(TS-NDCMNDHA-1)	50.9	-35.8	-38.8
PO + HOCl → $DCNDHMI^+$ + Cl^-	(TS-PO)	37.0	1.3	5.3
$DCNDHMI^+$ + Cl^- → NTCMNDHA	($TS\text{-}DCNDHMI^+$)	5.9	-35.1	-33.4
NTCMNDHA + $2H_2O$ → TCNSM + $3H_2O$	(TS-NTCMNDHA)	21.1	-12.2	-16.1
TCNSM + HOCl → TCNM + HCl	(TS-TCNSM)	35.8	-29.2	-28.4

Table S2. Energies (in hartree) of for *N*-Chlorination of MA and NCMA by hypochlorous acid assisted by n=0~3 water molecules

n	species	B3LYP/6-311+(d,p)			M06-2X/6-311+(d,p)		
		$\Delta\Delta G^*$	E**	$\Delta\Delta H^*$	$\Delta\Delta G^*$	E**	$\Delta\Delta H^*$
MA + HOCl → NCMA + H_2O							
	R	0.04267	-630.97926	0.087102	0.046079	-630.97890	0.08823
0	TS	0.04610	-631.85534	0.084273	0.049196	-630.90778	0.08646
	P	0.04611	-631.96269	0.087044	0.048485	-631.02306	0.08811
	R	0.06693	-707.302325	0.11505	0.06952	-707.30232	0.11515
1	TS	0.06977	-707.267186	0.113225	0.07040	-707.26723	0.11410
	P	0.065	-707.340991	0.114617	0.06953	707.34099	0.11494
	R	0.09066	-783.62276	0.14272	0.0921	-783.62208	0.14411
2	TS	0.0893	-783.60948	0.137	0.09087	-783.60913	0.13834
	P	0.08319	-783.65865	0.14206	0.08995	-783.65791	0.14392
	R	0.11108	-859.94509	0.17018	0.11331	-859.94452	0.17216
3	TS	0.10611	-859.93572	0.16302	0.11058	-859.93500	0.16541
	P	0.10545	-859.97802	0.16950	0.10963	-859.97755	0.17145
NCMA + HOCl → DCMA + H_2O							
	R	0.02671	-1090.02687	0.07833	0.03520	-1090.0270	0.07950
0	TS	0.03288	-1089.95865	0.07400	0.03659	-1089.9524	0.07692
	P	0.03315	-1090.06778	0.07739	0.03508	-1090.0668	0.07860
	R	0.05230	-1166.34928	0.10568	0.05128	-1166.3475	0.10714
1	TS	0.05712	-1166.29495	0.10270	0.05875	-1166.2949	0.10481
	P	0.05112	-1166.38513	0.10493	0.05617	-1166.3841	0.10553
	R	0.07648	-1242.66962	0.13351	0.07953	-1242.6688	0.13423
2	TS	0.07578	-1242.64214	0.12532	0.07753	-1242.6409	0.12583
	P	0.06958	-1242.70282	0.13238	0.07666	-1242.7019	0.13428
	R	0.09719	-1318.9915	0.16111	0.09855	-1318.9905	0.16311
3	TS	0.09281	-1318.9677	0.15066	0.09712	-1318.9672	0.15286
	P	0.09383	-1319.0230	0.16004	0.09704	-1319.0221	0.16219

* Thermal correction to Gibbs Free Energy (G)/Enthalpy(H) calculated at the B3LYP/6-311+(d,p) and M06-2X/6-311+(d,p) levels

** single point calculated at the CCSD(T)/6-311++(2d,p) level

Table S3. Energies (in hartree) of calculated at the CCSD(T)/6-311++G(2d,p)//M06-2X /6-311+G(d,p) level for elementary steps of TCNM formation from DCMA during chlorination

Reactions	species	$\Delta\Delta G^*$	E**	$\Delta\Delta H^*$
DCMA + $3H_2O$ → NCNMHA + HCl + $2H_2O$	R	0.052993	-1166.3841336	0.106563
	TS	0.057368	-1166.320135	0.104517
	P	0.054714	-1166.3703776	0.103042
CMHA + H_2O → NSM + HCl + H_2O	R	0.050749	-706.0822002	0.092702
	TS	0.050019	-706.0659196	0.089351
	P	0.043552	-706.0889814	0.088084
NSM + HOCl → NM + HCl	R	0.025154	-704.8108492	0.068062
	TS	0.027269	-704.7725137	0.066837
	P	0.025906	-704.8737997	0.067342
DCMA + H_2O → NCMI + HCl + H_2O	R	0.03424	-1090.062357	0.078147
	TS	0.031022	-1090.003188	0.071695
	P	0.028584	-1090.103315	0.073352
DCMA + ClO^- → NCMI + HOCl + Cl^-	R	0.03424	-1090.062357	0.078147
	TS	0.031022	-1090.003188	0.071695
	P	0.028584	-1090.103315	0.073352
DCMA + OH^- → NCMI + H_2O + Cl^-	R	0.010474	-1548.598946	0.057226
	TS	0.004724	-1548.571776	0.050528
	P	0.006396	-1548.69068	0.056916
NCMI + HOCl → $NCNMHI^+$ + Cl^-	R	0.012357	-1090.16415	0.053087
	TS	0.018	-1090.156636	0.055126
	P	0.020726	-1090.184868	0.057078
$NCNHMI^+$ + Cl^- → NCCMHA	R	0.013438	-1088.829526	0.053087
	TS	0.018	-1088.820369	0.055126
	P	0.020726	-1088.847711	0.057078
NCCMHA + H_2O → CNSM + HCl + H_2O	R	0.039168	-1165.16804	0.084795
	TS	0.036903	-1165.145925	0.08012
	P	0.029132	-1165.172798	0.079714
CNSM + HOCl → CNM + HCl	R	0.015224	-1163.894126	0.059304
	TS	0.017685	-1163.850303	0.057988
	P	0.015829	-1163.950531	0.059893
NM + HOCl + $2H_2O$ → CNM + $3H_2O$	R	0.060988	-932.5340545	0.128687
	TS	0.070475	-932.469428	0.12377
	P	0.061301	-932.6037444	0.128965
NM + HOCl + ClO^- → CNM + OH^- + HOCl	R	0.028937	-1314.759183	0.080533
	TS	0.019611	-1314.73825	0.075289
	P	0.024833	-1314.778186	0.081388
NM + HOCl + OH^- → CNM + OH^- + H_2O	R	0.034139	-855.7037828	0.087584
	TS	0.030702	-855.7018684	0.084951
	P	0.036901	-855.766977	0.089261
CNM^- + 2HOCl → DCNM + OH^- +	R	0.012942	-1773.841166	0.071632
	TS	0.016791	-1773.838674	0.07096

HOCl	P	0.01485	-1773.856375	0.072492
$DCNM^{-}$ + 2HOCl →	R	0.004561	-2232.92194	0.062668
TCNM + OH^{-} +	TS	0.005812	-2232.918799	0.062724
HOCl	P	0.00451	-2232.928487	0.061875

* Thermal correction to Gibbs Free Energy (G)/Enthalpy(H) calculated at the M06-2X/6-311+(d,p) level

** single point calculated at the CCSD(T)/6-311++(2d,p) level

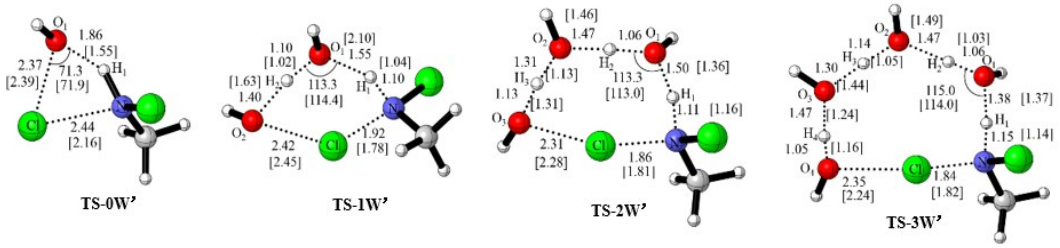

Figure S1. The optimized structures and important geometric parameters calculated at the B3LYP/6-311+G(d,p) and M06-2X/6-311+G(d,p) levels for the transition state in DCMA formation from *N*-chlorination of NCMA by hypochlorous acid assisted by 0~3 water molecules; distances in angstrom, angles in degree; values in the bracket from M06-2X method (atoms in green color represents chlorine atom, atom in blue color represents nitrogen atom; atom in red represents oxygen atom, atom in white represents hydrogen atom; atom in grey color represents carbon atom).

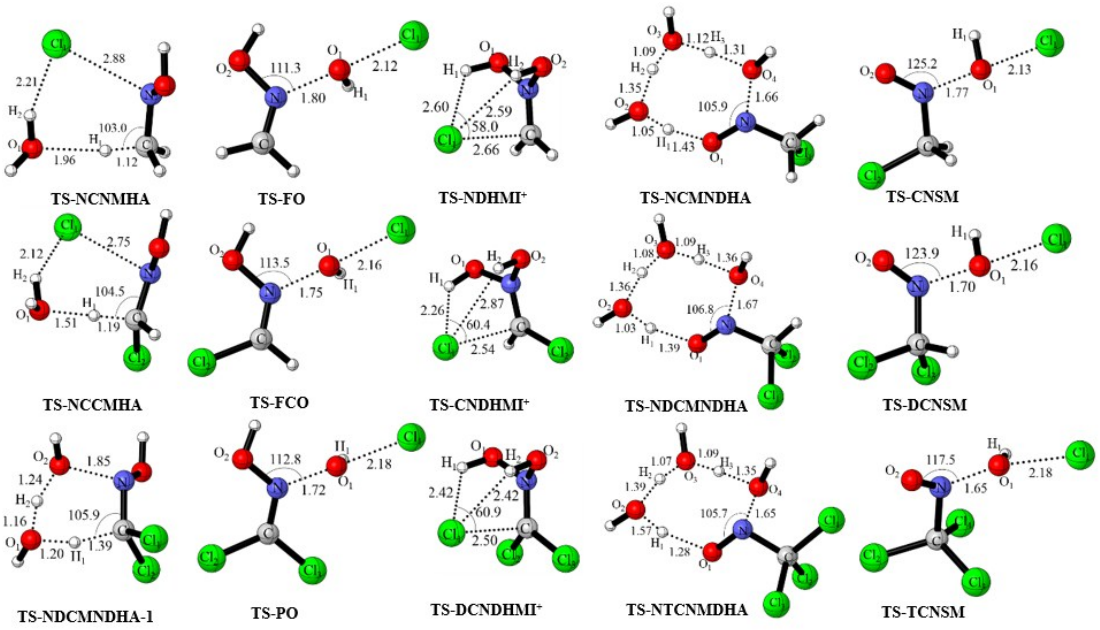

Figure S2. The optimized structures and important geometric parameters calculated at the M06-2X/6-311+G(d,p) level for the transition states in TCNM formation from NCNMHA, NCCMHA and NDCMNDHA during chlorination; distances in angstrom, angles in degree (atoms in green color represents chlorine atom, atom in blue color represents nitrogen atom; atom in red represents oxygen atom, atom in white represents hydrogen atom; atom in grey color represents carbon atom).

Standard orientation of TS-0W/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-0W/B3LYP

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -368.89 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.094455	0.004399	-0.328597
2	1	0	1.867613	0.258209	-1.362532
3	1	0	2.291004	-1.068132	-0.246063
4	1	0	3.003300	0.536612	-0.016713
5	7	0	0.984824	0.361914	0.515232
6	1	0	-2.042380	1.363532	0.412286
7	1	0	1.080028	0.165043	1.505053
8	17	0	-0.906906	-0.930279	-0.016794
9	1	0	0.396466	1.173215	0.295784
10	8	0	-1.329890	1.353309	-0.242169

Standard orientation of TS-0W/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:

Standard orientation of TS-0W/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -585.28 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.855218	0.071731	-0.453703
2	1	0	1.429567	0.788693	-1.152702
3	1	0	1.983663	-0.894969	-0.939851
4	1	0	2.827236	0.429444	-0.101878
5	7	0	0.935111	-0.075219	0.659117
6	1	0	-1.836649	1.570156	-0.253340
7	17	0	-0.974672	-0.778399	-0.104038
8	1	0	0.617092	0.796253	1.074041
9	8	0	-0.914934	1.427462	-0.011553
10	1	0	1.190902	-0.780337	1.343200

Standard orientation of TS-1W/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-1W/B3LYP

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -186.34 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.402982	0.223887	-0.462854
2	1	0	-0.881786	1.117358	-0.449541
3	6	0	-2.488877	0.177494	0.549217
4	1	0	-2.958197	-0.802004	0.517344
5	1	0	-2.057394	0.371511	1.527476
6	1	0	-3.208722	0.954579	0.290073
7	8	0	1.146298	1.664447	-0.010290
8	1	0	1.702784	2.414822	-0.239576
9	17	0	-0.015449	-0.918117	-0.164996
10	8	0	2.550039	-0.563488	0.179393
11	1	0	2.843303	-0.787874	1.070152
12	1	0	1.757742	0.850383	0.088118
13	1	0	-1.751646	0.049369	-1.407259

Standard orientation of TS-1W/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:

Standard orientation of TS-1W/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -166.96 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.471319	0.257983	-0.474402
2	1	0	-1.051031	1.196756	-0.509165
3	6	0	-2.520119	0.172979	0.576896
4	1	0	-2.915597	-0.838431	0.580587
5	1	0	-2.058493	0.416261	1.529662
6	1	0	-3.294835	0.894253	0.324657
7	8	0	1.427906	1.583561	0.001321
8	1	0	2.105280	2.262608	-0.027246
9	17	0	-0.083163	-0.782435	-0.182885
10	8	0	2.462273	-0.736056	0.168272
11	1	0	2.864155	-0.968355	1.009341
12	1	0	1.915855	0.670392	0.103376
13	1	0	-1.853056	0.044106	-1.399464

Standard orientation of TS-2W/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-2W/B3LYP

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -634.22 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.708728	0.035457	-0.417566
2	1	0	-1.293651	1.003500	-0.352545
3	6	0	-2.731656	-0.232431	0.619222
4	1	0	-3.060069	-1.266226	0.544342
5	1	0	-2.294963	-0.037877	1.595862
6	1	0	-3.569389	0.443283	0.441481
7	8	0	2.252548	0.968493	0.301367
8	1	0	3.054163	1.361535	-0.057278
9	17	0	-0.164682	-0.942505	-0.239179
10	8	0	-0.017798	2.149372	-0.199956
11	1	0	0.894873	1.733421	-0.000019
12	8	0	2.147018	-1.451897	0.027956
13	1	0	2.279878	-1.867568	0.887555
14	1	0	2.262356	-0.316588	0.167328
15	1	0	-2.066723	-0.131483	-1.358176
16	1	0	-0.109994	2.919226	0.370193

Standard orientation of TS-2W/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:

Standard orientation of TS-2W/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -616.02 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.677014	-0.019004	-0.450074
2	1	0	1.325607	0.975505	-0.425038
3	8	0	-2.214139	0.992299	0.124391
4	1	0	-2.895214	1.365726	0.687827
5	17	0	0.150167	-0.901107	-0.216848
6	8	0	0.127010	2.095815	-0.039016
7	1	0	0.062879	2.968571	-0.433928
8	1	0	-0.809933	1.719174	0.032879
9	8	0	-2.158435	-1.421711	0.227804
10	1	0	-2.593306	-1.804928	-0.538413
11	1	0	-2.252937	-0.165899	0.178140
12	1	0	2.040424	-0.243803	-1.377069
13	6	0	2.677765	-0.281179	0.608331
14	1	0	2.240873	0.004977	1.561812
15	1	0	2.931954	-1.337766	0.601757
16	1	0	3.555635	0.326146	0.393551

Standard orientation of TS-3W/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-3W/B3LYP

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -625.27 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.992785	-0.040881	-0.357822
2	1	0	-1.580123	0.954998	-0.287653
3	6	0	-2.983931	-0.314449	0.711278
4	1	0	-3.345551	-1.336034	0.622928
5	1	0	-2.506862	-0.154881	1.675112
6	1	0	-3.805565	0.390484	0.577800
7	8	0	1.748692	2.106299	0.031281
8	1	0	2.209538	2.574047	-0.672337
9	17	0	-0.538053	-1.106012	-0.280281
10	8	0	-0.795218	2.297457	-0.203895
11	1	0	-1.101224	2.940366	0.444696
12	1	0	0.224374	2.226556	-0.105847
13	8	0	1.660074	-2.275901	-0.144653
14	1	0	1.676028	-2.819514	0.650772
15	1	0	2.171023	-1.422190	0.085148
16	1	0	-2.400899	-0.177563	-1.283384
17	8	0	2.811899	-0.041417	0.407876
18	1	0	3.770973	0.023600	0.375750
19	1	0	2.284690	1.083691	0.194011

Standard orientation of TS-3W/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:

Standard orientation of TS-3W/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -657.58 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.970538	-0.105663	-0.389463
2	1	0	-1.665523	0.908529	-0.309250
3	6	0	-2.923552	-0.465604	0.681523
4	1	0	-3.163548	-1.523140	0.606298
5	1	0	-2.455003	-0.247838	1.638292
6	1	0	-3.820286	0.138852	0.552644
7	8	0	1.703373	2.117932	-0.033499
8	1	0	2.139701	2.490060	-0.804061
9	17	0	-0.436343	-1.035130	-0.288283
10	8	0	-0.916871	2.308226	-0.099290
11	1	0	-1.199490	2.889742	0.611947
12	1	0	0.076144	2.249386	-0.055266
13	8	0	1.611845	-2.127488	-0.155178
14	1	0	1.571591	-2.733675	0.589592
15	1	0	2.249156	-1.140847	0.172163
16	8	0	2.790643	-0.129736	0.467260
17	1	0	3.726931	-0.196136	0.266935
18	1	0	2.151182	1.218850	0.147175
19	1	0	-2.369880	-0.274764	-1.312900

Standard orientation of TS-0W'/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-0W'/B3LYP

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -375.00 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.899056	1.716360	-0.027328
2	1	0	0.032682	2.327208	0.224467
3	1	0	1.154175	1.846360	-1.081474
4	1	0	1.755930	2.013074	0.588290
5	7	0	0.538267	0.341195	0.232087
6	1	0	-1.863527	-1.065009	1.530234
7	17	0	-1.576560	-0.161606	-0.873798
8	1	0	-0.141482	0.090291	1.021643
9	8	0	-1.591433	-0.137035	1.511486
10	17	0	1.731353	-0.826757	-0.057713

Standard orientation of TS-0W'/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x /6-311+G** level:
Standard orientation of TS-0W'/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -563.10 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.452102	1.521107	-0.774944
2	1	0	-0.545234	1.957127	-0.783030
3	1	0	0.719964	1.145692	-1.761811
4	1	0	1.188980	2.250096	-0.431656
5	7	0	0.395105	0.398075	0.154576
6	1	0	-2.588161	0.160567	1.290427
7	17	0	-1.184275	-0.926081	-0.494898
8	1	0	-0.065145	0.610206	1.049574
9	8	0	-1.914517	0.720427	0.890115
10	17	0	1.838827	-0.473935	0.323322

Standard orientation of TS-1W’/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:
Standard orientation of TS-1W’/B3LYP

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -226.42 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.228861	0.948406	0.374049
2	8	0	3.070222	-0.287447	-0.235614
3	1	0	3.400052	-0.322641	-1.141937
4	17	0	0.633964	-1.007583	-0.164049
5	6	0	-1.381816	-0.314212	1.655796
6	7	0	-0.805546	0.059408	0.337152
7	1	0	-0.551855	-0.363635	2.358572
8	1	0	-2.083417	0.466052	1.947937
9	1	0	-1.878173	-1.276873	1.568096
10	8	0	1.372334	1.695668	0.216879
11	1	0	1.716761	2.323895	0.859794
12	1	0	2.099002	0.994296	0.043044
13	17	0	-2.050685	0.268416	-0.903864

Standard orientation of TS-1W’/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x /6-311+G** level:
Standard orientation of TS-1W’/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -221.38 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.399371	0.832034	1.451628
2	1	0	2.170890	1.558980	1.208606
3	1	0	1.802869	-0.007492	2.010954
4	1	0	0.571623	1.300174	1.979810
5	7	0	0.844955	0.308969	0.171602
6	1	0	-3.571934	-0.639972	0.689992
7	17	0	-0.574468	-0.742268	0.414972
8	1	0	0.390775	1.066602	-0.377175
9	8	0	-2.977273	-0.691916	-0.063664
10	8	0	-1.636213	1.455601	-0.773575
11	1	0	-2.152601	2.145679	-1.195207
12	1	0	-2.267329	0.698925	-0.517531
13	17	0	2.083450	-0.398165	-0.827473- ---

Standard orientation of TS-2W'/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-2W'/B3LYP

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -594.86 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.139938	0.070935	0.323711
2	1	0	0.628024	1.047440	0.233368
3	8	0	-2.698525	1.028685	-0.256997
4	1	0	-3.456186	1.455678	0.154452
5	17	0	-0.394552	-0.964065	0.117119
6	8	0	-0.445510	2.093942	0.172146
7	1	0	-0.300912	2.821215	-0.442418
8	1	0	-1.406705	1.695347	-0.008752
9	8	0	-2.658054	-1.410230	-0.070520
10	1	0	-2.821079	-1.793646	-0.940861
11	1	0	-2.755710	-0.288620	-0.165370
12	6	0	1.808440	-0.136748	1.629176
13	1	0	1.052630	0.020765	2.397501
14	1	0	2.206438	-1.147263	1.682900
15	1	0	2.604082	0.601014	1.726033
16	17	0	2.267253	-0.082239	-1.025055

Standard orientation of TS-2W'/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x /6-311+G** level:
Standard orientation of TS-2W'/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -626.69 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.111137	0.072029	0.318380
2	1	0	0.577556	1.102156	0.246367
3	8	0	-2.625963	1.018045	-0.253604
4	1	0	-3.397689	1.421603	0.150472
5	17	0	-0.395821	-0.914027	0.118949
6	8	0	-0.388668	2.057946	0.186709
7	1	0	-0.223106	2.790893	-0.413756
8	1	0	-1.345495	1.664737	0.000088
9	8	0	-2.618376	-1.405061	-0.066345
10	1	0	-2.805007	-1.827512	-0.909717
11	1	0	-2.699197	-0.106621	-0.181333
12	6	0	1.790575	-0.176045	1.605506
13	1	0	1.050076	-0.010399	2.386643
14	1	0	2.158746	-1.199636	1.634808
15	1	0	2.608161	0.536305	1.701073
16	17	0	2.196915	-0.096967	-1.025444

Standard orientation of TS-3W'/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-3W'/B3LYP

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -550.89 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.430518	0.024898	0.314265
2	1	0	-0.954311	1.066081	0.277224
3	6	0	-2.102907	-0.250203	1.607003
4	1	0	-2.493314	-1.265175	1.617434
5	1	0	-1.351819	-0.119713	2.385281
6	1	0	-2.904707	0.476305	1.731806
7	8	0	2.216358	2.062663	-0.165921
8	1	0	2.487304	2.490994	-0.984340
9	17	0	0.020586	-1.076091	0.062671
10	8	0	-0.262786	2.260635	0.182472
11	1	0	-0.421567	2.870338	0.912041
12	1	0	0.772725	2.175462	0.045296
13	8	0	2.057806	-2.208545	-0.227653
14	1	0	2.203467	-2.749522	0.557464
15	1	0	2.653582	-1.355382	-0.118541
16	8	0	3.360172	-0.075274	0.046962
17	1	0	4.249742	-0.048167	-0.318063
18	1	0	2.765462	1.068162	-0.093062
19	17	0	-2.570463	-0.076749	-1.035688

Standard orientation of TS-3W'/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x /6-311+G** level:
Standard orientation of TS-3W'/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -647.70 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.408697	0.004211	0.309251
2	1	0	-0.986087	1.063896	0.329676
3	6	0	-2.092721	-0.353552	1.569653
4	1	0	-2.426468	-1.388166	1.521759
5	1	0	-1.365268	-0.220305	2.369013
6	1	0	-2.934613	0.323044	1.705091
7	8	0	2.131905	2.051512	-0.221025
8	1	0	2.364523	2.398579	-1.086284
9	17	0	0.076971	-1.013092	0.055373
10	8	0	-0.326170	2.267423	0.272050
11	1	0	-0.449335	2.844537	1.032129
12	1	0	0.682422	2.182759	0.086164
13	8	0	2.009170	-2.116328	-0.232997
14	1	0	2.123121	-2.703684	0.519907
15	1	0	2.688259	-1.182776	-0.077103
16	8	0	3.301749	-0.120048	0.092654
17	1	0	4.177729	-0.158527	-0.297600
18	1	0	2.631849	1.134628	-0.109896
19	17	0	-2.490039	-0.096474	-1.047196

Standard orientation of TS-DCMA/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-DCMA/B3LYP

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -223.37 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.966903	-0.557504	1.590612
2	1	0	2.044688	-0.510407	1.755388
3	1	0	0.646908	-1.601813	1.665851
4	1	0	0.406806	0.036507	2.311583
5	7	0	0.566034	-0.116507	0.258650
6	1	0	-1.633249	2.425581	-1.195821
7	17	0	-2.111320	-1.018365	0.027721
8	1	0	-1.661945	1.137621	-0.312808
9	8	0	-1.339444	2.066153	-0.350672
10	8	0	1.171661	1.734497	0.202001
11	1	0	1.331822	2.060479	1.102767
12	1	0	0.224364	2.005886	-0.046775
13	17	0	1.535979	-0.852134	-0.936253

Standard orientation of TS-DCMA/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:

Standard orientation of TS-DCMA/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -441.57 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.408697	0.004211	0.309251
2	1	0	-0.986087	1.063896	0.329676
3	6	0	-2.092721	-0.353552	1.569653
4	1	0	-2.426468	-1.388166	1.521759
5	1	0	-1.365268	-0.220305	2.369013
6	1	0	-2.934613	0.323044	1.705091
7	8	0	2.131905	2.051512	-0.221025
8	1	0	2.364523	2.398579	-1.086284
9	17	0	0.076971	-1.013092	0.055373
10	8	0	-0.326170	2.267423	0.272050
11	1	0	-0.449335	2.844537	1.032129
12	1	0	0.682422	2.182759	0.086164
13	8	0	2.009170	-2.116328	-0.232997
14	1	0	2.123121	-2.703684	0.519907
15	1	0	2.688259	-1.182776	-0.077103
16	8	0	3.301749	-0.120048	0.092654
17	1	0	4.177729	-0.158527	-0.297600
18	1	0	2.631849	1.134628	-0.109896
19	17	0	-2.490039	-0.096474	-1.047196

Standard orientation of TS-NCNMHA/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-NCNMHA/B3LYP

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -216.80 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.230308	-0.388291	0.071314
2	7	0	-1.001800	0.299851	0.389589
3	1	0	-2.142059	-1.414518	0.421723
4	8	0	-0.737202	1.191521	-0.448470
5	8	0	1.591663	1.573082	0.060825
6	1	0	0.288964	1.554824	-0.177874
7	1	0	1.859483	1.993732	0.889385
8	1	0	1.773674	0.603268	0.139251
9	1	0	-2.499617	-0.310634	-0.982054
10	1	0	-2.989111	0.108515	0.695196
11	17	0	1.015731	-1.436542	-0.061145

Standard orientation of TS-NCNMHA/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:
Standard orientation of TS-NCNMHA/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -193.76 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.118879	0.370551	-0.116599
2	7	0	0.715208	0.604009	-0.389519
3	1	0	2.425183	-0.519859	-0.655568
4	8	0	0.199873	1.309505	0.498166
5	8	0	-2.115051	0.914936	-0.078275
6	1	0	-0.853780	1.342528	0.242858
7	1	0	-2.523185	1.281625	-0.871644
8	1	0	-1.992991	-0.042759	-0.221209
9	1	0	2.320655	0.316506	0.952445
10	1	0	2.622268	1.245372	-0.548930
11	17	0	-0.258615	-1.639430	0.068774

Standard orientation of TS-NSM/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-NSM/B3LYP

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -344.76 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.085085	1.143378	-0.037344
2	7	0	-1.495169	-0.191500	0.109482
3	8	0	0.411312	-0.075742	0.146321
4	8	0	-2.121400	-1.158065	-0.128374
5	1	0	0.493149	-0.961344	0.539237
6	17	0	2.512845	0.055255	-0.061392
7	1	0	-3.122756	1.064831	-0.356204
8	1	0	-1.974624	1.635363	0.931852
9	1	0	-1.456743	1.672515	-0.757105

Standard orientation of TS-NSM/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:
Standard orientation of TS-NSM/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -585.25 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.063286	1.136694	-0.019432
2	7	0	-1.447428	-0.187186	0.073022
3	8	0	0.387603	-0.073680	0.077436
4	8	0	-2.076063	-1.157384	-0.084788
5	1	0	0.482190	-0.980113	0.415641
6	17	0	2.472951	0.058236	-0.037485
7	1	0	-3.132319	1.035389	-0.191544
8	1	0	-1.824272	1.649055	0.913315
9	1	0	-1.546367	1.644316	-0.835909

Standard orientation of TS-DCMA-1/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-DCMA-1/B3LYP

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -511.66 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.359406	1.435297	0.740556
2	1	0	0.027698	1.726211	1.742368
3	1	0	-0.685890	1.477077	0.130895
4	1	0	0.971290	2.153867	0.191747
5	7	0	0.787206	0.135875	0.769237
6	17	0	1.893968	-0.228599	-0.483816
7	17	0	-1.180928	-1.408512	0.164342
8	8	0	-2.017272	1.365077	-0.556186
9	1	0	-2.052081	0.379122	-0.525909
10	1	0	-1.911397	1.611089	-1.486557

Standard orientation of TS-DCMA-1/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:
Standard orientation of TS-DCMA-1/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1123.03 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.261062	1.315961	0.911889
2	1	0	-0.115474	1.484972	1.921069
3	1	0	-0.746828	1.397941	0.202179
4	1	0	0.856340	2.104716	0.448026
5	7	0	0.745460	0.047322	0.793614
6	17	0	1.792812	-0.118958	-0.534873
7	17	0	-1.054792	-1.411158	0.143610
8	8	0	-1.938478	1.341347	-0.597498
9	1	0	-2.038868	0.373811	-0.683152
10	1	0	-1.778272	1.692716	-1.483298

Standard orientation of TS-DCMA-2/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-DCMA-2/B3LYP

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -413.05 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.415018	1.641469	-0.028445
2	1	0	-2.455470	1.917283	-0.170015
3	7	0	-1.041942	0.437542	0.077978
4	8	0	0.698624	0.136897	0.015316
5	1	0	0.730932	-0.375783	0.841492
6	1	0	-0.635448	2.393858	0.032189
7	17	0	2.898737	-0.184797	-0.039135
8	17	0	-2.160225	-0.870623	-0.031534

Standard orientation of TS-DCMA-2/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:
Standard orientation of TS-DCMA-2/M06-2X

Lowest Harmonic Vibrational Frequency (LHVF) = -624.87 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.422298	1.627154	-0.038397
2	1	0	-2.467086	1.876238	-0.201842
3	7	0	-1.026575	0.436256	0.087033
4	8	0	0.718720	0.139990	0.031285
5	1	0	0.735703	-0.284827	0.905713
6	1	0	-0.657084	2.394479	0.028436
7	17	0	2.830919	-0.179759	-0.046394
8	17	0	-2.103947	-0.874507	-0.033690

Standard orientation of TS-DCMA-3/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-DCMA-3/B3LYP

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -177.95 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.102657	0.096018	1.336102
2	1	0	-0.147200	-0.800695	1.884978
3	7	0	-0.655522	0.471527	0.355074
4	8	0	-0.204740	1.422787	-0.489108
5	1	0	0.694699	1.049772	-0.752672
6	1	0	0.822165	0.811076	1.702500
7	17	0	2.149609	-0.407983	-0.268734
8	17	0	-1.900141	-0.551973	-0.285623

Standard orientation of TS-DCMA-3/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:
Standard orientation of TS-DCMA-3/M06-2X

Lowest Harmonic Vibrational Frequency (LHVF) = -217.99 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.101814	0.314743	1.313594
2	1	0	-0.105931	-0.514748	1.976078
3	7	0	-0.657280	0.506059	0.293308
4	8	0	-0.284684	1.397184	-0.643661
5	1	0	0.597697	1.038871	-0.931138
6	1	0	0.802306	1.099509	1.558155
7	17	0	2.107273	-0.439833	-0.222144
8	17	0	-1.814716	-0.632637	-0.212475

Standard orientation of TS-NCMI/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-NCMI/B3LYP

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -413.05 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.415018	1.641469	-0.028445
2	1	0	-2.455470	1.917283	-0.170015
3	7	0	-1.041942	0.437542	0.077978
4	8	0	0.698624	0.136897	0.015316
5	1	0	0.730932	-0.375783	0.841492
6	1	0	-0.635448	2.393858	0.032189
7	17	0	2.898737	-0.184797	-0.039135
8	17	0	-2.160225	-0.870623	-0.031534

Standard orientation of TS-NCMI/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:
Standard orientation of TS-NCMI/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -624.87 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.422298	1.627154	-0.038397
2	1	0	-2.467086	1.876238	-0.201842
3	7	0	-1.026575	0.436256	0.087033
4	8	0	0.718720	0.139990	0.031285
5	1	0	0.735703	-0.284827	0.905713
6	1	0	-0.657084	2.394479	0.028436
7	17	0	2.830919	-0.179759	-0.046394
8	17	0	-2.103947	-0.874507	-0.033690

Standard orientation of TS-NCNHMI^{+}/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-NCNHMI^{+}/B3LYP

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -177.95 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.102657	0.096018	1.336102
2	1	0	-0.147200	-0.800695	1.884978
3	7	0	-0.655522	0.471527	0.355074
4	8	0	-0.204740	1.422787	-0.489108
5	1	0	0.694699	1.049772	-0.752672
6	1	0	0.822165	0.811076	1.702500
7	17	0	2.149609	-0.407983	-0.268734
8	17	0	-1.900141	-0.551973	-0.285623

Standard orientation of TS-NCNHMI^{+}/M06-2X

Cartesian coordinates of all the transition states optimized at the m62x/6-311+G** level:

Standard orientation of TS- NCNHMI^{+}/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -217.99 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.101814	0.314743	1.313594
2	1	0	-0.105931	-0.514748	1.976078
3	7	0	-0.657280	0.506059	0.293308
4	8	0	-0.284684	1.397184	-0.643661
5	1	0	0.597697	1.038871	-0.931138
6	1	0	0.802306	1.099509	1.558155
7	17	0	2.107273	-0.439833	-0.222144
8	17	0	-1.814716	-0.632637	-0.212475

Standard orientation of TS-NCCMHA/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-NCCMHA/B3LYP

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -660.79 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.215951	-0.624939	0.383620
2	7	0	0.138647	0.221454	-0.162117
3	1	0	1.124394	-1.617819	-0.038223
4	8	0	-0.176574	1.119947	0.650200
5	8	0	-2.361713	1.614084	-0.173617
6	1	0	-1.234489	1.571244	0.200769
7	1	0	-2.481721	2.087489	-1.010588
8	1	0	-2.568751	0.654111	-0.316598
9	1	0	1.243685	-0.607502	1.470102
10	17	0	-1.800794	-1.391593	-0.059805
11	17	0	2.739438	0.111575	-0.251079

Standard orientation of TS-NCCMHA/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:
Standard orientation of TS-NCCMHA/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -668.56 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.174918	-0.674067	0.253994
2	7	0	0.095655	0.218782	-0.212531
3	1	0	1.113733	-1.600915	-0.302445
4	8	0	-0.180243	1.059068	0.650056
5	8	0	-2.331455	1.652899	-0.153942
6	1	0	-1.206394	1.552018	0.244328
7	1	0	-2.437833	2.181095	-0.957150
8	1	0	-2.606655	0.729956	-0.341565
9	1	0	1.141005	-0.803622	1.332643
10	17	0	-1.723356	-1.411534	-0.040011
11	17	0	2.686335	0.162043	-0.194164

Standard orientation of TS-CNSM/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-CNSM/B3LYP

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -399.60 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.243730	-0.607777	0.395134
2	7	0	0.457280	0.645505	0.260765
3	8	0	-1.289709	0.200497	0.239424
4	8	0	0.897156	1.632248	-0.185360
5	1	0	-1.613281	1.082162	0.497176
6	17	0	-3.358971	-0.360216	-0.167044
7	17	0	2.898683	-0.487916	-0.211604
8	1	0	1.238202	-0.836137	1.461984
9	1	0	0.677064	-1.361618	-0.150814

Standard orientation of TS-CNSM/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:
Standard orientation of TS-CNSM/M06-2X

State=1-A
Charge = 0 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -609.33 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.225729	-0.666281	0.261993
2	7	0	0.432840	0.583343	0.195292
3	8	0	-1.287143	0.172341	0.143754
4	8	0	0.886542	1.602883	-0.118622
5	1	0	-1.586401	1.003832	0.552609
6	17	0	-3.349262	-0.327699	-0.120232
7	17	0	2.911809	-0.432346	-0.146891
8	1	0	1.109621	-1.025868	1.284535
9	1	0	0.734032	-1.344687	-0.436097

Standard orientation of TS-NM/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-NM/B3LYP

State=1-A

Charge = 0 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -270.46 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.462044	-0.193801	1.011002
2	1	0	1.222323	1.730673	-0.025479
3	8	0	2.644859	1.541892	-0.314475
4	17	0	0.995188	-1.074558	0.261017
5	1	0	2.982719	2.015445	-1.084825
6	7	0	-2.331273	-0.154536	-0.090718
7	8	0	0.201877	1.882139	0.173253
8	1	0	-0.302397	1.012966	0.495522
9	1	0	0.079098	2.594587	0.818978
10	8	0	2.684984	-1.302479	-0.326056
11	1	0	3.123068	-1.777223	0.397852
12	1	0	2.909940	0.605146	-0.411837
13	8	0	-2.451063	-1.161032	-0.821716
14	8	0	-2.926523	0.914313	-0.361211
15	1	0	-1.334340	-1.204350	1.377153
16	1	0	-1.740489	0.536139	1.766007

Standard orientation of TS-NM-1/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-NM-1/B3LYP

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -1123.56 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.308858	0.005733	-0.378486
2	1	0	-0.181059	-0.129259	-1.337494
3	1	0	1.657492	-0.133912	-0.626860
4	1	0	0.077743	-0.726069	0.389228
5	8	0	2.833216	-0.251594	-0.943039
6	8	0	-4.603172	-0.792996	0.136579
7	1	0	-4.731454	-1.750862	0.222906
8	17	0	-2.886866	-0.632352	-0.087075
9	17	0	3.667294	-1.049125	0.346301
10	7	0	0.123025	1.322936	0.104278
11	8	0	0.241652	1.548761	1.326362
12	8	0	-0.072237	2.249610	-0.709108

Standard orientation of TS-NM-1/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:
Standard orientation of TS-NM-1/M06-2X

State=1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -1162.22 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.316352	-0.189591	-0.555308
2	1	0	-0.196107	-0.213262	-1.511813
3	1	0	1.632957	-0.136268	-0.781220
4	1	0	0.119636	-1.028009	0.106341
5	8	0	2.878305	-0.066162	-0.980323
6	8	0	-4.411835	-0.638940	0.247299
7	1	0	-4.816990	-0.126435	-0.466476
8	17	0	-2.749129	-0.626610	-0.109289
9	17	0	3.595513	-0.777275	0.382464
10	7	0	0.025173	1.033990	0.118694
11	8	0	0.136296	1.083063	1.342659
12	8	0	-0.253058	2.030743	-0.545861

Standard orientation of TS-NM-2/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-NM-2/B3LYP

State=1-A

Charge = -1 Multiplicity = 1

Lowest Harmonic Vibrational Frequency (LHVF) = -272.05 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.253751	0.567208	0.029441
2	1	0	-0.689566	0.856216	-0.853764
3	1	0	-2.349061	1.080452	-0.015805
4	1	0	-0.768418	0.835980	0.964298
5	8	0	-3.676604	1.749414	-0.140499
6	1	0	-4.042300	1.808735	0.750128
7	8	0	4.202863	0.086409	-0.092876
8	1	0	4.577600	0.800489	0.446994
9	17	0	2.494318	0.338209	0.028463
10	7	0	-1.465022	-0.864341	0.004528
11	8	0	-1.657462	-1.456727	1.075678
12	8	0	-1.538047	-1.439632	-1.090312

Standard orientation of TS-NM-2/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:
Standard orientation of TS-NM-2/M06-2X

State=1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -174.38 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.242907	-0.782287	0.002903
2	1	0	0.817376	-1.220606	-0.895832
3	1	0	2.430898	-0.819016	-0.020510
4	1	0	0.854935	-1.213469	0.922362
5	8	0	3.955014	-0.778717	-0.134351
6	1	0	4.357893	-0.560420	0.710813
7	8	0	-3.525204	0.205045	-0.178255
8	1	0	-3.848795	0.385776	0.715648
9	17	0	-2.087024	-0.665045	0.055015
10	7	0	0.928764	0.641591	0.004716
11	8	0	0.882947	1.226191	1.076227
12	8	0	0.800781	1.214491	-1.065893

Standard orientation of TS-CNM^{-}/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-CNM^{-}/B3LYP

State=1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -105.46 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.017649	0.190600	-0.205573
2	8	0	-4.696772	-0.167844	-0.456410
3	1	0	-4.995286	0.662549	-0.053853
4	17	0	-2.948973	-0.028876	-0.415108
5	1	0	1.901507	0.004819	-0.910690
6	8	0	2.764097	-0.071859	-1.389108
7	17	0	3.953258	-0.054229	-0.133248
8	17	0	0.033715	1.794287	0.486773
9	7	0	0.031390	-0.899764	0.594747
10	8	0	-0.063967	-2.044277	0.037825
11	8	0	0.170707	-0.801741	1.847648
12	1	0	-0.270364	0.083038	-1.237990

Standard orientation of TS-CNM^{-}/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:

Standard orientation of TS-CNM^{-}/M06-2X

State=1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -223.02 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.426858	0.170671	-0.710615
2	8	0	-4.396111	0.024331	0.436830
3	1	0	-4.700431	-0.844267	0.147430
4	17	0	-2.639545	0.051399	-0.087140
5	1	0	2.068461	0.022024	1.293194
6	8	0	2.996427	0.306831	1.139266
7	17	0	3.270398	-0.199014	-0.455117
8	17	0	0.163174	1.716709	-0.180841
9	7	0	0.040303	-0.935941	-0.034928
10	8	0	-0.140701	-2.047167	-0.549470
11	8	0	0.526000	-0.829332	1.115958
12	1	0	-0.472376	0.037907	-1.780436

Standard orientation of TS-DCNM^{-}/B3LYP

Cartesian coordinates of all the transition states optimized at the b3lyp/6-311+G** level:

Standard orientation of TS-DCNM^{-}/B3LYP

State=1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -197.75 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.040918	0.354944	0.104277
2	8	0	-4.848753	-0.471443	-0.049751
3	1	0	-4.952602	-1.374542	0.289302
4	17	0	-3.130340	-0.207384	0.018075
5	17	0	-0.212919	1.898243	-0.676465
6	1	0	2.322589	0.458018	-0.134494
7	8	0	3.235332	0.719024	-0.353573
8	17	0	4.182997	-0.654813	0.099723
9	17	0	0.011973	0.339908	1.840822
10	7	0	0.029871	-0.784450	-0.608513
11	8	0	-0.011273	-0.734492	-1.883774
12	8	0	0.148111	-1.902238	-0.002588

Standard orientation of TS-DCNM^{-}/M06-2X

Cartesian coordinates of all the transition states optimized at the m062x/6-311+G** level:

Standard orientation of TS-DCNM^{-}/M06-2X

State=1-A
Charge = -1 Multiplicity = 1
Lowest Harmonic Vibrational Frequency (LHVF) = -145.25 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.415169	0.380090	0.178236
2	8	0	-4.325831	-0.837011	-0.029237
3	1	0	-4.292700	-1.686490	-0.484854
4	17	0	-2.561609	-0.320815	0.035678
5	1	0	2.171444	-1.626396	0.055503
6	8	0	3.089905	-1.411389	0.317007
7	17	0	3.263315	0.195879	-0.192903
8	17	0	0.224863	-0.174416	1.704903
9	7	0	0.129032	-0.293076	-0.951822
10	8	0	0.021116	0.221449	-2.055058
11	8	0	0.555749	-1.450417	-0.800590
12	17	0	-0.398244	2.117165	0.015012