An experimental and theoretical study on the substituent effect of the permanganate oxidation of styrenes

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Supplementary data

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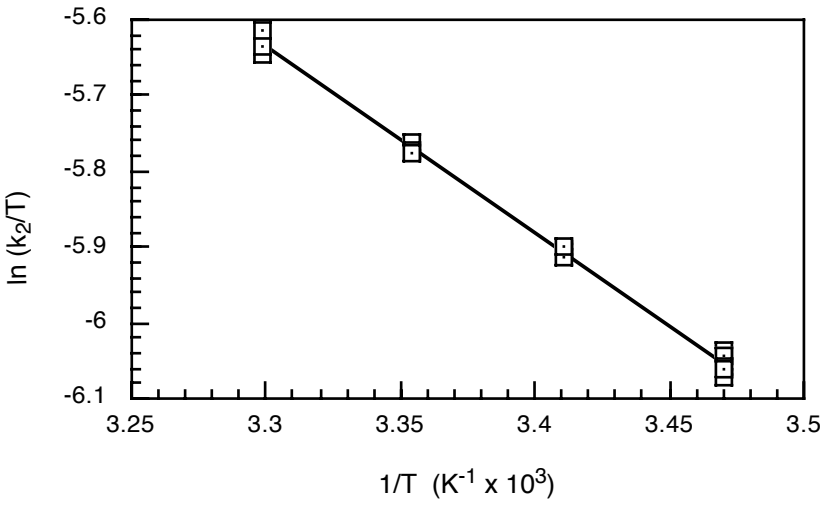

Figure S1. Eyring plot for the reaction of *p*-MePhCH=CH_2.

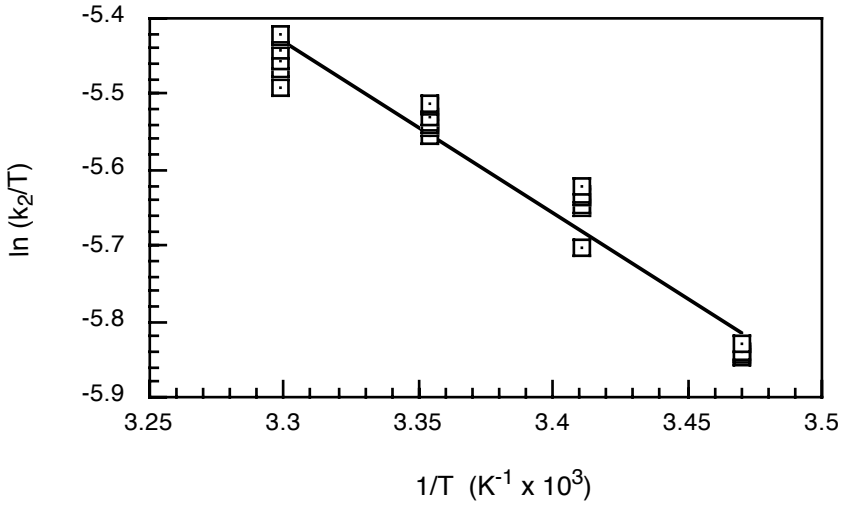

Figure S2. Eyring plot for the reaction of PhCH=CH_2.

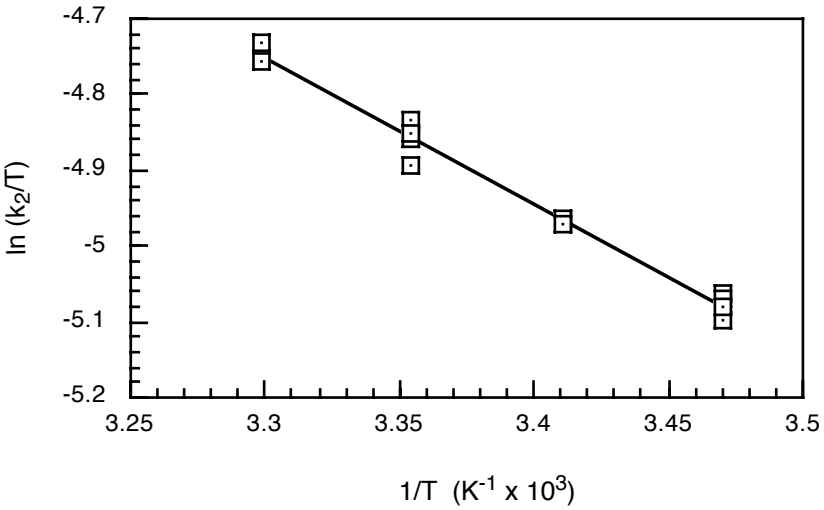

Figure S3. Eyring plot for the reaction of *p*-ClPhCH=CH_2.

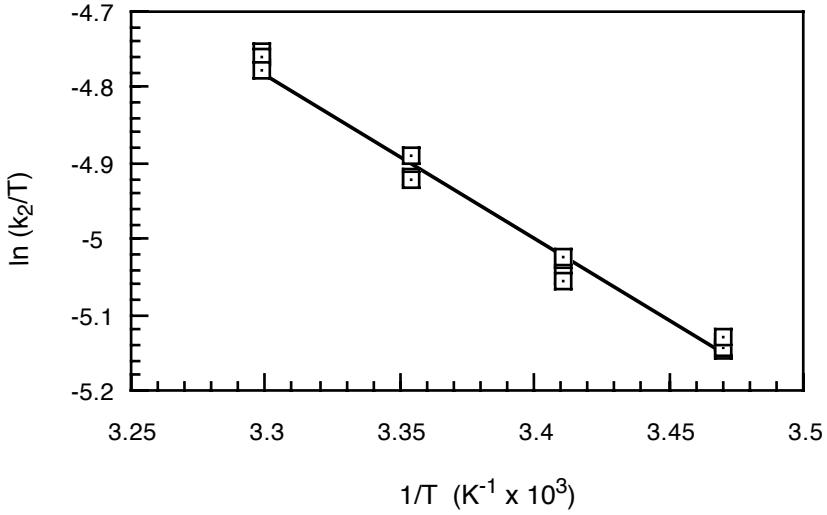

Figure S4. Eyring plot for the reaction of *m*-ClPhCH=CH_2.

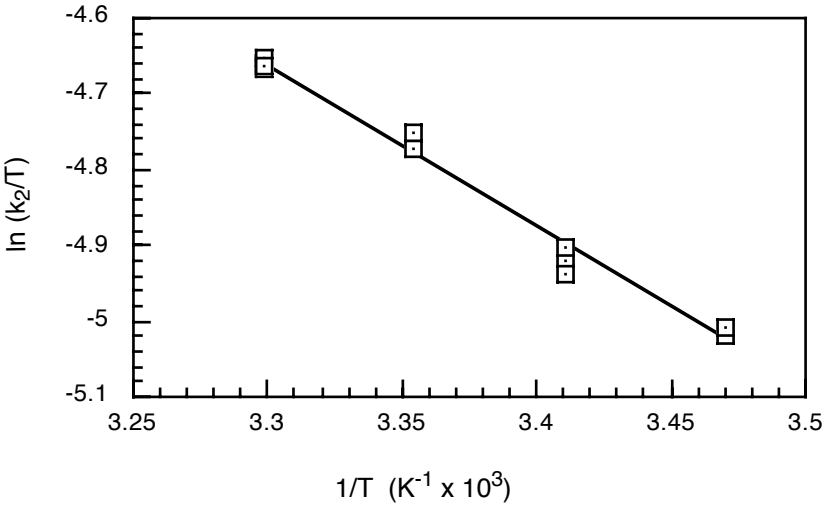

Figure S5. Eyring plot for the reaction of *m*-BrPhCH=CH_2.

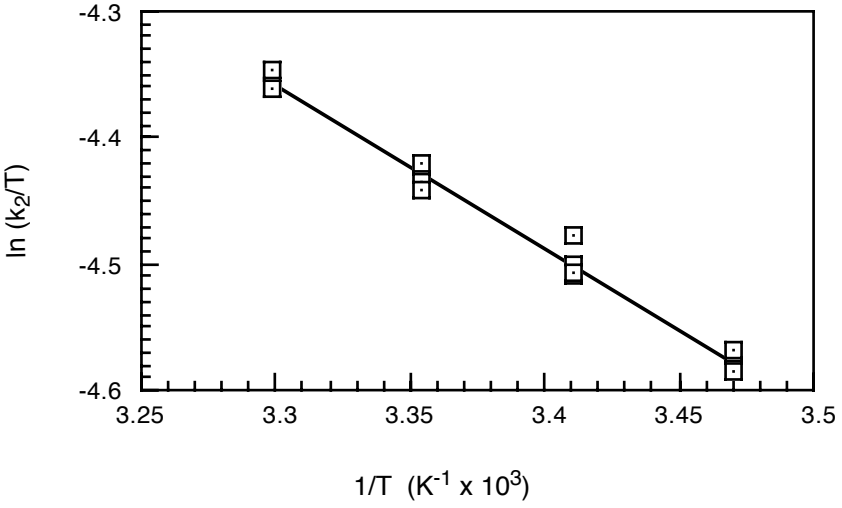

Figure S6. Eyring plot for the reaction of 3,4-diClPhCH=CH_2.

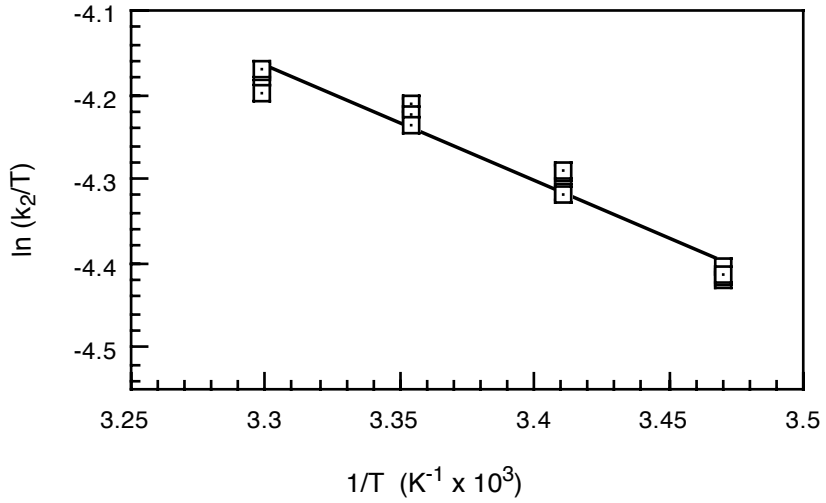

Figure S7. Eyring plot for the reaction of *m*-NO_2rPhCH=CH_2.

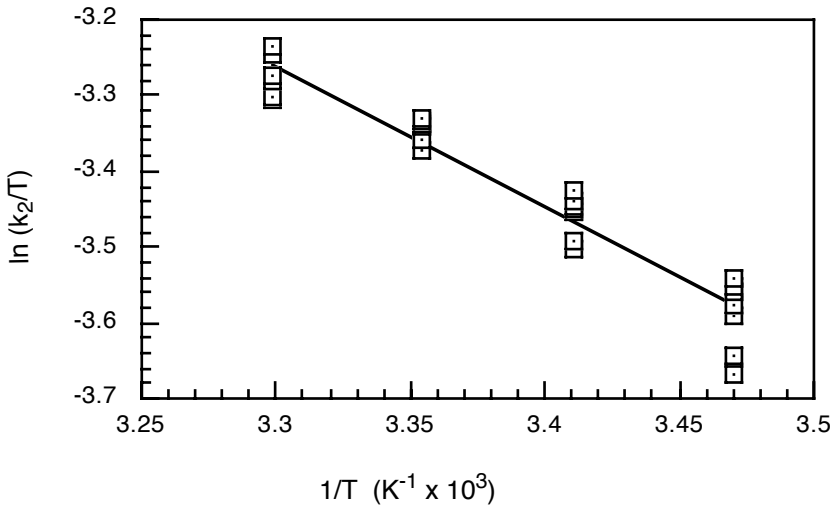

Figure S8. Eyring plot for the reaction of *p*-NO_2rPhCH=CH_2.

Electronic energies calculated at B3LYP/6-311+G(d,p) on B3LYP/LanL2DZ optimized geometries

X	X-PhCH=CH_2	QMnO4	TS^-Q^+	$\Delta E^{\ddagger}$/kJ mol^{-1}
p-Me	-349.0570483	-1823.6689174	-2172.7177616	21.5
H	-309.7293360	-1823.6689174	-2133.3908252	19.5
p-Cl	-769.3509423	-1823.6689174	-2593.0140856	15.2
m-Cl	-769.3507351	-1823.6689174	-2593.0138411	15.3
m-Br	-2883.2709688	-1823.6689174	-4706.9338656	15.8
3,4-diCl	-1228.96717	-1823.6689174	-3052.6315937	11.8
m-NO2	-514.2856388	-1823.6689174	-2337.9500955	11.7
p-NO2	-514.2863906	-1823.6689174	-2337.9534271	4.9

Electlnic energies calculated at B3LYP/6-311+G(d,p) on B3LYP/6-31G(d) optimized geometries

X	X-PhCH=CH_2	QMnO4	TS^-Q^+	$\Delta E^{\ddagger}$/kJ mol^{-1}
p-Me	-349.0584203	-1823.6725396	-2172.7187453	32.1
H	-309.7306977	-1823.6725396	-2133.3917621	30.1
p-Cl	-769.3536162	-1823.6725396	-2593.0164262	25.5
m-Cl	-769.3534076	-1823.6725396	-2593.0162074	25.6
m-Br	-2883.2731325	-1823.6725396	-4706.9351893	27.5
3,4-diCl	-1228.9711265	-1823.6725396	-3052.6352506	22.1
m-NO2	-514.2937481	-1823.6725396	-2337.9594307	18.0
p-NO2	-514.2945366	-1823.6725396	-2337.9622520	12.7

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MnO_4^- (GS) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.253144	0.058923	1.591360

2	25	0	0.000024	0.000006	-0.000010
3	8	0	-0.463715	1.391491	-0.669863
4	8	0	-0.852188	-1.212583	-0.635221
5	8	0	1.568974	-0.237849	-0.286244

D3LYP/LanL2DZ

Zero-point correction= 0.013194 (Hartree/Particle)
Thermal correction to Energy= 0.017804
Thermal correction to Enthalpy= 0.018748
Thermal correction to Gibbs Free Energy= -0.015153
Sum of electronic and zero-point Energies= -404.831789
Sum of electronic and thermal Energies= -404.827179
Sum of electronic and thermal Enthalpies= -404.826235
Sum of electronic and thermal Free Energies= -404.860136

B3LYP/6-311+G(d,p)

HF=-1452.0260993

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***p*-MePhCH=CH$_2$(GS) at B3LYP/LanL2DZ**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.503738	0.443463	0.000085
2	6	0	3.475913	-0.498423	0.000185
3	6	0	1.040986	0.228323	-0.000014
4	6	0	0.441388	-1.057027	-0.000108
5	6	0	-0.951979	-1.201370	-0.000234
6	6	0	-1.810164	-0.074387	-0.000203
7	6	0	-1.215718	1.204122	-0.000210
8	6	0	0.182885	1.352243	-0.000087
9	6	0	-3.317909	-0.248155	0.000349
10	1	0	2.811083	1.491213	0.000087
11	1	0	3.262415	-1.565179	0.000195
12	1	0	4.526139	-0.218953	0.000265
13	1	0	1.067371	-1.945929	-0.000164
14	1	0	-1.386553	-2.199986	-0.000389
15	1	0	-1.848837	2.089268	-0.000324
16	1	0	0.615985	2.351375	-0.000119
17	1	0	-3.832519	0.719364	-0.006287
18	1	0	-3.655256	-0.800931	0.888035
19	1	0	-3.654672	-0.812974	-0.879880

B3LYP/LanL2DZ

Zero-point correction= 0.162164 (Hartree/Particle)
Thermal correction to Energy= 0.170656
Thermal correction to Enthalpy= 0.171600
Thermal correction to Gibbs Free Energy= 0.127939
Sum of electronic and zero-point Energies= -348.752232
Sum of electronic and thermal Energies= -348.743740
Sum of electronic and thermal Enthalpies= -348.742796

Sum of electronic and thermal Free Energies= -348.786457

B3LYP/6-311+G(d,p)

HF=-349.0570483 (Hartree/Particle)

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PhCH=CH_2(GS) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.965126	-0.536595	-0.000015
2	6	0	-2.997469	0.338396	0.000002
3	6	0	-0.519106	-0.222913	-0.000007
4	6	0	-0.012732	1.101626	-0.000011
5	6	0	1.370015	1.341821	-0.000001
6	6	0	2.282030	0.265515	0.000012
7	6	0	1.794394	-1.054633	0.000015
8	6	0	0.408673	-1.293053	0.000005
9	1	0	-2.201240	-1.602493	-0.000037
10	1	0	-2.855896	1.416964	0.000027
11	1	0	-4.026695	-0.010512	-0.000007
12	1	0	-0.699580	1.944253	-0.000024
13	1	0	1.740479	2.364512	-0.000005
14	1	0	3.352729	0.455110	0.000020
15	1	0	2.488351	-1.891968	0.000024
16	1	0	0.037771	-2.316852	0.000007

B3LYP/LanL2DZ

Zero-point correction= 0.134623 (Hartree/Particle)
Thermal correction to Energy= 0.141238
Thermal correction to Enthalpy= 0.142182
Thermal correction to Gibbs Free Energy= 0.103624
Sum of electronic and zero-point Energies= -309.467928
Sum of electronic and thermal Energies= -309.461313
Sum of electronic and thermal Enthalpies= -309.460369
Sum of electronic and thermal Free Energies= -309.498927

B3LYP/6-311+G(d,p)

HF=-309.729336 (Hartree/Particle)

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***p*-ClPhCH=CH_2 (GS) at B3LYP/LanL2DZ**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.921079	0.412052	0.000018
2	6	0	3.870231	-0.552403	0.000023
3	6	0	1.453772	0.226768	0.000009
4	6	0	0.831257	-1.047242	0.000004
5	6	0	-0.566287	-1.173167	-0.000005
6	6	0	-1.354166	-0.011348	-0.000008

7	6	0	-0.779631	1.265563	-0.000004
8	6	0	0.622207	1.372899	0.000005
9	17	0	-3.168962	-0.171306	-0.000019
10	1	0	3.251674	1.452010	0.000022
11	1	0	3.633204	-1.614074	0.000021
12	1	0	4.926290	-0.296727	0.000031
13	1	0	1.436166	-1.949517	0.000007
14	1	0	-1.035330	-2.152142	-0.000009
15	1	0	-1.405860	2.151943	-0.000007
16	1	0	1.075443	2.361981	0.000009

B3LYP/LanL2DZ

Zero-point correction= 0.124762 (Hartree/Particle)
Thermal correction to Energy= 0.132631
Thermal correction to Enthalpy= 0.133575
Thermal correction to Gibbs Free Energy= 0.091462
Sum of electronic and zero-point Energies= -323.815489
Sum of electronic and thermal Energies= -323.807620
Sum of electronic and thermal Enthalpies= -323.806676
Sum of electronic and thermal Free Energies= -323.848789

B3LYP/6-311+G(d,p)

HF=-769.3509423 (Hartree/Particle)

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***m*-ClPhCH=CH$_2$ (GS) at B3LYP/LanL2DZ**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.401614	-1.056004	-0.000005
2	6	0	3.699098	-0.673002	0.000013
3	6	0	1.209786	-0.178785	-0.000003
4	6	0	1.283682	1.237088	-0.000001
5	6	0	0.116017	2.014656	0.000002
6	6	0	-1.157768	1.408466	0.000003
7	6	0	-1.218880	0.009883	-0.000001
8	6	0	-0.069369	-0.787772	-0.000004
9	17	0	-2.852404	-0.802717	-0.000002
10	1	0	2.185116	-2.125338	-0.000022
11	1	0	4.007271	0.370133	0.000032
12	1	0	4.497997	-1.409551	0.000009
13	1	0	2.251478	1.730205	-0.000003
14	1	0	0.185445	3.099424	0.000004
15	1	0	-2.064272	2.004834	0.000005
16	1	0	-0.157249	-1.870703	-0.000007

B3LYP/LanL2DZ

Zero-point correction= 0.124754 (Hartree/Particle)
Thermal correction to Energy= 0.132620
Thermal correction to Enthalpy= 0.133564
Thermal correction to Gibbs Free Energy= 0.091435

Sum of electronic and zero-point Energies= -323.815480
Sum of electronic and thermal Energies= -323.807614
Sum of electronic and thermal Enthalpies= -323.806669
Sum of electronic and thermal Free Energies= -323.848798

B3LYP/6-311+G(d,p)
HF=-769.3507351 (Hartree/Particle)

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***m*-BrPhCH=CH$_2$ (GS) at B3LYP/LanL2DZ**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.103317	-3.146273	0.000000
2	6	0	0.866387	-4.263247	0.000000
3	6	0	0.572787	-1.742785	0.000000
4	6	0	1.942845	-1.379391	0.000000
5	6	0	2.322972	-0.029381	0.000000
6	6	0	1.354214	0.996196	0.000000
7	6	0	0.000000	0.631430	0.000000
8	6	0	-0.399313	-0.712107	0.000000
9	35	0	-1.378440	2.041890	0.000000
10	1	0	-0.980992	-3.268199	0.000000
11	1	0	1.953747	-4.235480	0.000000
12	1	0	0.411432	-5.250053	0.000000
13	1	0	2.709318	-2.149142	0.000000
14	1	0	3.376423	0.239118	0.000000
15	1	0	1.651448	2.039981	0.000000
16	1	0	-1.455220	-0.969013	0.000000

B3LYP/LanL2DZ
Zero-point correction= 0.124229 (Hartree/Particle)
Thermal correction to Energy= 0.132316
Thermal correction to Enthalpy= 0.133260
Thermal correction to Gibbs Free Energy= 0.089829
Sum of electronic and zero-point Energies= -322.034232
Sum of electronic and thermal Energies= -322.026145
Sum of electronic and thermal Enthalpies= -322.025201
Sum of electronic and thermal Free Energies= -322.068631

B3LYP/6-311+G(d,p)
HF=-2883.2709688 (Hartree/Particle)

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3,4-diClPhCH=CH$_2$ (GS) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.270491	-0.363782	-0.000065

2	6	0	4.033643	0.752988	0.000398
3	6	0	1.793820	-0.439486	-0.000062
4	6	0	0.965759	0.708800	-0.000055
5	6	0	-0.427554	0.582641	-0.000031
6	6	0	-1.031578	-0.687165	-0.000028
7	6	0	-0.226229	-1.836300	-0.000060
8	6	0	1.171273	-1.710687	-0.000085
9	17	0	-2.827731	-0.884033	-0.000001
10	17	0	-1.424927	2.093677	-0.000031
11	1	0	3.777057	-1.329898	-0.000463
12	1	0	3.614069	1.756697	0.000868
13	1	0	5.118098	0.687440	0.000344
14	1	0	1.398842	1.703393	-0.000100
15	1	0	-0.695119	-2.815086	-0.000065
16	1	0	1.784490	-2.608553	-0.000106

B3LYP/LanL2DZ

Zero-point correction= 0.114912 (Hartree/Particle)
Thermal correction to Energy= 0.124051
Thermal correction to Enthalpy= 0.124995
Thermal correction to Gibbs Free Energy= 0.079321
Sum of electronic and zero-point Energies= -338.156699
Sum of electronic and thermal Energies= -338.147559
Sum of electronic and thermal Enthalpies= -338.146615
Sum of electronic and thermal Free Energies= -338.192290

B3LYP/6-311+G(d,p)

HF=-1228.96717 (Hartree/Particle)

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***m*-NO_2PhCH=CH_2 (GS) at B3LYP/LanL2DZ**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.613651	-1.063106	0.000010
2	6	0	3.919060	-0.710170	-0.000021
3	6	0	1.444041	-0.157007	0.000011
4	6	0	1.554048	1.257893	-0.000006
5	6	0	0.412971	2.075741	-0.000005
6	6	0	-0.874538	1.510972	0.000012
7	6	0	-0.975217	0.110464	0.000031
8	6	0	0.151626	-0.725749	0.000032
9	7	0	-2.318222	-0.508055	0.000052
10	8	0	-2.396026	-1.785201	-0.000035
11	8	0	-3.337911	0.264495	-0.000057
12	1	0	2.370188	-2.126320	0.000038
13	1	0	4.254018	0.324849	-0.000050
14	1	0	4.699633	-1.465819	-0.000017
15	1	0	2.536514	1.721531	-0.000019
16	1	0	0.523261	3.156529	-0.000018
17	1	0	-1.771698	2.119257	0.000012
18	1	0	0.013273	-1.802223	0.000046

B3LYP/LanL2DZ

Zero-point correction= 0.136290 (Hartree/Particle)
Thermal correction to Energy= 0.145442
Thermal correction to Enthalpy= 0.146386
Thermal correction to Gibbs Free Energy= 0.101097
Sum of electronic and zero-point Energies= -513.938751
Sum of electronic and thermal Energies= -513.929598
Sum of electronic and thermal Enthalpies= -513.928654
Sum of electronic and thermal Free Energies= -513.973944

B3LYP/6-311+G(d,p)

HF=-514.2856388 (Hartree/Particle)

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***p*-NO_2PhCH=CH_2 (GS) at B3LYP/LanL2DZ**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.182454	0.412565	-0.000005
2	6	0	4.122035	-0.561405	0.000470
3	6	0	1.716205	0.233436	-0.000020
4	6	0	1.090902	-1.041412	-0.000011
5	6	0	-0.301959	-1.161426	-0.000005
6	6	0	-1.085753	0.008772	-0.000024
7	6	0	-0.504586	1.288321	-0.000061
8	6	0	0.892334	1.387793	-0.000067
9	7	0	-2.552676	-0.112273	-0.000022
10	8	0	-3.063431	-1.287230	-0.000110
11	8	0	-3.249013	0.963049	-0.000172
12	1	0	3.519677	1.449742	-0.000396
13	1	0	3.876536	-1.621012	0.000927
14	1	0	5.180143	-0.314786	0.000434
15	1	0	1.696108	-1.942825	-0.000041
16	1	0	-0.790181	-2.129529	-0.000001
17	1	0	-1.140133	2.166639	-0.000087
18	1	0	1.356350	2.371260	-0.000095

B3LYP/LanL2DZ

Zero-point correction= 0.136268 (Hartree/Particle)
Thermal correction to Energy= 0.145430
Thermal correction to Enthalpy= 0.146374
Thermal correction to Gibbs Free Energy= 0.101038
Sum of electronic and zero-point Energies= -513.939609
Sum of electronic and thermal Energies= -513.930446
Sum of electronic and thermal Enthalpies= -513.929502
Sum of electronic and thermal Free Energies= -513.974838

B3LYP/6-311+G(d,p)

HF= HF=-514.2863906 (Hartree/Particle)

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TS^{-} (p-MePhCH=CH$_2$) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.903721	-0.211416	-0.770409
2	25	0	2.435677	-0.479468	-0.174733
3	8	0	2.112019	-2.038023	0.040425
4	8	0	1.296411	0.212163	-1.126053
5	8	0	2.232132	0.347162	1.241410
6	6	0	0.829789	1.873844	1.171447
7	6	0	0.042921	1.708757	0.038615
8	6	0	-1.217432	0.947238	0.021387
9	6	0	-3.432614	0.535147	-0.967245
10	6	0	-3.716293	-0.467258	-0.015761
11	6	0	-2.206760	1.224636	-0.951921
12	6	0	-1.495551	-0.079486	0.962237
13	6	0	-2.719417	-0.762453	0.944473
14	6	0	-5.031952	-1.228680	-0.034965
15	1	0	1.633947	2.602116	1.172118
16	1	0	0.494516	1.532143	2.145733
17	1	0	0.249788	2.312568	-0.840456
18	1	0	-4.174726	0.774553	-1.728814
19	1	0	-2.007280	1.988382	-1.702432
20	1	0	-0.727094	-0.362845	1.676398
21	1	0	-2.898694	-1.554566	1.671788
22	1	0	-4.875789	-2.293197	-0.264529
23	1	0	-5.714823	-0.822838	-0.792190
24	1	0	-5.542167	-1.179181	0.938099

B3LYP/LanL2DZ

Zero-point correction= 0.175956 (Hartree/Particle)
Thermal correction to Energy= 0.189656
Thermal correction to Enthalpy= 0.190600
Thermal correction to Gibbs Free Energy= 0.132908
Sum of electronic and zero-point Energies= -753.574638
Sum of electronic and thermal Energies= -753.560939
Sum of electronic and thermal Enthalpies= -753.559994
Sum of electronic and thermal Free Energies= -753.617687

B3LYP/6-311+G(d,p)
HF=-1801.0699345

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TS^{-} (PhCH=CH$_2$) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.539142	0.086023	-0.783809
2	25	0	2.114971	-0.343421	-0.176623
3	8	0	1.969982	-1.928046	0.039963

4	8	0	0.898797	0.216208	-1.118514
5	8	0	1.832480	0.454842	1.242015
6	6	0	0.261218	1.805208	1.195214
7	6	0	-0.502162	1.567652	0.059285
8	6	0	-1.670775	0.672116	0.027740
9	6	0	-3.815194	0.032253	-0.996811
10	6	0	-3.984387	-0.993676	-0.045409
11	6	0	-2.672257	0.849271	-0.960460
12	6	0	-1.841878	-0.382634	0.963104
13	6	0	-2.984638	-1.197210	0.929200
14	1	0	0.975558	2.621642	1.207698
15	1	0	-0.032977	1.414025	2.164165
16	1	0	-0.360725	2.200101	-0.812617
17	1	0	-4.569600	0.190365	-1.766516
18	1	0	-4.865719	-1.632249	-0.073225
19	1	0	-2.542834	1.634009	-1.704654
20	1	0	-1.053681	-0.584324	1.683539
21	1	0	-3.087057	-2.008143	1.648757

B3LYP/LanL2DZ

Zero-point correction= 0.148546 (Hartree/Particle)
Thermal correction to Energy= 0.160292
Thermal correction to Enthalpy= 0.161236
Thermal correction to Gibbs Free Energy= 0.108991
Sum of electronic and zero-point Energies= -714.291462
Sum of electronic and thermal Energies= -714.279717
Sum of electronic and thermal Enthalpies= -714.278773
Sum of electronic and thermal Free Energies= -714.331018

B3LYP/6-311+G(d,p)

HF=-1761.74360357 (Hartree/Particle)

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TS^{-} (*p*-ClPhCH=CH$_2$) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.203194	-0.410257	-0.762324
2	25	0	2.716459	-0.564162	-0.176454
3	8	0	2.277543	-2.092037	0.044586
4	8	0	1.638953	0.201850	-1.139954
5	8	0	2.567148	0.280416	1.236058
6	6	0	1.289203	1.903006	1.167895
7	6	0	0.489542	1.792042	0.038291
8	6	0	-0.806536	1.097173	0.022680
9	6	0	-3.043729	0.812325	-0.974920
10	6	0	-3.329592	-0.158793	-0.007173
11	6	0	-1.780449	1.429066	-0.952833
12	6	0	-1.130172	0.082825	0.963155
13	6	0	-2.387698	-0.542344	0.957751
14	17	0	-4.982056	-0.968266	-0.016926
15	1	0	2.138614	2.577880	1.164914

16	1	0	0.934847	1.588096	2.144522
17	1	0	0.731997	2.378732	-0.842764
18	1	0	-3.782418	1.078875	-1.724948
19	1	0	-1.542707	2.179852	-1.703832
20	1	0	-0.375487	-0.244901	1.671935
21	1	0	-2.619491	-1.325535	1.673258

B3LYP/LanL2DZ

Zero-point correction= 0.138709 (Hartree/Particle)
Thermal correction to Energy= 0.151794
Thermal correction to Enthalpy= 0.152738
Thermal correction to Gibbs Free Energy= 0.096731
Sum of electronic and zero-point Energies= -728.644901
Sum of electronic and thermal Energies= -728.631816
Sum of electronic and thermal Enthalpies= -728.630872
Sum of electronic and thermal Free Energies= -728.686878

B3LYP/6-311+G(d,p)

HF=-2221.3699819 (Hartree/Particle)

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TS^{-} (*m*-ClPhCH=CH2) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.011229	-0.926784	-0.813767
2	25	0	-2.720926	-0.027340	-0.493316
3	8	0	-2.646666	1.310197	-1.377417
4	8	0	-1.352423	-0.904012	-0.674673
5	8	0	-2.671422	0.350384	1.114286
6	6	0	-1.095101	-0.470329	2.170375
7	6	0	-0.149303	-0.942134	1.270161
8	6	0	0.970735	-0.131738	0.768413
9	6	0	3.223640	-0.002747	-0.141663
10	6	0	3.201469	1.397203	-0.165223
11	6	0	2.148293	-0.774103	0.303328
12	6	0	0.922518	1.287772	0.730356
13	6	0	2.020379	2.032827	0.276208
14	17	0	4.745886	-0.863816	-0.723114
15	1	0	-1.778918	-1.163525	2.648713
16	1	0	-0.985572	0.497929	2.648713
17	1	0	-0.116588	-2.003438	1.042871
18	1	0	4.053051	1.965788	-0.524893
19	1	0	2.206032	-1.858625	0.295516
20	1	0	0.004506	1.792946	1.015344
21	1	0	1.958726	3.118496	0.240433

B3LYP/LanL2DZ

Zero-point correction= 0.138710 (Hartree/Particle)
Thermal correction to Energy= 0.151777
Thermal correction to Enthalpy= 0.152721

Thermal correction to Gibbs Free Energy= 0.096838
Sum of electronic and zero-point Energies= -728.645267
Sum of electronic and thermal Energies= -728.632199
Sum of electronic and thermal Enthalpies= -728.631255
Sum of electronic and thermal Free Energies= -728.687139

B3LYP/6-311+G(d,p)
HF=-2221.3703013 (Hartree/Particle)

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TS^{-} (*m*-BrPhCH=CH2) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.527221	-1.327001	-0.533938
2	25	0	-3.312219	-0.279193	-0.484211
3	8	0	-3.276984	0.710106	-1.747724
4	8	0	-1.884703	-1.063702	-0.338791
5	8	0	-3.364005	0.593105	0.917790
6	6	0	-1.784062	0.282100	2.215332
7	6	0	-0.773220	-0.389370	1.540693
8	6	0	0.314691	0.291706	0.821857
9	6	0	2.603800	0.286302	-0.016911
10	6	0	2.481270	1.589767	-0.519738
11	6	0	1.556751	-0.371110	0.636640
12	6	0	0.170527	1.603870	0.297971
13	6	0	1.237370	2.237452	-0.354979
14	35	0	4.341463	-0.661876	-0.242398
15	1	0	-2.443245	-0.262547	2.882933
16	1	0	-1.754778	1.359112	2.347650
17	1	0	-0.664511	-1.461071	1.678361
18	1	0	3.305299	2.076724	-1.031684
19	1	0	1.682462	-1.385089	1.005744
20	1	0	-0.794450	2.097263	0.366695
21	1	0	1.104032	3.236748	-0.764374

B3LYP/LanL2DZ
Zero-point correction= 0.138094 (Hartree/Particle)
Thermal correction to Energy= 0.151448
Thermal correction to Enthalpy= 0.152392
Thermal correction to Gibbs Free Energy= 0.094782
Sum of electronic and zero-point Energies= -726.863783
Sum of electronic and thermal Energies= -726.850429
Sum of electronic and thermal Enthalpies= -726.849485
Sum of electronic and thermal Free Energies= -726.907095

B3LYP/6-311+G(d,p)
HF=-4335.2908064 (Hartree/Particle)

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TS^{-} (3,4-diClPhCH=CH2) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.568554	-0.276672	-1.082342
2	25	0	-3.190495	0.291461	-0.489160
3	8	0	-2.881194	1.799413	-0.941184
4	8	0	-1.945319	-0.686902	-0.895685
5	8	0	-3.187721	0.183560	1.159347
6	6	0	-1.786176	-1.102243	1.967785
7	6	0	-0.871899	-1.444035	0.981041
8	6	0	0.358849	-0.685643	0.719180
9	6	0	2.658592	-0.629839	-0.122888
10	6	0	2.779895	0.719216	0.237074
11	6	0	1.465757	-1.325103	0.108308
12	6	0	0.487665	0.689003	1.053402
13	17	0	4.043605	-1.528628	-0.896107
14	6	0	1.683611	1.379370	0.819347
15	17	0	4.314765	1.656883	-0.045180
16	1	0	-2.575208	-1.796088	2.237249
17	1	0	-1.571577	-0.320660	2.689973
18	1	0	-0.969404	-2.398551	0.473037
19	1	0	1.391556	-2.367878	-0.185767
20	1	0	-0.369049	1.222823	1.452325
21	1	0	1.768302	2.433961	1.063463

B3LYP/LanL2DZ

Zero-point correction= 0.128925 (Hartree/Particle)
Thermal correction to Energy= 0.143300
Thermal correction to Enthalpy= 0.144244
Thermal correction to Gibbs Free Energy= 0.084845
Sum of electronic and zero-point Energies= -742.990836
Sum of electronic and thermal Energies= -742.976461
Sum of electronic and thermal Enthalpies= -742.975517
Sum of electronic and thermal Free Energies= -743.034917

B3LYP/6-311+G(d,p)

HF=-2680.9903288 (Hartree/Particle)

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TS^- (*m*-$NO_2PhCH=CH_2$) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.183432	-0.625222	-1.125961
2	25	0	-2.903061	0.112667	-0.503611
3	8	0	-2.788822	1.655732	-0.929240
4	8	0	-1.531082	-0.683096	-0.901350
5	8	0	-2.908044	-0.017117	1.143457
6	6	0	-1.348186	-1.104492	1.956916
7	6	0	-0.382347	-1.295064	0.978430
8	6	0	0.713150	-0.346281	0.732349
9	6	0	2.987979	0.116182	-0.012125

10	6	0	2.865391	1.488361	0.281511
11	6	0	1.939991	-0.796321	0.195218
12	6	0	0.575248	1.042274	1.009359
13	6	0	1.636528	1.936855	0.792298
14	7	0	4.263250	-0.377114	-0.551795
15	8	0	4.385639	-1.628480	-0.806424
16	8	0	5.216311	0.462895	-0.744216
17	1	0	-2.026832	-1.911854	2.210713
18	1	0	-1.261926	-0.306520	2.688078
19	1	0	-0.319549	-2.251173	0.467675
20	1	0	3.696996	2.158666	0.098390
21	1	0	2.084016	-1.841388	-0.057391
22	1	0	-0.386055	1.413879	1.351711
23	1	0	1.496032	2.994733	0.999784

B3LYP/LanL2DZ

Zero-point correction= 0.150256 (Hartree/Particle)
Thermal correction to Energy= 0.164608
Thermal correction to Enthalpy= 0.165553
Thermal correction to Gibbs Free Energy= 0.106562
Sum of electronic and zero-point Energies= -918.775950
Sum of electronic and thermal Energies= -918.761598
Sum of electronic and thermal Enthalpies= -918.760654
Sum of electronic and thermal Free Energies= -918.819644

B3LYP/6-311+G(d,p)

HF=-1966.3124566 (Hartree/Particle)

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TS^{-} (*p*-NO$_2$ClPhCH=CH2) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.436673	-0.353694	-0.820842
2	25	0	2.957279	-0.570485	-0.242797
3	8	0	2.564463	-2.119559	-0.128960
4	8	0	1.869484	0.222742	-1.155249
5	8	0	2.811779	0.160862	1.230697
6	6	0	1.553676	1.785716	1.352707
7	6	0	0.730366	1.809564	0.234891
8	6	0	-0.562192	1.141586	0.153282
9	6	0	-2.745969	0.929095	-0.965208
10	6	0	-3.129179	-0.035423	-0.006098
11	6	0	-1.477081	1.500079	-0.879666
12	6	0	-0.968677	0.135059	1.080006
13	6	0	-2.234315	-0.444260	1.009728
14	7	0	-4.454659	-0.620582	-0.072196
15	8	0	-4.796510	-1.492234	0.815179
16	8	0	-5.254901	-0.245004	-1.013114
17	1	0	2.412536	2.446603	1.402384
18	1	0	1.212517	1.382709	2.300974
19	1	0	1.000277	2.443183	-0.604213

20	1	0	-3.445729	1.206185	-1.745898
21	1	0	-1.168100	2.238009	-1.616326
22	1	0	-0.264340	-0.210789	1.829876
23	1	0	-2.544214	-1.213108	1.708971

B3LYP/LanL2DZ

Zero-point correction= 0.150381 (Hartree/Particle)
Thermal correction to Energy= 0.164774
Thermal correction to Enthalpy= 0.165718
Thermal correction to Gibbs Free Energy= 0.106334
Sum of electronic and zero-point Energies= -918.780483
Sum of electronic and thermal Energies= -918.766090
Sum of electronic and thermal Enthalpies= -918.765145
Sum of electronic and thermal Free Energies= -918.824529

B3LYP/6-311+G(d,p)

HF=-1966.3174273 (Hartree/Particle)

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MnO_4^-—$^+NEt_4$ (GS) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.992247	1.380629	0.445870
2	25	0	-2.419877	-0.026093	-0.227268
3	8	0	-2.029451	-1.212990	0.801856
4	8	0	-1.547544	-0.220450	-1.571828
5	8	0	-3.977414	-0.050823	-0.557398
6	7	0	1.817849	0.016385	0.184995
7	6	0	1.001327	-1.263688	-0.144177
8	6	0	3.271084	-0.119869	-0.299265
9	6	0	1.103732	1.203214	-0.518195
10	6	0	1.875862	0.243034	1.714685
11	6	0	1.599978	-2.581297	0.355414
12	6	0	3.441523	-0.360810	-1.803900
13	6	0	0.528772	0.476465	2.410508
14	6	0	1.790852	2.563654	-0.361769
15	1	0	0.871003	-1.271562	-1.227884
16	1	0	0.008103	-1.123816	0.284353
17	1	0	3.708265	-0.944316	0.271229
18	1	0	3.785777	0.797000	0.001592
19	1	0	0.087515	1.240926	-0.119844
20	1	0	1.015773	0.923426	-1.569911
21	1	0	2.539722	1.100548	1.865788
22	1	0	2.376270	-0.638673	2.127235
23	1	0	1.704786	-2.618237	1.445601
24	1	0	2.561408	-2.835471	-0.105761
25	1	0	0.887574	-3.369092	0.083117
26	1	0	2.949733	-1.279116	-2.139119
27	1	0	4.513088	-0.464989	-2.013685
28	1	0	3.068029	0.472477	-2.407245
29	1	0	-0.172870	-0.354242	2.286674

30	1	0	0.020794	1.381316	2.066476
31	1	0	0.729102	0.590078	3.483845
32	1	0	2.788302	2.607921	-0.814903
33	1	0	1.859352	2.889277	0.682194
34	1	0	1.164733	3.299024	-0.880821

B3LYP/LanL2DZ

Zero-point correction= 0.294289 (Hartree/Particle)
Thermal correction to Energy= 0.312507
Thermal correction to Enthalpy= 0.313451
Thermal correction to Gibbs Free Energy= 0.247585
Sum of electronic and zero-point Energies= -776.040793
Sum of electronic and thermal Energies= -776.022574
Sum of electronic and thermal Enthalpies= -776.021630
Sum of electronic and thermal Free Energies= -776.087496

B3LYP/6-311+G(d,p)

HF=-1823.6689174 (Hartree/Particle)

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TS^{-}—$^{+}$NEt$_4$ (*p*-MePhCH=CH$_2$) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.991475	3.165785	0.395791
2	25	0	-0.743921	2.399273	-0.251992
3	8	0	-1.166263	1.505625	-1.540049
4	8	0	-0.062455	1.411837	0.866935
5	8	0	0.476981	3.421192	-0.607045
6	6	0	2.260198	3.164868	0.531954
7	6	0	2.191182	1.937634	1.170139
8	6	0	2.725834	0.677940	0.625445
9	6	0	3.520962	-1.618231	1.017717
10	6	0	3.838996	-1.784401	-0.348811
11	6	0	2.974637	-0.413678	1.493876
12	6	0	3.015547	0.497468	-0.751834
13	6	0	3.563654	-0.705785	-1.222713
14	6	0	4.482628	-3.062264	-0.858286
15	1	0	2.008782	4.073405	1.067659
16	1	0	2.796035	3.294762	-0.402551
17	1	0	1.872378	1.909340	2.208479
18	1	0	3.718672	-2.431471	1.715071
19	1	0	2.750503	-0.304943	2.554072
20	1	0	2.791825	1.295988	-1.454278
21	1	0	3.784426	-0.811306	-2.284190
22	1	0	4.244164	-3.918302	-0.214674
23	1	0	5.578388	-2.969795	-0.884318
24	1	0	4.155252	-3.301106	-1.878339
25	7	0	-2.193543	-1.676199	0.031878
26	6	0	-0.751815	-1.350211	-0.460547
27	6	0	-2.186335	-2.870358	1.000883
28	6	0	-2.719173	-0.391880	0.724427

29	6	0	-3.102869	-2.068425	-1.151578
30	6	0	-0.042216	-2.480422	-1.209564
31	6	0	-1.292169	-2.711466	2.236627
32	6	0	-3.363015	-0.962047	-2.182081
33	6	0	-4.104823	-0.507136	1.364737
34	1	0	-0.192246	-1.049419	0.425871
35	1	0	-0.837650	-0.451573	-1.079891
36	1	0	-1.874300	-3.740624	0.415293
37	1	0	-3.226172	-3.030852	1.300690
38	1	0	-2.704319	0.382584	-0.042663
39	1	0	-1.960007	-0.100681	1.453447
40	1	0	-4.045227	-2.414766	-0.713980
41	1	0	-2.622411	-2.930146	-1.623968
42	1	0	-0.510533	-2.721383	-2.170962
43	1	0	0.061748	-3.401989	-0.623516
44	1	0	0.971627	-2.122260	-1.422345
45	1	0	-0.233612	-2.614271	1.978040
46	1	0	-1.402545	-3.612160	2.853371
47	1	0	-1.576218	-1.852681	2.853116
48	1	0	-2.447615	-0.483886	-2.540952
49	1	0	-4.009421	-0.170722	-1.790569
50	1	0	-3.874903	-1.416241	-3.039969
51	1	0	-4.138639	-1.203880	2.210474
52	1	0	-4.888576	-0.782075	0.648991
53	1	0	-4.358230	0.486875	1.751858

B3LYP/LanL2DZ

Zero-point correction= 0.457518 (Hartree/Particle)
Thermal correction to Energy= 0.484888
Thermal correction to Enthalpy= 0.485832
Thermal correction to Gibbs Free Energy= 0.397514
Sum of electronic and zero-point Energies= -1124.787762
Sum of electronic and thermal Energies= -1124.760392
Sum of electronic and thermal Enthalpies= -1124.759448
Sum of electronic and thermal Free Energies= -1124.847766

B3LYP/6-311+G(d,p)

HF=-2172.7177616 (Hartree/Particle)

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TS^{-}—$^{+}NEt_4$ (PhCH=CH_2) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.574566	-3.418855	-0.607504
2	25	0	0.305401	-2.310835	0.141996
3	8	0	-0.435313	-1.719279	1.458809
4	8	0	0.615988	-1.069314	-0.883739
5	8	0	1.801709	-2.858711	0.492066
6	6	0	3.403500	-1.905078	-0.529150
7	6	0	2.915126	-0.742414	-1.101975
8	6	0	2.938974	0.583776	-0.460694

9	6	0	2.844947	3.032783	-0.693168
10	6	0	3.042976	3.188029	0.693810
11	6	0	2.790359	1.746947	-1.259215
12	6	0	3.114808	0.755420	0.937798
13	6	0	3.172922	2.039648	1.503776
14	1	0	3.516822	-2.801770	-1.128094
15	1	0	3.922433	-1.900186	0.423719
16	1	0	2.638926	-0.757169	-2.152664
17	1	0	2.749601	3.909922	-1.330483
18	1	0	3.101142	4.181136	1.134015
19	1	0	2.651383	1.633350	-2.333317
20	1	0	3.190829	-0.118189	1.579545
21	1	0	3.320403	2.147682	2.576553
22	7	0	-2.526742	0.966141	-0.000908
23	6	0	-1.074028	1.163887	0.525147
24	6	0	-2.929232	2.110694	-0.946443
25	6	0	-2.544630	-0.400863	-0.732898
26	6	0	-3.538570	0.974902	1.163714
27	6	0	-0.831150	2.451885	1.315077
28	6	0	-2.023443	2.308107	-2.167988
29	6	0	-3.390190	-0.165426	2.179002
30	6	0	-3.871684	-0.778935	-1.395417
31	1	0	-0.425423	1.105762	-0.349809
32	1	0	-0.844247	0.276909	1.123705
33	1	0	-2.949139	3.019777	-0.337651
34	1	0	-3.956019	1.903182	-1.262365
35	1	0	-2.253997	-1.139141	0.014810
36	1	0	-1.726724	-0.373294	-1.455828
37	1	0	-4.533521	0.954405	0.706738
38	1	0	-3.420774	1.945610	1.654011
39	1	0	-1.381566	2.487543	2.262534
40	1	0	-1.043390	3.365237	0.745725
41	1	0	0.237199	2.471444	1.558436
42	1	0	-1.000575	2.580097	-1.891249
43	1	0	-2.435564	3.130177	-2.766415
44	1	0	-1.982600	1.421650	-2.808688
45	1	0	-2.375606	-0.258544	2.575000
46	1	0	-3.666406	-1.137650	1.760303
47	1	0	-4.068373	0.041622	3.016576
48	1	0	-4.155080	-0.112956	-2.218902
49	1	0	-4.705493	-0.838158	-0.686109
50	1	0	-3.738729	-1.781454	-1.818968

B3LYP/LanL2DZ

Zero-point correction= 0.429881 (Hartree/Particle)
Thermal correction to Energy= 0.455407
Thermal correction to Enthalpy= 0.456352
Thermal correction to Gibbs Free Energy= 0.372258
Sum of electronic and zero-point Energies= -1085.504233
Sum of electronic and thermal Energies= -1085.478706
Sum of electronic and thermal Enthalpies= -1085.477762
Sum of electronic and thermal Free Energies= -1085.561855

B3LYP/6-311+G(d,p)

HF=-2133.3908252 (Hartree/Particle)

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TS^{-}—$^{+}NEt_4$ (*p*-ClPhCH=CH_2) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.701974	2.731294	0.187545
2	25	0	-1.270250	2.263643	-0.357982
3	8	0	-1.391503	1.262300	-1.626717
4	8	0	-0.452818	1.496909	0.839239
5	8	0	-0.299210	3.532102	-0.689544
6	6	0	1.451233	3.707134	0.491287
7	6	0	1.608656	2.521691	1.189786
8	6	0	2.374815	1.361272	0.707430
9	6	0	3.559935	-0.738966	1.219620
10	6	0	3.849119	-0.886888	-0.143727
11	6	0	2.821223	0.383708	1.632356
12	6	0	2.682357	1.167059	-0.664771
13	6	0	3.420875	0.052098	-1.094237
14	17	0	4.793292	-2.352487	-0.699766
15	1	0	1.017306	4.572779	0.979233
16	1	0	1.976592	3.898527	-0.438684
17	1	0	1.279725	2.478050	2.224210
18	1	0	3.908261	-1.473155	1.939644
19	1	0	2.595218	0.511072	2.689100
20	1	0	2.320256	1.876056	-1.403407
21	1	0	3.652824	-0.085609	-2.145988
22	7	0	-2.109084	-1.955181	0.090632
23	6	0	-0.689201	-1.468364	-0.322003
24	6	0	-2.026697	-3.020219	1.197690
25	6	0	-2.878699	-0.697968	0.575358
26	6	0	-2.834903	-2.610064	-1.102819
27	6	0	0.246425	-2.554897	-0.857286
28	6	0	-1.300790	-2.587368	2.476962
29	6	0	-3.116725	-1.688589	-2.296487
30	6	0	-4.290913	-0.948797	1.109509
31	1	0	-0.270487	-0.982054	0.560456
32	1	0	-0.841186	-0.669712	-1.054389
33	1	0	-1.530631	-3.888940	0.754109
34	1	0	-3.057705	-3.308527	1.423446
35	1	0	-2.897919	-0.017886	-0.275892
36	1	0	-2.245309	-0.218640	1.324752
37	1	0	-3.770328	-3.018138	-0.706148
38	1	0	-2.210122	-3.454552	-1.408028
39	1	0	-0.100494	-3.000085	-1.796888
40	1	0	0.446038	-3.357249	-0.136757
41	1	0	1.206657	-2.070678	-1.067275
42	1	0	-0.245691	-2.356851	2.303069
43	1	0	-1.344464	-3.420676	3.189245
44	1	0	-1.769222	-1.720772	2.953862
45	1	0	-2.222288	-1.181640	-2.667447

46	1	0	-3.858398	-0.918076	-2.066826
47	1	0	-3.519527	-2.307321	-3.108333
48	1	0	-4.311977	-1.544392	2.029647
49	1	0	-4.955510	-1.414046	0.371857
50	1	0	-4.713966	0.034077	1.348393

B3LYP/LanL2DZ

Zero-point correction= 0.419994 (Hartree/Particle)
Thermal correction to Energy= 0.446889
Thermal correction to Enthalpy= 0.447833
Thermal correction to Gibbs Free Energy= 0.359511
Sum of electronic and zero-point Energies= -1099.853694
Sum of electronic and thermal Energies= -1099.826799
Sum of electronic and thermal Enthalpies= -1099.825855
Sum of electronic and thermal Free Energies= -1099.914177

B3LYP/6-311+G(d,p)

HF=-2593.0140856

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TS^{-}—$^{+}$NEt$_4$ (*m*-ClPhCH=CH$_2$) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.846509	3.392285	0.058890
2	25	0	-0.646165	2.455185	-0.429215
3	8	0	-1.078717	1.487941	-1.654027
4	8	0	-0.126509	1.530954	0.824644
5	8	0	0.686201	3.321918	-0.799845
6	6	0	2.375929	3.028516	0.433372
7	6	0	2.115204	1.970887	1.288557
8	6	0	2.527915	0.577429	1.056990
9	6	0	3.044699	-1.644487	1.978111
10	6	0	3.368382	-2.130232	0.694858
11	6	0	2.624577	-0.315488	2.155027
12	6	0	2.839439	0.085398	-0.238907
13	6	0	3.248588	-1.241093	-0.384327
14	17	0	3.622355	-1.865432	-2.067038
15	1	0	2.236805	4.048634	0.772373
16	1	0	2.968257	2.903654	-0.467819
17	1	0	1.728510	2.188296	2.280349
18	1	0	3.135019	-2.306523	2.836283
19	1	0	3.704114	-3.150892	0.542754
20	1	0	2.383881	0.048415	3.151570
21	1	0	2.737798	0.727206	-1.107672
22	7	0	-2.376529	-1.528600	0.116447
23	6	0	-0.956158	-1.351497	-0.494731

24	6	0	-2.350729	-2.534428	1.281537
25	6	0	-2.827641	-0.124089	0.596231
26	6	0	-3.360740	-2.086037	-0.930949
27	6	0	-0.347071	-2.615008	-1.107677
28	6	0	-1.456021	-2.150301	2.466424
29	6	0	-3.532766	-1.235236	-2.195397
30	6	0	-4.188446	-0.067224	1.294704
31	1	0	-0.330604	-0.953329	0.306273
32	1	0	-1.039373	-0.545551	-1.229793
33	1	0	-2.028874	-3.489039	0.854514
34	1	0	-3.388200	-2.651725	1.609865
35	1	0	-2.813013	0.509994	-0.291074
36	1	0	-2.028030	0.252937	1.237360
37	1	0	-4.319695	-2.204486	-0.416611
38	1	0	-2.998836	-3.086045	-1.187614
39	1	0	-0.923878	-3.004202	-1.954620
40	1	0	-0.190167	-3.422981	-0.382848
41	1	0	0.640286	-2.340184	-1.495002
42	1	0	-0.400553	-2.067968	2.190762
43	1	0	-1.540852	-2.941105	3.222405
44	1	0	-1.762359	-1.210209	2.934867
45	1	0	-2.593347	-1.080395	-2.732990
46	1	0	-3.963489	-0.251667	-1.987577
47	1	0	-4.220964	-1.765685	-2.865470
48	1	0	-4.222236	-0.636333	2.231127
49	1	0	-5.018812	-0.389702	0.655362
50	1	0	-4.368283	0.984375	1.547863

B3LYP/LanL2DZ

Zero-point correction= 0.420204 (Hartree/Particle)
Thermal correction to Energy= 0.447002
Thermal correction to Enthalpy= 0.447946
Thermal correction to Gibbs Free Energy= 0.360336
Sum of electronic and zero-point Energies= -1099.853208
Sum of electronic and thermal Energies= -1099.826410
Sum of electronic and thermal Enthalpies= -1099.825466
Sum of electronic and thermal Free Energies= -1099.913077

B3LYP/6-311+G(d,p)

HF=-2593.0138411 (Hartree/Particle)

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TS^{-}—$^{+}NEt_4$ (*m*-BrPhCH=CH_2) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.773901	3.011182	-0.482988
2	25	0	-1.355077	2.298399	-0.677690
3	8	0	-1.390690	1.162459	-1.830080
4	8	0	-0.889500	1.606459	0.737639
5	8	0	-0.164541	3.382263	-0.945650
6	6	0	1.307017	3.557068	0.557112

7	6	0	1.130138	2.526780	1.465529
8	6	0	1.847988	1.242188	1.434172
9	6	0	2.643979	-0.751677	2.632063
10	6	0	3.272886	-1.232955	1.465865
11	6	0	1.937603	0.462250	2.615126
12	6	0	2.467526	0.749483	0.253813
13	6	0	3.161649	-0.463896	0.294096
14	35	0	4.006437	-1.140394	-1.364275
15	1	0	0.904870	4.541428	0.767729
16	1	0	2.056040	3.507875	-0.226976
17	1	0	0.550135	2.720229	2.363554
18	1	0	2.722227	-1.324889	3.553206
19	1	0	3.829741	-2.164564	1.473997
20	1	0	1.464657	0.827057	3.524519
21	1	0	2.381008	1.304124	-0.674745
22	7	0	-2.472292	-1.831286	0.132124
23	6	0	-1.011919	-1.451524	-0.249483
24	6	0	-2.507630	-2.631594	1.446303
25	6	0	-3.251040	-0.495791	0.269865
26	6	0	-3.108201	-2.725054	-0.950456
27	6	0	-0.063965	-2.634324	-0.460542
28	6	0	-1.909578	-1.922395	2.667128
29	6	0	-3.175523	-2.115512	-2.355943
30	6	0	-4.720858	-0.622456	0.677016
31	1	0	-0.655856	-0.787965	0.541090
32	1	0	-1.084933	-0.824388	-1.142076
33	1	0	-1.974030	-3.566378	1.249998
34	1	0	-3.557648	-2.882435	1.625731
35	1	0	-3.148028	0.008100	-0.692125
36	1	0	-2.688268	0.112699	0.980772
37	1	0	-4.112214	-2.973545	-0.592271
38	1	0	-2.524415	-3.650424	-0.963442
39	1	0	-0.358628	-3.284623	-1.292726
40	1	0	0.074584	-3.247422	0.437971
41	1	0	0.916579	-2.216308	-0.713625
42	1	0	-0.848024	-1.690080	2.541045
43	1	0	-2.003297	-2.596575	3.527785
44	1	0	-2.435427	-0.995272	2.914503
45	1	0	-2.190202	-1.854251	-2.751360
46	1	0	-3.802142	-1.220218	-2.399797
47	1	0	-3.617692	-2.864261	-3.025194
48	1	0	-4.861712	-1.056660	1.673720
49	1	0	-5.324786	-1.186787	-0.043260
50	1	0	-5.126240	0.395900	0.707655

B3LYP/LanL2DZ

Zero-point correction= 0.419193 (Hartree/Particle)
Thermal correction to Energy= 0.446449
Thermal correction to Enthalpy= 0.447393
Thermal correction to Gibbs Free Energy= 0.356893
Sum of electronic and zero-point Energies= -1098.072043
Sum of electronic and thermal Energies= -1098.044787
Sum of electronic and thermal Enthalpies= -1098.043842

Sum of electronic and thermal Free Energies= -1098.134342

B3LYP/6-311+G(d,p)
HF= -4706.9338656 (Hartree/Particle)

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TS^{-}—$^{+}NEt_4$ (3,4-diClPhCH=CH_2) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.268238	2.571483	-0.192413
2	25	0	1.798984	2.196561	0.316284
3	8	0	1.823716	1.169919	1.569321
4	8	0	0.949511	1.517485	-0.910873
5	8	0	0.916707	3.526793	0.659592
6	6	0	-0.774241	3.878465	-0.540725
7	6	0	-0.961911	2.776399	-1.358535
8	6	0	-1.844541	1.641680	-1.051147
9	6	0	-3.150407	-0.285518	-1.843322
10	6	0	-3.541047	-0.574092	-0.525314
11	6	0	-2.307509	0.806186	-2.098556
12	6	0	-2.247161	1.333438	0.273239
13	6	0	-3.084427	0.241093	0.523911
14	17	0	-3.538697	-0.115078	2.246399
15	17	0	-4.614795	-2.005823	-0.228912
16	1	0	-0.270746	4.758622	-0.923904
17	1	0	-1.343348	4.016939	0.373276
18	1	0	-0.559476	2.801712	-2.367218
19	1	0	-3.513034	-0.909267	-2.654724
20	1	0	-2.009551	1.021700	-3.121704
21	1	0	-1.880979	1.924105	1.106339
22	7	0	2.065151	-2.163455	-0.046936
23	6	0	0.751325	-1.497881	0.458985
24	6	0	1.763118	-3.276248	-1.065567
25	6	0	2.913206	-1.030827	-0.681152
26	6	0	2.829204	-2.824803	1.120133
27	6	0	-0.228275	-2.437240	1.167191
28	6	0	0.987132	-2.836656	-2.312469
29	6	0	3.296735	-1.875371	2.230713
30	6	0	4.223706	-1.472296	-1.337585
31	1	0	0.294874	-1.032227	-0.416763
32	1	0	1.059858	-0.674578	1.110413
33	1	0	1.208277	-4.047808	-0.523132
34	1	0	2.729441	-3.703327	-1.349563
35	1	0	3.100127	-0.318059	0.122147
36	1	0	2.261764	-0.514194	-1.389465
37	1	0	3.684566	-3.342260	0.673386
38	1	0	2.156778	-3.587406	1.523239
39	1	0	0.176036	-2.862565	2.092774
40	1	0	-0.595555	-3.252456	0.532288
41	1	0	-1.099872	-1.838057	1.452683
42	1	0	-0.015278	-2.468354	-2.075271
43	1	0	0.871942	-3.710909	-2.965072

44	1	0	1.512738	-2.065020	-2.883453
45	1	0	2.490919	-1.257296	2.635056
46	1	0	4.092253	-1.200903	1.900696
47	1	0	3.698528	-2.488989	3.046891
48	1	0	4.079113	-2.117880	-2.211685
49	1	0	4.909925	-1.968299	-0.641220
50	1	0	4.724593	-0.561164	-1.685623

B3LYP/LanL2DZ

Zero-point correction= 0.410188 (Hartree/Particle)
Thermal correction to Energy= 0.438331
Thermal correction to Enthalpy= 0.439275
Thermal correction to Gibbs Free Energy= 0.348275
Sum of electronic and zero-point Energies= -1114.196189
Sum of electronic and thermal Energies= -1114.168046
Sum of electronic and thermal Enthalpies= -1114.167102
Sum of electronic and thermal Free Energies= -1114.258102

B3LYP/6-311+G(d,p)

HF=-3052.6315937 (Hartree/Particle)

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TS^{-}—$^{+}$NEt$_4$ (*m*-NO$_2$PhCH=CH$_2$) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.642254	-3.402171	0.274035
2	25	0	-2.063364	-2.005352	-0.231724
3	8	0	-0.581303	-2.135779	-0.885284
4	8	0	-2.020196	-0.932150	0.999697
5	8	0	-3.091290	-1.288732	-1.284458
6	6	0	-3.965302	0.499775	-0.694759
7	6	0	-3.386088	0.895947	0.500686
8	6	0	-2.247732	1.816623	0.615463
9	6	0	-0.935743	3.385899	1.998396
10	6	0	-0.025107	3.595096	0.951793
11	6	0	-2.017560	2.502134	1.837276
12	6	0	-1.338653	2.035616	-0.447598
13	6	0	-0.249389	2.898675	-0.253674
14	7	0	0.734947	3.043618	-1.336937
15	8	0	0.474374	2.538319	-2.485180
16	8	0	1.847391	3.636350	-1.076687
17	1	0	-4.923959	-0.006471	-0.688980
18	1	0	-3.662435	0.927324	-1.646045
19	1	0	-3.880252	0.637407	1.432682
20	1	0	-0.801598	3.909574	2.941082
21	1	0	0.824208	4.261654	1.047410
22	1	0	-2.702092	2.334543	2.665636
23	1	0	-1.446731	1.511289	-1.390361
24	7	0	2.622078	-1.030932	0.254996
25	6	0	1.949556	-0.348594	-0.968097
26	6	0	3.782950	-0.175467	0.800825

27	6	0	1.497940	-1.206705	1.310174
28	6	0	3.236919	-2.393043	-0.139342
29	6	0	2.853557	-0.099462	-2.177864
30	6	0	3.428202	1.258685	1.211401
31	6	0	2.250220	-3.475317	-0.591085
32	6	0	1.923196	-1.873420	2.620946
33	1	0	1.556489	0.593725	-0.583064
34	1	0	1.086963	-0.973050	-1.223232
35	1	0	4.548591	-0.167460	0.019159
36	1	0	4.189213	-0.726306	1.654295
37	1	0	0.709380	-1.771392	0.807776
38	1	0	1.096206	-0.207290	1.495041
39	1	0	3.803536	-2.732865	0.734012
40	1	0	3.956271	-2.171057	-0.933052
41	1	0	3.177202	-1.025542	-2.665549
42	1	0	3.733511	0.513740	-1.950375
43	1	0	2.257485	0.462332	-2.906746
44	1	0	3.112629	1.882483	0.369711
45	1	0	4.331691	1.717732	1.632239
46	1	0	2.654459	1.294758	1.985224
47	1	0	1.592956	-3.152115	-1.401700
48	1	0	1.604556	-3.821239	0.220948
49	1	0	2.839175	-4.332795	-0.941491
50	1	0	2.658955	-1.291900	3.189139
51	1	0	2.309009	-2.888556	2.476443
52	1	0	1.023925	-1.958864	3.242259

B3LYP/LanL2DZ

Zero-point correction= 0.431103 (Hartree/Particle)
Thermal correction to Energy= 0.459373
Thermal correction to Enthalpy= 0.460317
Thermal correction to Gibbs Free Energy= 0.367612
Sum of electronic and zero-point Energies= -1289.979412
Sum of electronic and thermal Energies= -1289.951143
Sum of electronic and thermal Enthalpies= -1289.950198
Sum of electronic and thermal Free Energies= -1290.042903

B3LYP/6-311+G(d,p)

HF=-2337.9500955 (Hartree/Particle)

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TS^{-}—$^{+}NEt_4$ (*p*-$NO_2PhCH{=}CH_2$) at B3LYP/LanL2DZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.238471	0.539174	0.360122
2	25	0	2.949651	-0.204480	-0.215172
3	8	0	2.134750	0.703843	-1.280349
4	8	0	1.947793	-0.610810	1.006618
5	8	0	3.346437	-1.657607	-0.859916

6	6	0	2.599887	-3.368957	0.024582
7	6	0	1.612237	-2.971335	0.916439
8	6	0	0.216126	-2.738481	0.562799
9	6	0	-2.051225	-2.134119	1.304563
10	6	0	-2.463951	-2.092696	-0.046269
11	6	0	-0.726676	-2.459413	1.594207
12	6	0	-0.248071	-2.731262	-0.785368
13	6	0	-1.572346	-2.421339	-1.092055
14	7	0	-3.811136	-1.653364	-0.368260
15	8	0	-4.188873	-1.659747	-1.598638
16	8	0	-4.566599	-1.230140	0.589314
17	1	0	3.582708	-3.639306	0.395425
18	1	0	2.366723	-3.712035	-0.977976
19	1	0	1.864156	-2.880679	1.968413
20	1	0	-2.766265	-1.905901	2.087508
21	1	0	-0.390426	-2.476175	2.627832
22	1	0	0.446909	-2.931294	-1.594190
23	1	0	-1.926735	-2.404901	-2.117128
24	7	0	-0.779841	2.579331	0.060752
25	6	0	-0.951616	1.329595	-0.845589
26	6	0	-2.099897	2.943281	0.769431
27	6	0	0.329764	2.210841	1.078836
28	6	0	-0.375359	3.817553	-0.770058
29	6	0	-1.962402	1.477554	-1.986882
30	6	0	-2.721890	1.848013	1.643078
31	6	0	0.976703	3.732965	-1.488176
32	6	0	0.649227	3.280178	2.126520
33	1	0	-1.243062	0.519873	-0.173145
34	1	0	0.048354	1.087995	-1.220372
35	1	0	-2.798103	3.242422	-0.018253
36	1	0	-1.881731	3.830529	1.370991
37	1	0	1.208112	1.971057	0.479125
38	1	0	0.018624	1.276452	1.550025
39	1	0	-0.387623	4.664092	-0.075991
40	1	0	-1.185581	3.970174	-1.489019
41	1	0	-1.652837	2.214979	-2.735350
42	1	0	-2.976783	1.715446	-1.646884
43	1	0	-2.022583	0.509541	-2.497230
44	1	0	-3.063549	0.979836	1.072832
45	1	0	-3.607723	2.273631	2.130689
46	1	0	-2.046591	1.506378	2.434358
47	1	0	1.077019	2.846418	-2.119105
48	1	0	1.822639	3.730734	-0.794650
49	1	0	1.069386	4.621716	-2.125312
50	1	0	-0.183763	3.485347	2.808943
51	1	0	0.986130	4.225118	1.685099
52	1	0	1.479270	2.896823	2.731675

B3LYP/LanL2DZ

Zero-point correction= 0.431207 (Hartree/Particle)
Thermal correction to Energy= 0.459563
Thermal correction to Enthalpy= 0.460507
Thermal correction to Gibbs Free Energy= 0.368952

Sum of electronic and zero-point Energies= -1289.982705
Sum of electronic and thermal Energies= -1289.954349
Sum of electronic and thermal Enthalpies= -1289.953405
Sum of electronic and thermal Free Energies= -1290.044961

B3LYP/6-311+G(d,p)

HF=-2337.9534271 (Hartree/Particle)

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MnO_4^- (GS) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.570675	-0.261571	0.087446
2	25	0	0.000035	0.000021	-0.000012
3	8	0	-0.589053	-0.727767	-1.290838
4	8	0	-0.272939	1.567813	-0.102650
5	8	0	-0.708793	-0.578542	1.306079

B3LYP/6-31G(d)

Zero-point correction= 0.013508 (Hartree/Particle)
Thermal correction to Energy= 0.018053
Thermal correction to Enthalpy= 0.018997
Thermal correction to Gibbs Free Energy= -0.014762
Sum of electronic and zero-point Energies= -1451.827350
Sum of electronic and thermal Energies= -1451.822805
Sum of electronic and thermal Enthalpies= -1451.821861
Sum of electronic and thermal Free Energies= -1451.855620

B3LYP/6-311+G(d,p)

HF=-1452.02677462

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***p*-MePhCH=CH_2(GS) at B3LYP/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.490070	0.437368	0.000105
2	6	0	3.452870	-0.493561	0.000176
3	6	0	1.034136	0.226445	0.000004
4	6	0	0.435874	-1.048069	-0.000121
5	6	0	-0.945528	-1.190889	-0.000260
6	6	0	-1.797020	-0.073250	-0.000219
7	6	0	-1.205800	1.193605	-0.000199
8	6	0	0.181046	1.340494	-0.000062
9	6	0	-3.297407	-0.245294	0.000347
10	1	0	2.792865	1.484895	0.000140
11	1	0	3.243760	-1.560020	0.000151
12	1	0	4.501221	-0.211247	0.000266
13	1	0	1.059364	-1.937629	-0.000204
14	1	0	-1.377215	-2.189852	-0.000450
15	1	0	-1.837448	2.079175	-0.000316
16	1	0	0.612740	2.339072	-0.000092

17	1	0	-3.810828	0.721368	-0.006442
18	1	0	-3.637273	-0.797269	0.885850
19	1	0	-3.636634	-0.809592	-0.877530

B3LYP/6-31G(d)

Zero-point correction= 0.158091 (Hartree/Particle)
Thermal correction to Energy= 0.166880
Thermal correction to Enthalpy= 0.167824
Thermal correction to Gibbs Free Energy= 0.123022
Sum of electronic and zero-point Energies= -348.808396
Sum of electronic and thermal Energies= -348.799607
Sum of electronic and thermal Enthalpies= -348.798663
Sum of electronic and thermal Free Energies= -348.843465

B3LYP/6-311+G(d,p)

HF=- -349.058420325 (Hartree/Particle)

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PhCH=CH$_2$(GS) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.954787	-0.529289	-0.000026
2	6	0	-2.977368	0.334937	0.000013
3	6	0	-0.515179	-0.220355	-0.000013
4	6	0	-0.008790	1.092464	-0.000020
5	6	0	1.362297	1.329513	-0.000005
6	6	0	2.265302	0.261726	0.000018
7	6	0	1.780813	-1.046164	0.000022
8	6	0	0.406381	-1.281271	0.000006
9	1	0	-2.186126	-1.594694	-0.000063
10	1	0	-2.840452	1.412964	0.000062
11	1	0	-4.004510	-0.016800	0.000003
12	1	0	-0.693826	1.935370	-0.000042
13	1	0	1.730564	2.352199	-0.000012
14	1	0	3.335450	0.450293	0.000030
15	1	0	2.471965	-1.884977	0.000037
16	1	0	0.034912	-2.303717	0.000010

B3LYP/6-31G(d)

Zero-point correction= 0.131109 (Hartree/Particle)
Thermal correction to Energy= 0.137995
Thermal correction to Enthalpy= 0.138939
Thermal correction to Gibbs Free Energy= 0.099527
Sum of electronic and zero-point Energies= -309.517150
Sum of electronic and thermal Energies= -309.510264
Sum of electronic and thermal Enthalpies= -309.509320
Sum of electronic and thermal Free Energies= -309.548732

B3LYP/6-311+G(d,p)

HF=-309.730697659 (Hartree/Particle)

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***p*-ClPhCH=CH$_2$ (GS) at B3LYP/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.894321	0.407874	0.000030
2	6	0	3.836576	-0.543442	0.000034
3	6	0	1.434385	0.225113	0.000015
4	6	0	0.813927	-1.037647	0.000007
5	6	0	-0.570899	-1.163985	-0.000007
6	6	0	-1.363041	-0.013881	-0.000013
7	6	0	-0.783938	1.252716	-0.000006
8	6	0	0.605622	1.359555	0.000008
9	17	0	-3.114562	-0.169556	-0.000031
10	1	0	3.218079	1.448783	0.000037
11	1	0	3.605792	-1.605465	0.000026
12	1	0	4.890495	-0.283065	0.000045
13	1	0	1.419214	-1.939178	0.000013
14	1	0	-1.036880	-2.143680	-0.000013
15	1	0	-1.409348	2.139044	-0.000011
16	1	0	1.058473	2.348208	0.000015

B3LYP/6-31G(d)

Zero-point correction= 0.121696 (Hartree/Particle)
Thermal correction to Energy= 0.129768
Thermal correction to Enthalpy= 0.130712
Thermal correction to Gibbs Free Energy= 0.088021
Sum of electronic and zero-point Energies= -769.122792
Sum of electronic and thermal Energies= -769.114721
Sum of electronic and thermal Enthalpies= -769.113777
Sum of electronic and thermal Free Energies= -769.156467

B3LYP/6-311+G(d,p)

HF=-769.353616249 (Hartree/Particle)

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***m*-ClPhCH=CH$_2$ (GS) at B3LYP/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.386074	-1.036374	0.000021
2	6	0	-3.668697	-0.653324	-0.000018
3	6	0	-1.193530	-0.172534	0.000013
4	6	0	-1.255679	1.232778	0.000015
5	6	0	-0.092752	1.995519	0.000005
6	6	0	1.165662	1.386574	-0.000004
7	6	0	1.226665	-0.004436	-0.000003
8	6	0	0.072244	-0.782677	0.000006
9	17	0	2.797382	-0.800796	-0.000014
10	1	0	-2.169882	-2.104563	0.000058

11	1	0	-3.975753	0.389099	-0.000062
12	1	0	-4.468284	-1.387658	-0.000008
13	1	0	-2.219360	1.732429	0.000027
14	1	0	-0.158915	3.080157	0.000007
15	1	0	2.075917	1.975994	-0.000010
16	1	0	0.153744	-1.865089	0.000006

B3LYP/6-31G(d)

Zero-point correction= 0.121683 (Hartree/Particle)
Thermal correction to Energy= 0.129764
Thermal correction to Enthalpy= 0.130708
Thermal correction to Gibbs Free Energy= 0.087879
Sum of electronic and zero-point Energies= -769.122618
Sum of electronic and thermal Energies= -769.114538
Sum of electronic and thermal Enthalpies= -769.113594
Sum of electronic and thermal Free Energies= -769.156423

B3LYP/6-311+G(d,p)

HF=-769.353407575 (Hartree/Particle)

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***m*-BrPhCH=CH$_2$ (GS) at B3LYP/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.039632	-3.116923	0.000000
2	6	0	0.773412	-4.236294	0.000000
3	6	0	0.527940	-1.727489	0.000000
4	6	0	1.892739	-1.386636	0.000000
5	6	0	2.292713	-0.054554	0.000000
6	6	0	1.349929	0.977719	0.000000
7	6	0	0.000000	0.639959	0.000000
8	6	0	-0.416982	-0.687523	0.000000
9	35	0	-1.315609	2.031037	0.000000
10	1	0	-1.045756	-3.214018	0.000000
11	1	0	1.859960	-4.231689	0.000000
12	1	0	0.298920	-5.212669	0.000000
13	1	0	2.645880	-2.168219	0.000000
14	1	0	3.350979	0.191989	0.000000
15	1	0	1.657348	2.017402	0.000000
16	1	0	-1.477296	-0.918638	0.000000

B3LYP/6-31G(d)

Zero-point correction= 0.121299 (Hartree/Particle)
Thermal correction to Energy= 0.129589
Thermal correction to Enthalpy= 0.130533
Thermal correction to Gibbs Free Energy= 0.086442
Sum of electronic and zero-point Energies= -2880.631796
Sum of electronic and thermal Energies= -2880.623506
Sum of electronic and thermal Enthalpies= -2880.622562
Sum of electronic and thermal Free Energies= -2880.666653

B3LYP/6-311+G(d,p)
HF=-2883.27313255 (Hartree/Particle)

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3,4-diClPhCH=CH_2 (GS) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.159577	0.593027	0.000239
2	6	0	4.278470	-0.141780	-0.000527
3	6	0	1.771669	0.103673	0.000192
4	6	0	1.429419	-1.260573	0.000229
5	6	0	0.101399	-1.663417	0.000132
6	6	0	-0.930164	-0.717691	0.000021
7	6	0	-0.608561	0.643678	0.000029
8	6	0	0.728712	1.040999	0.000128
9	17	0	-2.585429	-1.272832	-0.000080
10	17	0	-1.848402	1.876592	-0.000070
11	1	0	3.256708	1.678350	0.000926
12	1	0	4.273588	-1.228442	-0.001334
13	1	0	5.255043	0.332259	-0.000399
14	1	0	2.206255	-2.018423	0.000391
15	1	0	-0.154338	-2.717774	0.000172
16	1	0	0.954762	2.102618	0.000128

B3LYP/6-31G(d)
Zero-point correction= 0.112263 (Hartree/Particle)
Thermal correction to Energy= 0.121546
Thermal correction to Enthalpy= 0.122490
Thermal correction to Gibbs Free Energy= 0.076498
Sum of electronic and zero-point Energies= -1228.722958
Sum of electronic and thermal Energies= -1228.713675
Sum of electronic and thermal Enthalpies= -1228.712731
Sum of electronic and thermal Free Energies= -1228.758723

B3LYP/6-311+G(d,p)
HF=-1228.97112654 (Hartree/Particle)

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***m*-NO_2PhCH=CH_2 (GS) at B3LYP/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.860704	-0.380307	-0.001334
2	6	0	3.152653	-1.686228	0.001752
3	6	0	1.521650	0.232528	-0.000705

4	6	0	0.338611	-0.523716	-0.000771
5	6	0	-0.888928	0.125278	-0.000032
6	6	0	-1.006579	1.515522	0.000684
7	6	0	0.164525	2.267583	0.000634
8	6	0	1.408049	1.634373	-0.000105
9	7	0	-2.118074	-0.689768	-0.000124
10	8	0	-3.195801	-0.095967	0.000186
11	8	0	-1.995026	-1.914183	-0.000473
12	1	0	3.684094	0.333217	-0.004415
13	1	0	2.392541	-2.462622	0.005340
14	1	0	4.183786	-2.025238	0.000926
15	1	0	0.353870	-1.606124	-0.001551
16	1	0	-1.987829	1.972780	0.001131
17	1	0	0.108544	3.351980	0.001154
18	1	0	2.314007	2.235393	-0.000156

B3LYP/6-31G(d)

Zero-point correction= 0.133743 (Hartree/Particle)
Thermal correction to Energy= 0.143136
Thermal correction to Enthalpy= 0.144080
Thermal correction to Gibbs Free Energy= 0.097879
Sum of electronic and zero-point Energies= -514.016129
Sum of electronic and thermal Energies= -514.006735
Sum of electronic and thermal Enthalpies= -514.005791
Sum of electronic and thermal Free Energies= -514.051992

B3LYP/6-311+G(d,p)

HF=-514.293748112 (Hartree/Particle)

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***p*-NO_2PhCH=CH_2 (GS) at B3LYP/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.160582	0.406912	-0.000354
2	6	0	4.092501	-0.554696	0.000958
3	6	0	1.701242	0.230677	-0.000314
4	6	0	1.076872	-1.032811	-0.000486
5	6	0	-0.305234	-1.151005	-0.000345
6	6	0	-1.083579	0.008216	-0.000074
7	6	0	-0.505247	1.275362	0.000013
8	6	0	0.881158	1.374501	-0.000130
9	7	0	-2.545849	-0.111881	0.000052
10	8	0	-3.027507	-1.245300	0.000089
11	8	0	-3.206386	0.927420	0.000360
12	1	0	3.492380	1.444700	-0.001465
13	1	0	3.850898	-1.614014	0.002297
14	1	0	5.148856	-0.304825	0.000799
15	1	0	1.679346	-1.935400	-0.000836
16	1	0	-0.792277	-2.118321	-0.000486
17	1	0	-1.139905	2.152874	0.000184
18	1	0	1.343018	2.358263	-0.000056

B3LYP/6-31G(d)

Zero-point correction= 0.133781 (Hartree/Particle)
Thermal correction to Energy= 0.143172
Thermal correction to Enthalpy= 0.144117
Thermal correction to Gibbs Free Energy= 0.097969
Sum of electronic and zero-point Energies= -514.016767
Sum of electronic and thermal Energies= -514.007375
Sum of electronic and thermal Enthalpies= -514.006431
Sum of electronic and thermal Free Energies= -514.052578

B3LYP/6-311+G(d,p)

HF= HF=-514.294536553 (Hartree/Particle)

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TS^- (p-MePhCH=CH_2) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.877022	-0.137648	-0.746350
2	25	0	2.424779	-0.458838	-0.187354
3	8	0	2.138065	-2.010632	-0.008007
4	8	0	1.293119	0.218411	-1.122512
5	8	0	2.171127	0.334886	1.235175
6	6	0	0.847017	1.747062	1.211322
7	6	0	0.056589	1.662224	0.075198
8	6	0	-1.201213	0.921853	0.031011
9	6	0	-3.445450	0.612871	-0.885684
10	6	0	-3.700520	-0.458654	-0.022836
11	6	0	-2.224173	1.284961	-0.863596
12	6	0	-1.453972	-0.175598	0.882705
13	6	0	-2.674704	-0.839023	0.857534
14	6	0	-5.016345	-1.202247	-0.053879
15	1	0	1.592730	2.532695	1.270409
16	1	0	0.455389	1.415000	2.167048
17	1	0	0.245597	2.338358	-0.751876
18	1	0	-4.216554	0.926875	-1.588707
19	1	0	-2.056152	2.115522	-1.546703
20	1	0	-0.661584	-0.522099	1.539398
21	1	0	-2.831701	-1.686506	1.524070
22	1	0	-4.896499	-2.230549	-0.423421
23	1	0	-5.740546	-0.703032	-0.708153
24	1	0	-5.468200	-1.276157	0.944699

B3LYP/6-31G(d)

Zero-point correction= 0.172340 (Hartree/Particle)
Thermal correction to Energy= 0.186177
Thermal correction to Enthalpy= 0.187122
Thermal correction to Gibbs Free Energy= 0.128986
Sum of electronic and zero-point Energies= -1800.623059
Sum of electronic and thermal Energies= -1800.609221
Sum of electronic and thermal Enthalpies= -1800.608277
Sum of electronic and thermal Free Energies= -1800.666412

B3LYP/6-311+G(d,p)
HF=-1801.07049332

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TS$^-$ (PhCH=CH$_2$) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.513845	0.178256	-0.738453
2	25	0	2.107918	-0.320329	-0.191367
3	8	0	2.001548	-1.898498	-0.049461
4	8	0	0.906910	0.244522	-1.113870
5	8	0	1.765257	0.405493	1.248727
6	6	0	0.289883	1.656833	1.255542
7	6	0	-0.482116	1.516872	0.112201
8	6	0	-1.653663	0.648216	0.039384
9	6	0	-3.847418	0.137657	-0.911359
10	6	0	-3.978392	-0.970057	-0.070307
11	6	0	-2.702309	0.930067	-0.858608
12	6	0	-1.791142	-0.490280	0.862435
13	6	0	-2.936607	-1.279170	0.810761
14	1	0	0.942908	2.518788	1.341151
15	1	0	-0.066407	1.257299	2.199206
16	1	0	-0.363367	2.231121	-0.695648
17	1	0	-4.641905	0.385882	-1.613270
18	1	0	-4.869709	-1.592556	-0.111710
19	1	0	-2.610555	1.791185	-1.517994
20	1	0	-0.968294	-0.766813	1.514882
21	1	0	-3.010519	-2.155696	1.451734

B3LYP/6-31G(d)
Zero-point correction= 0.145379 (Hartree/Particle)
Thermal correction to Energy= 0.157280
Thermal correction to Enthalpy= 0.158224
Thermal correction to Gibbs Free Energy= 0.105589
Sum of electronic and zero-point Energies= -1761.332671
Sum of electronic and thermal Energies= -1761.320770
Sum of electronic and thermal Enthalpies= -1761.319826
Sum of electronic and thermal Free Energies= -1761.372461

B3LYP/6-311+G(d,p)
HF=-1761.74402905 (Hartree/Particle)

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TS$^-$ (*p*-ClPhCH=CH$_2$) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	4.187382	-0.303687	-0.740575
2	25	0	2.716678	-0.533534	-0.188477
3	8	0	2.339822	-2.063922	-0.002205
4	8	0	1.633938	0.200676	-1.134435
5	8	0	2.505501	0.279408	1.230733
6	6	0	1.279918	1.769405	1.207094
7	6	0	0.479576	1.734313	0.075819
8	6	0	-0.810331	1.057232	0.033392
9	6	0	-3.067760	0.866745	-0.898981
10	6	0	-3.340288	-0.173090	-0.013282
11	6	0	-1.810750	1.466425	-0.870612
12	6	0	-1.116615	-0.022253	0.890560
13	6	0	-2.368484	-0.629390	0.877115
14	17	0	-4.942437	-0.938544	-0.030582
15	1	0	2.071460	2.509122	1.261071
16	1	0	0.872932	1.465925	2.165937
17	1	0	0.706712	2.392462	-0.755817
18	1	0	-3.827858	1.202154	-1.598064
19	1	0	-1.596943	2.279490	-1.560881
20	1	0	-0.342874	-0.408468	1.546684
21	1	0	-2.583686	-1.463216	1.538116

B3LYP/6-31G(d)

Zero-point correction= 0.136033 (Hartree/Particle)
Thermal correction to Energy= 0.149192
Thermal correction to Enthalpy= 0.150136
Thermal correction to Gibbs Free Energy= 0.094104
Sum of electronic and zero-point Energies= -2220.943823
Sum of electronic and thermal Energies= -2220.930664
Sum of electronic and thermal Enthalpies= -2220.929719
Sum of electronic and thermal Free Energies= -2220.985752

B3LYP/6-311+G(d,p)

HF=-2221.37176326 (Hartree/Particle)

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TS^{-} (*m*-ClPhCH=CH2) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.018109	-0.854531	-0.797215
2	25	0	-2.741356	0.025840	-0.458152
3	8	0	-2.748646	1.449293	-1.160156
4	8	0	-1.388094	-0.774403	-0.821600
5	8	0	-2.584722	0.198169	1.174441
6	6	0	-1.081703	-0.678826	2.002974
7	6	0	-0.141826	-1.061205	1.058372
8	6	0	0.979517	-0.217103	0.665438
9	6	0	3.254561	0.003089	-0.147640
10	6	0	3.220370	1.389920	-0.025623
11	6	0	2.169194	-0.798814	0.180253
12	6	0	0.930384	1.190684	0.765941

13	6	0	2.031914	1.970278	0.431925
14	17	0	4.746343	-0.768287	-0.734312
15	1	0	-1.700874	-1.444331	2.458056
16	1	0	-0.897249	0.189516	2.626714
17	1	0	-0.102641	-2.096398	0.737566
18	1	0	4.082138	1.991690	-0.293456
19	1	0	2.238111	-1.876696	0.072109
20	1	0	0.001840	1.661460	1.072501
21	1	0	1.966851	3.053274	0.510011

B3LYP/6-31G(d)

Zero-point correction= 0.136001 (Hartree/Particle)
Thermal correction to Energy= 0.149161
Thermal correction to Enthalpy= 0.150105
Thermal correction to Gibbs Free Energy= 0.094044
Sum of electronic and zero-point Energies= -2220.944067
Sum of electronic and thermal Energies= -2220.930908
Sum of electronic and thermal Enthalpies= -2220.929963
Sum of electronic and thermal Free Energies= -2220.986025

B3LYP/6-311+G(d,p)

HF= -2221.37211318 (Hartree/Particle)

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TS^{-} (*m*-BrPhCH=CH2) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.536241	-1.143491	-0.713324
2	25	0	-3.315548	-0.151423	-0.499621
3	8	0	-3.330456	1.095119	-1.481889
4	8	0	-1.913799	-0.942454	-0.617738
5	8	0	-3.264205	0.362785	1.066398
6	6	0	-1.764822	-0.224069	2.129332
7	6	0	-0.760128	-0.743266	1.327962
8	6	0	0.325003	0.067910	0.789955
9	6	0	2.616479	0.265752	0.023615
10	6	0	2.485756	1.634840	-0.189451
11	6	0	1.573808	-0.518734	0.496775
12	6	0	0.178028	1.452199	0.552549
13	6	0	1.240203	2.214100	0.079056
14	35	0	4.320278	-0.569955	-0.342855
15	1	0	-2.365463	-0.909129	2.717926
16	1	0	-1.659498	0.770024	2.550861
17	1	0	-0.645237	-1.818801	1.249113
18	1	0	3.316845	2.221549	-0.564731
19	1	0	1.719287	-1.583087	0.650280
20	1	0	-0.794410	1.908651	0.706396
21	1	0	1.099094	3.276719	-0.105723

B3LYP/6-31G(d)

Zero-point correction= 0.135501 (Hartree/Particle)
Thermal correction to Energy= 0.148917
Thermal correction to Enthalpy= 0.149861
Thermal correction to Gibbs Free Energy= 0.092353
Sum of electronic and zero-point Energies= -4332.453471
Sum of electronic and thermal Energies= -4332.440055
Sum of electronic and thermal Enthalpies= -4332.439111
Sum of electronic and thermal Free Energies= -4332.496619

B3LYP/6-311+G(d,p)
HF=-4335.29213344 (Hartree/Particle)

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TS^{-} (3,4-diClPhCH=CH2) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.581227	-0.296278	-0.973623
2	25	0	-3.200149	0.284847	-0.451577
3	8	0	-2.950869	1.795848	-0.865776
4	8	0	-1.972927	-0.639828	-0.942130
5	8	0	-3.093870	0.124145	1.186368
6	6	0	-1.760156	-1.092060	1.863819
7	6	0	-0.852802	-1.437152	0.874578
8	6	0	0.369490	-0.685810	0.627719
9	6	0	2.687829	-0.623118	-0.135622
10	6	0	2.788160	0.728298	0.208794
11	6	0	1.496878	-1.314569	0.067104
12	6	0	0.479918	0.686744	0.940231
13	17	0	4.058022	-1.495203	-0.820736
14	6	0	1.667857	1.375451	0.739934
15	17	0	4.274481	1.642103	-0.022017
16	1	0	-2.491504	-1.829087	2.177416
17	1	0	-1.478556	-0.374021	2.626889
18	1	0	-0.939642	-2.399583	0.382435
19	1	0	1.447691	-2.363716	-0.206848
20	1	0	-0.394317	1.217139	1.303176
21	1	0	1.735594	2.433005	0.975091

B3LYP/6-31G(d)
Zero-point correction= 0.126575 (Hartree/Particle)
Thermal correction to Energy= 0.141017
Thermal correction to Enthalpy= 0.141961
Thermal correction to Gibbs Free Energy= 0.082480
Sum of electronic and zero-point Energies= -2680.548480
Sum of electronic and thermal Energies= -2680.534038
Sum of electronic and thermal Enthalpies= -2680.533094
Sum of electronic and thermal Free Energies= -2680.592575

B3LYP/6-311+G(d,p)

HF=-2680.99329158 (Hartree/Particle)

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TS$^-$ (*m*-$NO_2PhCH{=}CH_2$) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.196512	-0.635549	-1.027913
2	25	0	-2.909943	0.108632	-0.473841
3	8	0	-2.836070	1.641344	-0.877271
4	8	0	-1.566153	-0.655065	-0.937678
5	8	0	-2.819155	-0.044129	1.165916
6	6	0	-1.344131	-1.071747	1.868875
7	6	0	-0.380208	-1.279737	0.895105
8	6	0	0.712544	-0.344902	0.660323
9	6	0	2.993218	0.116715	-0.019266
10	6	0	2.864033	1.478006	0.263933
11	6	0	1.950108	-0.788514	0.162328
12	6	0	0.570448	1.037895	0.920204
13	6	0	1.628900	1.923935	0.732624
14	7	0	4.279932	-0.377877	-0.517639
15	8	0	4.393483	-1.583383	-0.756586
16	8	0	5.197647	0.435518	-0.672096
17	1	0	-1.967039	-1.906959	2.170326
18	1	0	-1.183804	-0.320729	2.635377
19	1	0	-0.306293	-2.247032	0.410611
20	1	0	3.700067	2.146314	0.103707
21	1	0	2.107845	-1.833567	-0.075867
22	1	0	-0.400703	1.409456	1.231292
23	1	0	1.483580	2.982064	0.934334

B3LYP/6-31G(d)

Zero-point correction= 0.148128 (Hartree/Particle)
Thermal correction to Energy= 0.162567
Thermal correction to Enthalpy= 0.163512
Thermal correction to Gibbs Free Energy= 0.104391
Sum of electronic and zero-point Energies= -1965.844148
Sum of electronic and thermal Energies= -1965.829708
Sum of electronic and thermal Enthalpies= -1965.828764
Sum of electronic and thermal Free Energies= -1965.887884

B3LYP/6-311+G(d,p)

HF=-1966.31957351 (Hartree/Particle)

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TS$^-$ (*p*-$NO_2ClPhCH{=}CH_2$) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.239489	-0.646017	-0.850158

2	25	0	2.772989	-0.613061	-0.248269
3	8	0	2.165062	-2.056885	-0.015225
4	8	0	1.795962	0.252835	-1.181672
5	8	0	2.752950	0.233997	1.167477
6	6	0	1.664292	1.814107	1.278271
7	6	0	0.800914	1.910360	0.196950
8	1	0	2.502645	2.500569	1.333884
9	6	0	-0.480445	1.245201	0.140685
10	1	0	1.034207	2.594534	-0.612318
11	1	0	1.289483	1.476460	2.238387
12	1	0	0.010227	-0.299285	1.573962
13	6	0	-2.728202	1.077665	-0.809219
14	6	0	-2.987093	-0.023718	0.017415
15	6	0	-1.490584	1.692755	-0.745735
16	1	0	-2.216789	-1.387395	1.490372
17	1	0	-1.283318	2.544878	-1.388489
18	6	0	-0.771760	0.114010	0.946146
19	1	0	-3.502402	1.425908	-1.482158
20	6	0	-2.003729	-0.511350	0.889990
21	7	0	-4.275989	-0.673559	-0.044068
22	8	0	-4.485356	-1.643760	0.699089
23	8	0	-5.124008	-0.231222	-0.835192

B3LYP/6-31G(d)

Zero-point correction= 0.148186 (Hartree/Particle)
Thermal correction to Energy= 0.162651
Thermal correction to Enthalpy= 0.163595
Thermal correction to Gibbs Free Energy= 0.104408
Sum of electronic and zero-point Energies= -1965.848301
Sum of electronic and thermal Energies= -1965.833835
Sum of electronic and thermal Enthalpies= -1965.832891
Sum of electronic and thermal Free Energies= -1965.892078

B3LYP/6-311+G(d,p)

HF=-1966.32356022 (Hartree/Particle)

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MnO_4^- —$^+NEt_4$ (GS) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.972728	1.304700	0.588035
2	25	0	-2.410422	-0.001974	-0.232019
3	8	0	-1.967648	-1.294473	0.608206
4	8	0	-1.612368	-0.011104	-1.612951
5	8	0	-3.965606	-0.006962	-0.483803
6	7	0	1.811947	0.001230	0.182507
7	6	0	1.069022	-1.235625	-0.343726
8	6	0	3.264414	-0.001538	-0.269154
9	6	0	1.068801	1.231275	-0.358836
10	6	0	1.829506	0.010640	1.712952
11	6	0	1.681394	-2.580728	0.022421

12	6	0	3.494544	-0.012740	-1.776145
13	6	0	0.471754	0.020085	2.404323
14	6	0	1.679750	2.580749	-0.006700
15	1	0	1.010491	-1.109777	-1.424748
16	1	0	0.046898	-1.173163	0.033211
17	1	0	3.726201	-0.876636	0.192164
18	1	0	3.725502	0.880780	0.178862
19	1	0	0.046286	1.172120	0.017388
20	1	0	1.011777	1.093315	-1.438470
21	1	0	2.414610	0.889165	1.994498
22	1	0	2.407775	-0.868902	2.005089
23	1	0	1.720103	-2.752568	1.102217
24	1	0	2.678483	-2.745900	-0.398909
25	1	0	1.020136	-3.347344	-0.394038
26	1	0	3.087177	-0.904530	-2.259361
27	1	0	4.576263	-0.012617	-1.946819
28	1	0	3.084869	0.870538	-2.272871
29	1	0	-0.139309	-0.853925	2.167146
30	1	0	-0.126371	0.902862	2.167145
31	1	0	0.664797	0.018926	3.483091
32	1	0	2.676691	2.742445	-0.429742
33	1	0	1.718435	2.763499	1.071331
34	1	0	1.017809	3.342469	-0.430966

B3LYP/6-31G(d)

Zero-point correction= 0.289036 (Hartree/Particle)
Thermal correction to Energy= 0.307352
Thermal correction to Enthalpy= 0.308297
Thermal correction to Gibbs Free Energy= 0.242100
Sum of electronic and zero-point Energies= -1823.107040
Sum of electronic and thermal Energies= -1823.088724
Sum of electronic and thermal Enthalpies= -1823.087780
Sum of electronic and thermal Free Energies= -1823.153976

B3LYP/6-311+G(d,p)

HF=-1823.67253962 (Hartree/Particle)

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TS^{-}—$^{+}$NEt$_4$ (*p*-MePhCH=CH$_2$) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.107280	3.117006	0.441868
2	25	0	-0.888489	2.367620	-0.233479
3	8	0	-1.323425	1.476607	-1.502795
4	8	0	-0.155826	1.411825	0.857863
5	8	0	0.318775	3.398274	-0.601816
6	6	0	1.986467	3.232193	0.460275
7	6	0	1.985689	2.019892	1.127997
8	6	0	2.595907	0.796089	0.607982
9	6	0	3.525629	-1.427632	1.020102
10	6	0	3.849204	-1.592142	-0.333560

11	6	0	2.913584	-0.262794	1.480208
12	6	0	2.892555	0.613053	-0.757940
13	6	0	3.510515	-0.549645	-1.210851
14	6	0	4.564249	-2.828984	-0.825883
15	1	0	1.769019	4.138170	1.013496
16	1	0	2.577604	3.368701	-0.437685
17	1	0	1.719161	2.006265	2.179224
18	1	0	3.771604	-2.217744	1.727872
19	1	0	2.688033	-0.157679	2.539473
20	1	0	2.620168	1.386067	-1.470458
21	1	0	3.737207	-0.651274	-2.270946
22	1	0	4.334963	-3.702086	-0.204371
23	1	0	5.654957	-2.697689	-0.805477
24	1	0	4.290830	-3.069013	-1.859743
25	7	0	-2.015803	-1.779695	0.017948
26	6	0	-0.647961	-1.350880	-0.548049
27	6	0	-1.868939	-2.994937	0.919769
28	6	0	-2.567468	-0.575737	0.788785
29	6	0	-2.967218	-2.175415	-1.108373
30	6	0	0.085696	-2.401444	-1.368730
31	6	0	-0.917233	-2.832942	2.099970
32	6	0	-3.420014	-1.041650	-2.023952
33	6	0	-3.890863	-0.800683	1.505708
34	1	0	-0.056965	-1.038822	0.311087
35	1	0	-0.831631	-0.440796	-1.126676
36	1	0	-1.544190	-3.814638	0.275285
37	1	0	-2.873788	-3.238486	1.271003
38	1	0	-2.640597	0.224524	0.054631
39	1	0	-1.781540	-0.267536	1.477683
40	1	0	-3.827732	-2.648674	-0.628708
41	1	0	-2.447018	-2.950646	-1.673260
42	1	0	-0.428081	-2.663916	-2.298842
43	1	0	0.306812	-3.320468	-0.815346
44	1	0	1.047326	-1.956916	-1.642594
45	1	0	0.114921	-2.651580	1.790217
46	1	0	-0.933783	-3.767381	2.671061
47	1	0	-1.221274	-2.028639	2.775072
48	1	0	-2.600206	-0.405365	-2.365533
49	1	0	-4.155169	-0.393077	-1.540596
50	1	0	-3.900763	-1.493443	-2.898301
51	1	0	-3.824065	-1.523387	2.325265
52	1	0	-4.699980	-1.105610	0.834334
53	1	0	-4.179709	0.160768	1.942469

B3LYP/6-31G(d)

Zero-point correction= 0.448694 (Hartree/Particle)
Thermal correction to Energy= 0.476157
Thermal correction to Enthalpy= 0.477101
Thermal correction to Gibbs Free Energy= 0.388436
Sum of electronic and zero-point Energies= -2171.903478
Sum of electronic and thermal Energies= -2171.876016
Sum of electronic and thermal Enthalpies= -2171.875072
Sum of electronic and thermal Free Energies= -2171.963737

B3LYP/6-311+G(d,p)

HF=-2172.71874533 (Hartree/Particle)

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TS^{-}—$^{+}NEt_4$ ($PhCH{=}CH_2$) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.533112	-3.409789	-0.637119
2	25	0	0.298216	-2.304858	0.133433
3	8	0	-0.453895	-1.757269	1.446457
4	8	0	0.603466	-1.056382	-0.860988
5	8	0	1.810173	-2.811060	0.468656
6	6	0	3.290202	-1.904144	-0.491085
7	6	0	2.810916	-0.748626	-1.082863
8	6	0	2.855508	0.573929	-0.457622
9	6	0	2.822608	3.007372	-0.693427
10	6	0	2.990545	3.162277	0.685048
11	6	0	2.753696	1.732224	-1.253706
12	6	0	2.999995	0.748806	0.934369
13	6	0	3.075353	2.022899	1.493318
14	1	0	3.475134	-2.774877	-1.108985
15	1	0	3.864243	-1.857900	0.426953
16	1	0	2.585567	-0.763521	-2.143779
17	1	0	2.759847	3.882623	-1.336357
18	1	0	3.057919	4.154478	1.123841
19	1	0	2.638829	1.620911	-2.329914
20	1	0	3.039685	-0.124392	1.578717
21	1	0	3.201809	2.128283	2.568537
22	7	0	-2.466377	0.969731	0.013437
23	6	0	-1.056720	1.131587	0.615971
24	6	0	-2.828765	2.172461	-0.842391
25	6	0	-2.444098	-0.318860	-0.815475
26	6	0	-3.517745	0.877479	1.116135
27	6	0	-0.842815	2.367369	1.477587
28	6	0	-1.875652	2.478536	-1.992400
29	6	0	-3.460969	-0.377174	1.982891
30	6	0	-3.724055	-0.641099	-1.573351
31	1	0	-0.369947	1.115980	-0.228398
32	1	0	-0.858143	0.211042	1.171981
33	1	0	-2.891700	3.022805	-0.160275
34	1	0	-3.835609	1.986287	-1.221715
35	1	0	-2.188950	-1.109211	-0.112384
36	1	0	-1.588782	-0.235840	-1.485864
37	1	0	-4.487938	0.957030	0.619177
38	1	0	-3.390262	1.777012	1.720633
39	1	0	-1.438509	2.367784	2.396083
40	1	0	-1.011223	3.310745	0.947303
41	1	0	0.210810	2.354797	1.773236
42	1	0	-0.867465	2.726263	-1.651506
43	1	0	-2.269412	3.349143	-2.527618
44	1	0	-1.806383	1.655217	-2.708144

45	1	0	-2.455017	-0.616840	2.335068
46	1	0	-3.840872	-1.256974	1.457429
47	1	0	-4.104290	-0.208106	2.853048
48	1	0	-3.953317	0.078364	-2.365944
49	1	0	-4.599790	-0.738475	-0.923509
50	1	0	-3.568067	-1.613521	-2.051524

B3LYP/6-31G(d)

Zero-point correction= 0.421391 (Hartree/Particle)
Thermal correction to Energy= 0.447076
Thermal correction to Enthalpy= 0.448021
Thermal correction to Gibbs Free Energy= 0.363246
Sum of electronic and zero-point Energies= -2132.613100
Sum of electronic and thermal Energies= -2132.587415
Sum of electronic and thermal Enthalpies= -2132.586470
Sum of electronic and thermal Free Energies= -2132.671245

B3LYP/6-311+G(d,p)

HF=-2133.39176214 (Hartree/Particle)

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TS^{-}—$^{+}$NEt$_4$ (*p*-ClPhCH=CH$_2$) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.714905	2.699671	0.193790
2	25	0	-1.307847	2.215510	-0.348631
3	8	0	-1.430662	1.243441	-1.623207
4	8	0	-0.506238	1.439687	0.832794
5	8	0	-0.303955	3.466074	-0.638792
6	6	0	1.288562	3.627326	0.520456
7	6	0	1.468991	2.441488	1.210852
8	6	0	2.287396	1.332545	0.723713
9	6	0	3.596083	-0.681514	1.197449
10	6	0	3.881013	-0.810850	-0.161157
11	6	0	2.803232	0.381609	1.625330
12	6	0	2.582421	1.158925	-0.644353
13	6	0	3.375898	0.104051	-1.087406
14	17	0	4.879754	-2.155835	-0.718373
15	1	0	0.887548	4.486199	1.045716
16	1	0	1.894485	3.857629	-0.348093
17	1	0	1.168044	2.390666	2.251565
18	1	0	3.997181	-1.396680	1.908640
19	1	0	2.588739	0.488152	2.686194
20	1	0	2.165434	1.848592	-1.371676
21	1	0	3.598725	-0.012020	-2.143382
22	7	0	-2.052768	-1.963933	0.072076
23	6	0	-0.662109	-1.451403	-0.349632
24	6	0	-1.932390	-3.055262	1.123853
25	6	0	-2.819939	-0.752034	0.613685
26	6	0	-2.786954	-2.573300	-1.118968
27	6	0	0.290994	-2.501051	-0.902744

28	6	0	-1.181141	-2.669010	2.392731
29	6	0	-3.193438	-1.597720	-2.219601
30	6	0	-4.213211	-1.034915	1.155761
31	1	0	-0.246780	-0.963665	0.530748
32	1	0	-0.842299	-0.647037	-1.067318
33	1	0	-1.446498	-3.900796	0.632248
34	1	0	-2.952850	-3.361494	1.362806
35	1	0	-2.852143	-0.040903	-0.208697
36	1	0	-2.178943	-0.299914	1.370075
37	1	0	-3.666404	-3.077038	-0.709935
38	1	0	-2.124042	-3.347629	-1.508639
39	1	0	-0.050216	-2.948541	-1.841526
40	1	0	0.523158	-3.302713	-0.193894
41	1	0	1.230970	-1.983095	-1.116996
42	1	0	-0.134864	-2.418092	2.203031
43	1	0	-1.198365	-3.532708	3.065836
44	1	0	-1.648534	-1.831996	2.917838
45	1	0	-2.380899	-0.942473	-2.540531
46	1	0	-4.028327	-0.960392	-1.917811
47	1	0	-3.522230	-2.189623	-3.080501
48	1	0	-4.213556	-1.657986	2.055886
49	1	0	-4.882212	-1.486416	0.416109
50	1	0	-4.641732	-0.065346	1.429403

B3LYP/6-31G(d)

Zero-point correction= 0.412159 (Hartree/Particle)
Thermal correction to Energy= 0.439041
Thermal correction to Enthalpy= 0.439986
Thermal correction to Gibbs Free Energy= 0.352323
Sum of electronic and zero-point Energies= -2592.219898
Sum of electronic and thermal Energies= -2592.193015
Sum of electronic and thermal Enthalpies= -2592.192071
Sum of electronic and thermal Free Energies= -2592.279734

B3LYP/6-311+G(d,p)

HF=-2593.01642616

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TS^{-}—$^{+}NEt_4$ (*m*-ClPhCH=CH_2) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.036402	3.444481	0.204012
2	25	0	-0.903746	2.474763	-0.316073
3	8	0	-1.405987	1.491953	-1.487933
4	8	0	-0.322235	1.588417	0.911835
5	8	0	0.426496	3.308404	-0.760627
6	6	0	2.022011	3.135520	0.371668

7	6	0	1.856925	2.081592	1.253713
8	6	0	2.361918	0.727989	1.038368
9	6	0	2.951821	-1.455925	1.963357
10	6	0	3.389630	-1.901932	0.713459
11	6	0	2.444842	-0.168316	2.123737
12	6	0	2.787984	0.268402	-0.226293
13	6	0	3.295362	-1.017829	-0.362668
14	17	0	3.830754	-1.562101	-1.958740
15	1	0	1.900864	4.147806	0.738291
16	1	0	2.662493	3.036938	-0.497419
17	1	0	1.517680	2.297869	2.260619
18	1	0	3.024528	-2.119519	2.821790
19	1	0	3.799311	-2.896659	0.576424
20	1	0	2.118999	0.165833	3.105335
21	1	0	2.714965	0.911748	-1.096003
22	7	0	-2.127762	-1.736875	0.011941
23	6	0	-0.749889	-1.357800	-0.564027
24	6	0	-2.017347	-2.940358	0.936409
25	6	0	-2.637993	-0.501107	0.760451
26	6	0	-3.095229	-2.128413	-1.101225
27	6	0	-0.090058	-2.418141	-1.433645
28	6	0	-1.098521	-2.775662	2.141785
29	6	0	-3.439001	-1.032485	-2.103465
30	6	0	-3.968820	-0.665544	1.480303
31	1	0	-0.129295	-1.110891	0.296406
32	1	0	-0.900279	-0.420520	-1.108565
33	1	0	-1.683565	-3.772121	0.312583
34	1	0	-3.034438	-3.168098	1.262377
35	1	0	-2.679649	0.288603	0.011466
36	1	0	-1.842046	-0.209951	1.445475
37	1	0	-3.998295	-2.489758	-0.603264
38	1	0	-2.638817	-2.984603	-1.601078
39	1	0	-0.644082	-2.626764	-2.353954
40	1	0	0.098007	-3.362685	-0.911879
41	1	0	0.884515	-2.021700	-1.732597
42	1	0	-0.055870	-2.604454	1.863311
43	1	0	-1.139048	-3.707086	2.716742
44	1	0	-1.416710	-1.966267	2.804166
45	1	0	-2.559923	-0.550975	-2.535512
46	1	0	-4.057295	-0.245884	-1.664925
47	1	0	-4.013989	-1.496884	-2.912010
48	1	0	-3.936542	-1.398032	2.293261
49	1	0	-4.794522	-0.922079	0.809068
50	1	0	-4.208608	0.304918	1.926860

B3LYP/6-31G(d)

Zero-point correction= 0.412115 (Hartree/Particle)
Thermal correction to Energy= 0.439042
Thermal correction to Enthalpy= 0.439986
Thermal correction to Gibbs Free Energy= 0.352719
Sum of electronic and zero-point Energies= -2592.219648
Sum of electronic and thermal Energies= -2592.192721
Sum of electronic and thermal Enthalpies= -2592.191776

Sum of electronic and thermal Free Energies= -2592.279043

B3LYP/6-311+G(d,p)

HF=-2593.01620741 (Hartree/Particle)

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TS^{-}—$^{+}$NEt$_4$ (*m*-BrPhCH=CH$_2$) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.009462	3.030367	-0.332766
2	25	0	-1.636522	2.283148	-0.556905
3	8	0	-1.730599	1.110970	-1.655899
4	8	0	-1.105683	1.661535	0.843746
5	8	0	-0.442116	3.339031	-0.906243
6	6	0	0.937420	3.626740	0.459285
7	6	0	0.856238	2.633448	1.419949
8	6	0	1.642781	1.403504	1.401377
9	6	0	2.558914	-0.521742	2.596180
10	6	0	3.185205	-0.983439	1.434907
11	6	0	1.799126	0.646126	2.579924
12	6	0	2.263724	0.926528	0.226717
13	6	0	3.017494	-0.238004	0.267740
14	35	0	3.831713	-0.870264	-1.354843
15	1	0	0.551843	4.612294	0.691850
16	1	0	1.715903	3.604795	-0.294795
17	1	0	0.338153	2.847123	2.348260
18	1	0	2.679886	-1.076310	3.523751
19	1	0	3.786986	-1.885275	1.433949
20	1	0	1.324064	0.994073	3.493547
21	1	0	2.135711	1.455255	-0.710836
22	7	0	-2.029022	-2.078420	0.065385
23	6	0	-0.681567	-1.495068	-0.403292
24	6	0	-1.817478	-3.164127	1.109862
25	6	0	-2.834891	-0.905935	0.633869
26	6	0	-2.773347	-2.727636	-1.097511
27	6	0	0.248151	-2.479173	-1.099056
28	6	0	-1.087142	-2.737089	2.377862
29	6	0	-3.190010	-1.793192	-2.228407
30	6	0	-4.187943	-1.261627	1.233096
31	1	0	-0.217153	-1.074284	0.487886
32	1	0	-0.929908	-0.644377	-1.045697
33	1	0	-1.274497	-3.967343	0.607516
34	1	0	-2.810219	-3.548085	1.353644
35	1	0	-2.932721	-0.201990	-0.191062
36	1	0	-2.189052	-0.413150	1.360332
37	1	0	-3.648195	-3.216536	-0.662024
38	1	0	-2.114291	-3.515617	-1.466088
39	1	0	-0.138872	-2.825880	-2.062100
40	1	0	0.505115	-3.351006	-0.487358
41	1	0	1.185187	-1.952763	-1.303131
42	1	0	-0.062223	-2.408582	2.189502
43	1	0	-1.039268	-3.608130	3.040196

44	1	0	-1.611015	-1.942732	2.915852
45	1	0	-2.370174	-1.180044	-2.607130
46	1	0	-3.993107	-1.114170	-1.932763
47	1	0	-3.565148	-2.416976	-3.047026
48	1	0	-4.117704	-1.902363	2.118018
49	1	0	-4.869884	-1.728641	0.515298
50	1	0	-4.650348	-0.320890	1.549142

B3LYP/6-31G(d)

Zero-point correction= 0.411699 (Hartree/Particle)
Thermal correction to Energy= 0.438731
Thermal correction to Enthalpy= 0.439675
Thermal correction to Gibbs Free Energy= 0.352043
Sum of electronic and zero-point Energies= -4703.731630
Sum of electronic and thermal Energies= -4703.704598
Sum of electronic and thermal Enthalpies= -4703.703654
Sum of electronic and thermal Free Energies= -4703.791285

B3LYP/6-311+G(d,p)

HF=-4706.93518931 (Hartree/Particle)

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TS^{-}—$^{+}$NEt$_4$ (3,4-diClPhCH=CH$_2$) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.576977	2.435659	-0.311649
2	25	0	2.156876	2.028626	0.245844
3	8	0	2.237461	0.956806	1.442920
4	8	0	1.241683	1.426578	-0.949417
5	8	0	1.292081	3.344821	0.675262
6	6	0	-0.251611	3.818439	-0.432209
7	6	0	-0.556668	2.768969	-1.282038
8	6	0	-1.550665	1.738382	-1.004220
9	6	0	-2.995974	-0.052997	-1.824259
10	6	0	-3.501980	-0.266275	-0.539139
11	6	0	-2.038074	0.928806	-2.049984
12	6	0	-2.060030	1.501873	0.287889
13	6	0	-3.024534	0.524310	0.515767
14	17	0	-3.613396	0.295822	2.154280
15	17	0	-4.706177	-1.515697	-0.293518
16	1	0	0.262703	4.682976	-0.834561
17	1	0	-0.855681	4.013397	0.446665
18	1	0	-0.188694	2.801795	-2.301422
19	1	0	-3.373236	-0.655486	-2.644668
20	1	0	-1.663627	1.084125	-3.058189
21	1	0	-1.691493	2.074874	1.131348
22	7	0	1.642052	-2.339645	0.010276
23	6	0	0.530769	-1.453904	0.602865
24	6	0	1.052062	-3.427387	-0.876442
25	6	0	2.561037	-1.407302	-0.785389
26	6	0	2.422172	-3.049862	1.113063

27	6	0	-0.451841	-2.163822	1.523291
28	6	0	0.245484	-2.946435	-2.077635
29	6	0	3.173612	-2.148701	2.086337
30	6	0	3.710394	-2.079918	-1.521908
31	1	0	0.021108	-1.011912	-0.252340
32	1	0	1.041883	-0.631319	1.112278
33	1	0	0.434180	-4.048131	-0.224265
34	1	0	1.893470	-4.040395	-1.206224
35	1	0	2.921313	-0.675224	-0.063936
36	1	0	1.916177	-0.851309	-1.465557
37	1	0	3.112802	-3.726948	0.604876
38	1	0	1.692736	-3.668358	1.638894
39	1	0	0.016448	-2.557738	2.430457
40	1	0	-1.012802	-2.968544	1.036257
41	1	0	-1.183658	-1.416652	1.843788
42	1	0	-0.639574	-2.371254	-1.795457
43	1	0	-0.097593	-3.833613	-2.620525
44	1	0	0.842439	-2.347143	-2.770033
45	1	0	2.545223	-1.375536	2.531833
46	1	0	4.023706	-1.647031	1.618867
47	1	0	3.561671	-2.785769	2.888517
48	1	0	3.383549	-2.768081	-2.308367
49	1	0	4.398698	-2.609960	-0.856038
50	1	0	4.284200	-1.283000	-2.006044

B3LYP/6-31G(d)

Zero-point correction= 0.402671 (Hartree/Particle)
Thermal correction to Energy= 0.430857
Thermal correction to Enthalpy= 0.431802
Thermal correction to Gibbs Free Energy= 0.340892
Sum of electronic and zero-point Energies= -3051.821067
Sum of electronic and thermal Energies= -3051.792880
Sum of electronic and thermal Enthalpies= -3051.791936
Sum of electronic and thermal Free Energies= -3051.882846

B3LYP/6-311+G(d,p)

HF=-3052.63525061 (Hartree/Particle)

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TS^{-}—$^{+}NEt_4$ (*m*-$NO_2PhCH{=}CH_2$) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.642031	-2.379601	0.310670
2	25	0	-2.560459	-1.376467	-0.246256
3	8	0	-1.235244	-2.110338	-0.787577
4	8	0	-2.162360	-0.291452	0.886796
5	8	0	-3.198765	-0.416932	-1.404068
6	6	0	-3.411429	1.473543	-1.013503
7	6	0	-2.854521	1.783351	0.215974
8	6	0	-1.544764	2.398742	0.393418
9	6	0	-0.062603	3.834966	1.720182

10	6	0	0.966519	3.685225	0.794042
11	6	0	-1.287380	3.196942	1.528702
12	6	0	-0.496538	2.230116	-0.532470
13	6	0	0.722446	2.866101	-0.312767
14	7	0	1.825808	2.623828	-1.248363
15	8	0	1.667565	1.776377	-2.135676
16	8	0	2.876028	3.248175	-1.086555
17	1	0	-4.487627	1.374821	-1.088719
18	1	0	-2.912170	1.771263	-1.929689
19	1	0	-3.497678	1.788743	1.089666
20	1	0	0.091761	4.455094	2.598676
21	1	0	1.928472	4.166519	0.913137
22	1	0	-2.076984	3.323937	2.264763
23	1	0	-0.620641	1.590669	-1.397655
24	7	0	2.093483	-1.722031	0.387431
25	6	0	1.807601	-1.569711	-1.114355
26	6	0	3.463876	-1.161632	0.751111
27	6	0	0.967327	-0.965165	1.106024
28	6	0	2.115944	-3.192164	0.799745
29	6	0	2.759923	-2.303632	-2.048558
30	6	0	3.707559	0.306746	0.426249
31	6	0	0.829910	-3.981180	0.593379
32	6	0	1.002576	-0.994106	2.626294
33	1	0	1.829776	-0.497251	-1.312188
34	1	0	0.771857	-1.893222	-1.249276
35	1	0	4.193242	-1.790599	0.236111
36	1	0	3.583841	-1.337350	1.822250
37	1	0	0.037374	-1.382982	0.720532
38	1	0	1.021221	0.060308	0.740501
39	1	0	2.403139	-3.199055	1.853725
40	1	0	2.938800	-3.641344	0.239491
41	1	0	2.706952	-3.391845	-1.948513
42	1	0	3.803558	-1.988180	-1.947294
43	1	0	2.450395	-2.060844	-3.070227
44	1	0	3.636566	0.532131	-0.640422
45	1	0	4.728296	0.547252	0.742036
46	1	0	3.036160	0.976103	0.970310
47	1	0	0.482139	-3.978399	-0.440474
48	1	0	0.005168	-3.617693	1.208551
49	1	0	1.040065	-5.016353	0.885242
50	1	0	1.888203	-0.514299	3.056533
51	1	0	0.911134	-2.003504	3.038477
52	1	0	0.123219	-0.433505	2.957849

B3LYP/6-31G(d)

Zero-point correction= 0.423553 (Hartree/Particle)
Thermal correction to Energy= 0.451922
Thermal correction to Enthalpy= 0.452866
Thermal correction to Gibbs Free Energy= 0.362203
Sum of electronic and zero-point Energies= -2337.118007
Sum of electronic and thermal Energies= -2337.089638
Sum of electronic and thermal Enthalpies= -2337.088694
Sum of electronic and thermal Free Energies= -2337.179357

B3LYP/6-311+G(d,p)

HF=-2337.95943071 (Hartree/Particle)

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TS^{-}—$^{+}NEt_4$ (*p*-$NO_2PhCH{=}CH_2$) at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.922893	1.647667	0.319933
2	25	0	2.880181	0.590939	-0.216622
3	8	0	1.761444	1.238268	-1.164963
4	8	0	2.156416	-0.152661	1.017946
5	8	0	3.632222	-0.650698	-0.973706
6	6	0	3.458547	-2.439437	-0.268675
7	6	0	2.441087	-2.470036	0.674305
8	6	0	1.037786	-2.566160	0.339635
9	6	0	-1.278748	-2.839602	1.074683
10	6	0	-1.713086	-2.502909	-0.215220
11	6	0	0.079791	-2.863105	1.339940
12	6	0	0.560793	-2.293933	-0.967926
13	6	0	-0.793093	-2.256078	-1.244452
14	7	0	-3.123969	-2.317788	-0.465298
15	8	0	-3.464839	-1.820502	-1.552639
16	8	0	-3.928220	-2.612603	0.427457
17	1	0	4.484843	-2.519798	0.071702
18	1	0	3.283358	-2.803035	-1.274694
19	1	0	2.695547	-2.497404	1.728193
20	1	0	-2.011591	-3.050682	1.844481
21	1	0	0.423994	-3.092250	2.344862
22	1	0	1.267074	-2.046373	-1.752573
23	1	0	-1.157165	-2.013050	-2.235396
24	7	0	-1.541743	2.123172	0.243965
25	6	0	-1.449314	1.621577	-1.203557
26	6	0	-2.988063	2.144765	0.732144
27	6	0	-0.682358	1.160040	1.071788
28	6	0	-1.034364	3.559401	0.367926
29	6	0	-2.150445	2.476134	-2.251416
30	6	0	-3.738241	0.818788	0.720376
31	6	0	0.429397	3.803101	0.024824
32	6	0	-0.594001	1.453777	2.561314
33	1	0	-1.871329	0.615618	-1.191255
34	1	0	-0.380950	1.523797	-1.413606
35	1	0	-3.502296	2.879953	0.109280
36	1	0	-2.950788	2.549457	1.745650
37	1	0	0.305426	1.166731	0.614420
38	1	0	-1.099134	0.167172	0.899068
39	1	0	-1.238777	3.854856	1.399368
40	1	0	-1.688224	4.155026	-0.272485
41	1	0	-1.700680	3.466453	-2.366856
42	1	0	-3.224555	2.590430	-2.073548

43	1	0	-2.038309	1.960280	-3.210530
44	1	0	-3.855707	0.390614	-0.277869
45	1	0	-4.744311	1.012107	1.107771
46	1	0	-3.285367	0.066847	1.371049
47	1	0	0.708418	3.449994	-0.968873
48	1	0	1.115333	3.337210	0.735099
49	1	0	0.591119	4.886075	0.066266
50	1	0	-1.550786	1.355850	3.084658
51	1	0	-0.168287	2.437723	2.779615
52	1	0	0.095165	0.711517	2.974735

B3LYP/6-31G(d)

Zero-point correction= 0.424248 (Hartree/Particle)
Thermal correction to Energy= 0.452393
Thermal correction to Enthalpy= 0.453338
Thermal correction to Gibbs Free Energy= 0.364082
Sum of electronic and zero-point Energies= -2337.120665
Sum of electronic and thermal Energies= -2337.092519
Sum of electronic and thermal Enthalpies= -2337.091575
Sum of electronic and thermal Free Energies= -2337.180831

B3LYP/6-311+G(d,p)

HF=-2337.96225199 (Hartree/Particle)