Supporting Information

Direct Metal-Free Transformation of Alkynes to Nitriles: Computational Evidence for the Precise Reaction Mechanism

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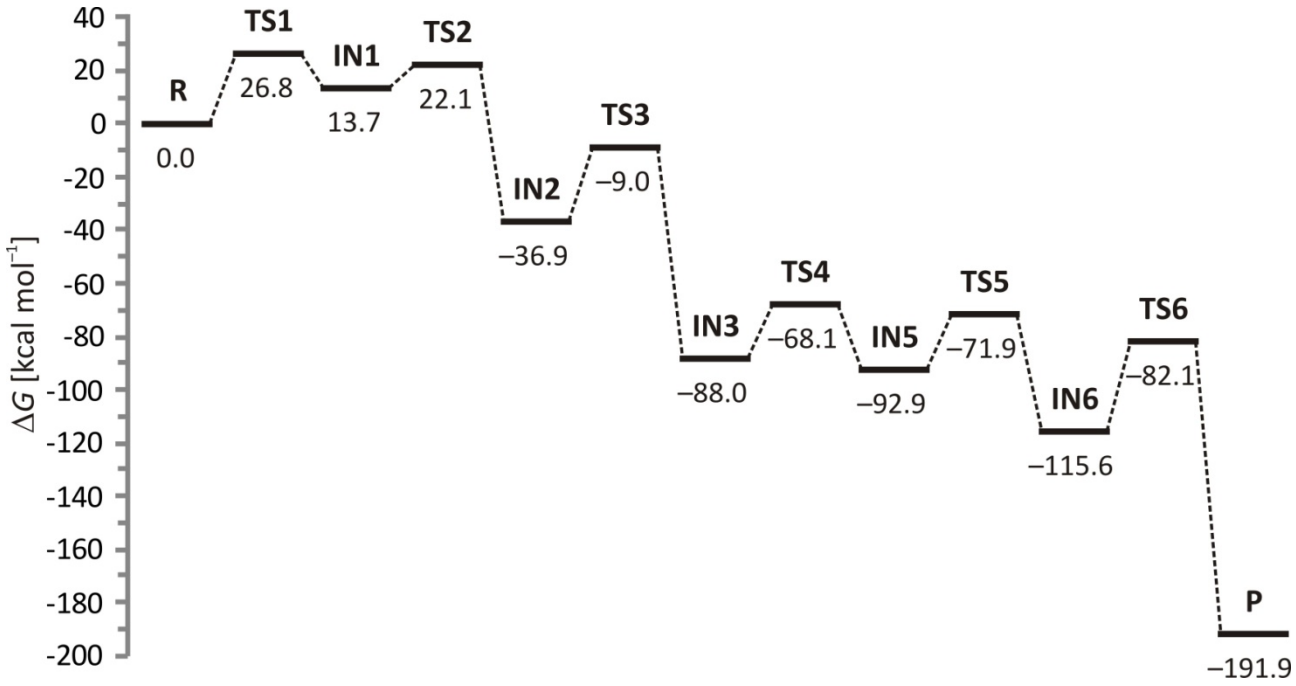

Figure S1. Graphical representation of the reaction profile for the conversion of diphenylacetylene **1** to benzonitrile with **NIS** as an oxidant and **$TMSN_3$** as a nitrogen source. Relative Gibbs free energies (in kcal mol^{-1}) correspond to the MeCN solution. **TS** and **IN** denote transition states and intermediates, while **R** and **P** stand for reactants and products. The matching chemical structures are given in Figure 2 in the main text.

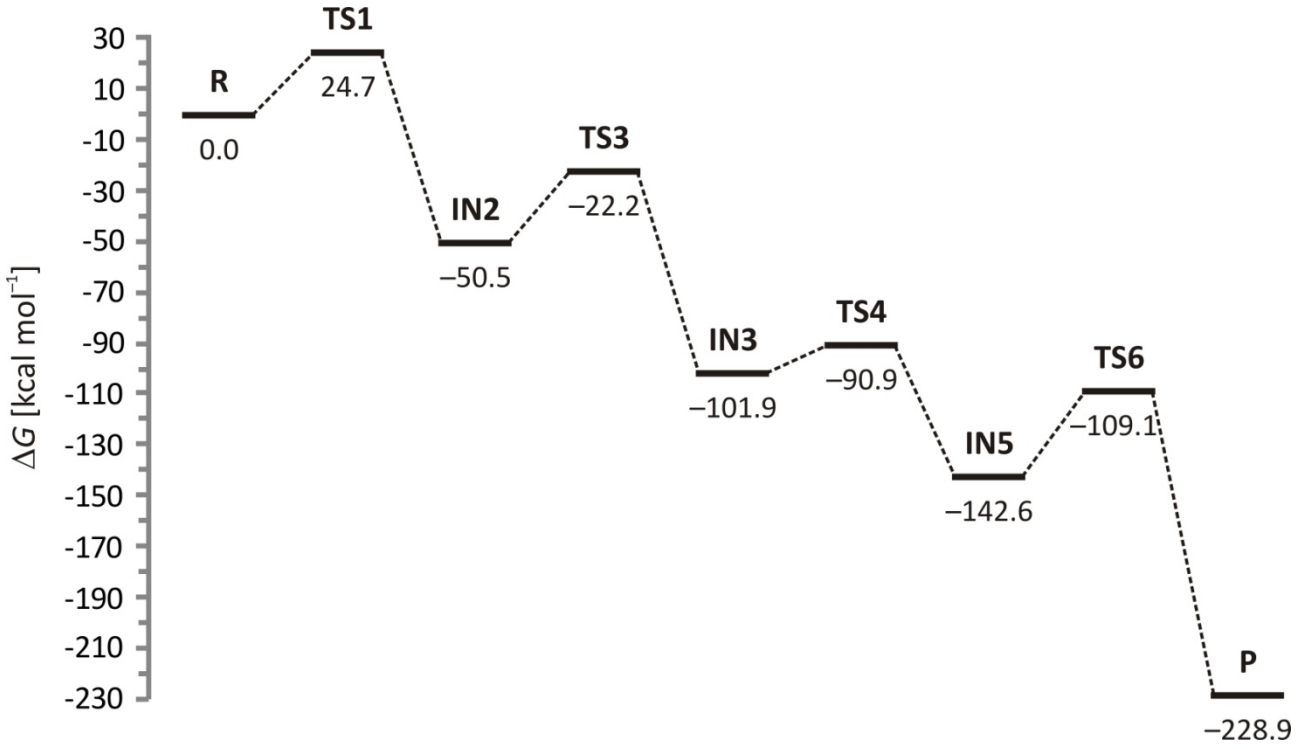

Figure S2. Graphical representation of the reaction profile for the conversion of **2** to *para*-Me-benzonitrile with **NIS** as an oxidant and **NaN_3** as a nitrogen source. Relative Gibbs free energies (in kcal mol^{-1}) correspond to the MeCN solution. **TS** and **IN** denote transition states and intermediates, while **R** and **P** stand for reactants and products. The matching chemical structures are given in Figure 4 in the main text.

System:	isolated **1**
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-539.239351949
Thermal correction to Gibbs Free Energy (in a.u.):	0.153991
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.606430	-0.000338	0.000520
2	6	0	-0.606432	-0.000107	0.000140
3	6	0	2.039148	-0.000144	0.000299
4	6	0	2.748731	-1.210928	-0.021133
5	6	0	2.748450	1.210823	0.021475
6	6	0	4.139608	-1.206723	-0.021429
7	1	0	2.198451	-2.146620	-0.037702
8	6	0	4.139336	1.206946	0.021108
9	1	0	2.197967	2.146387	0.038345
10	6	0	4.838720	0.000198	-0.000342
11	1	0	4.679921	-2.148594	-0.038310
12	1	0	4.679434	2.148947	0.037749
13	1	0	5.924642	0.000319	-0.000608
14	6	0	-2.039151	-0.000056	-0.000027
15	6	0	-2.748665	-1.210896	0.021215
16	6	0	-2.748519	1.210853	-0.021377
17	6	0	-4.139544	-1.206764	0.021176
18	1	0	-2.198349	-2.146561	0.037920
19	6	0	-4.139397	1.206904	-0.021377
20	1	0	-2.198083	2.146446	-0.038078
21	6	0	-4.838716	0.000111	-0.000086
22	1	0	-4.679808	-2.148665	0.037944
23	1	0	-4.679542	2.148872	-0.038158
24	1	0	-5.924636	0.000189	-0.000062

System:	isolated **2**
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-617.833944709
Thermal correction to Gibbs Free Energy (in a.u.):	0.203067
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.143010	-1.198778	0.009939
2	6	0	2.753706	-1.206254	0.005632
3	6	0	2.038489	0.001155	0.002987
4	6	0	2.752696	1.207928	0.005857
5	6	0	4.143094	1.201056	0.010239
6	6	0	4.861601	0.001771	0.009497
7	1	0	4.682678	-2.143318	0.015392
8	1	0	2.208240	-2.145211	0.007861
9	1	0	2.207238	2.146876	0.008253
10	1	0	4.681890	2.145874	0.016030
11	6	0	-2.038487	-0.001079	-0.002746
12	6	0	-2.753770	1.206297	-0.005773
13	6	0	-2.752629	-1.207885	-0.005391
14	6	0	-4.143069	1.198745	-0.010267
15	1	0	-2.208356	2.145283	-0.008174
16	6	0	-4.143032	-1.201088	-0.009964
17	1	0	-2.207124	-2.146806	-0.007477
18	6	0	-4.861602	-0.001845	-0.009640
19	1	0	-4.682783	2.143259	-0.016041
20	1	0	-4.681771	-2.145938	-0.015599
21	6	0	0.606493	0.000503	0.001380
22	6	0	-0.606492	-0.000370	-0.001045
23	6	0	-6.368831	0.001854	0.016464
24	1	0	-6.740439	0.124486	1.040517
25	1	0	-6.773865	0.824183	-0.581071
26	1	0	-6.774822	-0.935781	-0.373485
27	6	0	6.368826	-0.001964	-0.016928
28	1	0	6.774949	0.935124	0.374208
29	1	0	6.773952	-0.825118	0.579396
30	1	0	6.740185	-0.123198	-1.041242

System:	isolated **3**
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-723.671923818
Thermal correction to Gibbs Free Energy (in a.u.):	0.145910
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.133249	0.890725	-0.825666
2	6	0	2.745640	0.889519	-0.824301
3	6	0	2.040023	0.000011	0.000020
4	6	0	2.745653	-0.889521	0.824307
5	6	0	4.133260	-0.890724	0.825654
6	6	0	4.829112	0.000011	-0.000001
7	1	0	4.684255	1.576295	-1.461368
8	1	0	2.195904	1.575611	-1.460471
9	1	0	2.195924	-1.575626	1.460469
10	1	0	4.684279	-1.576299	1.461340
11	6	0	-2.040030	-0.000010	0.000009
12	6	0	-2.745652	-0.889523	-0.824303
13	6	0	-2.745643	0.889514	0.824313
14	6	0	-4.133259	-0.890738	-0.825639
15	1	0	-2.195914	-1.575629	-1.460457
16	6	0	-4.133252	0.890747	0.825648
17	1	0	-2.195902	1.575617	1.460467
18	6	0	-4.829111	0.000008	0.000007
19	1	0	-4.684283	-1.576312	-1.461322
20	1	0	-4.684267	1.576330	1.461329
21	6	0	0.605805	-0.000012	0.000009
22	6	0	-0.605795	-0.000018	0.000004
23	6	0	-6.269153	0.000018	0.000002
24	6	0	6.269153	0.000008	-0.000013
25	7	0	7.426680	-0.000004	-0.000010
26	7	0	-7.426679	-0.000008	-0.000031

System:	isolated **4**
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-422.747872085
Thermal correction to Gibbs Free Energy (in a.u.):	0.110335
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.698907	-1.003802	-0.000193
2	6	0	0.688224	-1.139729	-0.000159
3	6	0	1.523687	-0.019382	-0.000019
4	6	0	0.937645	1.258956	-0.000081
5	6	0	-0.438099	1.404343	-0.000124
6	6	0	-1.265539	0.273381	-0.000098
7	1	0	-1.318414	-1.893041	-0.000391
8	1	0	1.130537	-2.131227	-0.000196
9	1	0	1.577499	2.135923	-0.000099
10	1	0	-0.902837	2.385057	-0.000135
11	6	0	2.950700	-0.168460	0.000085
12	6	0	4.153068	-0.290713	0.000204
13	8	0	-2.600400	0.518332	0.000154
14	6	0	-3.475756	-0.590405	0.000176
15	1	0	-4.483768	-0.176761	0.000651
16	1	0	-3.332976	-1.206109	-0.895929
17	1	0	-3.332421	-1.206699	0.895828
18	1	0	5.215440	-0.398932	0.000289

System:	isolated **NIS**
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-7279.82166411
Thermal correction to Gibbs Free Energy (in a.u.):	0.047763
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	53	0	-1.497460	-0.000062	-0.000059
2	6	0	1.304219	1.175696	0.000652
3	6	0	1.304558	-1.175638	0.000755
4	6	0	2.770798	0.766613	-0.001622
5	6	0	2.771026	-0.766095	0.001107
6	1	0	3.244389	1.202009	-0.885147
7	1	0	3.248722	1.205724	0.877658
8	1	0	3.248067	-1.205124	-0.878696
9	1	0	3.245735	-1.201342	0.884106
10	7	0	0.545287	-0.000101	0.000945
11	8	0	0.853965	-2.291086	-0.001027
12	8	0	0.853264	2.290995	0.000184

System:	isolated **NCS**
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-820.080119376
Thermal correction to Gibbs Free Energy (in a.u.):	0.050594
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.883423	0.767488	-0.000156
2	6	0	1.883423	-0.767488	0.000157
3	6	0	0.421488	-1.185171	0.000048
4	6	0	0.421488	1.185171	-0.000052
5	1	0	2.361557	1.202049	0.881148
6	7	0	-0.327433	0.000000	-0.000001
7	8	0	-0.040100	2.293371	-0.000033
8	8	0	-0.040100	-2.293371	0.000034
9	1	0	2.361249	1.201634	-0.881837
10	1	0	2.361246	-1.201634	0.881839
11	1	0	2.361560	-1.202049	-0.881145
12	17	0	-2.010054	0.000000	0.000001

System:	isolated **NBS**
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-2934.06052282
Thermal correction to Gibbs Free Energy (in a.u.):	0.048897
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.367959	-0.767100	-0.000149
2	6	0	-2.367959	0.767100	0.000152
3	6	0	-0.904551	1.182489	0.000059
4	6	0	-0.904551	-1.182489	-0.000055
5	1	0	-2.845137	-1.202794	0.881159
6	7	0	-0.152535	0.000000	0.000001
7	8	0	-0.448818	-2.293855	-0.000061
8	8	0	-0.448818	2.293855	0.000061
9	1	0	-2.844858	-1.202399	-0.881808
10	1	0	-2.844858	1.202399	0.881811
11	1	0	-2.845137	1.202794	-0.881156
12	35	0	1.682827	0.000000	-0.000002

System:	isolated **$TMSN_3$**
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-573.324585061
Thermal correction to Gibbs Free Energy (in a.u.):	0.088855
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.658261	0.000001	0.024662
2	6	0	1.597093	1.542665	-0.462801
3	1	0	1.767887	1.563817	-1.544247
4	1	0	1.038960	2.445080	-0.192953
5	1	0	2.572408	1.583067	0.035385
6	6	0	1.596961	-1.542792	-0.462651
7	1	0	2.572258	-1.583257	0.035567
8	1	0	1.038731	-2.445135	-0.192762
9	1	0	1.767786	-1.564032	-1.544091
10	6	0	0.211632	0.000104	1.847144
11	1	0	-0.373006	0.886059	2.118969
12	1	0	-0.373082	-0.885782	2.119038
13	1	0	1.118787	0.000087	2.461858
14	7	0	-0.852581	0.000024	-0.917443
15	7	0	-1.958951	0.000015	-0.401400
16	7	0	-3.014253	-0.000006	0.008532

System:	isolated **NaN_3**
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-326.418631673
Thermal correction to Gibbs Free Energy (in a.u.):	-0.009621
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.066664	0.003279	0.000000
2	7	0	1.128754	0.000466	-0.000000
3	7	0	2.279816	-0.001877	0.000000
4	11	0	-2.126667	-0.001188	0.000000

System:	isolated **TMS–NS**
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-769.133940997
Thermal correction to Gibbs Free Energy (in a.u.):	0.156109
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.412342	0.033506	0.000000
2	6	0	2.020245	1.798602	-0.000028
3	1	0	1.677886	2.347919	-0.881129
4	1	0	1.677919	2.347934	0.881078
5	1	0	3.117243	1.788587	-0.000048
6	6	0	1.934082	-0.870490	-1.551987
7	1	0	3.027459	-0.919614	-1.612273
8	1	0	1.542828	-1.891962	-1.557022
9	1	0	1.573545	-0.353707	-2.448000
10	6	0	1.934069	-0.870446	1.552018
11	1	0	1.573528	-0.353635	2.448013
12	1	0	1.542807	-1.891914	1.557078
13	1	0	3.027445	-0.919578	1.612315
14	6	0	-1.119188	-1.152494	-0.000002
15	6	0	-1.268095	1.150236	-0.000000
16	6	0	-2.613827	-0.864558	-0.000002
17	6	0	-2.712528	0.659096	-0.000007
18	1	0	-3.056890	-1.336660	-0.880834
19	1	0	-3.056888	-1.336653	0.880834
20	1	0	-3.213827	1.069229	-0.880570
21	1	0	-3.213839	1.069236	0.880545
22	7	0	-0.408923	0.047633	-0.000004
23	8	0	-0.920695	2.307783	0.000008
24	8	0	-0.601568	-2.247954	0.000003

System:	isolated **Na–NS**
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-522.244053329
Thermal correction to Gibbs Free Energy (in a.u.):	0.049515
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.505234	0.726916	0.000003
2	6	0	1.204575	-0.709023	0.000002
3	6	0	0.703643	1.653926	0.000008
4	6	0	1.877352	0.675558	-0.000014
5	1	0	0.658582	2.301115	-0.880796
6	1	0	0.658596	2.301082	0.880837
7	1	0	2.519804	0.755929	-0.881026
8	1	0	2.519847	0.755935	0.880965
9	7	0	-0.171255	-0.576844	0.000005
10	8	0	1.812615	-1.760998	0.000006
11	8	0	-1.692141	1.124098	0.000000
12	11	0	-2.345804	-1.005930	-0.000005

System:	isolated **NS anion**
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-359.978917857
Thermal correction to Gibbs Free Energy (in a.u.):	0.049042
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.759869	-1.224558	-0.000173
2	6	0	-0.759869	-1.224558	0.000174
3	6	0	-1.108470	0.286181	-0.000040
4	6	0	1.108470	0.286181	0.000036
5	1	0	1.212266	-1.691073	0.881789
6	7	0	0.000000	1.066819	-0.000001
7	8	0	2.283508	0.659765	0.000031
8	8	0	-2.283508	0.659765	-0.000029
9	1	0	1.211769	-1.690651	-0.882620
10	1	0	-1.211769	-1.690648	0.882623
11	1	0	-1.212266	-1.691076	-0.881787

System:	isolated **1-product** (benzonitrile)
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-324.362339233
Thermal correction to Gibbs Free Energy (in a.u.):	0.069865
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.044333	-0.000166	-0.000081
2	6	0	0.603327	-0.000185	0.000099
3	6	0	-0.090306	1.215467	0.000120
4	6	0	-0.090445	-1.215597	0.000107
5	6	0	-1.481227	1.209585	-0.000042
6	1	0	0.463768	2.148744	0.000173
7	6	0	-1.481543	-1.209345	-0.000037
8	1	0	0.463151	-2.149142	0.000195
9	6	0	-2.175883	0.000105	-0.000045
10	1	0	-2.023749	2.149820	-0.000153
11	1	0	-2.024053	-2.149600	-0.000146
12	1	0	-3.261808	0.000263	-0.000188
13	7	0	3.201879	0.000105	-0.000086

System:	isolated **2-product** (*p*-tolunitrile)
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-363.660332725
Thermal correction to Gibbs Free Energy (in a.u.):	0.094678
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.552748	-0.000702	0.004487
2	6	0	1.112846	0.000319	0.000613
3	6	0	0.412532	-1.211431	-0.003159
4	6	0	0.414431	1.212042	-0.003103
5	6	0	-0.976596	-1.201314	-0.009570
6	1	0	0.960531	-2.148448	-0.004271
7	6	0	-0.975739	1.203682	-0.009564
8	1	0	0.963196	2.148604	-0.004135
9	6	0	-1.691215	0.002054	-0.010080
10	1	0	-1.518077	-2.144107	-0.015854
11	1	0	-1.515569	2.147205	-0.015926
12	7	0	3.710569	-0.001719	0.008162
13	6	0	-3.197803	-0.001222	0.013987
14	1	0	-3.566067	-0.116945	1.039804
15	1	0	-3.603609	0.933641	-0.381634
16	1	0	-3.601613	-0.828490	-0.576787

System:	isolated **3-product** (*p*-dicyanobenzene)
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-416.576126689
Thermal correction to Gibbs Free Energy (in a.u.):	0.065798
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.827218	-0.000017	0.000137
2	6	0	-1.386328	0.000012	0.000066
3	6	0	-0.694130	-1.216659	0.000031
4	6	0	-0.694141	1.216669	0.000036
5	6	0	0.694057	-1.216706	-0.000036
6	1	0	-1.246008	-2.150555	0.000055
7	6	0	0.694061	1.216721	-0.000031
8	1	0	-1.246000	2.150576	0.000064
9	6	0	1.386339	0.000016	-0.000066
10	1	0	1.245709	-2.150678	-0.000064
11	1	0	1.245691	2.150706	-0.000055
12	7	0	-3.984356	-0.000015	0.000193
13	6	0	2.827307	0.000001	-0.000137
14	7	0	3.984488	-0.000025	-0.000194

System:	isolated **4-product** (*p*-methoxybenzonitrile)
Oxidant:	
Nitrogen-donor:	
Stationary point:	
M06–2X/6–31+G(d) energy (in a.u.):	-438.845103072
Thermal correction to Gibbs Free Energy (in a.u.):	0.100022
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.962802	-0.180853	-0.000005
2	6	0	1.533503	-0.024822	-0.000069
3	6	0	0.963476	1.258796	-0.000202
4	6	0	0.705099	-1.148179	0.000008
5	6	0	-0.410818	1.406357	-0.000035
6	1	0	1.607975	2.131966	-0.000455
7	6	0	-0.680040	-1.006043	0.000132
8	1	0	1.146309	-2.139852	-0.000104
9	6	0	-1.240679	0.275291	0.000313
10	1	0	-0.874089	2.387412	-0.000234
11	1	0	-1.303556	-1.892073	-0.000157
12	7	0	4.114299	-0.305263	0.000057
13	8	0	-2.569604	0.523958	0.000371
14	6	0	-3.454976	-0.579847	-0.000310
15	1	0	-4.458670	-0.156635	-0.000645
16	1	0	-3.315303	-1.194713	-0.896946
17	1	0	-3.316125	-1.195125	0.896186

System:	**1**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	R
M06–2X/6–31+G(d) energy (in a.u.):	-8392.39413976
Thermal correction to Gibbs Free Energy (in a.u.):	0.326445
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.997025	0.016615	-0.040658
2	6	0	0.711167	1.196332	0.034633
3	6	0	1.297185	-1.383450	-0.111402
4	6	0	2.003312	-1.907258	-1.205284
5	6	0	0.871082	-2.240805	0.914972
6	6	0	2.279243	-3.269868	-1.263176
7	1	0	2.338764	-1.235394	-1.988800
8	6	0	1.156708	-3.600776	0.850681
9	1	0	0.316203	-1.832065	1.754337
10	6	0	1.861987	-4.118426	-0.236376
11	1	0	2.821089	-3.672759	-2.114075
12	1	0	0.824856	-4.257431	1.648948
13	1	0	2.081350	-5.180727	-0.286186
14	7	0	4.193377	0.417143	-0.755269
15	7	0	3.941429	1.548839	-0.365815
16	7	0	3.667754	2.606560	-0.069411
17	6	0	0.360676	2.583684	0.122596
18	6	0	0.603969	3.443709	-0.958232
19	6	0	-0.236355	3.085348	1.288702
20	6	0	0.255398	4.786576	-0.869422
21	1	0	1.069198	3.049125	-1.856258
22	6	0	-0.581434	4.430161	1.369294
23	1	0	-0.427489	2.412871	2.119690
24	6	0	-0.336236	5.282630	0.292622
25	1	0	0.447462	5.448437	-1.708259
26	1	0	-1.043329	4.813557	2.273918
27	1	0	-0.606853	6.332119	0.358565
28	53	0	-2.258933	-0.107108	-0.113620
29	14	0	5.312732	-0.649763	0.131804
30	6	0	6.690252	0.423028	0.823028
31	1	0	7.424521	-0.190228	1.357697
32	1	0	7.216338	0.959060	0.025816
33	1	0	6.304569	1.165429	1.531315
34	6	0	5.932985	-1.852150	-1.155861
35	1	0	5.093360	-2.390916	-1.607296
36	1	0	6.472998	-1.331395	-1.953103
37	1	0	6.606560	-2.591645	-0.708943
38	6	0	4.401363	-1.521261	1.516877
39	1	0	3.793583	-0.817083	2.096878
40	1	0	3.734290	-2.298028	1.128424
41	1	0	5.114448	-1.994859	2.202390
42	6	0	-4.810646	-1.304881	1.046672
43	6	0	-5.149256	-0.357548	-1.067201
44	6	0	-6.287316	-1.519273	0.739188
45	6	0	-6.508502	-0.900952	-0.644628
46	1	0	-6.492528	-2.592078	0.777697
47	1	0	-6.873537	-1.044086	1.529839
48	1	0	-6.837933	-1.620769	-1.398201
49	1	0	-7.222846	-0.073801	-0.645839
50	7	0	-4.246198	-0.633529	-0.038172
51	8	0	-4.879500	0.208863	-2.095285
52	8	0	-4.218011	-1.644568	2.039853

System:	**1**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS1
M06–2X/6–31+G(d) energy (in a.u.):	-8392.35128605
Thermal correction to Gibbs Free Energy (in a.u.):	0.334131
Number of imaginary frequencies:	1 (–355 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.225120	-0.367551	-0.294685
2	6	0	0.515125	0.680635	-0.063364
3	6	0	1.136286	-1.824383	-0.366765
4	6	0	1.797706	-2.560653	-1.358402
5	6	0	0.352613	-2.497631	0.581969
6	6	0	1.677967	-3.946468	-1.400940
7	1	0	2.399815	-2.042799	-2.099467
8	6	0	0.226561	-3.882304	0.527813
9	1	0	-0.164955	-1.930632	1.349067
10	6	0	0.892384	-4.610143	-0.458070
11	1	0	2.189482	-4.507425	-2.177512
12	1	0	-0.396805	-4.389034	1.257557
13	1	0	0.794525	-5.690826	-0.496097
14	7	0	3.013371	-0.038203	-0.581614
15	7	0	3.225823	0.912158	-1.350664
16	7	0	3.342729	1.771656	-2.066482
17	6	0	0.893892	2.080743	0.119893
18	6	0	0.289452	3.097515	-0.632905
19	6	0	1.873554	2.426775	1.064055
20	6	0	0.695670	4.419694	-0.479083
21	1	0	-0.495284	2.841685	-1.338823
22	6	0	2.264731	3.753494	1.226211
23	1	0	2.308762	1.646873	1.684615
24	6	0	1.685339	4.753541	0.446108
25	1	0	0.227139	5.195178	-1.077361
26	1	0	3.016522	4.007745	1.968556
27	1	0	1.991126	5.787880	0.569651
28	53	0	-1.908467	0.257660	0.002019
29	14	0	4.346780	-0.661433	0.505754
30	6	0	5.411231	0.835015	0.864517
31	1	0	6.202893	0.570281	1.574535
32	1	0	5.899081	1.213816	-0.040785
33	1	0	4.826488	1.652050	1.300589
34	6	0	5.278084	-1.964821	-0.453953
35	1	0	4.634297	-2.824305	-0.667158
36	1	0	5.655065	-1.570839	-1.404239
37	1	0	6.138940	-2.320535	0.123975
38	6	0	3.471342	-1.346923	2.000290
39	1	0	2.688092	-0.672270	2.362035
40	1	0	3.005600	-2.311975	1.776845
41	1	0	4.193577	-1.495984	2.811262
42	6	0	-4.667527	-1.143359	0.673072
43	6	0	-5.012142	0.818163	-0.481074
44	6	0	-6.187900	-1.040285	0.532962
45	6	0	-6.417117	0.264930	-0.230290
46	1	0	-6.547803	-1.928247	0.006263
47	1	0	-6.629392	-1.050501	1.533119
48	1	0	-6.914163	0.131285	-1.194785
49	1	0	-6.986430	1.010068	0.331835
50	7	0	-4.087618	-0.046441	0.070662
51	8	0	-4.755573	1.847315	-1.068964
52	8	0	-4.071565	-2.045754	1.225377

System:	**1**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN1
M06–2X/6–31+G(d) energy (in a.u.):	-8392.35918413
Thermal correction to Gibbs Free Energy (in a.u.):	0.336647
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.330752	-0.369352	-0.276432
2	6	0	0.507700	0.662466	-0.052261
3	6	0	1.058719	-1.821306	-0.370874
4	6	0	1.661294	-2.595546	-1.371257
5	6	0	0.199712	-2.443914	0.544912
6	6	0	1.403638	-3.961110	-1.464177
7	1	0	2.320708	-2.124133	-2.097258
8	6	0	-0.064735	-3.806192	0.444782
9	1	0	-0.273638	-1.857622	1.325265
10	6	0	0.537754	-4.568936	-0.555958
11	1	0	1.866554	-4.545203	-2.254168
12	1	0	-0.753550	-4.265258	1.146635
13	1	0	0.326137	-5.631012	-0.633297
14	7	0	2.806498	-0.116470	-0.490679
15	7	0	3.102033	0.790991	-1.315894
16	7	0	3.369861	1.599640	-2.040018
17	6	0	1.003284	2.045416	0.092587
18	6	0	0.521849	3.064624	-0.742843
19	6	0	1.947462	2.375478	1.077628
20	6	0	1.009829	4.363280	-0.625726
21	1	0	-0.242807	2.829122	-1.477880
22	6	0	2.421436	3.679691	1.204638
23	1	0	2.284334	1.604943	1.768462
24	6	0	1.963177	4.676360	0.343835
25	1	0	0.630109	5.138084	-1.284787
26	1	0	3.137584	3.920793	1.985684
27	1	0	2.330424	5.693272	0.441358
28	53	0	-1.735604	0.395257	0.021464
29	14	0	4.176382	-0.830136	0.571620
30	6	0	5.314782	0.634135	0.796521
31	1	0	6.098595	0.377508	1.518405
32	1	0	5.818223	0.914409	-0.135716
33	1	0	4.782295	1.512104	1.177697
34	6	0	4.979042	-2.192368	-0.413833
35	1	0	4.321076	-3.062005	-0.499745
36	1	0	5.243451	-1.856527	-1.422978
37	1	0	5.905309	-2.507810	0.080810
38	6	0	3.295239	-1.393366	2.106891
39	1	0	2.566640	-0.655572	2.458102
40	1	0	2.763535	-2.333291	1.930327
41	1	0	4.028102	-1.555810	2.905767
42	6	0	-4.606633	-1.073746	0.632635
43	6	0	-5.032117	0.906247	-0.400640
44	6	0	-6.137008	-1.035175	0.518898
45	6	0	-6.423341	0.297457	-0.170506
46	1	0	-6.467327	-1.908793	-0.050317
47	1	0	-6.564801	-1.117274	1.522108
48	1	0	-6.926189	0.198818	-1.136612
49	1	0	-7.011877	0.992029	0.435552
50	7	0	-4.068690	0.064018	0.093440
51	8	0	-4.832792	1.978419	-0.944558
52	8	0	-3.977726	-1.993368	1.133989

System:	**1**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS2
M06–2X/6–31+G(d) energy (in a.u.):	-8392.38637197
Thermal correction to Gibbs Free Energy (in a.u.):	0.346592
Number of imaginary frequencies:	1 (–33 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.432760	0.375575	-0.630881
2	6	0	1.610516	0.001871	-0.106303
3	6	0	-0.144339	1.730332	-0.780312
4	6	0	-0.492811	2.185413	-2.056280
5	6	0	-0.363899	2.547791	0.332774
6	6	0	-1.048612	3.449845	-2.224037
7	1	0	-0.330901	1.544026	-2.920473
8	6	0	-0.931554	3.807864	0.162027
9	1	0	-0.099452	2.178380	1.318596
10	6	0	-1.273816	4.260731	-1.112161
11	1	0	-1.312156	3.798069	-3.218012
12	1	0	-1.109826	4.437448	1.028530
13	1	0	-1.717042	5.243914	-1.238950
14	7	0	-0.437388	-0.650842	-1.209070
15	7	0	0.162701	-1.459777	-1.972603
16	7	0	0.659633	-2.203638	-2.641907
17	6	0	2.034501	-1.405344	0.086862
18	6	0	3.268321	-1.859865	-0.395379
19	6	0	1.167804	-2.308827	0.719444
20	6	0	3.622053	-3.200339	-0.268417
21	1	0	3.949689	-1.160178	-0.872223
22	6	0	1.529953	-3.647521	0.847073
23	1	0	0.227869	-1.941135	1.120589
24	6	0	2.752879	-4.098207	0.350860
25	1	0	4.578536	-3.542393	-0.651686
26	1	0	0.854401	-4.337784	1.343755
27	1	0	3.031129	-5.142823	0.452572
28	53	0	2.985214	1.475591	0.520917
29	14	0	-2.383470	-0.984226	-1.134745
30	6	0	-2.581667	-2.746062	-0.495345
31	1	0	-3.459700	-3.186773	-0.981331
32	1	0	-1.709663	-3.328149	-0.828659
33	1	0	-2.685316	-2.846242	0.583136
34	6	0	-2.435834	-1.439552	-3.017995
35	1	0	-1.971751	-0.686468	-3.669942
36	1	0	-2.035224	-2.424263	-3.287938
37	1	0	-3.500558	-1.461615	-3.289966
38	6	0	-3.315441	0.643282	-1.288445
39	1	0	-4.383571	0.402761	-1.285277
40	1	0	-3.116146	1.350455	-0.481407
41	1	0	-3.068661	1.106209	-2.248434
42	6	0	-3.559336	-0.562691	1.537883
43	6	0	-1.468778	-0.081358	2.180920
44	6	0	-3.723301	-0.200130	3.011526
45	6	0	-2.308900	0.162855	3.438705
46	1	0	-4.444747	0.617266	3.095455
47	1	0	-4.141404	-1.060894	3.541103
48	1	0	-2.191141	1.211171	3.730247

49	1	0	-1.910763	-0.447887	4.253190
50	7	0	-2.253805	-0.439891	1.115421
51	8	0	-0.249032	0.038655	2.176411
52	8	0	-4.481262	-0.934301	0.821956

System:	**1**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN2
M06–2X/6–31+G(d) energy (in a.u.):	-7623.31808876
Thermal correction to Gibbs Free Energy (in a.u.):	0.164029
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.468578	0.997297	0.047850
2	6	0	-0.396310	-0.040975	0.031556
3	6	0	1.949783	0.914451	0.132629
4	6	0	2.733728	1.606816	-0.794656
5	6	0	2.572983	0.195340	1.156449
6	6	0	4.122866	1.550894	-0.722363
7	1	0	2.248297	2.187259	-1.574205
8	6	0	3.961902	0.150400	1.236525
9	1	0	1.966765	-0.321955	1.894761
10	6	0	4.739308	0.821115	0.293270
11	1	0	4.723109	2.081857	-1.455097
12	1	0	4.437691	-0.405060	2.039100
13	1	0	5.822903	0.782074	0.354854
14	7	0	0.049451	2.360559	0.007615
15	7	0	-1.003774	2.635286	-0.589668
16	6	0	-1.864671	0.087317	0.180769
17	6	0	-2.753517	-0.431439	-0.768980
18	6	0	-2.378386	0.749976	1.303095
19	6	0	-4.125990	-0.270257	-0.609691
20	1	0	-2.363076	-0.957957	-1.636126
21	6	0	-3.753372	0.905709	1.462919
22	1	0	-1.690344	1.142975	2.047612
23	6	0	-4.630334	0.398142	0.506183
24	1	0	-4.804755	-0.668593	-1.357768
25	1	0	-4.138095	1.419751	2.338769
26	1	0	-5.702286	0.518848	0.630697
27	53	0	0.297538	-2.032941	-0.229865
28	7	0	-1.924129	3.026720	-1.108391

System:	**1**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS3
M06–2X/6–31+G(d) energy (in a.u.):	-7623.27067785
Thermal correction to Gibbs Free Energy (in a.u.):	0.160160
Number of imaginary frequencies:	1 (–572 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.550190	-0.799826	0.214186
2	6	0	-0.620023	-0.066506	0.059966
3	6	0	1.902292	-0.254226	-0.084185
4	6	0	2.994010	-0.610353	0.714715
5	6	0	2.102744	0.560672	-1.203280
6	6	0	4.270313	-0.147458	0.403796
7	1	0	2.828440	-1.233404	1.590207
8	6	0	3.378587	1.019826	-1.513997
9	1	0	1.253010	0.827354	-1.826744
10	6	0	4.464463	0.667772	-0.710360
11	1	0	5.112769	-0.420714	1.032199
12	1	0	3.528562	1.649767	-2.385810
13	1	0	5.459852	1.026828	-0.954699
14	6	0	-0.672453	1.395839	0.225861
15	6	0	-1.527951	2.191797	-0.553214
16	6	0	0.169174	2.026322	1.156814
17	6	0	-1.508047	3.576731	-0.433289
18	1	0	-2.202429	1.720625	-1.262023
19	6	0	0.177518	3.411911	1.281954
20	1	0	0.811152	1.421152	1.790109
21	6	0	-0.656103	4.193475	0.483518
22	1	0	-2.165585	4.177620	-1.054426
23	1	0	0.832515	3.879427	2.011138
24	1	0	-0.650995	5.274802	0.582676
25	7	0	0.354191	-1.965747	0.826426
26	7	0	1.437020	-3.141259	0.179188
27	53	0	-2.469803	-1.070219	-0.176477
28	7	0	1.915070	-4.121235	0.362348

System:	**1**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN3
M06–2X/6–31+G(d) energy (in a.u.):	-7513.88727644
Thermal correction to Gibbs Free Energy (in a.u.):	0.156399
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.937844	0.146406	0.768542
2	6	0	0.459856	-0.089291	0.545980
3	7	0	-0.269841	0.002941	1.835322
4	6	0	-2.267585	0.382929	0.250476
5	6	0	-2.461371	0.417072	-1.133560
6	6	0	-3.340307	0.576723	1.129390
7	6	0	-3.736438	0.646703	-1.641573
8	1	0	-1.612726	0.259323	-1.794199
9	6	0	-4.609788	0.809579	0.614655
10	1	0	-3.165037	0.544123	2.201049
11	6	0	-4.806095	0.843761	-0.768438
12	1	0	-3.897000	0.672106	-2.714659
13	1	0	-5.447704	0.963887	1.287342
14	1	0	-5.800205	1.023738	-1.167034
15	6	0	1.437143	0.987776	0.182813
16	6	0	2.095218	1.014195	-1.049346
17	6	0	1.656973	2.020697	1.098450
18	6	0	2.954961	2.063472	-1.363145
19	1	0	1.943409	0.207040	-1.760111
20	6	0	2.525190	3.064706	0.785489
21	1	0	1.146867	1.999335	2.057321
22	6	0	3.174252	3.091635	-0.446781
23	1	0	3.459538	2.073436	-2.324846
24	1	0	2.694190	3.856421	1.509393
25	1	0	3.849944	3.905740	-0.691486
26	53	0	1.053823	-2.101583	-0.062033

System:	**1**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS4
M06–2X/6–31+G(d) energy (in a.u.):	-8087.18465593
Thermal correction to Gibbs Free Energy (in a.u.):	0.269473
Number of imaginary frequencies:	1 (–227 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.547799	1.148998	1.150299
2	6	0	0.830894	1.269837	1.190292
3	7	0	0.154082	1.232152	2.317501
4	6	0	-1.817304	1.627521	0.659451
5	6	0	-2.012270	1.818206	-0.714023
6	6	0	-2.841911	1.876349	1.585931
7	6	0	-3.244641	2.294882	-1.155531
8	1	0	-1.225733	1.545368	-1.414965
9	6	0	-4.063192	2.350978	1.130547
10	1	0	-2.664572	1.700058	2.643375
11	6	0	-4.259888	2.561559	-0.239250
12	1	0	-3.412676	2.436662	-2.217874
13	1	0	-4.863962	2.554440	1.834023
14	1	0	-5.220161	2.926493	-0.591598
15	6	0	2.175726	1.452470	0.738528
16	6	0	2.469027	1.527232	-0.629658
17	6	0	3.185243	1.560634	1.712515
18	6	0	3.792877	1.705494	-1.020458
19	1	0	1.678919	1.391658	-1.362955
20	6	0	4.497335	1.741388	1.307851
21	1	0	2.924890	1.498513	2.765891
22	6	0	4.796666	1.810746	-0.059143
23	1	0	4.036594	1.745159	-2.076774
24	1	0	5.289459	1.824041	2.044694
25	1	0	5.828001	1.944090	-0.372791
26	53	0	0.225786	-0.812572	-2.328976
27	7	0	-1.055085	-0.971001	1.080484
28	7	0	-2.049511	-1.142120	0.369940
29	7	0	-2.974520	-1.193143	-0.269413
30	14	0	0.014563	-2.399974	1.447768
31	6	0	-0.331262	-2.783627	3.251059
32	1	0	-1.374515	-3.078960	3.405578
33	1	0	0.307407	-3.601060	3.605547
34	1	0	-0.132680	-1.905403	3.875923
35	6	0	1.792145	-1.876758	1.233019
36	1	0	2.424547	-2.769273	1.318281
37	1	0	1.954446	-1.440054	0.241546
38	1	0	2.116094	-1.174777	2.009304
39	6	0	-0.510135	-3.784074	0.313312
40	1	0	-0.381712	-3.483972	-0.732740
41	1	0	0.107451	-4.670282	0.500217
42	1	0	-1.556177	-4.068968	0.474294

System:	**1**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN4
M06–2X/6–31+G(d) energy (in a.u.):	-1167.06440988
Thermal correction to Gibbs Free Energy (in a.u.):	0.272801
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.186504	0.167090	-0.241858
2	6	0	-1.165307	-0.210105	-0.589958
3	7	0	-0.319521	-0.385671	-1.517018
4	6	0	0.709098	1.564678	-0.154214
5	6	0	1.819821	1.903157	0.623451
6	6	0	0.049111	2.561930	-0.881685
7	6	0	2.266372	3.222790	0.672628
8	1	0	2.359882	1.147752	1.189688
9	6	0	0.500224	3.876836	-0.831823
10	1	0	-0.812608	2.310736	-1.494170
11	6	0	1.608614	4.211522	-0.054169
12	1	0	3.130974	3.474203	1.278710
13	1	0	-0.016267	4.641688	-1.402917
14	1	0	1.957419	5.238384	-0.015711
15	6	0	-2.563529	-0.287033	-0.244953
16	6	0	-2.997778	0.217018	0.987793
17	6	0	-3.469140	-0.856519	-1.152102
18	6	0	-4.347055	0.150170	1.315152
19	1	0	-2.282380	0.672373	1.668781
20	6	0	-4.814181	-0.921865	-0.814101
21	1	0	-3.111353	-1.236877	-2.104735
22	6	0	-5.249526	-0.420627	0.416071
23	1	0	-4.696939	0.542651	2.264147
24	1	0	-5.526305	-1.360486	-1.505289
25	1	0	-6.302807	-0.473122	0.673980
26	7	0	1.013761	-0.842361	0.494904
27	7	0	0.813182	-0.906074	1.739530
28	7	0	0.647008	-0.966733	2.842105
29	14	0	2.353993	-1.897768	-0.361156
30	6	0	1.421821	-3.294424	-1.151735
31	1	0	2.127755	-3.997402	-1.609384
32	1	0	0.826577	-3.851836	-0.421199
33	1	0	0.757371	-2.923270	-1.937605
34	6	0	3.403293	-2.387293	1.097896
35	1	0	4.272722	-2.950418	0.739203
36	1	0	3.789843	-1.518533	1.642630
37	1	0	2.874897	-3.041125	1.800617
38	6	0	3.108903	-0.679259	-1.537093
39	1	0	3.620075	0.136481	-1.017586
40	1	0	3.842943	-1.194377	-2.167768
41	1	0	2.347822	-0.250598	-2.197663

System:	**1**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS5
M06–2X/6–31+G(d) energy (in a.u.):	-1527.20016280
Thermal correction to Gibbs Free Energy (in a.u.):	0.349979
Number of imaginary frequencies:	1 (–58 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.114524	-0.582066	0.289432
2	6	0	-1.249248	0.800173	0.705077
3	7	0	-1.046566	-0.008734	1.655116
4	6	0	-2.272352	-1.448802	-0.096239
5	6	0	-2.109301	-2.626771	-0.830261
6	6	0	-3.560467	-1.060085	0.290298
7	6	0	-3.215570	-3.403286	-1.171213
8	1	0	-1.117324	-2.957717	-1.125357
9	6	0	-4.662213	-1.838638	-0.048752
10	1	0	-3.701187	-0.146746	0.862355
11	6	0	-4.494229	-3.012780	-0.782493
12	1	0	-3.072634	-4.318328	-1.737997
13	1	0	-5.654967	-1.525895	0.260472
14	1	0	-5.354942	-3.618994	-1.047711
15	6	0	-1.641164	2.168714	0.436086
16	6	0	-1.763394	2.620941	-0.879483
17	6	0	-1.925763	3.013009	1.514784
18	6	0	-2.178574	3.925998	-1.116716
19	1	0	-1.504320	1.956219	-1.697921
20	6	0	-2.337119	4.318351	1.270261
21	1	0	-1.822869	2.637996	2.529451
22	6	0	-2.464383	4.771851	-0.043955
23	1	0	-2.269720	4.288711	-2.135579
24	1	0	-2.558591	4.982096	2.100198
25	1	0	-2.785323	5.792118	-0.232906
26	7	0	0.195131	-1.052093	-0.207219
27	7	0	0.411995	-0.810225	-1.424414
28	7	0	0.606946	-0.666259	-2.512294
29	14	0	1.588666	-1.791708	0.886798
30	6	0	2.595812	-2.869753	-0.261276
31	1	0	2.891871	-2.358958	-1.179550
32	1	0	3.529432	-3.140263	0.243576
33	1	0	2.041854	-3.786598	-0.493718
34	6	0	0.413465	-2.983955	1.778759
35	1	0	1.017676	-3.610556	2.449003
36	1	0	-0.321675	-2.460181	2.399584
37	1	0	-0.123909	-3.655115	1.099838
38	6	0	2.246045	-0.698494	2.255419
39	1	0	1.785593	0.292247	2.194345
40	1	0	2.000713	-1.135445	3.229234
41	1	0	3.329275	-0.584135	2.160300
42	7	0	2.717117	0.109223	-0.371355
43	6	0	4.089533	0.146499	-0.296234
44	6	0	4.627341	1.549867	-0.606568
45	6	0	3.361921	2.385107	-0.769284
46	6	0	2.239187	1.357375	-0.603509
47	8	0	1.040440	1.656120	-0.680799
48	1	0	3.243186	3.161385	-0.007256

49	1	0	5.277114	1.871103	0.211836
50	8	0	4.800172	-0.802374	0.002658
51	1	0	3.261110	2.868820	-1.745033
52	1	0	5.241025	1.499277	-1.510838

System:	**1**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN5
M06–2X/6–31+G(d) energy (in a.u.):	-758.109104162
Thermal correction to Gibbs Free Energy (in a.u.):	0.169376
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.722235	0.864736	-0.275842
2	6	0	0.606900	0.374467	-0.566237
3	7	0	0.021419	0.861043	-1.578665
4	6	0	-1.900337	-0.041094	-0.119353
5	6	0	-2.993727	0.316651	0.673310
6	6	0	-1.907566	-1.275644	-0.778001
7	6	0	-4.076253	-0.551332	0.806162
8	1	0	-2.994710	1.275245	1.180258
9	6	0	-2.991632	-2.138069	-0.645209
10	1	0	-1.066752	-1.559725	-1.404845
11	6	0	-4.080197	-1.779707	0.149249
12	1	0	-4.921170	-0.261571	1.424097
13	1	0	-2.985688	-3.091554	-1.165122
14	1	0	-4.925641	-2.453263	0.253461
15	6	0	1.850093	-0.258694	-0.163492
16	6	0	2.000781	-0.708938	1.151238
17	6	0	2.882658	-0.416626	-1.096079
18	6	0	3.190434	-1.321385	1.534985
19	1	0	1.184057	-0.577868	1.856271
20	6	0	4.068043	-1.027573	-0.705565
21	1	0	2.742700	-0.056441	-2.111606
22	6	0	4.220627	-1.478786	0.608083
23	1	0	3.314882	-1.674692	2.553746
24	1	0	4.875102	-1.152950	-1.420715
25	1	0	5.148764	-1.955526	0.909352
26	7	0	-0.938884	2.147146	0.384797
27	7	0	-0.026413	2.963177	0.242978
28	7	0	0.764295	3.765823	0.163120

System:	**1**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS6
M06–2X/6–31+G(d) energy (in a.u.):	-758.048676779
Thermal correction to Gibbs Free Energy (in a.u.):	0.163760
Number of imaginary frequencies:	1 (–619 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.582102	0.122194	1.140537
2	6	0	-0.711497	0.829772	0.878712
3	7	0	-0.010662	0.229844	2.216307
4	6	0	1.728998	-0.362707	0.393641
5	6	0	1.672900	-0.363249	-1.002925
6	6	0	2.867466	-0.818352	1.067826
7	6	0	2.763877	-0.828633	-1.730605
8	1	0	0.772097	-0.011910	-1.501038
9	6	0	3.953653	-1.277814	0.332301
10	1	0	2.889118	-0.805438	2.153744
11	6	0	3.901363	-1.282560	-1.063334
12	1	0	2.727621	-0.837108	-2.815408
13	1	0	4.842642	-1.632422	0.844821
14	1	0	4.753635	-1.641469	-1.632889
15	6	0	-1.837054	-0.002360	0.335283
16	6	0	-2.763860	0.589482	-0.529523
17	6	0	-1.974376	-1.358563	0.652930
18	6	0	-3.804846	-0.162063	-1.068599
19	1	0	-2.662703	1.645613	-0.760233
20	6	0	-3.019887	-2.106199	0.115463
21	1	0	-1.271875	-1.830108	1.334113
22	6	0	-3.937459	-1.512839	-0.749535
23	1	0	-4.518795	0.311369	-1.736941
24	1	0	-3.116238	-3.156656	0.375229
25	1	0	-4.751222	-2.097142	-1.169193
26	7	0	-0.714841	2.179594	0.800351
27	7	0	0.397882	2.728314	-0.399888
28	7	0	0.871542	3.613479	-0.863234

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	R
M06–2X/6–31+G(d) energy (in a.u.):	-8470.98861381
Thermal correction to Gibbs Free Energy (in a.u.):	0.378218
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.267728	1.654868	-1.085051
2	6	0	-0.937843	0.656620	-1.269265
3	6	0	0.484005	2.856844	-0.874193
4	6	0	0.511604	3.852867	-1.862041
5	6	0	1.193955	3.064166	0.318476
6	6	0	1.232718	5.022784	-1.656543
7	1	0	-0.039034	3.700190	-2.785054
8	6	0	1.911680	4.239023	0.509060
9	1	0	1.178852	2.299956	1.090251
10	6	0	1.946718	5.235151	-0.472339
11	1	0	1.242084	5.786817	-2.430121
12	1	0	2.456694	4.385633	1.438427
13	7	0	-3.853152	1.028531	0.598618
14	7	0	-4.574441	0.204981	0.059191
15	7	0	-5.245306	-0.514886	-0.501157
16	6	0	-1.746045	-0.504305	-1.495984
17	6	0	-2.463475	-0.640519	-2.693372
18	6	0	-1.834564	-1.520944	-0.531931
19	6	0	-3.252025	-1.764007	-2.913207
20	1	0	-2.396599	0.141220	-3.443759
21	6	0	-2.630666	-2.635729	-0.764198
22	1	0	-1.265364	-1.439183	0.390284
23	6	0	-3.356652	-2.773741	-1.952476
24	1	0	-3.808685	-1.851889	-3.842956
25	1	0	-2.691029	-3.414391	-0.007153
26	53	0	1.853609	-0.690639	-0.327581
27	14	0	-3.263797	0.860199	2.266564
28	6	0	-3.593018	-0.896706	2.839334
29	1	0	-3.225668	-1.041404	3.861644
30	1	0	-4.665455	-1.123231	2.836838
31	1	0	-3.093495	-1.630051	2.197191
32	6	0	-4.205459	2.094713	3.316587
33	1	0	-4.062616	3.111760	2.936548
34	1	0	-5.279628	1.881500	3.311816
35	1	0	-3.859069	2.069339	4.356235
36	6	0	-1.446136	1.292873	2.236146
37	1	0	-0.851573	0.536423	1.712927
38	1	0	-1.303641	2.245933	1.713902
39	1	0	-1.053444	1.395128	3.254570
40	6	0	2.933475	-2.969528	1.375686
41	6	0	4.583998	-2.029618	0.007457
42	6	0	4.201737	-3.759689	1.671849
43	6	0	5.281882	-3.144876	0.776182
44	1	0	4.417293	-3.673933	2.739901
45	1	0	4.005107	-4.813770	1.460102
46	1	0	6.115229	-2.707890	1.332110
47	1	0	5.702450	-3.847459	0.052314
48	7	0	3.248910	-2.007445	0.416608
49	8	0	5.072700	-1.290191	-0.807948
50	8	0	1.844721	-3.128440	1.869317
51	6	0	-4.272402	-3.949523	-2.164680
52	1	0	-5.274693	-3.717700	-1.784800
53	1	0	-4.367634	-4.195118	-3.226216
54	1	0	-3.912424	-4.837009	-1.636404
55	6	0	2.756450	6.490201	-0.271690
56	1	0	3.782351	6.350617	-0.631768

57	1	0	2.325377	7.332740	-0.819860
58	1	0	2.811789	6.762062	0.786294

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS1
M06–2X/6–31+G(d) energy (in a.u.):	-8470.94572985
Thermal correction to Gibbs Free Energy (in a.u.):	0.385349
Number of imaginary frequencies:	1 (–354 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.104602	0.462675	-0.285578
2	6	0	-0.475047	-0.643667	-0.090200
3	6	0	-0.913047	1.909529	-0.299209
4	6	0	-1.506483	2.733172	-1.261946
5	6	0	-0.095833	2.493665	0.681352
6	6	0	-1.285954	4.107450	-1.246261
7	1	0	-2.139038	2.294892	-2.028899
8	6	0	0.127050	3.864071	0.680081
9	1	0	0.372559	1.865644	1.432525
10	6	0	-0.464146	4.694698	-0.279898
11	1	0	-1.750577	4.732142	-2.005314
12	1	0	0.777302	4.295446	1.437017
13	7	0	-2.910867	0.270794	-0.593638
14	7	0	-3.184072	-0.629914	-1.401776
15	7	0	-3.354088	-1.451035	-2.151362
16	6	0	-0.958125	-2.016801	0.046627
17	6	0	-0.420365	-3.056559	-0.726628
18	6	0	-1.973913	-2.323705	0.962071
19	6	0	-0.924154	-4.346448	-0.616506
20	1	0	0.391128	-2.842699	-1.416247
21	6	0	-2.460466	-3.624417	1.076335
22	1	0	-2.366933	-1.536861	1.601990
23	6	0	-1.952032	-4.655367	0.283257
24	1	0	-0.502144	-5.135981	-1.234207
25	1	0	-3.242432	-3.842612	1.800780
26	53	0	1.958213	-0.396974	-0.009505
27	14	0	-4.205295	0.954042	0.502771
28	6	0	-5.380393	-0.471048	0.803662
29	1	0	-6.159021	-0.171852	1.514412
30	1	0	-5.883721	-0.784374	-0.118096
31	1	0	-4.861564	-1.342000	1.218212
32	6	0	-5.030787	2.352343	-0.420170
33	1	0	-4.324677	3.169489	-0.600061
34	1	0	-5.425536	2.017484	-1.385836
35	1	0	-5.869748	2.750253	0.162487
36	6	0	-3.298929	1.524828	2.026647
37	1	0	-2.570497	0.783330	2.371836
38	1	0	-2.761812	2.459845	1.838550
39	1	0	-4.017106	1.699318	2.836172
40	6	0	4.822350	0.783054	0.691890
41	6	0	5.022026	-1.180875	-0.487908
42	6	0	6.331730	0.566049	0.558284
43	6	0	6.464606	-0.741043	-0.223918
44	1	0	6.762315	1.431671	0.047646
45	1	0	6.766105	0.527033	1.560880
46	1	0	6.974654	-0.631096	-1.184659
47	1	0	6.972997	-1.535892	0.328445
48	7	0	4.163222	-0.256110	0.070666
49	8	0	4.691727	-2.180177	-1.091205
50	8	0	4.295357	1.721240	1.255575
51	6	0	-2.463955	-6.067782	0.406961
52	1	0	-2.736824	-6.475799	-0.571630
53	1	0	-1.698412	-6.724928	0.833992
54	1	0	-3.345131	-6.115840	1.052739
55	6	0	-0.195316	6.177055	-0.276767
56	1	0	0.842182	6.380197	-0.563772

57	1	0	-0.848330	6.702417	-0.978720
58	1	0	-0.348191	6.603916	0.719460

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN1
M06–2X/6–31+G(d) energy (in a.u.):	-8470.95343535
Thermal correction to Gibbs Free Energy (in a.u.):	0.386187
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.190978	0.536212	-0.267568
2	6	0	-0.514127	-0.604662	-0.082705
3	6	0	-0.730217	1.941203	-0.302994
4	6	0	-1.214463	2.831349	-1.267484
5	6	0	0.197171	2.413089	0.637839
6	6	0	-0.773668	4.152794	-1.303270
7	1	0	-1.928017	2.487593	-2.013993
8	6	0	0.638385	3.728422	0.590398
9	1	0	0.585610	1.742413	1.396987
10	6	0	0.163784	4.620699	-0.379768
11	1	0	-1.151552	4.823326	-2.071412
12	1	0	1.378087	4.062324	1.313657
13	7	0	-2.685689	0.488519	-0.489762
14	7	0	-3.096626	-0.342642	-1.344961
15	7	0	-3.466369	-1.086444	-2.093450
16	6	0	-1.189261	-1.913591	0.016687
17	6	0	-0.841583	-2.965788	-0.844822
18	6	0	-2.178696	-2.150726	0.980537
19	6	0	-1.496891	-4.189066	-0.767787
20	1	0	-0.047509	-2.815523	-1.571189
21	6	0	-2.819132	-3.386351	1.062597
22	1	0	-2.425570	-1.366609	1.694046
23	6	0	-2.496583	-4.423575	0.184698
24	1	0	-1.214420	-4.986908	-1.450872
25	1	0	-3.570634	-3.551084	1.832130
26	53	0	1.735606	-0.632164	0.003742
27	14	0	-3.949158	1.344147	0.598288
28	6	0	-5.278741	0.041832	0.765061
29	1	0	-6.023666	0.373434	1.497479
30	1	0	-5.811311	-0.129211	-0.177375
31	1	0	-4.872673	-0.915367	1.109570
32	6	0	-4.551982	2.841640	-0.331836
33	1	0	-3.779337	3.614415	-0.382147
34	1	0	-4.853513	2.585875	-1.353973
35	1	0	-5.429050	3.261379	0.174823
36	6	0	-3.007780	1.720683	2.155033
37	1	0	-2.380063	0.880653	2.469554
38	1	0	-2.359179	2.591261	2.017672
39	1	0	-3.715426	1.939237	2.963194
40	6	0	4.771287	0.450178	0.671850
41	6	0	4.964449	-1.544656	-0.397409
42	6	0	6.287271	0.224568	0.579104
43	6	0	6.417367	-1.117302	-0.138467
44	1	0	6.733437	1.063080	0.036685
45	1	0	6.704352	0.229775	1.590217
46	1	0	6.940652	-1.059131	-1.097044
47	1	0	6.908788	-1.892493	0.456256
48	7	0	4.104770	-0.599827	0.100985
49	8	0	4.643727	-2.574463	-0.965439
50	8	0	4.254431	1.431944	1.184745
51	6	0	-3.167341	-5.770112	0.278560
52	1	0	-3.513084	-6.109231	-0.703120
53	1	0	-2.471261	-6.525484	0.659460
54	1	0	-4.028819	-5.739516	0.951392
55	6	0	0.677271	6.036115	-0.430757
56	1	0	1.735665	6.050374	-0.712240

57	1	0	0.125158	6.635289	-1.159857
58	1	0	0.593312	6.521959	0.546595

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS2
M06–2X/6–31+G(d) energy (in a.u.):	-8470.98093101
Thermal correction to Gibbs Free Energy (in a.u.):	0.395126
Number of imaginary frequencies:	1 (–32 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.002147	0.583481	-0.579161
2	6	0	1.153092	1.078467	-0.106558
3	6	0	-1.350751	1.188794	-0.600064
4	6	0	-2.014575	1.345052	-1.818915
5	6	0	-1.987841	1.584118	0.581916
6	6	0	-3.291964	1.896082	-1.861449
7	1	0	-1.531483	1.030089	-2.742000
8	6	0	-3.268219	2.121528	0.529827
9	1	0	-1.474199	1.449269	1.528695
10	6	0	-3.940688	2.286878	-0.687838
11	1	0	-3.794203	2.015636	-2.818035
12	1	0	-3.760459	2.417131	1.453685
13	7	0	0.012169	-0.728792	-1.231141
14	7	0	0.947663	-0.874177	-2.068091
15	7	0	1.770757	-1.046529	-2.803781
16	6	0	2.424382	0.322969	-0.032628
17	6	0	3.612836	0.848138	-0.551069
18	6	0	2.438901	-0.967204	0.519572
19	6	0	4.783032	0.094518	-0.537673
20	1	0	3.619767	1.850541	-0.970896
21	6	0	3.615113	-1.708472	0.529845
22	1	0	1.524916	-1.365384	0.950660
23	6	0	4.805273	-1.194447	0.002207
24	1	0	5.694589	0.516995	-0.952992
25	1	0	3.609417	-2.705652	0.964620
26	53	0	1.211286	3.064671	0.608732
27	14	0	-1.191276	-2.292306	-1.167576
28	6	0	-0.100577	-3.758400	-0.704037
29	1	0	-0.492899	-4.647121	-1.211591
30	1	0	0.904562	-3.577644	-1.113048
31	1	0	-0.019576	-3.965263	0.361138
32	6	0	-1.068134	-2.540229	-3.086033
33	1	0	-1.285275	-1.631244	-3.664091
34	1	0	-0.130489	-2.970569	-3.458437
35	1	0	-1.856242	-3.261036	-3.345838
36	6	0	-2.987042	-1.727514	-1.144306
37	1	0	-3.607466	-2.629173	-1.115152
38	1	0	-3.244170	-1.100247	-0.288742
39	1	0	-3.203604	-1.186554	-2.070128
40	6	0	-2.133459	-2.960562	1.550859
41	6	0	-0.893673	-1.212735	2.203442
42	6	0	-2.390139	-2.893310	3.054285
43	6	0	-1.577965	-1.683248	3.491260
44	1	0	-3.466339	-2.800985	3.224435
45	1	0	-2.066901	-3.834219	3.508648
46	1	0	-2.186247	-0.858903	3.876246
47	1	0	-0.810980	-1.898779	4.239721
48	7	0	-1.296418	-1.954419	1.122399

49	8	0	-0.090381	-0.287545	2.190525
50	8	0	-2.607817	-3.820130	0.818014
51	6	0	-5.328629	2.873249	-0.718563
52	1	0	-6.019677	2.272913	-0.117577
53	1	0	-5.333185	3.888465	-0.307723
54	1	0	-5.718827	2.918816	-1.738624
55	6	0	6.077631	-2.000524	0.046941
56	1	0	6.820985	-1.609360	-0.652919
57	1	0	6.517122	-1.974678	1.050546
58	1	0	5.890195	-3.049273	-0.202470

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN2
M06–2X/6–31+G(d) energy (in a.u.):	-7701.91227979
Thermal correction to Gibbs Free Energy (in a.u.):	0.213655
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.471283	0.929932	0.012851
2	6	0	0.403493	-0.100727	0.016084
3	6	0	-1.949338	0.839579	-0.089053
4	6	0	-2.753056	1.518459	0.831979
5	6	0	-2.562229	0.126384	-1.121376
6	6	0	-4.138579	1.452306	0.741644
7	1	0	-2.284655	2.095570	1.624511
8	6	0	-3.949978	0.074825	-1.214055
9	1	0	-1.950233	-0.385542	-1.858785
10	6	0	-4.759861	0.730361	-0.283368
11	1	0	-4.749667	1.972931	1.475527
12	1	0	-4.411522	-0.481948	-2.026010
13	7	0	-0.059922	2.295484	0.085638
14	7	0	0.982498	2.563276	0.703727
15	7	0	1.894583	2.948366	1.241913
16	6	0	1.870220	0.042599	-0.122337
17	6	0	2.763589	-0.491719	0.815573
18	6	0	2.389922	0.737340	-1.220021
19	6	0	4.132481	-0.311460	0.667101
20	1	0	2.378478	-1.047628	1.666759
21	6	0	3.764915	0.909906	-1.363435
22	1	0	1.707747	1.144342	-1.962609
23	6	0	4.658047	0.393217	-0.423025
24	1	0	4.810140	-0.726422	1.409926
25	1	0	4.147564	1.451119	-2.225471
26	53	0	-0.277203	-2.102885	0.244715
27	6	0	6.145670	0.589201	-0.563255
28	1	0	6.522439	1.273439	0.205185
29	1	0	6.681135	-0.358989	-0.450638
30	1	0	6.399962	1.009492	-1.540116
31	6	0	-6.262850	0.692128	-0.392533
32	1	0	-6.727055	0.565306	0.590287
33	1	0	-6.645917	1.626122	-0.819379
34	1	0	-6.593748	-0.128728	-1.034665

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS3
M06–2X/6–31+G(d) energy (in a.u.):	-7701.86496209
Thermal correction to Gibbs Free Energy (in a.u.):	0.210699
Number of imaginary frequencies:	1 (–567 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.167006	-1.165495	0.259616
2	6	0	-0.898575	-0.302766	0.036020
3	6	0	1.581579	-0.768342	0.024592
4	6	0	2.591971	-1.186153	0.896137
5	6	0	1.925243	-0.011201	-1.099633
6	6	0	3.917045	-0.836051	0.654357
7	1	0	2.326194	-1.763063	1.778629
8	6	0	3.251897	0.329772	-1.337328
9	1	0	1.145116	0.312218	-1.784438
10	6	0	4.268682	-0.074523	-0.465332
11	1	0	4.691575	-1.153962	1.348826
12	1	0	3.505121	0.920733	-2.214260
13	6	0	-0.777065	1.158285	0.164488
14	6	0	-1.450607	2.029571	-0.706221
15	6	0	0.054412	1.714585	1.146891
16	6	0	-1.262382	3.401871	-0.617853
17	1	0	-2.112069	1.621958	-1.465419
18	6	0	0.225051	3.092459	1.236762
19	1	0	0.564399	1.060059	1.848086
20	6	0	-0.425403	3.959871	0.356801
21	1	0	-1.780762	4.056986	-1.314674
22	1	0	0.872912	3.499345	2.009489
23	7	0	-0.182271	-2.291807	0.878645
24	7	0	0.812644	-3.583065	0.299035
25	53	0	-2.854957	-1.063779	-0.243282
26	7	0	1.207610	-4.589563	0.530637
27	6	0	-0.266133	5.454077	0.466796
28	1	0	-0.147579	5.912563	-0.519949
29	1	0	-1.148306	5.905991	0.934849
30	1	0	0.604942	5.717635	1.072773
31	6	0	5.708662	0.278205	-0.737296
32	1	0	5.786327	1.179948	-1.351280
33	1	0	6.257142	0.449651	0.193676
34	1	0	6.213521	-0.533721	-1.273345

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN3
M06–2X/6–31+G(d) energy (in a.u.):	-7592.48200169
Thermal correction to Gibbs Free Energy (in a.u.):	0.206497
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.823446	0.049971	0.895099
2	6	0	-0.520675	0.448978	0.595613
3	7	0	0.149227	0.387348	1.914797
4	6	0	2.126623	-0.395038	0.460141
5	6	0	2.352352	-0.639513	-0.896664
6	6	0	3.158392	-0.576203	1.390561
7	6	0	3.607347	-1.065207	-1.319930
8	1	0	1.543194	-0.492602	-1.607433
9	6	0	4.404650	-1.001315	0.955153
10	1	0	2.969009	-0.381191	2.442465
11	6	0	4.647871	-1.249449	-0.404315
12	1	0	3.783834	-1.256947	-2.374962
13	1	0	5.206787	-1.144704	1.674917
14	6	0	-1.640039	-0.497068	0.292348
15	6	0	-2.178135	-0.624414	-0.992031
16	6	0	-2.137096	-1.302695	1.316398
17	6	0	-3.187615	-1.546091	-1.240496
18	1	0	-1.813204	0.009752	-1.795911
19	6	0	-3.156665	-2.218921	1.059713
20	1	0	-1.722383	-1.208989	2.316283
21	6	0	-3.697457	-2.357063	-0.218911
22	1	0	-3.594890	-1.635292	-2.245359
23	1	0	-3.537211	-2.834310	1.871537
24	53	0	-0.803884	2.459915	-0.229305
25	6	0	6.015619	-1.683338	-0.863068
26	1	0	6.703978	-0.830576	-0.878290
27	1	0	6.437761	-2.434771	-0.189144
28	1	0	5.982467	-2.104843	-1.871065
29	6	0	-4.804308	-3.340327	-0.504033
30	1	0	-5.050436	-3.929208	0.383689
31	1	0	-5.714231	-2.823394	-0.828057
32	1	0	-4.519281	-4.033696	-1.302531

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS4
M06–2X/6–31+G(d) energy (in a.u.):	-8165.78206794
Thermal correction to Gibbs Free Energy (in a.u.):	0.318230
Number of imaginary frequencies:	1 (–231 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.611780	-0.808434	-1.313181
2	6	0	0.758316	-1.014722	-1.361173
3	7	0	0.097063	-0.832331	-2.482505
4	6	0	-1.906669	-1.268480	-0.877548
5	6	0	-2.129990	-1.587646	0.466324
6	6	0	-2.941194	-1.368235	-1.822185
7	6	0	-3.389987	-2.037310	0.851627
8	1	0	-1.339425	-1.436193	1.198634
9	6	0	-4.186787	-1.816703	-1.417887
10	1	0	-2.750843	-1.099797	-2.857924
11	6	0	-4.427957	-2.157819	-0.075345
12	1	0	-3.569886	-2.277214	1.895533
13	1	0	-4.991536	-1.904271	-2.143397
14	6	0	2.079312	-1.314492	-0.911932
15	6	0	2.351290	-1.503576	0.448659
16	6	0	3.104132	-1.407778	-1.873225
17	6	0	3.656770	-1.778843	0.841121
18	1	0	1.560868	-1.379914	1.184416
19	6	0	4.393216	-1.687148	-1.462500
20	1	0	2.871207	-1.256193	-2.924060
21	6	0	4.687393	-1.872779	-0.097965
22	1	0	3.875740	-1.905310	1.897286
23	1	0	5.192910	-1.759849	-2.195033
24	53	0	0.192215	0.762779	2.396921
25	7	0	-0.964710	1.292907	-1.025706
26	7	0	-1.965805	1.461456	-0.322972
27	7	0	-2.903294	1.512533	0.297366
28	14	0	0.199182	2.682154	-1.230224
29	6	0	-0.052242	3.229461	-3.006704
30	1	0	-1.069078	3.601021	-3.172330
31	1	0	0.648171	4.029971	-3.271820
32	1	0	0.117181	2.391885	-3.693046
33	6	0	1.939508	2.055787	-0.991199
34	1	0	2.610391	2.923846	-0.965876
35	1	0	2.036614	1.523818	-0.038535
36	1	0	2.270588	1.412896	-1.813925
37	6	0	-0.301915	3.992226	-0.000735
38	1	0	-0.231923	3.596895	1.019029
39	1	0	0.368477	4.855363	-0.086150
40	1	0	-1.324085	4.347591	-0.174106
41	6	0	-5.796636	-2.620956	0.346876
42	1	0	-6.520878	-1.803470	0.260950
43	1	0	-6.147428	-3.439107	-0.290246
44	1	0	-5.798001	-2.966098	1.383283
45	6	0	6.101576	-2.161261	0.327176
46	1	0	6.478115	-3.063862	-0.165679
47	1	0	6.763795	-1.335007	0.047204
48	1	0	6.172153	-2.304164	1.407632

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN4
M06–2X/6–31+G(d) energy (in a.u.):	-1245.66316522
Thermal correction to Gibbs Free Energy (in a.u.):	0.323932
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.384923	0.156415	0.269807
2	6	0	-1.003736	0.238686	0.662063
3	7	0	-0.183199	0.602627	1.558750
4	6	0	1.195298	-1.093320	0.162518
5	6	0	0.775731	-2.219888	0.881573
6	6	0	2.347533	-1.183192	-0.619507
7	6	0	1.501455	-3.401208	0.816270
8	1	0	-0.116286	-2.170504	1.500672
9	6	0	3.067320	-2.375992	-0.680429
10	1	0	2.713000	-0.327771	-1.183596
11	6	0	2.659871	-3.503123	0.034102
12	1	0	1.163788	-4.264576	1.384179
13	1	0	3.962811	-2.425527	-1.293985
14	6	0	-2.392621	0.010653	0.362937
15	6	0	-2.751876	-0.579022	-0.854605
16	6	0	-3.378624	0.371206	1.295593
17	6	0	-4.092746	-0.806017	-1.138454
18	1	0	-1.980141	-0.872444	-1.562840
19	6	0	-4.710791	0.141145	0.996677
20	1	0	-3.088467	0.824279	2.239497
21	6	0	-5.088803	-0.449187	-0.221546
22	1	0	-4.373672	-1.268473	-2.080147
23	1	0	-5.479206	0.418766	1.713403
24	7	0	0.948942	1.314775	-0.500655
25	7	0	0.726540	1.300406	-1.742597
26	7	0	0.537662	1.292012	-2.843281
27	14	0	2.035779	2.655570	0.308213
28	6	0	3.073584	1.661290	1.479698
29	1	0	3.748065	0.976581	0.957282
30	1	0	3.681969	2.340834	2.087999
31	1	0	2.444076	1.079503	2.161178
32	6	0	0.834488	3.824777	1.105237
33	1	0	1.376343	4.675534	1.534759
34	1	0	0.113495	4.221611	0.383185
35	1	0	0.287396	3.329412	1.912706
36	6	0	2.917354	3.342992	-1.182224
37	1	0	2.240211	3.847343	-1.880549
38	1	0	3.644610	4.093982	-0.852534
39	1	0	3.478235	2.573540	-1.724760
40	6	0	3.430793	-4.795234	-0.025832
41	1	0	4.309340	-4.705923	-0.668901
42	1	0	3.768118	-5.093685	0.971817
43	1	0	2.804755	-5.603986	-0.416184
44	6	0	-6.542665	-0.695015	-0.518037
45	1	0	-6.970107	-1.392866	0.209571
46	1	0	-7.114170	0.236233	-0.451941
47	1	0	-6.683619	-1.114374	-1.516367

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS5
M06–2X/6–31+G(d) energy (in a.u.):	-1605.79574355
Thermal correction to Gibbs Free Energy (in a.u.):	0.399005
Number of imaginary frequencies:	1 (–58 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.888639	-0.535968	0.394353
2	6	0	-0.803976	0.855049	0.792733
3	7	0	-0.690106	0.033195	1.747856
4	6	0	-2.171132	-1.227277	0.054915
5	6	0	-2.209843	-2.443246	-0.628153
6	6	0	-3.380830	-0.632760	0.436096
7	6	0	-3.430358	-3.051340	-0.920853
8	1	0	-1.288803	-2.938983	-0.923273
9	6	0	-4.590996	-1.246865	0.142962
10	1	0	-3.373999	0.314831	0.968860
11	6	0	-4.638760	-2.467346	-0.542149
12	1	0	-3.436900	-4.001231	-1.449587
13	1	0	-5.519232	-0.770033	0.449950
14	6	0	-0.994472	2.262638	0.518427
15	6	0	-1.081584	2.725558	-0.797140
16	6	0	-1.126155	3.151365	1.589535
17	6	0	-1.305253	4.074103	-1.034167
18	1	0	-0.945291	2.028148	-1.618086
19	6	0	-1.346782	4.500309	1.338433
20	1	0	-1.059459	2.777334	2.607713
21	6	0	-1.438041	4.979770	0.026707
22	1	0	-1.368449	4.437716	-2.056727
23	1	0	-1.451316	5.193042	2.169462
24	7	0	0.320860	-1.198868	-0.138981
25	7	0	0.510816	-1.026166	-1.371759
26	7	0	0.671494	-0.942281	-2.471714
27	14	0	1.647923	-2.099992	0.916230
28	6	0	2.430734	-3.350002	-0.234101
29	1	0	2.736016	-2.920539	-1.190437
30	1	0	3.348934	-3.724930	0.230329
31	1	0	1.745392	-4.190380	-0.393527
32	6	0	0.358842	-3.091069	1.895806
33	1	0	0.901693	-3.782033	2.555501
34	1	0	-0.264210	-2.454898	2.533760
35	1	0	-0.300007	-3.694926	1.262085
36	6	0	2.512062	-1.082055	2.228525
37	1	0	2.198083	-0.036362	2.153649
38	1	0	2.244528	-1.453710	3.223308
39	1	0	3.595987	-1.129167	2.092127
40	7	0	2.975648	-0.437330	-0.437159
41	6	0	4.340569	-0.603959	-0.421911
42	6	0	5.065210	0.692480	-0.807443
43	6	0	3.932174	1.703575	-0.943820
44	6	0	2.677628	0.861733	-0.694772
45	8	0	1.535353	1.335015	-0.733159
46	1	0	3.966792	2.508671	-0.203527
47	1	0	5.796021	0.935783	-0.031639
48	8	0	4.916984	-1.638427	-0.118349

49	1	0	3.858143	2.170766	-1.929938
50	1	0	5.618134	0.523064	-1.736152
51	6	0	-5.961389	-3.119268	-0.854633
52	1	0	-6.525273	-3.321017	0.062136
53	1	0	-6.579557	-2.470752	-1.484487
54	1	0	-5.821644	-4.067173	-1.380804
55	6	0	-1.648444	6.446125	-0.248108
56	1	0	-2.368558	6.597065	-1.057858
57	1	0	-2.013684	6.969654	0.639214
58	1	0	-0.707314	6.918075	-0.552335

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN5
M06–2X/6–31+G(d) energy (in a.u.):	-836.704529787
Thermal correction to Gibbs Free Energy (in a.u.):	0.220562
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.591456	0.739856	0.615241
2	6	0	-0.720805	1.223178	0.248608
3	7	0	-0.013062	1.319482	1.566590
4	6	0	1.821256	0.040525	0.297489
5	6	0	1.992909	-0.511254	-0.973713
6	6	0	2.828439	-0.090073	1.262959
7	6	0	3.167832	-1.192367	-1.277649
8	1	0	1.203167	-0.403986	-1.712917
9	6	0	3.994575	-0.770803	0.947147
10	1	0	2.683680	0.346619	2.247518
11	6	0	4.181211	-1.332498	-0.325393
12	1	0	3.300976	-1.621193	-2.267410
13	1	0	4.778555	-0.873087	1.693893
14	6	0	-1.903571	0.318578	0.131195
15	6	0	-2.956828	0.594438	-0.745440
16	6	0	-1.961176	-0.840504	0.908687
17	6	0	-4.036063	-0.278715	-0.840827
18	1	0	-2.928948	1.495440	-1.348840
19	6	0	-3.047339	-1.705621	0.808325
20	1	0	-1.157894	-1.066780	1.604863
21	6	0	-4.101557	-1.442674	-0.068820
22	1	0	-4.847700	-0.048264	-1.528171
23	1	0	-3.074004	-2.600831	1.425177
24	7	0	-0.900576	2.446902	-0.526061
25	7	0	0.011092	3.268045	-0.414913
26	7	0	0.804825	4.070745	-0.368979
27	6	0	5.449470	-2.081433	-0.642659
28	1	0	6.331240	-1.494016	-0.368085
29	1	0	5.493714	-3.021873	-0.082215
30	1	0	5.515237	-2.320199	-1.707171
31	6	0	-5.276335	-2.380162	-0.190988
32	1	0	-6.219329	-1.857678	0.001846
33	1	0	-5.337567	-2.805163	-1.198900
34	1	0	-5.197935	-3.208033	0.518980

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS6
M06–2X/6–31+G(d) energy (in a.u.):	-836.643853191
Thermal correction to Gibbs Free Energy (in a.u.):	0.214732
Number of imaginary frequencies:	1 (–625 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.560162	0.660352	1.236226
2	6	0	-0.696997	1.318698	0.759147
3	7	0	-0.053445	1.067169	2.226088
4	6	0	1.707788	-0.018999	0.667126
5	6	0	1.670596	-0.402820	-0.675818
6	6	0	2.842085	-0.276472	1.445279
7	6	0	2.767403	-1.048747	-1.235628
8	1	0	0.777231	-0.204086	-1.263658
9	6	0	3.931117	-0.917070	0.870520
10	1	0	2.859111	0.028534	2.487749
11	6	0	3.911899	-1.309567	-0.475123
12	1	0	2.736335	-1.355273	-2.278029
13	1	0	4.813936	-1.120317	1.471801
14	6	0	-1.843983	0.416227	0.408215
15	6	0	-2.667374	0.755247	-0.670637
16	6	0	-2.109344	-0.765141	1.106530
17	6	0	-3.725182	-0.069003	-1.039521
18	1	0	-2.473525	1.679567	-1.206726
19	6	0	-3.177020	-1.580140	0.734529
20	1	0	-1.490579	-1.047024	1.953758
21	6	0	-4.002480	-1.249257	-0.341985
22	1	0	-4.352371	0.212783	-1.883031
23	1	0	-3.370428	-2.492475	1.294705
24	7	0	-0.635544	2.597154	0.321652
25	7	0	0.518805	2.758178	-0.946534
26	7	0	1.028195	3.466430	-1.626367
27	6	0	5.114472	-1.974531	-1.092516
28	1	0	4.836304	-2.563124	-1.970662
29	1	0	5.846080	-1.223438	-1.412101
30	1	0	5.611677	-2.636384	-0.377601
31	6	0	-5.174288	-2.117957	-0.724795
32	1	0	-6.112321	-1.699293	-0.342303
33	1	0	-5.270340	-2.200145	-1.812034
34	1	0	-5.070320	-3.126751	-0.315025

System:	**3**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	R
M06–2X/6–31+G(d) energy (in a.u.):	-8576.82618702
Thermal correction to Gibbs Free Energy (in a.u.):	0.318466
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.678915	0.728732	0.861505
2	6	0	1.404122	-0.243322	0.803343
3	6	0	-0.136731	1.902486	0.928452
4	6	0	0.157053	2.892192	1.880867
5	6	0	-1.214823	2.075300	0.046606
6	6	0	-0.616604	4.040680	1.950588
7	1	0	0.994725	2.750297	2.557312
8	6	0	-1.995876	3.220165	0.122320
9	1	0	-1.454579	1.311757	-0.685680
10	6	0	-1.695891	4.204314	1.071758
11	1	0	-0.394241	4.812459	2.679866
12	1	0	-2.838967	3.347554	-0.548707
13	7	0	2.876638	2.917395	-0.266791
14	7	0	3.316348	2.428658	0.756924
15	7	0	3.690205	2.033028	1.752156
16	6	0	2.306308	-1.349652	0.710686
17	6	0	3.383908	-1.447172	1.606656
18	6	0	2.146016	-2.315396	-0.296841
19	6	0	4.287642	-2.494021	1.495328
20	1	0	3.507906	-0.688730	2.372747
21	6	0	3.048308	-3.363891	-0.407187
22	1	0	1.316566	-2.231075	-0.992857
23	6	0	4.121846	-3.453136	0.487826
24	1	0	5.125019	-2.573534	2.180554
25	1	0	2.931183	-4.113017	-1.183178
26	53	0	-1.844235	-1.611940	0.415749
27	14	0	3.067566	2.178551	-1.880173
28	6	0	4.280593	0.756278	-1.725977
29	1	0	4.407921	0.256444	-2.693069
30	1	0	5.266424	1.107543	-1.401059
31	1	0	3.937474	0.002465	-1.007998
32	6	0	3.722648	3.544596	-2.975428
33	1	0	3.037747	4.399141	-2.974761
34	1	0	4.698937	3.896478	-2.626923
35	1	0	3.832795	3.200035	-4.009722
36	6	0	1.382876	1.617499	-2.471723
37	1	0	1.020016	0.753934	-1.904249
38	1	0	0.650691	2.425405	-2.363759
39	1	0	1.424746	1.339245	-3.531427
40	6	0	-4.297523	-0.669540	-1.079326
41	6	0	-4.549996	-2.858119	-0.267772
42	6	0	-5.695652	-1.098863	-1.498674
43	6	0	-5.857501	-2.531415	-0.976458
44	1	0	-6.411864	-0.394132	-1.068310
45	1	0	-5.768266	-1.017713	-2.586115
46	1	0	-6.673357	-2.645557	-0.258416
47	1	0	-6.010588	-3.269445	-1.767876
48	7	0	-3.724425	-1.732182	-0.381386
49	8	0	-4.249122	-3.878860	0.291874
50	8	0	-3.756969	0.387504	-1.296002
51	6	0	5.062224	-4.536730	0.368651
52	6	0	-2.505383	5.392709	1.150366
53	7	0	5.818775	-5.407242	0.270462
54	7	0	-3.156386	6.347804	1.214491

System:	**3**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS1
M06–2X/6–31+G(d) energy (in a.u.):	-8576.78101296
Thermal correction to Gibbs Free Energy (in a.u.):	0.325839
Number of imaginary frequencies:	1 (–356 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.019914	0.622112	-0.276621
2	6	0	-0.570031	-0.567517	-0.091893
3	6	0	-0.569839	2.013674	-0.283182
4	6	0	-1.036483	2.940722	-1.224886
5	6	0	0.370318	2.419253	0.676181
6	6	0	-0.576359	4.250455	-1.211463
7	1	0	-1.756804	2.631162	-1.975572
8	6	0	0.842745	3.724987	0.688025
9	1	0	0.736280	1.705911	1.406688
10	6	0	0.363991	4.644875	-0.251828
11	1	0	-0.931887	4.968257	-1.943537
12	1	0	1.579978	4.031884	1.422316
13	7	0	-2.816271	0.746990	-0.594023
14	7	0	-3.226908	-0.091744	-1.413084
15	7	0	-3.520544	-0.871489	-2.168091
16	6	0	-1.244536	-1.853137	0.012545
17	6	0	-0.876024	-2.934952	-0.803198
18	6	0	-2.275874	-2.028493	0.951438
19	6	0	-1.556536	-4.141481	-0.720878
20	1	0	-0.054918	-2.819349	-1.504009
21	6	0	-2.948915	-3.238831	1.049391
22	1	0	-2.530784	-1.209299	1.618639
23	6	0	-2.599459	-4.296679	0.201817
24	1	0	-1.279070	-4.971887	-1.361764
25	1	0	-3.740870	-3.374559	1.779541
26	53	0	1.947316	-0.729896	0.001275
27	14	0	-3.998306	1.605672	0.519001
28	6	0	-5.368661	0.366554	0.805429
29	1	0	-6.094075	0.771000	1.520318
30	1	0	-5.914551	0.140877	-0.117604
31	1	0	-4.987664	-0.576078	1.212560
32	6	0	-4.598690	3.122332	-0.387891
33	1	0	-3.780391	3.829799	-0.556391
34	1	0	-5.037668	2.863220	-1.357653
35	1	0	-5.370135	3.634190	0.198904
36	6	0	-3.000238	2.007997	2.039528
37	1	0	-2.404536	1.153886	2.378985
38	1	0	-2.317539	2.844239	1.858046
39	1	0	-3.675534	2.294561	2.853910
40	6	0	4.895960	0.047764	0.691427
41	6	0	4.822099	-1.947327	-0.473905
42	6	0	6.357039	-0.378633	0.555950
43	6	0	6.308152	-1.700880	-0.213282
44	1	0	6.901316	0.413638	0.035170
45	1	0	6.785755	-0.467294	1.557643
46	1	0	6.827191	-1.670296	-1.174820
47	1	0	6.705848	-2.550858	0.347420
48	7	0	4.100541	-0.904577	0.081566
49	8	0	4.349387	-2.891644	-1.066077
50	8	0	4.494809	1.051911	1.240382
51	6	0	-3.308174	-5.545779	0.290315
52	6	0	0.831449	6.006901	-0.233537
53	7	0	-3.887477	-6.545614	0.362311
54	7	0	1.193931	7.105927	-0.220639

System:	**3**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN1
M06–2X/6–31+G(d) energy (in a.u.):	-8576.78787820
Thermal correction to Gibbs Free Energy (in a.u.):	0.328163
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.028234	0.768451	-0.236776
2	6	0	-0.598286	-0.485224	-0.061239
3	6	0	-0.271864	2.040049	-0.273686
4	6	0	-0.582552	3.024459	-1.222652
5	6	0	0.765166	2.278303	0.639502
6	6	0	0.127314	4.217114	-1.270834
7	1	0	-1.374569	2.851233	-1.947013
8	6	0	1.488509	3.462992	0.592136
9	1	0	1.016526	1.529912	1.382551
10	6	0	1.166447	4.437712	-0.359812
11	1	0	-0.107913	4.972010	-2.014117
12	1	0	2.304556	3.628955	1.287441
13	7	0	-2.500627	1.042825	-0.466435
14	7	0	-3.063547	0.337436	-1.348788
15	7	0	-3.567344	-0.296752	-2.119495
16	6	0	-1.518675	-1.630115	-0.000144
17	6	0	-1.384963	-2.696646	-0.905011
18	6	0	-2.527044	-1.698171	0.976548
19	6	0	-2.266056	-3.768968	-0.871696
20	1	0	-0.578336	-2.677532	-1.632045
21	6	0	-3.401417	-2.776455	1.028064
22	1	0	-2.602437	-0.907482	1.719396
23	6	0	-3.283172	-3.809645	0.090989
24	1	0	-2.164460	-4.584498	-1.580242
25	1	0	-4.170461	-2.830518	1.792685
26	53	0	1.646457	-1.007615	0.030338
27	14	0	-3.581065	2.114015	0.638668
28	6	0	-5.138497	1.095676	0.785771
29	1	0	-5.808604	1.560249	1.518155
30	1	0	-5.689411	1.041339	-0.160001
31	1	0	-4.932796	0.074436	1.123726
32	6	0	-3.866688	3.713010	-0.272398
33	1	0	-2.958577	4.321710	-0.309200
34	1	0	-4.210115	3.537899	-1.298292
35	1	0	-4.645101	4.291901	0.238490
36	6	0	-2.575970	2.270633	2.192771
37	1	0	-2.170084	1.309269	2.523463
38	1	0	-1.738644	2.961228	2.052938
39	1	0	-3.211600	2.664067	2.994552
40	6	0	4.767720	-0.548645	0.673527
41	6	0	4.534932	-2.558225	-0.386795
42	6	0	6.198910	-1.086491	0.569362
43	6	0	6.042741	-2.434438	-0.134823
44	1	0	6.803212	-0.364335	0.013308
45	1	0	6.619372	-1.158573	1.576222
46	1	0	6.563277	-2.495950	-1.094372
47	1	0	6.365711	-3.287540	0.468193
48	7	0	3.895673	-1.448436	0.114220

49	8	0	3.996277	-3.494939	-0.945209
50	8	0	4.459014	0.518372	1.178013
51	6	0	-4.204448	-4.914374	0.127954
52	6	0	1.894893	5.679219	-0.403556
53	7	0	-4.957489	-5.793156	0.157365
54	7	0	2.463082	6.686770	-0.441263

System:	**3**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS2
M06–2X/6–31+G(d) energy (in a.u.):	-8576.81454842
Thermal correction to Gibbs Free Energy (in a.u.):	0.338389
Number of imaginary frequencies:	1 (–34 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.129310	-0.546710	-0.569342
2	6	0	-0.901194	-1.273815	-0.108760
3	6	0	1.573234	-0.874756	-0.563391
4	6	0	2.269310	-0.906239	-1.776279
5	6	0	2.246095	-1.132264	0.635650
6	6	0	3.625147	-1.203430	-1.802713
7	1	0	1.747080	-0.694532	-2.706372
8	6	0	3.605802	-1.417046	0.618189
9	1	0	1.696319	-1.089807	1.570506
10	6	0	4.294814	-1.454273	-0.600030
11	1	0	4.168707	-1.236130	-2.741021
12	1	0	4.139785	-1.609191	1.542925
13	7	0	-0.134586	0.729141	-1.229767
14	7	0	-1.071063	0.682529	-2.078817
15	7	0	-1.902399	0.690656	-2.824931
16	6	0	-2.301737	-0.791365	-0.056761
17	6	0	-3.347666	-1.552535	-0.594635
18	6	0	-2.578511	0.462318	0.509499
19	6	0	-4.648085	-1.065251	-0.591059
20	1	0	-3.140207	-2.530273	-1.019829
21	6	0	-3.879038	0.951360	0.520374
22	1	0	-1.766997	1.028012	0.957415
23	6	0	-4.915005	0.191033	-0.034403
24	1	0	-5.457656	-1.650454	-1.014339
25	1	0	-4.097213	1.917585	0.963788
26	53	0	-0.574049	-3.223609	0.623310
27	14	0	0.731571	2.518258	-1.158996
28	6	0	-0.633793	3.727982	-0.689483
29	1	0	-0.434599	4.677100	-1.200145
30	1	0	-1.582592	3.346568	-1.095285
31	1	0	-0.751404	3.917210	0.375491
32	6	0	0.556543	2.731747	-3.075171
33	1	0	0.947187	1.885543	-3.657368
34	1	0	-0.447105	2.972295	-3.445930
35	1	0	1.187444	3.593296	-3.335463
36	6	0	2.602392	2.311103	-1.141328
37	1	0	2.987534	1.776945	-0.270917
38	1	0	2.916248	1.799767	-2.056265
39	1	0	3.034478	3.317154	-1.147043
40	6	0	1.515043	3.331235	1.557917
41	6	0	0.614901	1.386155	2.207325
42	6	0	1.758249	3.321296	3.063688
43	6	0	1.166143	1.989491	3.501924
44	1	0	2.831619	3.419179	3.247989
45	1	0	1.270069	4.194125	3.505947
46	1	0	1.900430	1.294674	3.920908
47	1	0	0.351197	2.074504	4.225617
48	7	0	0.891386	2.178420	1.125447

49	8	0	0.003460	0.321774	2.187529
50	8	0	1.822002	4.258292	0.820243
51	6	0	-6.262214	0.699813	-0.029281
52	6	0	5.703820	-1.753605	-0.617080
53	7	0	-7.344896	1.108740	-0.028994
54	7	0	6.835446	-1.995471	-0.631703

System:	**3**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN2
M06–2X/6–31+G(d) energy (in a.u.):	-7807.74742823
Thermal correction to Gibbs Free Energy (in a.u.):	0.156014
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.461751	-0.906512	-0.051165
2	6	0	0.401569	0.134470	-0.045406
3	6	0	-1.941345	-0.819659	0.059153
4	6	0	-2.742546	-1.498440	-0.864278
5	6	0	-2.541866	-0.114286	1.106666
6	6	0	-4.127264	-1.443215	-0.770083
7	1	0	-2.275282	-2.070323	-1.659899
8	6	0	-3.924999	-0.063617	1.218487
9	1	0	-1.921990	0.388456	1.842483
10	6	0	-4.719268	-0.722517	0.273075
11	1	0	-4.752469	-1.956943	-1.492652
12	1	0	-4.394229	0.477215	2.033473
13	7	0	-0.053848	-2.266730	-0.145663
14	7	0	0.991237	-2.521497	-0.769565
15	6	0	1.869715	-0.010152	0.085557
16	6	0	2.755831	0.555119	-0.840617
17	6	0	2.385427	-0.733631	1.170614
18	6	0	4.125919	0.380175	-0.704415
19	1	0	2.365616	1.130052	-1.675309
20	6	0	3.755761	-0.908400	1.318227
21	1	0	1.702390	-1.160481	1.900068
22	6	0	4.629136	-0.353379	0.377112
23	1	0	4.810886	0.808126	-1.428850
24	1	0	4.153077	-1.467253	2.159098
25	53	0	-0.281818	2.130348	-0.250365
26	7	0	1.904698	-2.891335	-1.313516
27	6	0	6.050238	-0.531838	0.524057
28	6	0	-6.154549	-0.667330	0.380807
29	7	0	-7.307825	-0.622273	0.466993
30	7	0	7.192639	-0.675026	0.642346

System:	**3**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS3
M06–2X/6–31+G(d) energy (in a.u.):	-7807.70016448
Thermal correction to Gibbs Free Energy (in a.u.):	0.151959
Number of imaginary frequencies:	1 (–546 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.057678	-1.306048	0.284843
2	6	0	-1.074623	-0.393672	0.028429
3	6	0	1.382846	-0.988703	0.079655
4	6	0	2.341389	-1.469748	0.978332
5	6	0	1.789191	-0.263092	-1.045900
6	6	0	3.691220	-1.215735	0.767363
7	1	0	2.018227	-2.025224	1.854626
8	6	0	3.135407	-0.006866	-1.266859
9	1	0	1.043858	0.096162	-1.750308
10	6	0	4.088464	-0.482729	-0.357039
11	1	0	4.438769	-1.576900	1.466152
12	1	0	3.456449	0.554080	-2.138429
13	6	0	-0.870661	1.060956	0.141914
14	6	0	-1.480128	1.952136	-0.756645
15	6	0	-0.028820	1.576995	1.140587
16	6	0	-1.220339	3.312449	-0.689151
17	1	0	-2.151177	1.570809	-1.520202
18	6	0	0.225674	2.939200	1.222453
19	1	0	0.416666	0.903008	1.865978
20	6	0	-0.364328	3.811112	0.301467
21	1	0	-1.678472	3.995778	-1.396740
22	1	0	0.873781	3.332533	1.998821
23	7	0	-0.480281	-2.402537	0.907080
24	7	0	0.447829	-3.770406	0.353234
25	53	0	-3.058690	-1.049258	-0.277461
26	7	0	0.747264	-4.810303	0.573929
27	6	0	-0.102293	5.224156	0.378569
28	6	0	5.486474	-0.219782	-0.581990
29	7	0	6.610051	-0.009217	-0.762434
30	7	0	0.109669	6.360555	0.438098

System:	**3**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN3
M06–2X/6–31+G(d) energy (in a.u.):	-7698.31469140
Thermal correction to Gibbs Free Energy (in a.u.):	0.147838
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.778589	0.218272	0.931384
2	6	0	-0.546705	0.658472	0.594771
3	7	0	0.110821	0.617678	1.928812
4	6	0	2.074716	-0.290890	0.534128
5	6	0	2.309633	-0.581784	-0.812852
6	6	0	3.074112	-0.479255	1.496934
7	6	0	3.550535	-1.067359	-1.205214
8	1	0	1.519897	-0.421697	-1.541342
9	6	0	4.313867	-0.964884	1.109303
10	1	0	2.869270	-0.241999	2.536529
11	6	0	4.548352	-1.258038	-0.242029
12	1	0	3.754363	-1.298501	-2.245095
13	1	0	5.103233	-1.119011	1.837132
14	6	0	-1.684124	-0.277662	0.323246
15	6	0	-2.246726	-0.403063	-0.950568
16	6	0	-2.167130	-1.066548	1.371516
17	6	0	-3.270811	-1.312033	-1.180032
18	1	0	-1.889394	0.221115	-1.764156
19	6	0	-3.200316	-1.970724	1.153315
20	1	0	-1.732281	-0.964934	2.361246
21	6	0	-3.751717	-2.097627	-0.125439
22	1	0	-3.705602	-1.414330	-2.168797
23	1	0	-3.583285	-2.576927	1.967707
24	53	0	-0.760427	2.629713	-0.298915
25	6	0	5.836559	-1.762224	-0.644937
26	6	0	-4.817834	-3.037058	-0.358836
27	7	0	6.870988	-2.167430	-0.968172
28	7	0	-5.673179	-3.793691	-0.547622

System:	**3**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS4
M06–2X/6–31+G(d) energy (in a.u.):	-8271.60554183
Thermal correction to Gibbs Free Energy (in a.u.):	0.260702
Number of imaginary frequencies:	1 (–224 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.597706	-0.519159	-1.312158
2	6	0	0.774479	-0.670275	-1.376143
3	7	0	0.112287	-0.303253	-2.453052
4	6	0	-1.896855	-1.048970	-0.968608
5	6	0	-2.124309	-1.594264	0.299997
6	6	0	-2.913678	-0.983970	-1.934093
7	6	0	-3.382250	-2.112338	0.593184
8	1	0	-1.338991	-1.561463	1.052522
9	6	0	-4.163503	-1.500110	-1.638351
10	1	0	-2.711073	-0.534325	-2.901861
11	6	0	-4.390969	-2.067523	-0.373445
12	1	0	-3.586192	-2.533631	1.571474
13	1	0	-4.965865	-1.470043	-2.367364
14	6	0	2.119150	-1.017969	-1.016951
15	6	0	2.420557	-1.550355	0.243089
16	6	0	3.114503	-0.829185	-1.991916
17	6	0	3.737059	-1.891899	0.530364
18	1	0	1.642783	-1.646653	0.993752
19	6	0	4.423628	-1.168185	-1.702219
20	1	0	2.849470	-0.418412	-2.962072
21	6	0	4.728399	-1.698531	-0.437082
22	1	0	3.998374	-2.292582	1.503499
23	1	0	5.212240	-1.029719	-2.433454
24	53	0	0.301363	0.423192	2.339230
25	7	0	-1.112251	1.571324	-0.774415
26	7	0	-2.080921	1.574394	-0.010802
27	7	0	-2.984500	1.474672	0.653987
28	14	0	-0.008162	3.023384	-0.801470
29	6	0	-0.443444	3.909494	-2.394819
30	1	0	-1.481186	4.259412	-2.388710
31	1	0	0.204372	4.780937	-2.544866
32	1	0	-0.316016	3.242938	-3.255255
33	6	0	1.748147	2.395255	-0.873034
34	1	0	2.425849	3.253771	-0.789677
35	1	0	1.957352	1.717934	-0.037757
36	1	0	1.970560	1.901191	-1.825661
37	6	0	-0.391804	4.044824	0.709552
38	1	0	-0.209737	3.463012	1.619634
39	1	0	0.250735	4.932774	0.728732
40	1	0	-1.432016	4.390033	0.713561
41	6	0	6.093259	-2.052487	-0.138593
42	6	0	-5.693156	-2.605904	-0.070956
43	7	0	-6.739082	-3.041910	0.161896
44	7	0	7.190512	-2.338431	0.090673

System:	**3**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN4
M06–2X/6–31+G(d) energy (in a.u.):	-1351.47778194
Thermal correction to Gibbs Free Energy (in a.u.):	0.264771
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.424183	0.350359	0.265669
2	6	0	-0.959318	0.306461	0.689992
3	7	0	-0.158354	0.719439	1.577751
4	6	0	1.332123	-0.831428	0.145214
5	6	0	1.208768	-1.863018	1.082496
6	6	0	2.283315	-0.932377	-0.874214
7	6	0	2.028888	-2.981278	1.003692
8	1	0	0.479225	-1.790423	1.883611
9	6	0	3.103923	-2.051204	-0.961104
10	1	0	2.405079	-0.139242	-1.607356
11	6	0	2.977638	-3.077950	-0.020324
12	1	0	1.940196	-3.779858	1.732772
13	1	0	3.842429	-2.132835	-1.751763
14	6	0	-2.336964	-0.036532	0.420506
15	6	0	-2.669795	-0.657198	-0.789775
16	6	0	-3.316492	0.247005	1.383021
17	6	0	-3.990794	-0.997380	-1.044822
18	1	0	-1.894266	-0.887685	-1.515904
19	6	0	-4.637039	-0.088629	1.127651
20	1	0	-3.036963	0.723957	2.317818
21	6	0	-4.970335	-0.708229	-0.085985
22	1	0	-4.271698	-1.484306	-1.972415
23	1	0	-5.413867	0.121133	1.855126
24	7	0	0.891157	1.548900	-0.493515
25	7	0	0.395836	1.697509	-1.646687
26	7	0	-0.022645	1.844519	-2.671362
27	14	0	2.045883	2.875322	0.273831
28	6	0	3.159894	1.825026	1.318769
29	1	0	3.769817	1.141961	0.720187
30	1	0	3.836911	2.477304	1.883028
31	1	0	2.586601	1.240153	2.046037
32	6	0	0.899059	3.996952	1.206996
33	1	0	1.467764	4.826472	1.643526
34	1	0	0.132575	4.431675	0.556830
35	1	0	0.405862	3.460935	2.023491
36	6	0	2.801407	3.617543	-1.255811
37	1	0	2.072104	4.151766	-1.874870
38	1	0	3.558024	4.353780	-0.960146
39	1	0	3.309397	2.866899	-1.871264
40	6	0	-6.342998	-1.054582	-0.350938
41	6	0	3.828612	-4.236388	-0.107697
42	7	0	4.514116	-5.165048	-0.180814
43	7	0	-7.445253	-1.330906	-0.565709

System:	**3**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS5
M06–2X/6–31+G(d) energy (in a.u.):	-1711.62988089
Thermal correction to Gibbs Free Energy (in a.u.):	0.341799
Number of imaginary frequencies:	1 (–62 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.853657	-0.403662	0.393087
2	6	0	-0.370601	0.906286	0.788439
3	7	0	-0.470823	0.085235	1.742022
4	6	0	-2.292876	-0.696412	0.106939
5	6	0	-2.689784	-1.821038	-0.622564
6	6	0	-3.268041	0.187245	0.586434
7	6	0	-4.036157	-2.062262	-0.871729
8	1	0	-1.952042	-2.529639	-0.986687
9	6	0	-4.614022	-0.047436	0.344575
10	1	0	-2.974815	1.063013	1.158249
11	6	0	-5.001810	-1.174895	-0.388837
12	1	0	-4.342323	-2.938040	-1.434382
13	1	0	-5.368192	0.637062	0.718686
14	6	0	-0.173530	2.320073	0.526082
15	6	0	-0.149124	2.800726	-0.784714
16	6	0	-0.044150	3.187685	1.615435
17	6	0	-0.001259	4.161189	-1.011487
18	1	0	-0.213086	2.102624	-1.612793
19	6	0	0.108507	4.549048	1.393098
20	1	0	-0.064851	2.789526	2.625840
21	6	0	0.126829	5.031849	0.078399
22	1	0	0.026631	4.555868	-2.021385
23	1	0	0.211899	5.240350	2.222672
24	7	0	0.095957	-1.382291	-0.163003
25	7	0	0.345856	-1.234640	-1.391244
26	7	0	0.540229	-1.177494	-2.486637
27	14	0	1.116465	-2.638823	0.880839
28	6	0	1.570799	-4.003997	-0.309556
29	1	0	1.951484	-3.629226	-1.262157
30	1	0	2.390521	-4.585937	0.124884
31	1	0	0.712176	-4.664523	-0.474109
32	6	0	-0.404651	-3.256800	1.826967
33	1	0	-0.080836	-4.069559	2.490899
34	1	0	-0.848093	-2.480996	2.461274
35	1	0	-1.186838	-3.661669	1.175399
36	6	0	2.223989	-1.908793	2.198035
37	1	0	2.204224	-0.816281	2.146327
38	1	0	1.872540	-2.216065	3.188757
39	1	0	3.254211	-2.243297	2.048040
40	7	0	2.866104	-1.308915	-0.459876
41	6	0	4.145783	-1.818164	-0.445136
42	6	0	5.178958	-0.737187	-0.787323
43	6	0	4.338843	0.530825	-0.900621
44	6	0	2.912145	0.025302	-0.678285
45	8	0	1.922912	0.774996	-0.703622
46	1	0	4.569202	1.283275	-0.140238
47	1	0	5.936780	-0.706168	-0.000107
48	8	0	4.432331	-2.973542	-0.171069

49	1	0	4.395219	1.025280	-1.874563
50	1	0	5.684515	-1.014685	-1.716865
51	6	0	-6.397235	-1.420354	-0.646666
52	6	0	0.280071	6.445480	-0.155916
53	7	0	-7.518584	-1.616825	-0.854985
54	7	0	0.400557	7.581035	-0.343406

System:	**3**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN5
M06–2X/6–31+G(d) energy (in a.u.):	-942.540097599
Thermal correction to Gibbs Free Energy (in a.u.):	0.160989
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.578267	0.869861	0.615826
2	6	0	-0.722164	1.369411	0.223443
3	7	0	-0.025759	1.472857	1.550254
4	6	0	1.820276	0.168310	0.336068
5	6	0	2.020408	-0.407844	-0.921476
6	6	0	2.798697	0.075291	1.333610
7	6	0	3.204357	-1.083892	-1.188285
8	1	0	1.246580	-0.324412	-1.679383
9	6	0	3.982186	-0.598173	1.071259
10	1	0	2.621148	0.533463	2.302268
11	6	0	4.181727	-1.176562	-0.190602
12	1	0	3.378941	-1.538790	-2.157447
13	1	0	4.754346	-0.681946	1.828731
14	6	0	-1.921729	0.485402	0.119560
15	6	0	-2.959599	0.776544	-0.770312
16	6	0	-2.006991	-0.653827	0.928448
17	6	0	-4.064835	-0.062137	-0.857279
18	1	0	-2.900257	1.663385	-1.390720
19	6	0	-3.109226	-1.493629	0.849772
20	1	0	-1.212948	-0.881547	1.633294
21	6	0	-4.142202	-1.199676	-0.047776
22	1	0	-4.871467	0.162200	-1.547660
23	1	0	-3.177174	-2.374680	1.479489
24	7	0	-0.878155	2.577420	-0.570519
25	7	0	0.053318	3.382444	-0.476417
26	7	0	0.861718	4.168970	-0.448201
27	6	0	5.411176	-1.877063	-0.463456
28	6	0	-5.284995	-2.071388	-0.138289
29	7	0	6.398319	-2.439934	-0.681650
30	7	0	-6.202482	-2.773391	-0.212271

System:	**3**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS6
M06–2X/6–31+G(d) energy (in a.u.):	-942.479838425
Thermal correction to Gibbs Free Energy (in a.u.):	0.155591
Number of imaginary frequencies:	1 (–602 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.550405	0.956963	1.182248
2	6	0	-0.704544	1.559961	0.630270
3	7	0	-0.066221	1.454615	2.125817
4	6	0	1.706402	0.213442	0.710058
5	6	0	1.692433	-0.305992	-0.587572
6	6	0	2.810935	0.030598	1.549883
7	6	0	2.788692	-1.021273	-1.051968
8	1	0	0.819724	-0.155279	-1.217735
9	6	0	3.908765	-0.679589	1.086201
10	1	0	2.800955	0.446688	2.552614
11	6	0	3.894825	-1.203950	-0.213776
12	1	0	2.796598	-1.437350	-2.053698
13	1	0	4.776833	-0.833209	1.718460
14	6	0	-1.851528	0.625002	0.382196
15	6	0	-2.701735	0.874952	-0.701327
16	6	0	-2.087013	-0.492058	1.193324
17	6	0	-3.762739	0.022720	-0.977944
18	1	0	-2.526403	1.754015	-1.312883
19	6	0	-3.150402	-1.345872	0.926528
20	1	0	-1.448127	-0.689920	2.048326
21	6	0	-3.989432	-1.093390	-0.164095
22	1	0	-4.422055	0.217971	-1.817703
23	1	0	-3.335363	-2.208352	1.558806
24	7	0	-0.657713	2.790978	0.075765
25	7	0	0.541536	2.852134	-1.181532
26	7	0	1.083006	3.501967	-1.892341
27	6	0	-5.086562	-1.981372	-0.448278
28	6	0	5.036307	-1.941081	-0.693676
29	7	0	-5.966869	-2.697138	-0.678812
30	7	0	5.953259	-2.532403	-1.078699

System:	**4**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	R
M06–2X/6–31+G(d) energy (in a.u.):	-8275.90538929
Thermal correction to Gibbs Free Energy (in a.u.):	0.283132
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.888977	-0.889248	-0.763892
2	6	0	-0.525656	-2.036487	-0.911153
3	6	0	-1.313464	0.471562	-0.600414
4	6	0	-2.200596	1.043529	-1.518091
5	6	0	-0.845958	1.251937	0.472974
6	6	0	-2.616713	2.365294	-1.382913
7	1	0	-2.579501	0.439013	-2.335655
8	6	0	-1.258191	2.565385	0.616071
9	1	0	-0.149234	0.824557	1.188423
10	6	0	-2.144462	3.130735	-0.311684
11	1	0	-3.308622	2.778208	-2.107339
12	1	0	-0.902393	3.180131	1.436207
13	7	0	-4.017574	-1.605728	-0.732007
14	7	0	-3.602035	-2.695612	-1.093595
15	7	0	-3.206362	-3.677594	-1.496866
16	53	0	2.345626	-0.750974	-0.318197
17	14	0	-4.352643	-1.270306	0.989902
18	6	0	-5.890345	-2.239364	1.460159
19	1	0	-6.149533	-2.072657	2.512103
20	1	0	-6.747051	-1.938999	0.847988
21	1	0	-5.738515	-3.316033	1.322235
22	6	0	-4.643303	0.569617	1.087756
23	1	0	-3.708456	1.127286	0.969438
24	1	0	-5.334750	0.893367	0.302218
25	1	0	-5.079171	0.836543	2.057169
26	6	0	-2.891768	-1.834486	2.020517
27	1	0	-2.624442	-2.874720	1.799475
28	1	0	-2.008503	-1.216232	1.831731
29	1	0	-3.131770	-1.773116	3.088448
30	6	0	4.435935	0.875739	1.182336
31	6	0	5.398743	-0.570208	-0.386863
32	6	0	5.937918	1.106651	1.288613
33	6	0	6.568160	0.160023	0.261979
34	1	0	6.136484	2.162900	1.089883
35	1	0	6.243684	0.902871	2.317936
36	1	0	7.127512	0.675236	-0.523010
37	1	0	7.233817	-0.585321	0.704527
38	7	0	4.225873	-0.094071	0.202079
39	8	0	5.451218	-1.408518	-1.250243
40	8	0	3.568195	1.419531	1.818797
41	1	0	-0.255304	-3.062545	-1.044547
42	8	0	-2.489756	4.420915	-0.085763
43	6	0	-3.386919	5.034886	-0.988910
44	1	0	-3.525605	6.053142	-0.627100
45	1	0	-2.970495	5.059619	-2.002805
46	1	0	-4.352295	4.514874	-1.000005

System:	**4**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS1
M06–2X/6–31+G(d) energy (in a.u.):	-8275.86169668
Thermal correction to Gibbs Free Energy (in a.u.):	0.289234
Number of imaginary frequencies:	1 (–344 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.262228	-0.916555	-0.487608
2	6	0	-0.313851	-1.787715	-0.460428
3	6	0	-1.468269	0.525545	-0.401287
4	6	0	-2.210986	1.211061	-1.364770
5	6	0	-0.892280	1.249749	0.657413
6	6	0	-2.393043	2.588772	-1.287321
7	1	0	-2.656256	0.658930	-2.188025
8	6	0	-1.066094	2.619949	0.744857
9	1	0	-0.280251	0.735177	1.392315
10	6	0	-1.820119	3.297364	-0.223989
11	1	0	-2.969538	3.093796	-2.053309
12	1	0	-0.608596	3.193043	1.544257
13	7	0	-2.955934	-1.561712	-0.573405
14	7	0	-2.984296	-2.670639	-1.129406
15	7	0	-2.883427	-3.651217	-1.671595
16	53	0	1.906776	-0.954800	-0.209574
17	14	0	-4.035137	-1.257794	0.897177
18	6	0	-5.373833	-2.556460	0.746993
19	1	0	-6.086416	-2.443475	1.571887
20	1	0	-5.936124	-2.456835	-0.187872
21	1	0	-4.973110	-3.574648	0.802277
22	6	0	-4.697597	0.475683	0.748537
23	1	0	-3.921949	1.224700	0.938251
24	1	0	-5.115129	0.660547	-0.246428
25	1	0	-5.498177	0.616505	1.484737
26	6	0	-2.933520	-1.519058	2.376917
27	1	0	-2.471715	-2.511979	2.359313
28	1	0	-2.130997	-0.775261	2.406425
29	1	0	-3.513373	-1.429448	3.302742
30	6	0	4.199511	0.965214	0.903158
31	6	0	5.130053	-0.692319	-0.380836
32	6	0	5.703278	1.253634	0.938974
33	6	0	6.323673	0.148453	0.084441
34	1	0	5.872699	2.261278	0.549593
35	1	0	6.033732	1.245073	1.981236
36	1	0	6.853255	0.516829	-0.798299
37	1	0	7.011930	-0.500379	0.632837
38	7	0	3.970119	-0.150568	0.130952
39	8	0	5.202283	-1.676950	-1.086983
40	8	0	3.349021	1.623664	1.471686
41	1	0	-0.388111	-2.870240	-0.489034
42	8	0	-1.937266	4.633285	-0.051197
43	6	0	-2.638598	5.374251	-1.029864
44	1	0	-2.589113	6.414146	-0.709276
45	1	0	-2.166865	5.270816	-2.013867
46	1	0	-3.687187	5.058497	-1.087801

System:	**4**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN1
M06–2X/6–31+G(d) energy (in a.u.):	-8275.91345176
Thermal correction to Gibbs Free Energy (in a.u.):	0.297460
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.780026	-0.839574	0.182779
2	6	0	-1.539151	-1.931373	0.027663
3	6	0	-1.102089	0.587825	0.047084
4	6	0	-2.280849	1.128507	0.567386
5	6	0	-0.178597	1.438450	-0.585021
6	6	0	-2.555786	2.487045	0.441496
7	1	0	-2.984506	0.491474	1.095346
8	6	0	-0.441850	2.788478	-0.716733
9	1	0	0.775524	1.064760	-0.951393
10	6	0	-1.636736	3.320093	-0.211963
11	1	0	-3.473048	2.882383	0.861233
12	1	0	0.285265	3.441643	-1.188695
13	7	0	0.618647	-1.051084	0.554075
14	7	0	1.244309	-1.906780	-0.150115
15	7	0	1.788772	-2.667372	-0.754599
16	53	0	-3.489458	-1.969034	-0.708710
17	14	0	1.426097	-0.285088	2.094913
18	6	0	-0.010235	-0.524582	3.279406
19	1	0	0.296258	-0.195996	4.280098
20	1	0	-0.881912	0.073434	2.992244
21	1	0	-0.315360	-1.574259	3.350419
22	6	0	1.814665	1.520378	1.907034
23	1	0	2.159399	1.779951	0.902322
24	1	0	0.934528	2.126279	2.148575
25	1	0	2.610869	1.768554	2.620942
26	6	0	2.807428	-1.464325	2.484295
27	1	0	2.409521	-2.433994	2.805873
28	1	0	3.486625	-1.624888	1.639764
29	1	0	3.388388	-1.055427	3.319858
30	6	0	4.269567	-0.915743	-0.748408
31	6	0	3.504482	1.122443	-1.187792
32	6	0	5.406757	-0.288167	-1.563328
33	6	0	4.881150	1.109288	-1.866674
34	1	0	6.321999	-0.301901	-0.964304
35	1	0	5.589650	-0.901520	-2.450298
36	1	0	5.489361	1.917109	-1.449506
37	1	0	4.752188	1.316721	-2.932857
38	7	0	3.226932	-0.059506	-0.561654
39	8	0	2.758308	2.101672	-1.218374
40	8	0	4.313825	-2.073308	-0.320853
41	1	0	-1.147617	-2.919601	0.243691
42	8	0	-1.812981	4.649138	-0.384029
43	6	0	-3.000264	5.236650	0.108877
44	1	0	-2.938155	6.294032	-0.145685
45	1	0	-3.884592	4.796215	-0.366556
46	1	0	-3.073079	5.125859	1.197280

System:	**4**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS2
M06–2X/6–31+G(d) energy (in a.u.):	-8275.91092942
Thermal correction to Gibbs Free Energy (in a.u.):	0.299068
Number of imaginary frequencies:	1 (–77 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.682379	-0.780795	0.123600
2	6	0	-1.305408	-1.966451	0.081344
3	6	0	-1.210611	0.582830	-0.031213
4	6	0	-2.428148	0.960252	0.542103
5	6	0	-0.459863	1.543904	-0.729307
6	6	0	-2.911538	2.257636	0.406062
7	1	0	-2.996564	0.246070	1.129622
8	6	0	-0.932971	2.836109	-0.872079
9	1	0	0.517102	1.302956	-1.143737
10	6	0	-2.164358	3.200613	-0.311875
11	1	0	-3.853617	2.522527	0.870981
12	1	0	-0.351839	3.581749	-1.405102
13	7	0	0.763718	-0.798007	0.339626
14	7	0	1.380628	-1.685237	-0.330218
15	7	0	1.916633	-2.481768	-0.896199
16	53	0	-3.284217	-2.311521	-0.478801
17	14	0	1.700416	0.098873	1.785082
18	6	0	0.210489	-0.006859	2.952124
19	1	0	0.559238	0.305285	3.945361
20	1	0	-0.609575	0.662540	2.673200
21	1	0	-0.188442	-1.023515	3.049542
22	6	0	2.108018	1.910890	1.648028
23	1	0	1.706275	2.359753	0.737020
24	1	0	1.690776	2.429204	2.518793
25	1	0	3.192845	2.047977	1.621382
26	6	0	2.966594	-1.081279	2.482115
27	1	0	2.885811	-2.090808	2.067277
28	1	0	3.984157	-0.749636	2.267868
29	1	0	2.818045	-1.141065	3.566648
30	6	0	4.360241	-0.781564	-0.483637
31	6	0	3.436202	1.134666	-1.160568
32	6	0	5.423510	-0.188501	-1.413811
33	6	0	4.788665	1.115072	-1.882976
34	1	0	6.349498	-0.053324	-0.846892
35	1	0	5.633930	-0.900595	-2.216275
36	1	0	5.348207	2.011934	-1.601044
37	1	0	4.616248	1.165164	-2.961564
38	7	0	3.303386	0.072475	-0.305599
39	8	0	2.587534	1.999282	-1.362620
40	8	0	4.440759	-1.905655	0.004205
41	1	0	-0.770661	-2.884573	0.298637
42	8	0	-2.544269	4.484234	-0.500324
43	6	0	-3.772478	4.906675	0.058221
44	1	0	-3.879837	5.955624	-0.215410
45	1	0	-4.610716	4.332544	-0.353587
46	1	0	-3.761712	4.812285	1.150439

System:	**4**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN2
M06–2X/6–31+G(d) energy (in a.u.):	-7506.83711345
Thermal correction to Gibbs Free Energy (in a.u.):	0.118923
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.741155	1.232548	0.176050
2	6	0	-1.886261	0.532224	0.113331
3	6	0	0.640768	0.704014	0.186018
4	6	0	1.614197	1.291209	-0.621721
5	6	0	1.014327	-0.354000	1.027069
6	6	0	2.926702	0.821540	-0.631105
7	1	0	1.344745	2.130153	-1.256493
8	6	0	2.316264	-0.824100	1.036496
9	1	0	0.281733	-0.798885	1.692829
10	6	0	3.279401	-0.244401	0.200687
11	1	0	3.654857	1.294249	-1.279525
12	1	0	2.618398	-1.636261	1.689457
13	7	0	-0.740522	2.660871	0.230166
14	7	0	-1.839158	3.219950	0.116853
15	53	0	-2.061414	-1.530166	-0.175270
16	7	0	-2.789937	3.820140	0.027736
17	8	0	4.524405	-0.776462	0.276083
18	6	0	5.533197	-0.216779	-0.539341
19	1	0	6.439362	-0.783079	-0.326478
20	1	0	5.281353	-0.314681	-1.602054
21	1	0	5.696055	0.839989	-0.296257
22	1	0	-2.854134	1.018770	0.150966

System:	**4**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS3
M06–2X/6–31+G(d) energy (in a.u.):	-7506.78547981
Thermal correction to Gibbs Free Energy (in a.u.):	0.113953
Number of imaginary frequencies:	1 (–534 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.371911	0.265781	0.165953
2	6	0	1.319550	-0.729881	0.254092
3	6	0	-1.071975	-0.063124	0.077576
4	6	0	-2.023609	0.712891	0.739566
5	6	0	-1.503628	-1.150748	-0.694948
6	6	0	-3.382687	0.416686	0.648690
7	1	0	-1.693218	1.545300	1.355296
8	6	0	-2.850042	-1.457946	-0.793594
9	1	0	-0.770859	-1.743094	-1.237354
10	6	0	-3.798226	-0.674731	-0.120898
11	1	0	-4.097937	1.030917	1.183014
12	1	0	-3.200393	-2.291044	-1.394173
13	7	0	0.854734	1.479123	0.431026
14	7	0	-0.028638	2.658895	-0.562983
15	53	0	3.376126	-0.477763	0.036860
16	7	0	-0.291679	3.723382	-0.689253
17	8	0	-5.090972	-1.050144	-0.278710
18	6	0	-6.087070	-0.288849	0.373535
19	1	0	-7.037437	-0.753962	0.113874
20	1	0	-5.952716	-0.312845	1.461428
21	1	0	-6.080350	0.750657	0.024853
22	1	0	1.039768	-1.713618	0.617780

System:	**4**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN3
M06–2X/6–31+G(d) energy (in a.u.):	-7397.40581569
Thermal correction to Gibbs Free Energy (in a.u.):	0.111904
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.357886	1.066072	0.471988
2	6	0	-1.721166	0.887840	0.864703
3	7	0	-1.109531	2.049334	0.189918
4	6	0	0.989259	0.571166	0.340801
5	6	0	1.321121	-0.700487	0.832663
6	6	0	1.966872	1.351630	-0.282503
7	6	0	2.611711	-1.179050	0.704749
8	1	0	0.553499	-1.305691	1.307005
9	6	0	3.267729	0.880494	-0.414354
10	1	0	1.700180	2.332664	-0.665518
11	6	0	3.591440	-0.390333	0.081844
12	1	0	2.895391	-2.159155	1.072879
13	1	0	4.013129	1.498677	-0.899904
14	53	0	-3.045054	-0.412172	-0.257174
15	8	0	4.821648	-0.941239	0.004336
16	6	0	5.852601	-0.197289	-0.617735
17	1	0	6.035645	0.742362	-0.084161
18	1	0	6.742258	-0.823741	-0.569299
19	1	0	5.607967	0.012704	-1.665167
20	1	0	-2.096781	0.991584	1.877309

System:	**4**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS4
M06–2X/6–31+G(d) energy (in a.u.):	-7970.69051297
Thermal correction to Gibbs Free Energy (in a.u.):	0.223591
Number of imaginary frequencies:	1 (–280 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.246235	-0.543751	-1.489773
2	6	0	-0.711530	0.085824	-2.251969
3	7	0	-0.516742	-1.184625	-2.451588
4	6	0	1.588774	-0.492999	-0.994617
5	6	0	2.059769	0.722004	-0.479648
6	6	0	2.405863	-1.639966	-0.981848
7	6	0	3.357193	0.812019	0.012110
8	1	0	1.390249	1.581106	-0.450647
9	6	0	3.691168	-1.553673	-0.495495
10	1	0	2.018483	-2.581177	-1.361681
11	6	0	4.173619	-0.325613	0.003997
12	1	0	3.709131	1.755576	0.410306
13	1	0	4.355022	-2.411293	-0.478692
14	53	0	-1.685347	2.199796	0.034062
15	7	0	-0.697194	-1.239030	0.276062
16	7	0	-0.107006	-0.769387	1.252564
17	7	0	0.517286	-0.320308	2.074707
18	14	0	-2.429938	-1.792310	0.482314
19	6	0	-2.307845	-3.661678	0.543324
20	1	0	-1.699089	-3.998308	1.389174
21	1	0	-3.302232	-4.112083	0.642870
22	1	0	-1.854960	-4.047754	-0.376699
23	6	0	-3.426745	-1.256640	-1.000703
24	1	0	-4.466177	-1.562102	-0.826251
25	1	0	-3.411070	-0.167658	-1.111840
26	1	0	-3.095720	-1.735162	-1.927507
27	6	0	-3.031205	-1.060109	2.089155
28	1	0	-2.977600	0.033634	2.047388
29	1	0	-4.074364	-1.349585	2.261050
30	1	0	-2.444886	-1.411127	2.945952
31	8	0	5.437470	-0.350323	0.459468
32	6	0	5.985138	0.842387	0.998867
33	1	0	6.998980	0.589527	1.304959
34	1	0	6.014316	1.634156	0.242609
35	1	0	5.408830	1.176922	1.867942
36	1	0	-1.283202	0.937678	-2.594962

System:	**4**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN4
M06–2X/6–31+G(d) energy (in a.u.):	-1050.56050129
Thermal correction to Gibbs Free Energy (in a.u.):	0.228955
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.502249	1.101387	0.183901
2	6	0	-0.880328	2.476160	0.392734
3	7	0	-1.124772	2.055375	-0.768247
4	6	0	0.876297	0.570335	0.033772
5	6	0	1.114364	-0.641328	-0.635948
6	6	0	1.957257	1.288821	0.538941
7	6	0	2.402501	-1.113652	-0.793778
8	1	0	0.284522	-1.211242	-1.049151
9	6	0	3.262889	0.829306	0.381563
10	1	0	1.789266	2.227021	1.063399
11	6	0	3.490156	-0.379170	-0.287445
12	1	0	2.606987	-2.043862	-1.313316
13	1	0	4.084274	1.410833	0.782425
14	7	0	-1.511232	0.051053	0.587380
15	7	0	-1.144232	-0.674194	1.557410
16	7	0	-0.810858	-1.319077	2.404243
17	14	0	-3.090801	-0.411202	-0.394120
18	6	0	-4.205542	1.065315	-0.234371
19	1	0	-5.210547	0.790245	-0.576136
20	1	0	-4.292801	1.396759	0.805618
21	1	0	-3.862033	1.903079	-0.847016
22	6	0	-3.662004	-1.905614	0.558870
23	1	0	-4.575186	-2.286650	0.086404
24	1	0	-2.935205	-2.725218	0.543455
25	1	0	-3.918423	-1.675474	1.598765
26	6	0	-2.464061	-0.760548	-2.105630
27	1	0	-1.892235	-1.692462	-2.151488
28	1	0	-3.317937	-0.863181	-2.785938
29	1	0	-1.843659	0.059858	-2.480511
30	8	0	4.700400	-0.918933	-0.494212
31	6	0	5.846169	-0.224341	-0.020454
32	1	0	6.700010	-0.836506	-0.304423
33	1	0	5.925116	0.760640	-0.492619
34	1	0	5.813591	-0.119679	1.069270
35	1	0	-0.962760	3.381998	0.984198

System:	**4**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS5
M06–2X/6–31+G(d) energy (in a.u.):	-1410.70496037
Thermal correction to Gibbs Free Energy (in a.u.):	0.305923
Number of imaginary frequencies:	1 (–56 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.704240	-0.814828	0.608173
2	6	0	0.144326	-2.030362	1.150863
3	7	0	0.246548	-1.103642	1.993469
4	6	0	2.153261	-0.589497	0.325444
5	6	0	2.597124	0.409671	-0.536939
6	6	0	3.109881	-1.404232	0.950650
7	6	0	3.957700	0.602393	-0.785867
8	1	0	1.884778	1.071697	-1.021590
9	6	0	4.460825	-1.222592	0.716057
10	1	0	2.792963	-2.183116	1.638612
11	6	0	4.895929	-0.216319	-0.157086
12	1	0	4.263387	1.392440	-1.461651
13	1	0	5.205691	-1.846560	1.199246
14	7	0	-0.213159	0.083175	-0.125822
15	7	0	-0.442546	-0.270751	-1.314090
16	7	0	-0.627613	-0.509746	-2.386918
17	14	0	-1.315872	1.445492	0.684733
18	6	0	-1.709082	2.619641	-0.717350
19	1	0	-2.180175	2.132664	-1.573009
20	1	0	-2.428165	3.364191	-0.359003
21	1	0	-0.795557	3.140032	-1.028315
22	6	0	0.185365	2.224286	1.553164
23	1	0	-0.153142	3.133930	2.067495
24	1	0	0.612580	1.562950	2.315918
25	1	0	0.986168	2.514351	0.863952
26	6	0	-2.431843	0.986394	2.118214
27	1	0	-2.388146	-0.092601	2.295118
28	1	0	-2.098421	1.498175	3.027150
29	1	0	-3.466546	1.260124	1.895081
30	7	0	-2.963239	-0.062889	-0.384049
31	6	0	-4.238323	0.440458	-0.524693
32	6	0	-5.256700	-0.682314	-0.755513
33	6	0	-4.422250	-1.950912	-0.617454
34	6	0	-3.005579	-1.418570	-0.393646
35	8	0	-2.026617	-2.163561	-0.248149
36	1	0	-4.702489	-2.573177	0.237842
37	1	0	-6.060953	-0.589695	-0.021024
38	8	0	-4.532403	1.623496	-0.453218
39	1	0	-4.424996	-2.593436	-1.502430
40	1	0	-5.701965	-0.554333	-1.746495
41	1	0	-0.156911	-3.064240	1.049166
42	8	0	6.237553	-0.117349	-0.323949
43	6	0	6.723042	0.890976	-1.187654
44	1	0	7.808452	0.798471	-1.175697
45	1	0	6.354027	0.745311	-2.209849
46	1	0	6.435932	1.887061	-0.830540

System:	**4**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN5
M06–2X/6–31+G(d) energy (in a.u.):	-641.611479186
Thermal correction to Gibbs Free Energy (in a.u.):	0.124360
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.316890	1.506988	0.642489
2	6	0	1.725795	0.328339	0.048199
3	7	0	2.239433	1.575153	-0.613601
4	6	0	0.255248	0.072637	0.037429
5	6	0	-0.261120	-1.228274	0.105632
6	6	0	-0.636273	1.140946	-0.042721
7	6	0	-1.629412	-1.446371	0.100288
8	1	0	0.419309	-2.071182	0.158016
9	6	0	-2.015844	0.934204	-0.053548
10	1	0	-0.260703	2.157867	-0.112563
11	6	0	-2.516699	-0.366976	0.020367
12	1	0	-2.039034	-2.450098	0.152196
13	1	0	-2.678255	1.789191	-0.123221
14	7	0	2.482511	-0.900618	-0.138340
15	7	0	3.707166	-0.773202	-0.082351
16	7	0	4.835556	-0.743772	-0.044188
17	1	0	2.652185	2.116710	1.477044
18	8	0	-3.838041	-0.682582	0.020138
19	6	0	-4.767816	0.376370	-0.071460
20	1	0	-4.637818	0.936855	-1.005094
21	1	0	-5.753659	-0.087727	-0.060162
22	1	0	-4.674967	1.058942	0.781987

System:	**4**
Oxidant:	NIS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS6
M06–2X/6–31+G(d) energy (in a.u.):	-641.550012902
Thermal correction to Gibbs Free Energy (in a.u.):	0.118441
Number of imaginary frequencies:	1 (–618 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.481027	1.568577	0.556191
2	6	0	1.804516	0.524165	-0.272641
3	7	0	2.342235	2.031386	-0.572241
4	6	0	0.313589	0.413269	-0.150536
5	6	0	-0.294745	-0.824448	-0.352551
6	6	0	-0.500141	1.510828	0.168901
7	6	0	-1.676074	-0.982739	-0.236631
8	1	0	0.325436	-1.675238	-0.617139
9	6	0	-1.874497	1.368325	0.281886
10	1	0	-0.061434	2.493811	0.312312
11	6	0	-2.472220	0.118931	0.082959
12	1	0	-2.111943	-1.961199	-0.403345
13	1	0	-2.510668	2.214626	0.521154
14	7	0	2.552091	-0.444514	-0.849291
15	7	0	3.366165	-1.391801	0.367153
16	7	0	4.056995	-2.234948	0.548125
17	1	0	2.810999	1.776680	1.569303
18	8	0	-3.824449	0.078367	0.219071
19	6	0	-4.468622	-1.160564	0.010424
20	1	0	-5.532104	-0.975325	0.159630
21	1	0	-4.300434	-1.526933	-1.009511
22	1	0	-4.123647	-1.912289	0.730803

System:	**2**
Oxidant:	NCS
Nitrogen-donor:	$TMSN_3$
Stationary point:	R
M06–2X/6–31+G(d) energy (in a.u.):	-2011.24416299
Thermal correction to Gibbs Free Energy (in a.u.):	0.382148
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.057903	0.411363	-0.845762
2	6	0	-0.680575	1.362032	-0.679850
3	6	0	1.011868	-0.636955	-1.069973
4	6	0	2.213289	-0.331676	-1.726217
5	6	0	0.798877	-1.954067	-0.628811
6	6	0	3.183879	-1.310915	-1.915461
7	1	0	2.377538	0.680053	-2.085468
8	6	0	1.773278	-2.923504	-0.833719
9	1	0	-0.122395	-2.218613	-0.120231
10	6	0	2.983522	-2.620642	-1.470998
11	1	0	4.112966	-1.045875	-2.415091
12	1	0	1.590905	-3.937378	-0.484178
13	7	0	4.609033	1.374861	-0.142814
14	7	0	3.642347	2.117715	-0.195838
15	7	0	2.765405	2.824496	-0.320715
16	6	0	-1.467322	2.546596	-0.485954
17	6	0	-2.870358	2.511759	-0.440638
18	6	0	-0.813155	3.779711	-0.345887
19	6	0	-3.590213	3.685881	-0.258529
20	1	0	-3.395821	1.568436	-0.550060
21	6	0	-1.549586	4.946123	-0.164715
22	1	0	0.271557	3.809455	-0.380652
23	6	0	-2.945943	4.920630	-0.117105
24	1	0	-4.676570	3.642213	-0.225616
25	1	0	-1.027861	5.894136	-0.058136
26	14	0	4.866995	0.255037	1.223520
27	6	0	5.662830	1.236694	2.611147
28	1	0	5.889029	0.589536	3.466548
29	1	0	6.597651	1.699767	2.278800
30	1	0	4.997849	2.033424	2.962863
31	6	0	6.032841	-1.041970	0.554987
32	1	0	5.557915	-1.602922	-0.256549
33	1	0	6.945506	-0.580291	0.163683
34	1	0	6.318828	-1.751865	1.339050
35	6	0	3.220035	-0.450354	1.763785
36	1	0	2.454736	0.329870	1.859559
37	1	0	2.851554	-1.189433	1.044846
38	1	0	3.315513	-0.940883	2.739630
39	6	0	-3.427044	-3.490684	0.641816
40	6	0	-5.111956	-1.848996	0.403397
41	6	0	-4.738592	-4.196463	0.948045
42	6	0	-5.832755	-3.129770	0.795063
43	1	0	-4.847433	-5.032349	0.252559
44	1	0	-4.676058	-4.612770	1.956498
45	1	0	-6.561475	-3.364175	0.015218
46	1	0	-6.386823	-2.941367	1.717954
47	7	0	-3.749767	-2.163499	0.346156
48	8	0	-5.578470	-0.764454	0.179058
49	8	0	-2.313042	-3.944389	0.642377
50	6	0	-3.747618	6.181798	0.081370
51	1	0	-3.097222	7.057044	0.161046
52	1	0	-4.435408	6.346188	-0.755043
53	1	0	-4.350574	6.124202	0.994061
54	6	0	4.036720	-3.682823	-1.659208
55	1	0	4.437375	-4.014403	-0.694052
56	1	0	3.622567	-4.563865	-2.160422

57	1	0	4.871863	-3.312419	-2.260560
58	17	0	-2.571189	-1.024888	-0.056191

System:	**2**
Oxidant:	NCS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS1
M06–2X/6–31+G(d) energy (in a.u.):	-2011.18322325
Thermal correction to Gibbs Free Energy (in a.u.):	0.385619
Number of imaginary frequencies:	1 (–424 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.657328	0.502510	-0.319839
2	6	0	-0.220035	-0.694001	-0.130964
3	6	0	-0.178871	1.883007	-0.339850
4	6	0	-0.699080	2.848479	-1.209038
5	6	0	0.864859	2.246888	0.528290
6	6	0	-0.192693	4.145917	-1.208773
7	1	0	-1.496924	2.582618	-1.896661
8	6	0	1.372414	3.538909	0.505971
9	1	0	1.297515	1.512279	1.199006
10	6	0	0.851228	4.512297	-0.355409
11	1	0	-0.607730	4.880900	-1.894521
12	1	0	2.197936	3.786869	1.168735
13	7	0	-2.444896	0.631093	-0.595207
14	7	0	-2.883624	-0.197893	-1.407784
15	7	0	-3.199294	-0.968441	-2.163946
16	6	0	-0.866248	-1.992134	-0.005249
17	6	0	-0.402692	-3.095526	-0.739492
18	6	0	-1.951028	-2.177002	0.863113
19	6	0	-1.046074	-4.322497	-0.641757
20	1	0	0.466940	-2.978969	-1.380008
21	6	0	-2.578967	-3.416704	0.964653
22	1	0	-2.285376	-1.345897	1.479722
23	6	0	-2.145716	-4.506497	0.206594
24	1	0	-0.678280	-5.163113	-1.225964
25	1	0	-3.413352	-3.540868	1.651892
26	14	0	-3.563188	1.466733	0.589076
27	6	0	-4.983356	0.271536	0.831530
28	1	0	-5.664398	0.652467	1.600992
29	1	0	-5.567840	0.145967	-0.087034
30	1	0	-4.636049	-0.717218	1.149727
31	6	0	-4.133342	3.058256	-0.204842
32	1	0	-3.299111	3.756666	-0.324813
33	1	0	-4.578103	2.877871	-1.189793
34	1	0	-4.893877	3.540218	0.420610
35	6	0	-2.525171	1.746540	2.109145
36	1	0	-2.005335	0.836482	2.425925
37	1	0	-1.768911	2.517567	1.929116
38	1	0	-3.164328	2.081093	2.934490
39	6	0	4.545782	0.094973	0.720436
40	6	0	4.599221	-1.914780	-0.418542
41	6	0	6.031512	-0.264996	0.639649
42	6	0	6.066516	-1.602079	-0.106440
43	1	0	6.555378	0.541482	0.119444
44	1	0	6.432362	-0.316470	1.655454
45	1	0	6.621088	-1.566742	-1.047794
46	1	0	6.475915	-2.424377	0.486421
47	7	0	3.827450	-0.897792	0.099478
48	8	0	4.191164	-2.886812	-1.015971
49	8	0	4.081595	1.089116	1.243600
50	6	0	-2.816399	-5.852664	0.309697
51	1	0	-3.678291	-5.816663	0.981794
52	1	0	-3.165047	-6.195259	-0.670314
53	1	0	-2.122050	-6.608478	0.692424
54	6	0	1.420821	5.907341	-0.365916
55	1	0	0.862215	6.561353	-1.040995
56	1	0	1.397350	6.349770	0.635378

57	1	0	2.466135	5.896082	-0.692768
58	17	0	1.925009	-0.792572	-0.027891

System:	**2**
Oxidant:	NCS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN1
M06–2X/6–31+G(d) energy (in a.u.):	-2011.26739891
Thermal correction to Gibbs Free Energy (in a.u.):	0.396900
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.259463	-1.146754	0.160050
2	6	0	0.723769	-1.568847	-0.655153
3	6	0	-1.714370	-1.323740	0.011467
4	6	0	-2.483656	-1.802506	1.074324
5	6	0	-2.342712	-0.963842	-1.187245
6	6	0	-3.864436	-1.926447	0.943680
7	1	0	-2.002981	-2.079264	2.011085
8	6	0	-3.721392	-1.086128	-1.303583
9	1	0	-1.735595	-0.574923	-2.001203
10	6	0	-4.504062	-1.566993	-0.245179
11	1	0	-4.452310	-2.304646	1.776328
12	1	0	-4.205706	-0.794768	-2.232877
13	7	0	0.102862	-0.428343	1.382665
14	7	0	1.036672	-0.956580	2.051528
15	7	0	1.869548	-1.378126	2.666483
16	6	0	2.151772	-1.214965	-0.516479
17	6	0	3.143308	-2.200190	-0.514373
18	6	0	2.515302	0.127854	-0.352507
19	6	0	4.477069	-1.848306	-0.324201
20	1	0	2.869611	-3.241862	-0.659857
21	6	0	3.850953	0.464906	-0.163763
22	1	0	1.739218	0.889497	-0.396842
23	6	0	4.852314	-0.513628	-0.144890
24	1	0	5.239066	-2.623738	-0.317768
25	1	0	4.123174	1.511376	-0.042996
26	14	0	-0.555653	1.224419	2.156093
27	6	0	0.927939	2.344597	2.082131
28	1	0	0.682197	3.278687	2.599364
29	1	0	1.775520	1.877000	2.600920
30	1	0	1.201870	2.595335	1.058831
31	6	0	-0.692084	0.622655	3.940869
32	1	0	-1.354431	-0.246489	4.029562
33	1	0	0.267641	0.383333	4.412657
34	1	0	-1.141019	1.427686	4.536387
35	6	0	-2.280272	1.520214	1.543870
36	1	0	-2.538963	2.551347	1.807124
37	1	0	-2.354801	1.423325	0.460731
38	1	0	-2.970476	0.825829	2.033330
39	6	0	-0.664057	3.206819	-0.730920
40	6	0	-0.111702	1.593113	-2.160052
41	6	0	-0.759586	3.902270	-2.095753
42	6	0	-0.378329	2.799051	-3.073928
43	1	0	-1.775730	4.285817	-2.226940
44	1	0	-0.084120	4.762754	-2.104192
45	1	0	-1.168095	2.537741	-3.784581
46	1	0	0.524566	3.007688	-3.655298
47	7	0	-0.289611	1.897509	-0.840104
48	8	0	0.220417	0.492982	-2.600122

49	8	0	-0.905418	3.786960	0.328757
50	6	0	-5.997754	-1.695117	-0.399153
51	1	0	-6.443279	-0.742767	-0.704531
52	1	0	-6.248284	-2.435169	-1.166901
53	1	0	-6.469503	-2.006655	0.536547
54	6	0	6.299426	-0.128920	0.025707
55	1	0	6.717264	0.230257	-0.921671
56	1	0	6.411934	0.674528	0.759780
57	1	0	6.901820	-0.980474	0.353689
58	17	0	0.335671	-2.654391	-1.946387

System:	**2**
Oxidant:	NCS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS2
M06–2X/6–31+G(d) energy (in a.u.):	-2011.26349316
Thermal correction to Gibbs Free Energy (in a.u.):	0.398413
Number of imaginary frequencies:	1 (–29 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.009035	-1.109797	0.298170
2	6	0	1.052687	-1.686866	-0.320993
3	6	0	-1.413305	-1.501845	0.256425
4	6	0	-2.109898	-1.715141	1.447922
5	6	0	-2.086137	-1.646249	-0.963553
6	6	0	-3.455416	-2.070585	1.426001
7	1	0	-1.598867	-1.596257	2.401509
8	6	0	-3.431768	-1.991363	-0.974341
9	1	0	-1.546234	-1.470831	-1.888892
10	6	0	-4.138370	-2.209023	0.215760
11	1	0	-3.983077	-2.234317	2.362153
12	1	0	-3.949092	-2.092194	-1.925907
13	7	0	0.261108	0.035293	1.167148
14	7	0	1.213540	-0.148887	1.978739
15	7	0	2.065542	-0.271509	2.690837
16	6	0	2.438036	-1.169124	-0.337805
17	6	0	3.517818	-2.014179	-0.063103
18	6	0	2.684188	0.187129	-0.598046
19	6	0	4.815176	-1.509673	-0.028152
20	1	0	3.340703	-3.069347	0.126612
21	6	0	3.984071	0.677452	-0.561971
22	1	0	1.851017	0.835474	-0.853378
23	6	0	5.070251	-0.158369	-0.274994
24	1	0	5.642590	-2.178765	0.194286
25	1	0	4.160387	1.730179	-0.771885
26	14	0	-0.638974	1.778690	1.420264
27	6	0	0.642488	3.126558	1.104487
28	1	0	0.482372	3.932302	1.829926
29	1	0	1.634618	2.701072	1.318510
30	1	0	0.645629	3.545937	0.100251
31	6	0	-0.350959	1.692085	3.339814
32	1	0	-0.686041	0.754332	3.804810
33	1	0	0.667932	1.904117	3.686816
34	1	0	-0.984526	2.483907	3.764034
35	6	0	-2.503739	1.521628	1.495751
36	1	0	-2.956450	2.495650	1.707525
37	1	0	-2.938890	1.128602	0.574847
38	1	0	-2.737143	0.846079	2.324025
39	6	0	-1.640057	2.968725	-1.061982
40	6	0	-0.644680	1.217629	-2.044961
41	6	0	-1.989082	3.150897	-2.536342
42	6	0	-1.360163	1.932653	-3.195024
43	1	0	-3.076278	3.210081	-2.636579
44	1	0	-1.576356	4.103795	-2.879654
45	1	0	-2.090786	1.238583	-3.622695
46	1	0	-0.632048	2.162810	-3.976807
47	7	0	-0.916848	1.816085	-0.838932
48	8	0	0.072718	0.243069	-2.229204

49	8	0	-1.950612	3.765969	-0.186322
50	6	0	-5.597662	-2.583538	0.178407
51	1	0	-6.184740	-1.817887	-0.339583
52	1	0	-5.745354	-3.527846	-0.356408
53	1	0	-6.004792	-2.697995	1.186365
54	6	0	6.474859	0.387156	-0.263055
55	1	0	6.825875	0.575707	-1.283844
56	1	0	6.525822	1.334946	0.281629
57	1	0	7.170043	-0.314551	0.205479
58	17	0	0.796755	-3.173611	-1.182804

System:	**2**
Oxidant:	NCS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN2
M06–2X/6–31+G(d) energy (in a.u.):	-1242.19443514
Thermal correction to Gibbs Free Energy (in a.u.):	0.216578
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.564826	0.409380	0.009517
2	6	0	-0.343285	-0.573633	-0.185401
3	6	0	2.035814	0.243612	0.073937
4	6	0	2.867434	1.162085	-0.571822
5	6	0	2.623590	-0.787180	0.817696
6	6	0	4.252394	1.033165	-0.504698
7	1	0	2.424863	1.983799	-1.127096
8	6	0	4.005756	-0.902889	0.889722
9	1	0	1.993602	-1.491296	1.352622
10	6	0	4.844207	-0.001290	0.222878
11	1	0	4.882504	1.752713	-1.021476
12	1	0	4.444965	-1.704054	1.479801
13	7	0	0.183768	1.771608	0.202448
14	7	0	-0.821231	2.177458	-0.401003
15	7	0	-1.706807	2.671358	-0.892992
16	6	0	-1.805685	-0.438657	-0.013094
17	6	0	-2.701534	-0.891299	-0.990297
18	6	0	-2.320186	0.137874	1.153188
19	6	0	-4.071123	-0.746597	-0.810416
20	1	0	-2.316857	-1.356104	-1.893752
21	6	0	-3.695333	0.276228	1.326218
22	1	0	-1.636289	0.476449	1.927723
23	6	0	-4.592513	-0.158671	0.348809
24	1	0	-4.751742	-1.096199	-1.583443
25	1	0	-4.075346	0.724894	2.240578
26	6	0	-6.081366	-0.003782	0.524180
27	1	0	-6.495500	0.669860	-0.233845
28	1	0	-6.592312	-0.966796	0.421832
29	1	0	-6.324585	0.406211	1.507936
30	6	0	6.342054	-0.153527	0.293951
31	1	0	6.850076	0.710166	-0.143316
32	1	0	6.679160	-0.258316	1.330246
33	1	0	6.669402	-1.046903	-0.249398
34	17	0	0.182803	-2.163312	-0.698458

System:	**2**
Oxidant:	NCS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS3
M06–2X/6–31+G(d) energy (in a.u.):	-1242.14580123
Thermal correction to Gibbs Free Energy (in a.u.):	0.213242
Number of imaginary frequencies:	1 (–589 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.823971	-1.282123	-0.151326
2	6	0	0.501284	-1.612127	0.112190
3	6	0	-1.363184	0.095072	-0.004322
4	6	0	-2.316311	0.579846	-0.903221
5	6	0	-0.975248	0.901017	1.073002
6	6	0	-2.858097	1.852869	-0.736767
7	1	0	-2.612285	-0.039170	-1.746584
8	6	0	-1.521676	2.167331	1.233986
9	1	0	-0.241740	0.526031	1.782546
10	6	0	-2.471144	2.665469	0.331588
11	1	0	-3.590141	2.221938	-1.451006
12	1	0	-1.211979	2.782961	2.075526
13	6	0	1.626183	-0.680008	-0.046791
14	6	0	2.771915	-0.778606	0.757589
15	6	0	1.570771	0.348731	-1.000851
16	6	0	3.802710	0.145666	0.636282
17	1	0	2.845450	-1.575313	1.491078
18	6	0	2.611364	1.261256	-1.119923
19	1	0	0.710117	0.424738	-1.658255
20	6	0	3.743708	1.180585	-0.302830
21	1	0	4.673260	0.059488	1.282161
22	1	0	2.546703	2.047159	-1.868681
23	7	0	-1.507697	-2.277584	-0.714995
24	7	0	-3.121938	-2.265888	-0.126199
25	7	0	-4.161238	-2.568577	-0.356042
26	6	0	4.883719	2.153099	-0.459712
27	1	0	5.433932	2.274086	0.477741
28	1	0	5.593389	1.799933	-1.216963
29	1	0	4.525410	3.136758	-0.776668
30	6	0	-3.065988	4.036401	0.528574
31	1	0	-2.284972	4.785228	0.694620
32	1	0	-3.652737	4.343321	-0.341333
33	1	0	-3.727177	4.052825	1.402205
34	17	0	0.931334	-3.250736	0.502909

System:	**2**
Oxidant:	NCS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN3
M06–2X/6–31+G(d) energy (in a.u.):	-1132.76553543
Thermal correction to Gibbs Free Energy (in a.u.):	0.208350
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.658699	0.884121	0.660857
2	6	0	-0.655778	1.326999	0.292284
3	7	0	0.018590	1.433429	1.606821
4	6	0	1.914330	0.248364	0.326762
5	6	0	2.116551	-0.244040	-0.964049
6	6	0	2.920999	0.124953	1.293987
7	6	0	3.322504	-0.860244	-1.285648
8	1	0	1.328117	-0.139095	-1.704597
9	6	0	4.117641	-0.491100	0.960517
10	1	0	2.751632	0.515300	2.293626
11	6	0	4.335974	-0.992359	-0.332239
12	1	0	3.480432	-1.242741	-2.290331
13	1	0	4.901299	-0.588211	1.708050
14	6	0	-1.832369	0.412323	0.145843
15	6	0	-2.684971	0.450061	-0.957680
16	6	0	-2.066578	-0.541154	1.144266
17	6	0	-3.745544	-0.449194	-1.059531
18	1	0	-2.529258	1.187212	-1.738262
19	6	0	-3.130570	-1.428794	1.036379
20	1	0	-1.417307	-0.578287	2.014137
21	6	0	-3.988848	-1.400831	-0.068401
22	1	0	-4.398570	-0.402559	-1.927674
23	1	0	-3.300438	-2.156377	1.827094
24	6	0	5.643598	-1.658886	-0.672156
25	1	0	6.484613	-0.980234	-0.495710
26	1	0	5.802011	-2.545762	-0.049419
27	1	0	5.671764	-1.970136	-1.719304
28	6	0	-5.142599	-2.366162	-0.169388
29	1	0	-4.797273	-3.402835	-0.096939
30	1	0	-5.862626	-2.202981	0.639862
31	1	0	-5.672654	-2.251976	-1.118848
32	17	0	-0.780594	2.861196	-0.629426

System:	**2**
Oxidant:	NCS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS4
M06–2X/6–31+G(d) energy (in a.u.):	-1706.05189513
Thermal correction to Gibbs Free Energy (in a.u.):	0.322073
Number of imaginary frequencies:	1 (–237 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.542810	-0.455703	-0.910988
2	6	0	0.831195	-0.631460	-0.952221
3	7	0	0.196083	-0.298168	-2.053010
4	6	0	-1.826135	-1.035470	-0.590875
5	6	0	-2.072061	-1.557666	0.683625
6	6	0	-2.819871	-1.057642	-1.582582
7	6	0	-3.313214	-2.133738	0.944768
8	1	0	-1.312596	-1.456822	1.457178
9	6	0	-4.047513	-1.631900	-1.300013
10	1	0	-2.612037	-0.631972	-2.560713
11	6	0	-4.309962	-2.179919	-0.032390
12	1	0	-3.513311	-2.535785	1.933860
13	1	0	-4.820288	-1.660291	-2.064145
14	6	0	2.151827	-1.006066	-0.547173
15	6	0	2.431638	-1.400952	0.766996
16	6	0	3.163266	-0.985581	-1.525273
17	6	0	3.731963	-1.775331	1.090133
18	1	0	1.648498	-1.349668	1.519789
19	6	0	4.448669	-1.361371	-1.181872
20	1	0	2.923306	-0.675902	-2.539233
21	6	0	4.750368	-1.760501	0.132724
22	1	0	3.960266	-2.070385	2.110214
23	1	0	5.236965	-1.347368	-1.930174
24	7	0	-1.016987	1.564244	-0.390071
25	7	0	-2.003272	1.557492	0.353647
26	7	0	-2.927726	1.461971	0.987901
27	14	0	0.153711	2.954098	-0.189340
28	6	0	-0.134628	3.996278	-1.724087
29	1	0	-1.161114	4.376273	-1.763820
30	1	0	0.544899	4.856364	-1.744643
31	1	0	0.041232	3.405341	-2.630089
32	6	0	1.904132	2.312005	-0.182114
33	1	0	2.570533	3.170075	-0.025899
34	1	0	2.049383	1.605166	0.640708
35	1	0	2.190799	1.848994	-1.132626
36	6	0	-0.318302	3.855483	1.373553
37	1	0	-0.242092	3.171587	2.226369
38	1	0	0.364110	4.698346	1.534184
39	1	0	-1.336390	4.258520	1.324987
40	6	0	-5.657385	-2.785766	0.258576
41	1	0	-5.908413	-3.554387	-0.479656
42	1	0	-5.682721	-3.241592	1.251112
43	1	0	-6.440693	-2.021193	0.215859
44	6	0	6.158172	-2.155840	0.489359
45	1	0	6.231503	-2.472326	1.532281
46	1	0	6.503234	-2.978962	-0.145225
47	1	0	6.844844	-1.316014	0.338036
48	17	0	0.167961	0.416042	2.354839

System:	**2**
Oxidant:	NCS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN4
M06–2X/6–31+G(d) energy (in a.u.):	-1245.66316522
Thermal correction to Gibbs Free Energy (in a.u.):	0.323932
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.384923	0.156415	0.269807
2	6	0	-1.003736	0.238686	0.662063
3	7	0	-0.183199	0.602627	1.558750
4	6	0	1.195298	-1.093320	0.162518
5	6	0	0.775731	-2.219888	0.881573
6	6	0	2.347533	-1.183192	-0.619507
7	6	0	1.501455	-3.401208	0.816270
8	1	0	-0.116286	-2.170504	1.500672
9	6	0	3.067320	-2.375992	-0.680429
10	1	0	2.713000	-0.327771	-1.183596
11	6	0	2.659871	-3.503123	0.034102
12	1	0	1.163788	-4.264576	1.384179
13	1	0	3.962811	-2.425527	-1.293985
14	6	0	-2.392621	0.010653	0.362937
15	6	0	-2.751876	-0.579022	-0.854605
16	6	0	-3.378624	0.371206	1.295593
17	6	0	-4.092746	-0.806017	-1.138454
18	1	0	-1.980141	-0.872444	-1.562840
19	6	0	-4.710791	0.141145	0.996677
20	1	0	-3.088467	0.824279	2.239497
21	6	0	-5.088803	-0.449187	-0.221546
22	1	0	-4.373672	-1.268473	-2.080147
23	1	0	-5.479206	0.418766	1.713403
24	7	0	0.948942	1.314775	-0.500655
25	7	0	0.726540	1.300406	-1.742597
26	7	0	0.537662	1.292012	-2.843281
27	14	0	2.035779	2.655570	0.308213
28	6	0	3.073584	1.661290	1.479698
29	1	0	3.748065	0.976581	0.957282
30	1	0	3.681969	2.340834	2.087999
31	1	0	2.444076	1.079503	2.161178
32	6	0	0.834488	3.824777	1.105237
33	1	0	1.376343	4.675534	1.534759
34	1	0	0.113495	4.221611	0.383185
35	1	0	0.287396	3.329412	1.912706
36	6	0	2.917354	3.342992	-1.182224
37	1	0	2.240211	3.847343	-1.880549
38	1	0	3.644610	4.093982	-0.852534
39	1	0	3.478235	2.573540	-1.724760
40	6	0	3.430793	-4.795234	-0.025832
41	1	0	4.309340	-4.705923	-0.668901
42	1	0	3.768118	-5.093685	0.971817
43	1	0	2.804755	-5.603986	-0.416184
44	6	0	-6.542665	-0.695015	-0.518037
45	1	0	-6.970107	-1.392866	0.209571
46	1	0	-7.114170	0.236233	-0.451941
47	1	0	-6.683619	-1.114374	-1.516367

System:	**2**
Oxidant:	NCS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS5
M06–2X/6–31+G(d) energy (in a.u.):	-1605.79574355
Thermal correction to Gibbs Free Energy (in a.u.):	0.399005
Number of imaginary frequencies:	1 (–58 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.888639	-0.535968	0.394353
2	6	0	-0.803976	0.855049	0.792733
3	7	0	-0.690106	0.033195	1.747856
4	6	0	-2.171132	-1.227277	0.054915
5	6	0	-2.209843	-2.443246	-0.628153
6	6	0	-3.380830	-0.632760	0.436096
7	6	0	-3.430358	-3.051340	-0.920853
8	1	0	-1.288803	-2.938983	-0.923273
9	6	0	-4.590996	-1.246865	0.142962
10	1	0	-3.373999	0.314831	0.968860
11	6	0	-4.638760	-2.467346	-0.542149
12	1	0	-3.436900	-4.001231	-1.449587
13	1	0	-5.519232	-0.770033	0.449950
14	6	0	-0.994472	2.262638	0.518427
15	6	0	-1.081584	2.725558	-0.797140
16	6	0	-1.126155	3.151365	1.589535
17	6	0	-1.305253	4.074103	-1.034167
18	1	0	-0.945291	2.028148	-1.618086
19	6	0	-1.346782	4.500309	1.338433
20	1	0	-1.059459	2.777334	2.607713
21	6	0	-1.438041	4.979770	0.026707
22	1	0	-1.368449	4.437716	-2.056727
23	1	0	-1.451316	5.193042	2.169462
24	7	0	0.320860	-1.198868	-0.138981
25	7	0	0.510816	-1.026166	-1.371759
26	7	0	0.671494	-0.942281	-2.471714
27	14	0	1.647923	-2.099992	0.916230
28	6	0	2.430734	-3.350002	-0.234101
29	1	0	2.736016	-2.920539	-1.190437
30	1	0	3.348934	-3.724930	0.230329
31	1	0	1.745392	-4.190380	-0.393527
32	6	0	0.358842	-3.091069	1.895806
33	1	0	0.901693	-3.782033	2.555501
34	1	0	-0.264210	-2.454898	2.533760
35	1	0	-0.300007	-3.694926	1.262085
36	6	0	2.512062	-1.082055	2.228525
37	1	0	2.198083	-0.036362	2.153649
38	1	0	2.244528	-1.453710	3.223308
39	1	0	3.595987	-1.129167	2.092127
40	7	0	2.975648	-0.437330	-0.437159
41	6	0	4.340569	-0.603959	-0.421911
42	6	0	5.065210	0.692480	-0.807443
43	6	0	3.932174	1.703575	-0.943820
44	6	0	2.677628	0.861733	-0.694772
45	8	0	1.535353	1.335015	-0.733159
46	1	0	3.966792	2.508671	-0.203527
47	1	0	5.796021	0.935783	-0.031639
48	8	0	4.916984	-1.638427	-0.118349

49	1	0	3.858143	2.170766	-1.929938
50	1	0	5.618134	0.523064	-1.736152
51	6	0	-5.961389	-3.119268	-0.854633
52	1	0	-6.525273	-3.321017	0.062136
53	1	0	-6.579557	-2.470752	-1.484487
54	1	0	-5.821644	-4.067173	-1.380804
55	6	0	-1.648444	6.446125	-0.248108
56	1	0	-2.368558	6.597065	-1.057858
57	1	0	-2.013684	6.969654	0.639214
58	1	0	-0.707314	6.918075	-0.552335

System:	**2**
Oxidant:	NCS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN5
M06–2X/6–31+G(d) energy (in a.u.):	-836.704529787
Thermal correction to Gibbs Free Energy (in a.u.):	0.220562
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.591456	0.739856	0.615241
2	6	0	-0.720805	1.223178	0.248608
3	7	0	-0.013062	1.319482	1.566590
4	6	0	1.821256	0.040525	0.297489
5	6	0	1.992909	-0.511254	-0.973713
6	6	0	2.828439	-0.090073	1.262959
7	6	0	3.167832	-1.192367	-1.277649
8	1	0	1.203167	-0.403986	-1.712917
9	6	0	3.994575	-0.770803	0.947147
10	1	0	2.683680	0.346619	2.247518
11	6	0	4.181211	-1.332498	-0.325393
12	1	0	3.300976	-1.621193	-2.267410
13	1	0	4.778555	-0.873087	1.693893
14	6	0	-1.903571	0.318578	0.131195
15	6	0	-2.956828	0.594438	-0.745440
16	6	0	-1.961176	-0.840504	0.908687
17	6	0	-4.036063	-0.278715	-0.840827
18	1	0	-2.928948	1.495440	-1.348840
19	6	0	-3.047339	-1.705621	0.808325
20	1	0	-1.157894	-1.066780	1.604863
21	6	0	-4.101557	-1.442674	-0.068820
22	1	0	-4.847700	-0.048264	-1.528171
23	1	0	-3.074004	-2.600831	1.425177
24	7	0	-0.900576	2.446902	-0.526061
25	7	0	0.011092	3.268045	-0.414913
26	7	0	0.804825	4.070745	-0.368979
27	6	0	5.449470	-2.081433	-0.642659
28	1	0	6.331240	-1.494016	-0.368085
29	1	0	5.493714	-3.021873	-0.082215
30	1	0	5.515237	-2.320199	-1.707171
31	6	0	-5.276335	-2.380162	-0.190988
32	1	0	-6.219329	-1.857678	0.001846
33	1	0	-5.337567	-2.805163	-1.198900
34	1	0	-5.197935	-3.208033	0.518980

System:	**2**
Oxidant:	NCS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS6
M06–2X/6–31+G(d) energy (in a.u.):	-836.643853191
Thermal correction to Gibbs Free Energy (in a.u.):	0.214732
Number of imaginary frequencies:	1 (–625 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.560162	0.660352	1.236226
2	6	0	-0.696997	1.318698	0.759147
3	7	0	-0.053445	1.067169	2.226088
4	6	0	1.707788	-0.018999	0.667126
5	6	0	1.670596	-0.402820	-0.675818
6	6	0	2.842085	-0.276472	1.445279
7	6	0	2.767403	-1.048747	-1.235628
8	1	0	0.777231	-0.204086	-1.263658
9	6	0	3.931117	-0.917070	0.870520
10	1	0	2.859111	0.028534	2.487749
11	6	0	3.911899	-1.309567	-0.475123
12	1	0	2.736335	-1.355273	-2.278029
13	1	0	4.813936	-1.120317	1.471801
14	6	0	-1.843983	0.416227	0.408215
15	6	0	-2.667374	0.755247	-0.670637
16	6	0	-2.109344	-0.765141	1.106530
17	6	0	-3.725182	-0.069003	-1.039521
18	1	0	-2.473525	1.679567	-1.206726
19	6	0	-3.177020	-1.580140	0.734529
20	1	0	-1.490579	-1.047024	1.953758
21	6	0	-4.002480	-1.249257	-0.341985
22	1	0	-4.352371	0.212783	-1.883031
23	1	0	-3.370428	-2.492475	1.294705
24	7	0	-0.635544	2.597154	0.321652
25	7	0	0.518805	2.758178	-0.946534
26	7	0	1.028195	3.466430	-1.626367
27	6	0	5.114472	-1.974531	-1.092516
28	1	0	4.836304	-2.563124	-1.970662
29	1	0	5.846080	-1.223438	-1.412101
30	1	0	5.611677	-2.636384	-0.377601
31	6	0	-5.174288	-2.117957	-0.724795
32	1	0	-6.112321	-1.699293	-0.342303
33	1	0	-5.270340	-2.200145	-1.812034
34	1	0	-5.070320	-3.126751	-0.315025

System:	**2**
Oxidant:	NBS
Nitrogen-donor:	$TMSN_3$
Stationary point:	R
M06–2X/6–31+G(d) energy (in a.u.):	-4125.22778057
Thermal correction to Gibbs Free Energy (in a.u.):	0.381279
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.496090	1.192449	-1.037352
2	6	0	0.866582	0.039277	-1.133948
3	6	0	0.071085	2.556496	-0.895098
4	6	0	0.576051	3.345976	0.146604
5	6	0	-0.858713	3.111926	-1.787986
6	6	0	0.157049	4.666815	0.282457
7	1	0	1.293062	2.914578	0.840276
8	6	0	-1.268583	4.429598	-1.636313
9	1	0	-1.257927	2.499477	-2.591137
10	6	0	-0.768283	5.228788	-0.600465
11	1	0	0.554515	5.270340	1.094797
12	1	0	-1.994014	4.847521	-2.330559
13	7	0	2.499303	1.025478	1.885233
14	7	0	1.554891	0.264803	2.032850
15	7	0	0.635574	-0.372583	2.204591
16	6	0	1.374131	-1.300084	-1.238120
17	6	0	0.868657	-2.334636	-0.432680
18	6	0	2.416368	-1.582033	-2.133416
19	6	0	1.412490	-3.610372	-0.521029
20	1	0	0.055614	-2.139053	0.259050
21	6	0	2.953250	-2.863836	-2.205363
22	1	0	2.802735	-0.789661	-2.767953
23	6	0	2.465453	-3.896115	-1.398712
24	1	0	1.007758	-4.400243	0.107533
25	1	0	3.764305	-3.065127	-2.900926
26	14	0	4.073106	0.556326	1.196217
27	6	0	4.195793	-1.313792	1.152511
28	1	0	5.150690	-1.616878	0.706948
29	1	0	4.152053	-1.731307	2.165001
30	1	0	3.395657	-1.770664	0.560044
31	6	0	5.347881	1.293975	2.352657
32	1	0	5.197757	2.374370	2.451954
33	1	0	5.278497	0.851721	3.351817
34	1	0	6.363016	1.127332	1.974778
35	6	0	4.209574	1.347582	-0.494386
36	1	0	3.405776	1.014479	-1.157476
37	1	0	4.139111	2.437925	-0.408805
38	1	0	5.171192	1.105505	-0.962109
39	6	0	-4.933196	-0.664377	0.351973
40	6	0	-3.545123	-2.496789	0.869845
41	6	0	-5.851919	-1.723306	0.946462
42	6	0	-4.947818	-2.914782	1.286120
43	1	0	-6.349655	-1.291790	1.818447
44	1	0	-6.623661	-1.958373	0.209273
45	1	0	-4.928834	-3.157074	2.351671
46	1	0	-5.207900	-3.827991	0.745080
47	7	0	-3.642020	-1.201102	0.357231
48	8	0	-2.528598	-3.136478	0.952124
49	8	0	-5.231152	0.427653	-0.052971
50	6	0	3.054719	-5.281965	-1.459600
51	1	0	3.595782	-5.516004	-0.535934
52	1	0	2.271581	-6.037249	-1.580334
53	1	0	3.754876	-5.380389	-2.293547
54	6	0	-1.229574	6.655871	-0.449464
55	1	0	-2.311537	6.701969	-0.285587
56	1	0	-0.738701	7.144164	0.396575

57	1	0	-1.009582	7.237646	-1.350976
58	35	0	-2.159533	-0.294267	-0.255876

System:	**2**
Oxidant:	NBS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS1
M06–2X/6–31+G(d) energy (in a.u.):	-4125.17640824
Thermal correction to Gibbs Free Energy (in a.u.):	0.386047
Number of imaginary frequencies:	1 (–367 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.849219	0.490583	-0.316933
2	6	0	-0.331217	-0.673045	-0.138451
3	6	0	-0.512571	1.909961	-0.336403
4	6	0	-1.091443	2.805217	-1.242986
5	6	0	0.447821	2.389667	0.570181
6	6	0	-0.720931	4.147168	-1.243187
7	1	0	-1.829609	2.448613	-1.955660
8	6	0	0.820187	3.726896	0.548980
9	1	0	0.919118	1.708672	1.271164
10	6	0	0.241373	4.629500	-0.351870
11	1	0	-1.178009	4.827309	-1.957996
12	1	0	1.583740	4.070374	1.242540
13	7	0	-2.681964	0.471065	-0.584546
14	7	0	-3.054646	-0.395092	-1.389394
15	7	0	-3.312558	-1.192194	-2.140290
16	6	0	-0.902392	-2.008672	-0.004352
17	6	0	-0.408408	-3.081266	-0.762328
18	6	0	-1.950383	-2.251943	0.893427
19	6	0	-0.987254	-4.339335	-0.656712
20	1	0	0.431627	-2.916748	-1.430981
21	6	0	-2.513174	-3.521907	1.002702
22	1	0	-2.307621	-1.442023	1.525097
23	6	0	-2.049900	-4.583560	0.222767
24	1	0	-0.597536	-5.155929	-1.260350
25	1	0	-3.319573	-3.691799	1.713095
26	14	0	-3.860901	1.233639	0.585521
27	6	0	-5.175342	-0.070057	0.862978
28	1	0	-5.888268	0.272065	1.621675
29	1	0	-5.744640	-0.271667	-0.051569
30	1	0	-4.744178	-1.015864	1.208221
31	6	0	-4.560988	2.756053	-0.239621
32	1	0	-3.780885	3.508502	-0.393800
33	1	0	-5.007200	2.516401	-1.211127
34	1	0	-5.343674	3.200774	0.385986
35	6	0	-2.848672	1.633657	2.096906
36	1	0	-2.229376	0.787739	2.413071
37	1	0	-2.183687	2.482948	1.909366
38	1	0	-3.514767	1.898161	2.926334
39	6	0	4.607962	0.470867	0.715196
40	6	0	4.801854	-1.530704	-0.412955
41	6	0	6.115350	0.213424	0.642076
42	6	0	6.244072	-1.117662	-0.101985
43	1	0	6.585570	1.054097	0.124751
44	1	0	6.513170	0.189969	1.660184
45	1	0	6.794139	-1.044912	-1.043929
46	1	0	6.709959	-1.909539	0.490597
47	7	0	3.954820	-0.568890	0.095032
48	8	0	4.466777	-2.533647	-1.005760
49	8	0	4.079794	1.434312	1.234877
50	6	0	-2.650010	-5.961903	0.334190
51	1	0	-3.009409	-6.314650	-0.638266
52	1	0	-1.908127	-6.684587	0.690707
53	1	0	-3.492703	-5.973196	1.030965
54	6	0	0.665505	6.075200	-0.361913
55	1	0	1.724097	6.165374	-0.627832
56	1	0	0.084396	6.656519	-1.082776

57	1	0	0.537546	6.529733	0.625978
58	35	0	1.919516	-0.606447	-0.039987

System:	**2**
Oxidant:	NBS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN1
M06–2X/6–31+G(d) energy (in a.u.):	-4125.23869663
Thermal correction to Gibbs Free Energy (in a.u.):	0.395910
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.256181	-0.807445	-0.606260
2	6	0	-0.748108	-1.459867	0.004357
3	6	0	1.708312	-1.048384	-0.528568
4	6	0	2.466811	-1.176528	-1.694102
5	6	0	2.344386	-1.099898	0.717673
6	6	0	3.845150	-1.360763	-1.619781
7	1	0	1.979554	-1.132370	-2.666576
8	6	0	3.720751	-1.276388	0.779128
9	1	0	1.745460	-0.981984	1.617442
10	6	0	4.492793	-1.409018	-0.382928
11	1	0	4.424507	-1.465385	-2.533712
12	1	0	4.211500	-1.304575	1.749374
13	7	0	-0.075451	0.296945	-1.512889
14	7	0	-1.018409	0.056747	-2.319846
15	7	0	-1.855180	-0.105937	-3.042947
16	6	0	-2.164011	-1.037369	-0.011903
17	6	0	-3.184029	-1.917425	-0.386125
18	6	0	-2.485282	0.286150	0.317503
19	6	0	-4.501375	-1.472374	-0.454477
20	1	0	-2.944239	-2.950012	-0.625702
21	6	0	-3.805713	0.716737	0.246054
22	1	0	-1.688745	0.953402	0.640683
23	6	0	-4.833954	-0.150998	-0.140731
24	1	0	-5.284533	-2.164649	-0.753571
25	1	0	-4.043922	1.745363	0.508716
26	14	0	0.630174	2.097254	-1.679594
27	6	0	-0.829317	3.158075	-1.225952
28	1	0	-0.559720	4.207439	-1.388443
29	1	0	-1.682397	2.917343	-1.874396
30	1	0	-1.106224	3.045718	-0.179014
31	6	0	0.767621	2.133205	-3.562533
32	1	0	1.405965	1.325801	-3.940264
33	1	0	-0.193421	2.097208	-4.087792
34	1	0	1.245850	3.078323	-3.849388
35	6	0	2.356941	2.126829	-1.005888
36	1	0	2.646940	3.179836	-0.923371
37	1	0	2.420445	1.684106	-0.012142
38	1	0	3.031328	1.608166	-1.694692
39	6	0	0.762606	2.987807	1.708726
40	6	0	0.163464	1.003155	2.517343
41	6	0	0.859157	3.186682	3.227579
42	6	0	0.447075	1.829133	3.781488
43	1	0	1.881279	3.482793	3.481459
44	1	0	0.200409	4.009405	3.520737
45	1	0	1.225555	1.328316	4.364784
46	1	0	-0.455918	1.851893	4.398582
47	7	0	0.359813	1.725851	1.374779
48	8	0	-0.195211	-0.173075	2.564035

49	8	0	1.026362	3.881814	0.903212
50	6	0	5.984249	-1.603518	-0.288085
51	1	0	6.446282	-1.631054	-1.278475
52	1	0	6.449167	-0.792484	0.281962
53	1	0	6.223280	-2.542185	0.223256
54	6	0	-6.264759	0.320649	-0.179150
55	1	0	-6.880210	-0.325641	-0.810975
56	1	0	-6.699653	0.315665	0.826835
57	1	0	-6.334778	1.343121	-0.562083
58	35	0	-0.376129	-3.065742	0.930549

System:	**2**
Oxidant:	NBS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS2
M06–2X/6–31+G(d) energy (in a.u.):	-4125.23486588
Thermal correction to Gibbs Free Energy (in a.u.):	0.397889
Number of imaginary frequencies:	1 (–30 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.015023	-0.852552	-0.477062
2	6	0	-1.073379	-1.435484	0.052147
3	6	0	1.418995	-1.310402	-0.462779
4	6	0	2.115863	-1.439447	-1.666324
5	6	0	2.075264	-1.593786	0.741316
6	6	0	3.445242	-1.851613	-1.671999
7	1	0	1.618421	-1.209577	-2.606689
8	6	0	3.405738	-1.993673	0.725333
9	1	0	1.535856	-1.479357	1.676361
10	6	0	4.112033	-2.130125	-0.476921
11	1	0	3.973441	-1.949328	-2.617043
12	1	0	3.911226	-2.201965	1.665693
13	7	0	-0.157529	0.394118	-1.220927
14	7	0	-1.104518	0.359472	-2.057590
15	7	0	-1.947032	0.372438	-2.791283
16	6	0	-2.425101	-0.837394	0.104287
17	6	0	-3.550365	-1.560604	-0.303608
18	6	0	-2.588425	0.489949	0.530107
19	6	0	-4.808460	-0.963967	-0.306247
20	1	0	-3.439689	-2.593536	-0.622245
21	6	0	-3.850078	1.072741	0.524647
22	1	0	-1.721648	1.041814	0.882309
23	6	0	-4.980181	0.359918	0.105961
24	1	0	-5.671010	-1.539007	-0.633474
25	1	0	-3.960929	2.100937	0.862265
26	14	0	0.842517	2.097953	-1.279352
27	6	0	-0.411783	3.454537	-0.900435
28	1	0	-0.151888	4.336405	-1.497093
29	1	0	-1.396446	3.112878	-1.253192
30	1	0	-0.489726	3.744026	0.145707
31	6	0	0.661135	2.195576	-3.209064
32	1	0	0.977374	1.282488	-3.732577
33	1	0	-0.325946	2.486737	-3.588719
34	1	0	1.353992	2.985601	-3.531719
35	6	0	2.695392	1.758196	-1.269958
36	1	0	3.201894	2.727550	-1.319428
37	1	0	3.044946	1.227722	-0.382079
38	1	0	2.958970	1.184210	-2.163094
39	6	0	1.741650	3.050024	1.351688
40	6	0	0.713446	1.219605	2.136072
41	6	0	2.032199	3.101299	2.849177
42	6	0	1.374549	1.833878	3.374127
43	1	0	3.114718	3.144645	2.996989
44	1	0	1.609142	4.023505	3.257641
45	1	0	2.083875	1.104873	3.778280
46	1	0	0.609596	2.001556	4.136602
47	7	0	1.015857	1.932193	1.002549
48	8	0	0.007553	0.221033	2.199974

49	8	0	2.100614	3.912227	0.559239
50	6	0	5.553208	-2.570654	-0.468798
51	1	0	5.975342	-2.568989	-1.477105
52	1	0	6.161703	-1.908084	0.155396
53	1	0	5.649427	-3.583493	-0.062969
54	6	0	-6.343051	1.002335	0.128233
55	1	0	-7.074506	0.402607	-0.419861
56	1	0	-6.702804	1.112661	1.157339
57	1	0	-6.315824	2.001195	-0.318255
58	35	0	-0.908886	-3.166376	0.810273

System:	**2**
Oxidant:	NBS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN2
M06–2X/6–31+G(d) energy (in a.u.):	-3356.16611197
Thermal correction to Gibbs Free Energy (in a.u.):	0.215236
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.530138	0.667923	-0.003987
2	6	0	-0.368080	-0.340222	-0.070551
3	6	0	2.004170	0.537499	0.088523
4	6	0	2.824575	1.339996	-0.707712
5	6	0	2.601900	-0.337111	1.003525
6	6	0	4.210939	1.244183	-0.616958
7	1	0	2.372346	2.044468	-1.399751
8	6	0	3.985262	-0.418854	1.097591
9	1	0	1.977818	-0.944752	1.651901
10	6	0	4.813575	0.363060	0.283373
11	1	0	4.833562	1.869771	-1.251672
12	1	0	4.433297	-1.096881	1.820447
13	7	0	0.135989	2.040483	0.010110
14	7	0	-0.885712	2.355817	-0.619356
15	7	0	-1.783526	2.776592	-1.154940
16	6	0	-1.830994	-0.190731	0.085454
17	6	0	-2.731915	-0.713242	-0.851509
18	6	0	-2.339714	0.485241	1.199900
19	6	0	-4.099654	-0.539435	-0.685360
20	1	0	-2.352111	-1.255139	-1.713263
21	6	0	-3.713566	0.651665	1.360206
22	1	0	-1.651796	0.881043	1.943092
23	6	0	-4.615102	0.146918	0.421520
24	1	0	-4.783961	-0.944507	-1.427459
25	1	0	-4.088673	1.178643	2.233959
26	6	0	-6.102326	0.330784	0.582104
27	1	0	-6.507564	0.952706	-0.223505
28	1	0	-6.624085	-0.631241	0.548235
29	1	0	-6.342209	0.813456	1.533154
30	6	0	6.313164	0.248066	0.383360
31	1	0	6.655177	-0.725370	0.014709
32	1	0	6.810951	1.023571	-0.204880
33	1	0	6.647381	0.341224	1.421725
34	35	0	0.213096	-2.130619	-0.400408

System:	**2**
Oxidant:	NBS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS3
M06–2X/6–31+G(d) energy (in a.u.):	-3356.11784251
Thermal correction to Gibbs Free Energy (in a.u.):	0.210041
Number of imaginary frequencies:	1 (–582 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.637534	-1.129507	0.233425
2	6	0	-0.730742	-1.077052	-0.008178
3	6	0	1.538365	0.035813	0.028302
4	6	0	2.601425	0.271584	0.903607
5	6	0	1.371722	0.876038	-1.078970
6	6	0	3.471248	1.337582	0.683154
7	1	0	2.726591	-0.371362	1.771360
8	6	0	2.244837	1.934268	-1.293958
9	1	0	0.551894	0.692471	-1.769057
10	6	0	3.308576	2.183732	-0.416563
11	1	0	4.286737	1.517175	1.379576
12	1	0	2.104348	2.579412	-2.158276
13	6	0	-1.533845	0.146341	0.129182
14	6	0	-2.642540	0.393913	-0.697493
15	6	0	-1.188273	1.115152	1.082710
16	6	0	-3.346125	1.586040	-0.596768
17	1	0	-2.940625	-0.349694	-1.430068
18	6	0	-1.907600	2.301761	1.182731
19	1	0	-0.356184	0.931434	1.755756
20	6	0	-2.993846	2.562026	0.344398
21	1	0	-4.191243	1.763284	-1.258255
22	1	0	-1.622557	3.034633	1.933442
23	7	0	1.023228	-2.253341	0.835456
24	7	0	2.578939	-2.707419	0.249619
25	7	0	3.489758	-3.289928	0.483875
26	6	0	-3.786463	3.838429	0.458119
27	1	0	-4.794039	3.640084	0.840302
28	1	0	-3.303389	4.546419	1.136752
29	1	0	-3.896050	4.322546	-0.517756
30	6	0	4.259239	3.325180	-0.672095
31	1	0	3.716715	4.244679	-0.913200
32	1	0	4.889512	3.519631	0.199852
33	1	0	4.918298	3.101294	-1.518499
34	35	0	-1.701559	-2.675000	-0.346406

System:	**2**
Oxidant:	NBS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN3
M06–2X/6–31+G(d) energy (in a.u.):	-3246.73710489
Thermal correction to Gibbs Free Energy (in a.u.):	0.206223
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.739898	0.424262	0.816523
2	6	0	-0.587401	0.859707	0.496433
3	7	0	0.083241	0.853781	1.813274
4	6	0	2.019940	-0.112690	0.414212
5	6	0	2.228535	-0.467941	-0.920006
6	6	0	3.045657	-0.273843	1.355684
7	6	0	3.459906	-0.985769	-1.310798
8	1	0	1.425113	-0.333503	-1.639464
9	6	0	4.267441	-0.790876	0.953079
10	1	0	2.870958	0.010170	2.389604
11	6	0	4.492549	-1.154070	-0.383977
12	1	0	3.622882	-1.261940	-2.348933
13	1	0	5.066000	-0.916979	1.680186
14	6	0	-1.745973	-0.056157	0.250714
15	6	0	-2.422806	-0.095089	-0.972007
16	6	0	-2.137311	-0.929923	1.266251
17	6	0	-3.463911	-0.995021	-1.168846
18	1	0	-2.140354	0.588197	-1.767158
19	6	0	-3.188413	-1.822545	1.062359
20	1	0	-1.619712	-0.905962	2.221031
21	6	0	-3.867918	-1.872114	-0.155551
22	1	0	-3.978619	-1.013274	-2.127046
23	1	0	-3.484500	-2.489868	1.868143
24	6	0	5.829549	-1.710353	-0.799373
25	1	0	6.627854	-0.984184	-0.612990
26	1	0	6.069595	-2.614476	-0.230156
27	1	0	5.842869	-1.963977	-1.862231
28	6	0	-5.013754	-2.826297	-0.378909
29	1	0	-5.118527	-3.522494	0.457612
30	1	0	-5.959777	-2.283978	-0.484941
31	1	0	-4.867693	-3.412389	-1.292117
32	35	0	-0.767849	2.628015	-0.345691

System:	**2**
Oxidant:	NBS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS4
M06–2X/6–31+G(d) energy (in a.u.):	-3820.03100923
Thermal correction to Gibbs Free Energy (in a.u.):	0.320247
Number of imaginary frequencies:	1 (–233 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.570157	-0.564872	-1.135025
2	6	0	0.802759	-0.749234	-1.185277
3	7	0	0.155741	-0.447843	-2.288833
4	6	0	-1.859727	-1.105978	-0.780321
5	6	0	-2.099915	-1.578852	0.514409
6	6	0	-2.868593	-1.135293	-1.756837
7	6	0	-3.350664	-2.114082	0.812696
8	1	0	-1.329273	-1.474704	1.276448
9	6	0	-4.105305	-1.668987	-1.437827
10	1	0	-2.665117	-0.747093	-2.751323
11	6	0	-4.362423	-2.167491	-0.148589
12	1	0	-3.545434	-2.476609	1.817908
13	1	0	-4.890050	-1.702960	-2.189367
14	6	0	2.123774	-1.104558	-0.770966
15	6	0	2.401316	-1.447880	0.558040
16	6	0	3.139795	-1.107941	-1.745288
17	6	0	3.704286	-1.792430	0.902497
18	1	0	1.615900	-1.382929	1.307528
19	6	0	4.427001	-1.455386	-1.381359
20	1	0	2.901740	-0.837787	-2.770917
21	6	0	4.726797	-1.800289	-0.050260
22	1	0	3.929775	-2.044412	1.934617
23	1	0	5.219358	-1.460237	-2.125417
24	7	0	-0.994293	1.483072	-0.645939
25	7	0	-1.987868	1.529078	0.085931
26	7	0	-2.918903	1.475936	0.715617
27	14	0	0.171639	2.886007	-0.577952
28	6	0	-0.093720	3.769095	-2.212485
29	1	0	-1.115714	4.153009	-2.300018
30	1	0	0.595619	4.615269	-2.315415
31	1	0	0.082956	3.085924	-3.051059
32	6	0	1.916838	2.236757	-0.481319
33	1	0	2.586918	3.095534	-0.347366
34	1	0	2.033511	1.571821	0.380697
35	1	0	2.226939	1.723053	-1.397797
36	6	0	-0.319890	3.934656	0.884064
37	1	0	-0.249473	3.342326	1.803388
38	1	0	0.355714	4.793926	0.967394
39	1	0	-1.340112	4.322993	0.786184
40	6	0	-5.720203	-2.728079	0.181478
41	1	0	-6.002341	-3.512802	-0.527992
42	1	0	-5.742152	-3.150952	1.188510
43	1	0	-6.483676	-1.944543	0.125329
44	6	0	6.137815	-2.162413	0.327456
45	1	0	6.811906	-1.316562	0.154442
46	1	0	6.208899	-2.444997	1.380147
47	1	0	6.500075	-2.998930	-0.279377
48	35	0	0.169418	0.473297	2.382481

System:	**2**
Oxidant:	NBS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN4
M06–2X/6–31+G(d) energy (in a.u.):	-1245.66316522
Thermal correction to Gibbs Free Energy (in a.u.):	0.323932
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.384923	0.156415	0.269807
2	6	0	-1.003736	0.238686	0.662063
3	7	0	-0.183199	0.602627	1.558750
4	6	0	1.195298	-1.093320	0.162518
5	6	0	0.775731	-2.219888	0.881573
6	6	0	2.347533	-1.183192	-0.619507
7	6	0	1.501455	-3.401208	0.816270
8	1	0	-0.116286	-2.170504	1.500672
9	6	0	3.067320	-2.375992	-0.680429
10	1	0	2.713000	-0.327771	-1.183596
11	6	0	2.659871	-3.503123	0.034102
12	1	0	1.163788	-4.264576	1.384179
13	1	0	3.962811	-2.425527	-1.293985
14	6	0	-2.392621	0.010653	0.362937
15	6	0	-2.751876	-0.579022	-0.854605
16	6	0	-3.378624	0.371206	1.295593
17	6	0	-4.092746	-0.806017	-1.138454
18	1	0	-1.980141	-0.872444	-1.562840
19	6	0	-4.710791	0.141145	0.996677
20	1	0	-3.088467	0.824279	2.239497
21	6	0	-5.088803	-0.449187	-0.221546
22	1	0	-4.373672	-1.268473	-2.080147
23	1	0	-5.479206	0.418766	1.713403
24	7	0	0.948942	1.314775	-0.500655
25	7	0	0.726540	1.300406	-1.742597
26	7	0	0.537662	1.292012	-2.843281
27	14	0	2.035779	2.655570	0.308213
28	6	0	3.073584	1.661290	1.479698
29	1	0	3.748065	0.976581	0.957282
30	1	0	3.681969	2.340834	2.087999
31	1	0	2.444076	1.079503	2.161178
32	6	0	0.834488	3.824777	1.105237
33	1	0	1.376343	4.675534	1.534759
34	1	0	0.113495	4.221611	0.383185
35	1	0	0.287396	3.329412	1.912706
36	6	0	2.917354	3.342992	-1.182224
37	1	0	2.240211	3.847343	-1.880549
38	1	0	3.644610	4.093982	-0.852534
39	1	0	3.478235	2.573540	-1.724760
40	6	0	3.430793	-4.795234	-0.025832
41	1	0	4.309340	-4.705923	-0.668901
42	1	0	3.768118	-5.093685	0.971817
43	1	0	2.804755	-5.603986	-0.416184
44	6	0	-6.542665	-0.695015	-0.518037
45	1	0	-6.970107	-1.392866	0.209571
46	1	0	-7.114170	0.236233	-0.451941
47	1	0	-6.683619	-1.114374	-1.516367

System:	**2**
Oxidant:	NBS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS5
M06–2X/6–31+G(d) energy (in a.u.):	-1605.79574355
Thermal correction to Gibbs Free Energy (in a.u.):	0.399005
Number of imaginary frequencies:	1 (–58 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.888639	-0.535968	0.394353
2	6	0	-0.803976	0.855049	0.792733
3	7	0	-0.690106	0.033195	1.747856
4	6	0	-2.171132	-1.227277	0.054915
5	6	0	-2.209843	-2.443246	-0.628153
6	6	0	-3.380830	-0.632760	0.436096
7	6	0	-3.430358	-3.051340	-0.920853
8	1	0	-1.288803	-2.938983	-0.923273
9	6	0	-4.590996	-1.246865	0.142962
10	1	0	-3.373999	0.314831	0.968860
11	6	0	-4.638760	-2.467346	-0.542149
12	1	0	-3.436900	-4.001231	-1.449587
13	1	0	-5.519232	-0.770033	0.449950
14	6	0	-0.994472	2.262638	0.518427
15	6	0	-1.081584	2.725558	-0.797140
16	6	0	-1.126155	3.151365	1.589535
17	6	0	-1.305253	4.074103	-1.034167
18	1	0	-0.945291	2.028148	-1.618086
19	6	0	-1.346782	4.500309	1.338433
20	1	0	-1.059459	2.777334	2.607713
21	6	0	-1.438041	4.979770	0.026707
22	1	0	-1.368449	4.437716	-2.056727
23	1	0	-1.451316	5.193042	2.169462
24	7	0	0.320860	-1.198868	-0.138981
25	7	0	0.510816	-1.026166	-1.371759
26	7	0	0.671494	-0.942281	-2.471714
27	14	0	1.647923	-2.099992	0.916230
28	6	0	2.430734	-3.350002	-0.234101
29	1	0	2.736016	-2.920539	-1.190437
30	1	0	3.348934	-3.724930	0.230329
31	1	0	1.745392	-4.190380	-0.393527
32	6	0	0.358842	-3.091069	1.895806
33	1	0	0.901693	-3.782033	2.555501
34	1	0	-0.264210	-2.454898	2.533760
35	1	0	-0.300007	-3.694926	1.262085
36	6	0	2.512062	-1.082055	2.228525
37	1	0	2.198083	-0.036362	2.153649
38	1	0	2.244528	-1.453710	3.223308
39	1	0	3.595987	-1.129167	2.092127
40	7	0	2.975648	-0.437330	-0.437159
41	6	0	4.340569	-0.603959	-0.421911
42	6	0	5.065210	0.692480	-0.807443
43	6	0	3.932174	1.703575	-0.943820
44	6	0	2.677628	0.861733	-0.694772
45	8	0	1.535353	1.335015	-0.733159
46	1	0	3.966792	2.508671	-0.203527
47	1	0	5.796021	0.935783	-0.031639
48	8	0	4.916984	-1.638427	-0.118349

49	1	0	3.858143	2.170766	-1.929938
50	1	0	5.618134	0.523064	-1.736152
51	6	0	-5.961389	-3.119268	-0.854633
52	1	0	-6.525273	-3.321017	0.062136
53	1	0	-6.579557	-2.470752	-1.484487
54	1	0	-5.821644	-4.067173	-1.380804
55	6	0	-1.648444	6.446125	-0.248108
56	1	0	-2.368558	6.597065	-1.057858
57	1	0	-2.013684	6.969654	0.639214
58	1	0	-0.707314	6.918075	-0.552335

System:	**2**
Oxidant:	NBS
Nitrogen-donor:	$TMSN_3$
Stationary point:	IN5
M06–2X/6–31+G(d) energy (in a.u.):	-836.704529787
Thermal correction to Gibbs Free Energy (in a.u.):	0.220562
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.591456	0.739856	0.615241
2	6	0	-0.720805	1.223178	0.248608
3	7	0	-0.013062	1.319482	1.566590
4	6	0	1.821256	0.040525	0.297489
5	6	0	1.992909	-0.511254	-0.973713
6	6	0	2.828439	-0.090073	1.262959
7	6	0	3.167832	-1.192367	-1.277649
8	1	0	1.203167	-0.403986	-1.712917
9	6	0	3.994575	-0.770803	0.947147
10	1	0	2.683680	0.346619	2.247518
11	6	0	4.181211	-1.332498	-0.325393
12	1	0	3.300976	-1.621193	-2.267410
13	1	0	4.778555	-0.873087	1.693893
14	6	0	-1.903571	0.318578	0.131195
15	6	0	-2.956828	0.594438	-0.745440
16	6	0	-1.961176	-0.840504	0.908687
17	6	0	-4.036063	-0.278715	-0.840827
18	1	0	-2.928948	1.495440	-1.348840
19	6	0	-3.047339	-1.705621	0.808325
20	1	0	-1.157894	-1.066780	1.604863
21	6	0	-4.101557	-1.442674	-0.068820
22	1	0	-4.847700	-0.048264	-1.528171
23	1	0	-3.074004	-2.600831	1.425177
24	7	0	-0.900576	2.446902	-0.526061
25	7	0	0.011092	3.268045	-0.414913
26	7	0	0.804825	4.070745	-0.368979
27	6	0	5.449470	-2.081433	-0.642659
28	1	0	6.331240	-1.494016	-0.368085
29	1	0	5.493714	-3.021873	-0.082215
30	1	0	5.515237	-2.320199	-1.707171
31	6	0	-5.276335	-2.380162	-0.190988
32	1	0	-6.219329	-1.857678	0.001846
33	1	0	-5.337567	-2.805163	-1.198900
34	1	0	-5.197935	-3.208033	0.518980

System:	**2**
Oxidant:	NBS
Nitrogen-donor:	$TMSN_3$
Stationary point:	TS6
M06–2X/6–31+G(d) energy (in a.u.):	-836.643853191
Thermal correction to Gibbs Free Energy (in a.u.):	0.214732
Number of imaginary frequencies:	1 (–625 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.560162	0.660352	1.236226
2	6	0	-0.696997	1.318698	0.759147
3	7	0	-0.053445	1.067169	2.226088
4	6	0	1.707788	-0.018999	0.667126
5	6	0	1.670596	-0.402820	-0.675818
6	6	0	2.842085	-0.276472	1.445279
7	6	0	2.767403	-1.048747	-1.235628
8	1	0	0.777231	-0.204086	-1.263658
9	6	0	3.931117	-0.917070	0.870520
10	1	0	2.859111	0.028534	2.487749
11	6	0	3.911899	-1.309567	-0.475123
12	1	0	2.736335	-1.355273	-2.278029
13	1	0	4.813936	-1.120317	1.471801
14	6	0	-1.843983	0.416227	0.408215
15	6	0	-2.667374	0.755247	-0.670637
16	6	0	-2.109344	-0.765141	1.106530
17	6	0	-3.725182	-0.069003	-1.039521
18	1	0	-2.473525	1.679567	-1.206726
19	6	0	-3.177020	-1.580140	0.734529
20	1	0	-1.490579	-1.047024	1.953758
21	6	0	-4.002480	-1.249257	-0.341985
22	1	0	-4.352371	0.212783	-1.883031
23	1	0	-3.370428	-2.492475	1.294705
24	7	0	-0.635544	2.597154	0.321652
25	7	0	0.518805	2.758178	-0.946534
26	7	0	1.028195	3.466430	-1.626367
27	6	0	5.114472	-1.974531	-1.092516
28	1	0	4.836304	-2.563124	-1.970662
29	1	0	5.846080	-1.223438	-1.412101
30	1	0	5.611677	-2.636384	-0.377601
31	6	0	-5.174288	-2.117957	-0.724795
32	1	0	-6.112321	-1.699293	-0.342303
33	1	0	-5.270340	-2.200145	-1.812034
34	1	0	-5.070320	-3.126751	-0.315025

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	NaN_3
Stationary point:	R
M06–2X/6–31+G(d) energy (in a.u.):	-8224.16073717
Thermal correction to Gibbs Free Energy (in a.u.):	0.272738
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.585790	-0.501778	-0.356598
2	6	0	-0.953952	-1.539548	-0.307968
3	6	0	-2.336690	0.717901	-0.400829
4	6	0	-3.021852	1.096662	-1.567920
5	6	0	-2.422868	1.538095	0.739134
6	6	0	-3.779663	2.268070	-1.586431
7	1	0	-2.970814	0.464331	-2.449256
8	6	0	-3.182380	2.705667	0.706534
9	1	0	-1.904552	1.246827	1.648263
10	6	0	-3.869575	3.095198	-0.455731
11	1	0	-4.311750	2.543997	-2.493284
12	1	0	-3.245917	3.325766	1.597157
13	7	0	-4.625416	-1.425800	0.918541
14	7	0	-4.020716	-2.420166	1.119803
15	7	0	-3.425597	-3.402716	1.319639
16	6	0	-0.190773	-2.751098	-0.253541
17	6	0	0.106363	-3.459119	-1.426565
18	6	0	0.273837	-3.237750	0.980755
19	6	0	0.852585	-4.633262	-1.360979
20	1	0	-0.248441	-3.086403	-2.383234
21	6	0	1.017850	-4.409237	1.029596
22	1	0	0.044001	-2.691763	1.891703
23	6	0	1.318778	-5.127008	-0.137771
24	1	0	1.077554	-5.174920	-2.276447
25	1	0	1.372934	-4.778533	1.989124
26	53	0	1.426741	0.700843	-0.089253
27	6	0	3.199184	3.059831	0.688590
28	6	0	4.407973	1.322223	-0.288492
29	6	0	4.637243	3.537047	0.663651
30	6	0	5.433771	2.387875	0.040369
31	1	0	4.681690	4.458724	0.077190
32	1	0	4.942138	3.770711	1.686922
33	1	0	5.950308	2.667777	-0.881408
34	1	0	6.169379	1.954533	0.723441
35	7	0	3.159878	1.789472	0.118250
36	8	0	4.599166	0.244820	-0.807937
37	8	0	2.230603	3.647981	1.116913
38	6	0	2.120753	-6.398926	-0.062539
39	1	0	3.080028	-6.226861	0.437635
40	1	0	1.585557	-7.161735	0.514319
41	1	0	2.318925	-6.801161	-1.059712
42	6	0	-4.660532	4.374433	-0.490851
43	1	0	-4.002238	5.217653	-0.731662
44	1	0	-5.443517	4.333395	-1.252796
45	1	0	-5.120736	4.580935	0.479609
46	11	0	-5.093870	0.637497	0.317539

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	NaN_3
Stationary point:	TS1
M06–2X/6–31+G(d) energy (in a.u.):	-8224.06859497
Thermal correction to Gibbs Free Energy (in a.u.):	0.275725
Number of imaginary frequencies:	1 (–334 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.177554	1.224681	0.199207
2	6	0	1.401695	-0.017390	0.144040
3	6	0	0.164652	2.268837	0.175797
4	6	0	0.018634	3.162363	1.248711
5	6	0	-0.611794	2.465434	-0.976705
6	6	0	-0.872501	4.230036	1.161059
7	1	0	0.624312	3.016031	2.138273
8	6	0	-1.501561	3.537999	-1.054560
9	1	0	-0.525526	1.760027	-1.798288
10	6	0	-1.647331	4.437023	0.009152
11	1	0	-0.981126	4.907139	2.005099
12	1	0	-2.109948	3.660787	-1.947113
13	7	0	2.782980	2.520036	0.078123
14	7	0	3.711610	2.058915	0.705546
15	7	0	4.568313	1.596752	1.303943
16	6	0	2.476462	-0.979007	-0.042380
17	6	0	2.463266	-2.223148	0.596520
18	6	0	3.542738	-0.672503	-0.903538
19	6	0	3.508020	-3.123316	0.403244
20	1	0	1.632944	-2.483402	1.246301
21	6	0	4.570141	-1.584499	-1.100703
22	1	0	3.554373	0.290258	-1.408141
23	6	0	4.574369	-2.822837	-0.446498
24	1	0	3.485842	-4.081776	0.915784
25	1	0	5.391164	-1.330382	-1.767821
26	53	0	-0.966975	-1.011311	0.138300
27	6	0	-4.006883	-1.245159	-0.599451
28	6	0	-3.284715	-3.137024	0.508165
29	6	0	-5.241529	-2.143757	-0.518747
30	6	0	-4.762614	-3.398301	0.213632
31	1	0	-6.030561	-1.600422	0.008118
32	1	0	-5.596935	-2.335015	-1.534793
33	1	0	-5.276994	-3.579159	1.161089
34	1	0	-4.839484	-4.312078	-0.381455
35	7	0	-2.948501	-1.890808	0.007496
36	8	0	-2.533214	-3.891653	1.083473
37	8	0	-3.966315	-0.145565	-1.112226
38	6	0	5.706507	-3.795115	-0.660014
39	1	0	5.829539	-4.030827	-1.722520
40	1	0	6.654376	-3.375980	-0.304807
41	1	0	5.530625	-4.731770	-0.124168
42	6	0	-2.652434	5.557526	-0.056927
43	1	0	-3.629104	5.207395	0.295341
44	1	0	-2.356015	6.400509	0.573536
45	1	0	-2.783379	5.918271	-1.080897
46	11	0	1.612265	4.195664	-0.712653

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	NaN_3
Stationary point:	IN2
M06–2X/6–31+G(d) energy (in a.u.):	-7701.91227979
Thermal correction to Gibbs Free Energy (in a.u.):	0.213655
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.471283	0.929932	0.012851
2	6	0	0.403493	-0.100727	0.016084
3	6	0	-1.949338	0.839579	-0.089053
4	6	0	-2.753056	1.518459	0.831979
5	6	0	-2.562229	0.126384	-1.121376
6	6	0	-4.138579	1.452306	0.741644
7	1	0	-2.284655	2.095570	1.624511
8	6	0	-3.949978	0.074825	-1.214055
9	1	0	-1.950233	-0.385542	-1.858785
10	6	0	-4.759861	0.730361	-0.283368
11	1	0	-4.749667	1.972931	1.475527
12	1	0	-4.411522	-0.481948	-2.026010
13	7	0	-0.059922	2.295484	0.085638
14	7	0	0.982498	2.563276	0.703727
15	7	0	1.894583	2.948366	1.241913
16	6	0	1.870220	0.042599	-0.122337
17	6	0	2.763589	-0.491719	0.815573
18	6	0	2.389922	0.737340	-1.220021
19	6	0	4.132481	-0.311460	0.667101
20	1	0	2.378478	-1.047628	1.666759
21	6	0	3.764915	0.909906	-1.363435
22	1	0	1.707747	1.144342	-1.962609
23	6	0	4.658047	0.393217	-0.423025
24	1	0	4.810140	-0.726422	1.409926
25	1	0	4.147564	1.451119	-2.225471
26	53	0	-0.277203	-2.102885	0.244715
27	6	0	6.145670	0.589201	-0.563255
28	1	0	6.522439	1.273439	0.205185
29	1	0	6.681135	-0.358989	-0.450638
30	1	0	6.399962	1.009492	-1.540116
31	6	0	-6.262850	0.692128	-0.392533
32	1	0	-6.727055	0.565306	0.590287
33	1	0	-6.645917	1.626122	-0.819379
34	1	0	-6.593748	-0.128728	-1.034665

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	NaN_3
Stationary point:	TS3
M06–2X/6–31+G(d) energy (in a.u.):	-7701.86496209
Thermal correction to Gibbs Free Energy (in a.u.):	0.210699
Number of imaginary frequencies:	1 (–567 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.167006	-1.165495	0.259616
2	6	0	-0.898575	-0.302766	0.036020
3	6	0	1.581579	-0.768342	0.024592
4	6	0	2.591971	-1.186153	0.896137
5	6	0	1.925243	-0.011201	-1.099633
6	6	0	3.917045	-0.836051	0.654357
7	1	0	2.326194	-1.763063	1.778629
8	6	0	3.251897	0.329772	-1.337328
9	1	0	1.145116	0.312218	-1.784438
10	6	0	4.268682	-0.074523	-0.465332
11	1	0	4.691575	-1.153962	1.348826
12	1	0	3.505121	0.920733	-2.214260
13	6	0	-0.777065	1.158285	0.164488
14	6	0	-1.450607	2.029571	-0.706221
15	6	0	0.054412	1.714585	1.146891
16	6	0	-1.262382	3.401871	-0.617853
17	1	0	-2.112069	1.621958	-1.465419
18	6	0	0.225051	3.092459	1.236762
19	1	0	0.564399	1.060059	1.848086
20	6	0	-0.425403	3.959871	0.356801
21	1	0	-1.780762	4.056986	-1.314674
22	1	0	0.872912	3.499345	2.009489
23	7	0	-0.182271	-2.291807	0.878645
24	7	0	0.812644	-3.583065	0.299035
25	53	0	-2.854957	-1.063779	-0.243282
26	7	0	1.207610	-4.589563	0.530637
27	6	0	-0.266133	5.454077	0.466796
28	1	0	-0.147579	5.912563	-0.519949
29	1	0	-1.148306	5.905991	0.934849
30	1	0	0.604942	5.717635	1.072773
31	6	0	5.708662	0.278205	-0.737296
32	1	0	5.786327	1.179948	-1.351280
33	1	0	6.257142	0.449651	0.193676
34	1	0	6.213521	-0.533721	-1.273345

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	NaN_3
Stationary point:	IN3
M06–2X/6–31+G(d) energy (in a.u.):	-7592.48200169
Thermal correction to Gibbs Free Energy (in a.u.):	0.206497
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.823446	0.049971	0.895099
2	6	0	-0.520675	0.448978	0.595613
3	7	0	0.149227	0.387348	1.914797
4	6	0	2.126623	-0.395038	0.460141
5	6	0	2.352352	-0.639513	-0.896664
6	6	0	3.158392	-0.576203	1.390561
7	6	0	3.607347	-1.065207	-1.319930
8	1	0	1.543194	-0.492602	-1.607433
9	6	0	4.404650	-1.001315	0.955153
10	1	0	2.969009	-0.381191	2.442465
11	6	0	4.647871	-1.249449	-0.404315
12	1	0	3.783834	-1.256947	-2.374962
13	1	0	5.206787	-1.144704	1.674917
14	6	0	-1.640039	-0.497068	0.292348
15	6	0	-2.178135	-0.624414	-0.992031
16	6	0	-2.137096	-1.302695	1.316398
17	6	0	-3.187615	-1.546091	-1.240496
18	1	0	-1.813204	0.009752	-1.795911
19	6	0	-3.156665	-2.218921	1.059713
20	1	0	-1.722383	-1.208989	2.316283
21	6	0	-3.697457	-2.357063	-0.218911
22	1	0	-3.594890	-1.635292	-2.245359
23	1	0	-3.537211	-2.834310	1.871537
24	53	0	-0.803884	2.459915	-0.229305
25	6	0	6.015619	-1.683338	-0.863068
26	1	0	6.703978	-0.830576	-0.878290
27	1	0	6.437761	-2.434771	-0.189144
28	1	0	5.982467	-2.104843	-1.871065
29	6	0	-4.804308	-3.340327	-0.504033
30	1	0	-5.050436	-3.929208	0.383689
31	1	0	-5.714231	-2.823394	-0.828057
32	1	0	-4.519281	-4.033696	-1.302531

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	NaN_3
Stationary point:	TS4
M06–2X/6–31+G(d) energy (in a.u.):	-7918.91240763
Thermal correction to Gibbs Free Energy (in a.u.):	0.211547
Number of imaginary frequencies:	1 (–250 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.573800	-0.569193	-0.699681
2	6	0	0.491359	0.399717	-0.663182
3	7	0	-0.054662	-0.103516	-1.841439
4	6	0	-1.980120	-0.597299	-0.244931
5	6	0	-2.329208	-0.886772	1.074929
6	6	0	-2.978573	-0.276104	-1.166098
7	6	0	-3.663013	-0.850281	1.467492
8	1	0	-1.550486	-1.143017	1.789058
9	6	0	-4.310892	-0.247157	-0.766397
10	1	0	-2.691440	-0.034533	-2.185592
11	6	0	-4.673207	-0.530805	0.554158
12	1	0	-3.926773	-1.073229	2.498473
13	1	0	-5.083735	0.003638	-1.489608
14	6	0	1.909485	0.170960	-0.264764
15	6	0	2.344307	0.258065	1.065499
16	6	0	2.812621	-0.263397	-1.241523
17	6	0	3.642623	-0.118062	1.410623
18	1	0	1.652767	0.614554	1.824862
19	6	0	4.119733	-0.620105	-0.892714
20	1	0	2.460482	-0.344323	-2.266494
21	6	0	4.556756	-0.560170	0.437831
22	1	0	3.961350	-0.052748	2.448700
23	1	0	4.811898	-0.944513	-1.666766
24	53	0	-0.075597	2.534123	-0.013295
25	6	0	-6.119098	-0.475422	0.978270
26	1	0	-6.253110	-0.876055	1.986820
27	1	0	-6.487182	0.556620	0.975045
28	1	0	-6.752231	-1.052043	0.296273
29	6	0	5.979217	-0.896489	0.809079
30	1	0	6.423418	-1.600084	0.099445
31	1	0	6.596234	0.008862	0.805320
32	1	0	6.041610	-1.330271	1.811441
33	7	0	0.099998	-2.223602	-0.156960
34	7	0	-0.729873	-3.086116	-0.396093
35	7	0	-1.537002	-3.857815	-0.619887
36	11	0	2.271405	-2.342630	0.338799

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	NaN_3
Stationary point:	IN5
M06–2X/6–31+G(d) energy (in a.u.):	-836.704529787
Thermal correction to Gibbs Free Energy (in a.u.):	0.220562
Number of imaginary frequencies:	0

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.591456	0.739856	0.615241
2	6	0	-0.720805	1.223178	0.248608
3	7	0	-0.013062	1.319482	1.566590
4	6	0	1.821256	0.040525	0.297489
5	6	0	1.992909	-0.511254	-0.973713
6	6	0	2.828439	-0.090073	1.262959
7	6	0	3.167832	-1.192367	-1.277649
8	1	0	1.203167	-0.403986	-1.712917
9	6	0	3.994575	-0.770803	0.947147
10	1	0	2.683680	0.346619	2.247518
11	6	0	4.181211	-1.332498	-0.325393
12	1	0	3.300976	-1.621193	-2.267410
13	1	0	4.778555	-0.873087	1.693893
14	6	0	-1.903571	0.318578	0.131195
15	6	0	-2.956828	0.594438	-0.745440
16	6	0	-1.961176	-0.840504	0.908687
17	6	0	-4.036063	-0.278715	-0.840827
18	1	0	-2.928948	1.495440	-1.348840
19	6	0	-3.047339	-1.705621	0.808325
20	1	0	-1.157894	-1.066780	1.604863
21	6	0	-4.101557	-1.442674	-0.068820
22	1	0	-4.847700	-0.048264	-1.528171
23	1	0	-3.074004	-2.600831	1.425177
24	7	0	-0.900576	2.446902	-0.526061
25	7	0	0.011092	3.268045	-0.414913
26	7	0	0.804825	4.070745	-0.368979
27	6	0	5.449470	-2.081433	-0.642659
28	1	0	6.331240	-1.494016	-0.368085
29	1	0	5.493714	-3.021873	-0.082215
30	1	0	5.515237	-2.320199	-1.707171
31	6	0	-5.276335	-2.380162	-0.190988
32	1	0	-6.219329	-1.857678	0.001846
33	1	0	-5.337567	-2.805163	-1.198900
34	1	0	-5.197935	-3.208033	0.518980

System:	**2**
Oxidant:	NIS
Nitrogen-donor:	NaN_3
Stationary point:	TS6
M06–2X/6–31+G(d) energy (in a.u.):	-836.643853191
Thermal correction to Gibbs Free Energy (in a.u.):	0.214732
Number of imaginary frequencies:	1 (–625 cm^{-1})

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.560162	0.660352	1.236226
2	6	0	-0.696997	1.318698	0.759147
3	7	0	-0.053445	1.067169	2.226088
4	6	0	1.707788	-0.018999	0.667126
5	6	0	1.670596	-0.402820	-0.675818
6	6	0	2.842085	-0.276472	1.445279
7	6	0	2.767403	-1.048747	-1.235628
8	1	0	0.777231	-0.204086	-1.263658
9	6	0	3.931117	-0.917070	0.870520
10	1	0	2.859111	0.028534	2.487749
11	6	0	3.911899	-1.309567	-0.475123
12	1	0	2.736335	-1.355273	-2.278029
13	1	0	4.813936	-1.120317	1.471801
14	6	0	-1.843983	0.416227	0.408215
15	6	0	-2.667374	0.755247	-0.670637
16	6	0	-2.109344	-0.765141	1.106530
17	6	0	-3.725182	-0.069003	-1.039521
18	1	0	-2.473525	1.679567	-1.206726
19	6	0	-3.177020	-1.580140	0.734529
20	1	0	-1.490579	-1.047024	1.953758
21	6	0	-4.002480	-1.249257	-0.341985
22	1	0	-4.352371	0.212783	-1.883031
23	1	0	-3.370428	-2.492475	1.294705
24	7	0	-0.635544	2.597154	0.321652
25	7	0	0.518805	2.758178	-0.946534
26	7	0	1.028195	3.466430	-1.626367
27	6	0	5.114472	-1.974531	-1.092516
28	1	0	4.836304	-2.563124	-1.970662
29	1	0	5.846080	-1.223438	-1.412101
30	1	0	5.611677	-2.636384	-0.377601
31	6	0	-5.174288	-2.117957	-0.724795
32	1	0	-6.112321	-1.699293	-0.342303
33	1	0	-5.270340	-2.200145	-1.812034
34	1	0	-5.070320	-3.126751	-0.315025