Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Intriguing Roles of Reactive Intermediates in Dissociation Chemistry of *N*-phenylcinnamides

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Supplementary information

Fig. S1 The CID spectrum of $[M + D]^+$ ion of compound **1**.

Scheme S1 Proposed mechanism to explain the formations of ions at *m/z* 132, 131, 104, 103, 95, 94, 78 and 77 from $[M + D]^+$ ion of compound **1**.

Scheme S2 Proposed mechanism to explain the formations of ions at *m/z* 121, 120, 106 and 105 from $[M + D]^+$ ion of compound **1**

Scheme S3 Proposed mechanism to explain the formations of ions at *m/z* 147 and 146 from $[M + D]^+$ ion of compound **1**

Scheme S4 Proposed mechanism to explain the formations of ions at *m/z* 183 and 182 from $[M + D]^+$ ion of compound **1**

- ^{1}H NMR, ^{13}C NMR spectra of *N*-phenylcinnamide (compound **1**)

- Cartesian coordinates, total energies, zero point energy corrections and the number of imaginary frequencies of all structures discussed in the text.

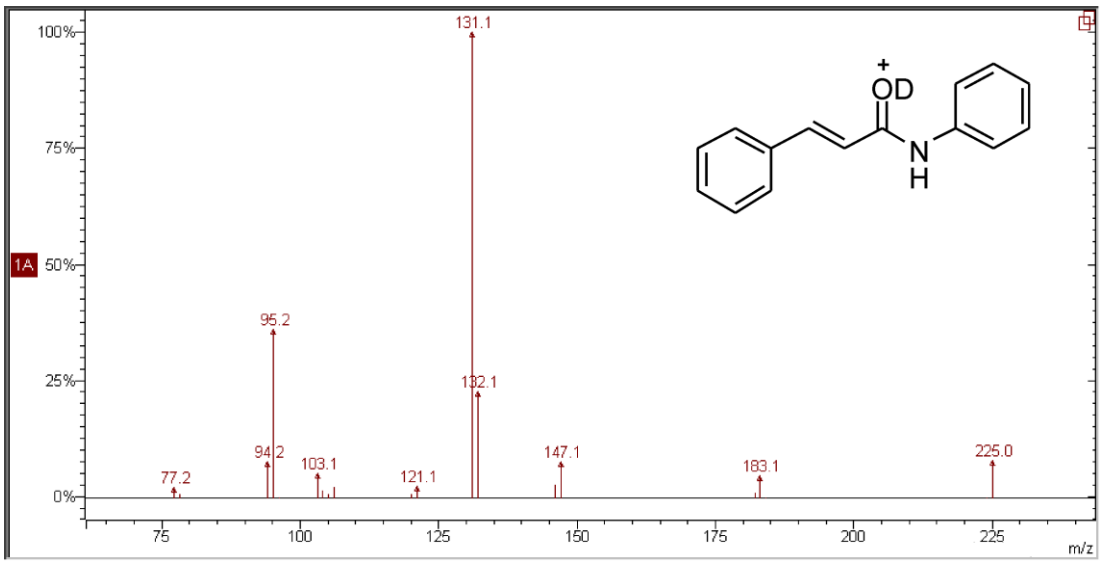
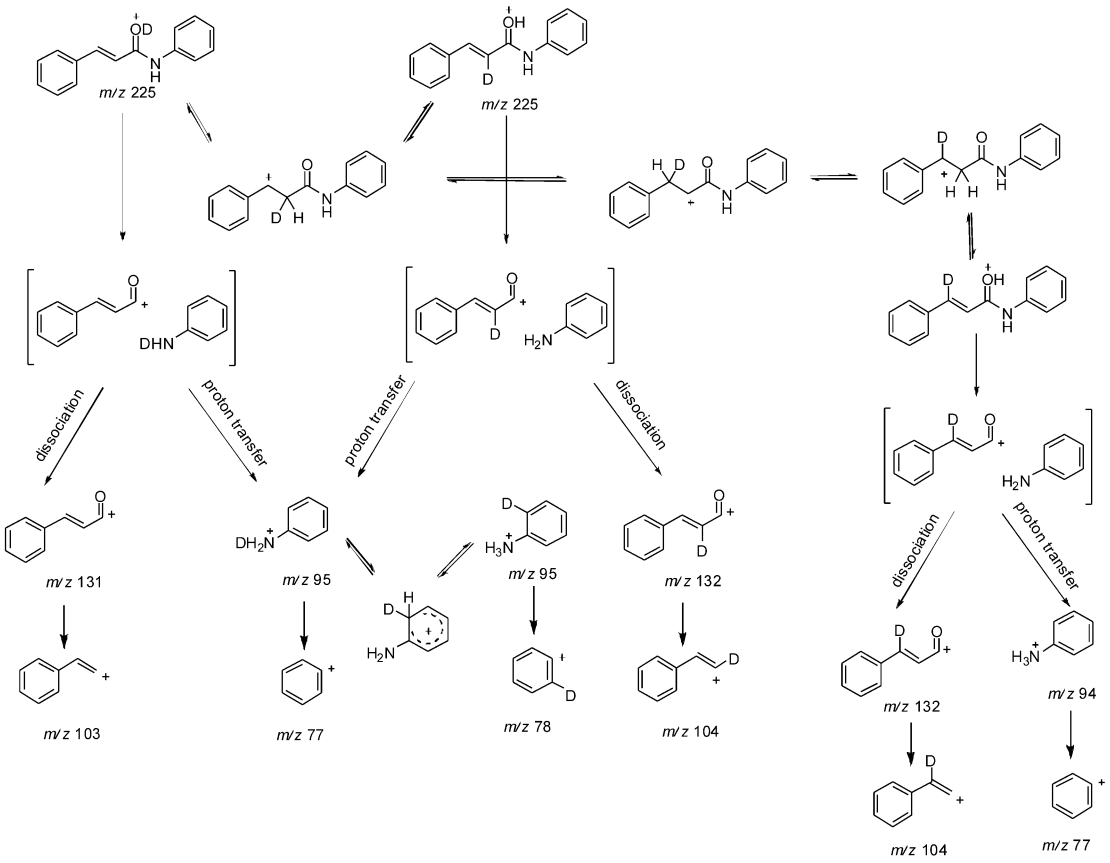
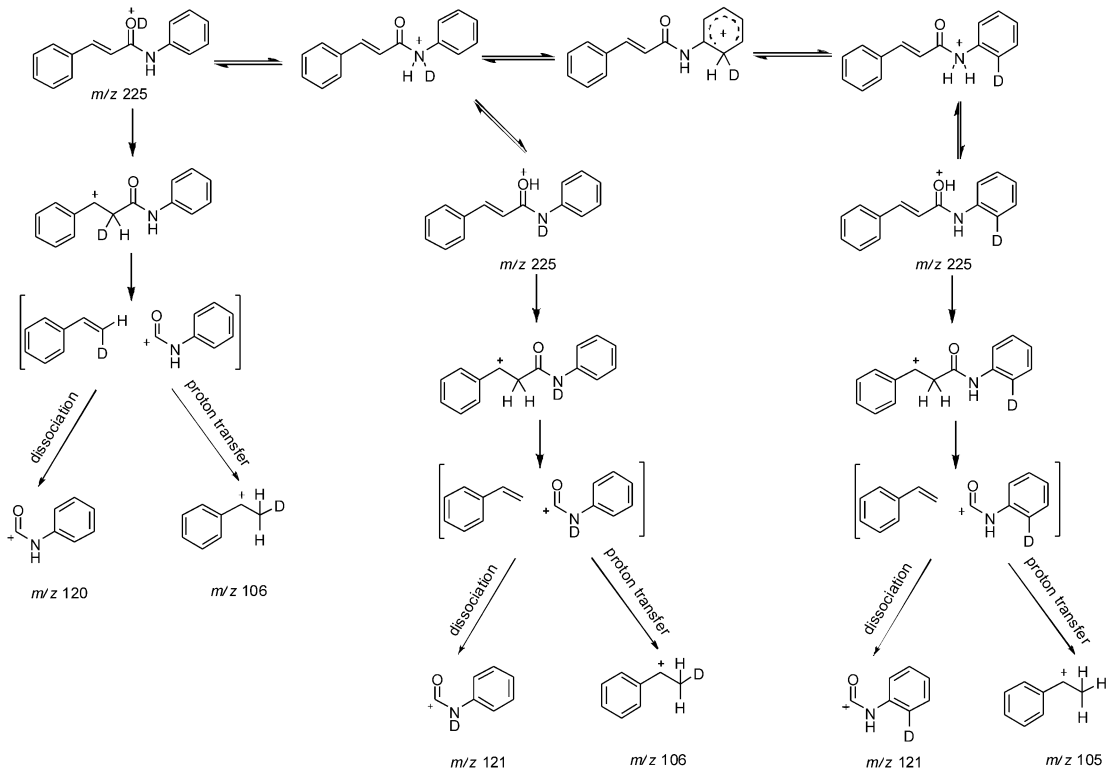


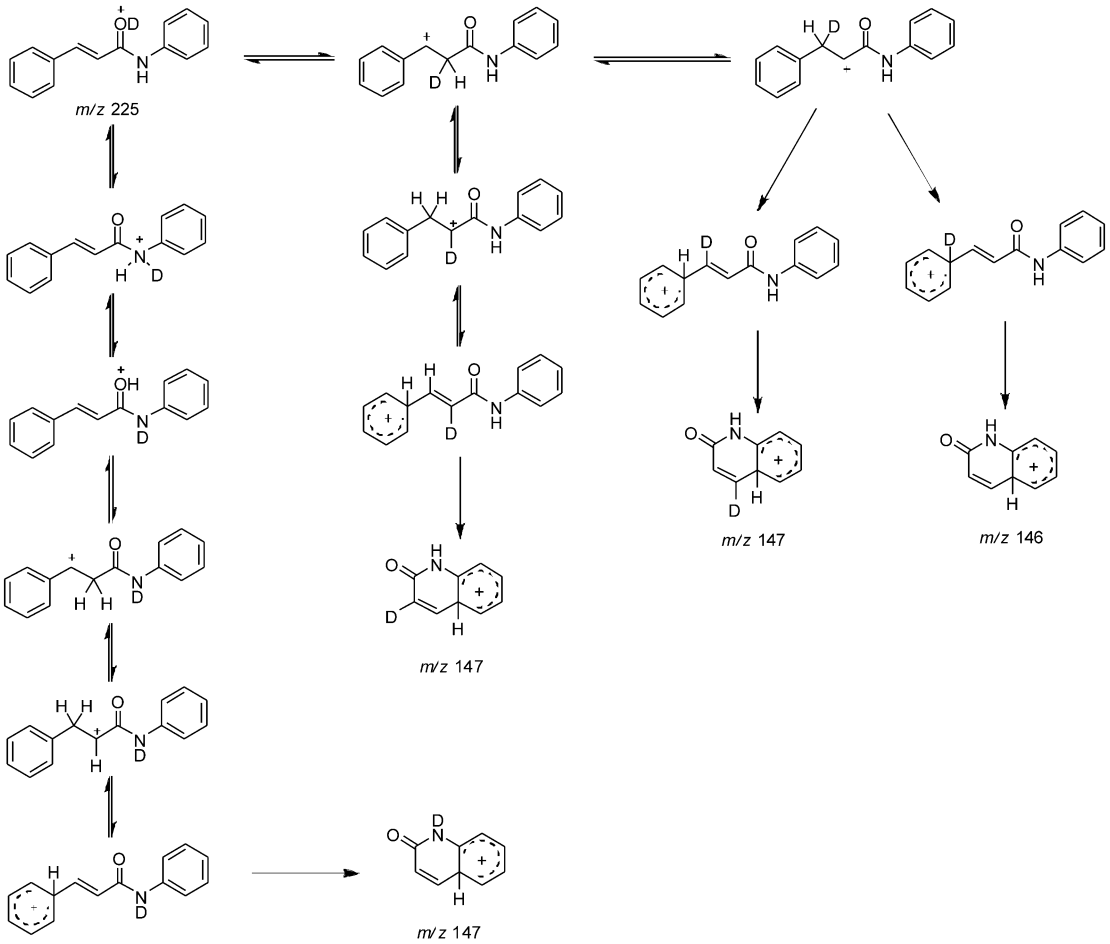
Fig. S1 The CID spectrum of $[M + D]^+$ ion of compound **1**.



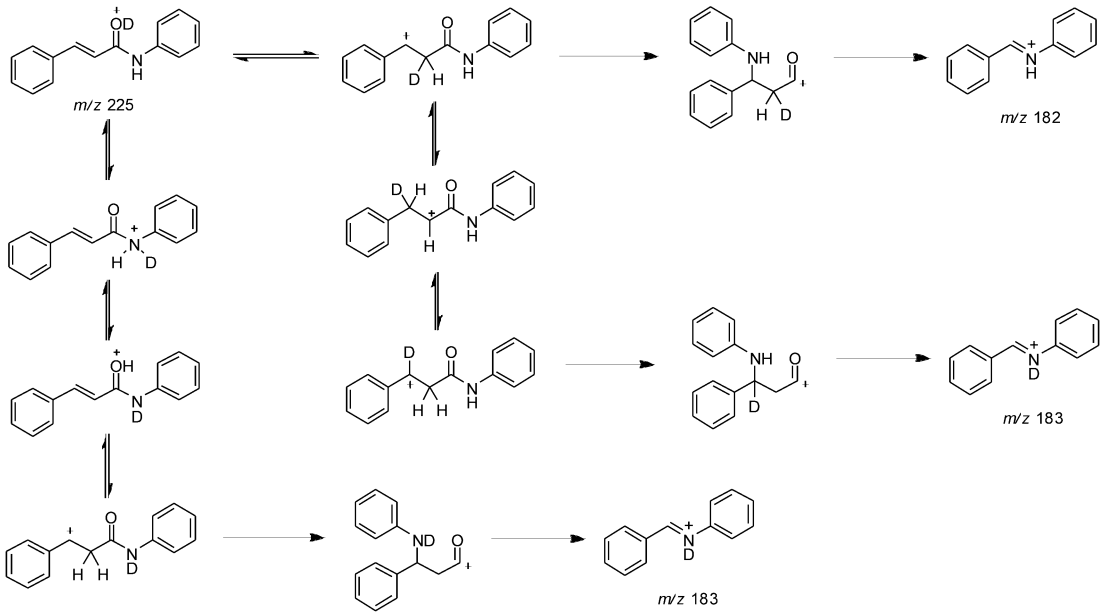
Scheme S1 Proposed mechanism to explain the formations of ions at *m/z* 132, 131, 104, 103, 95, 94, 78 and 77 from $[M + D]^+$ ion of compound **1**.



Scheme S2 Proposed mechanism to explain the formations of ions at *m/z* 121, 120, 106 and 105 from $[M + D]^+$ ion of compound **1**

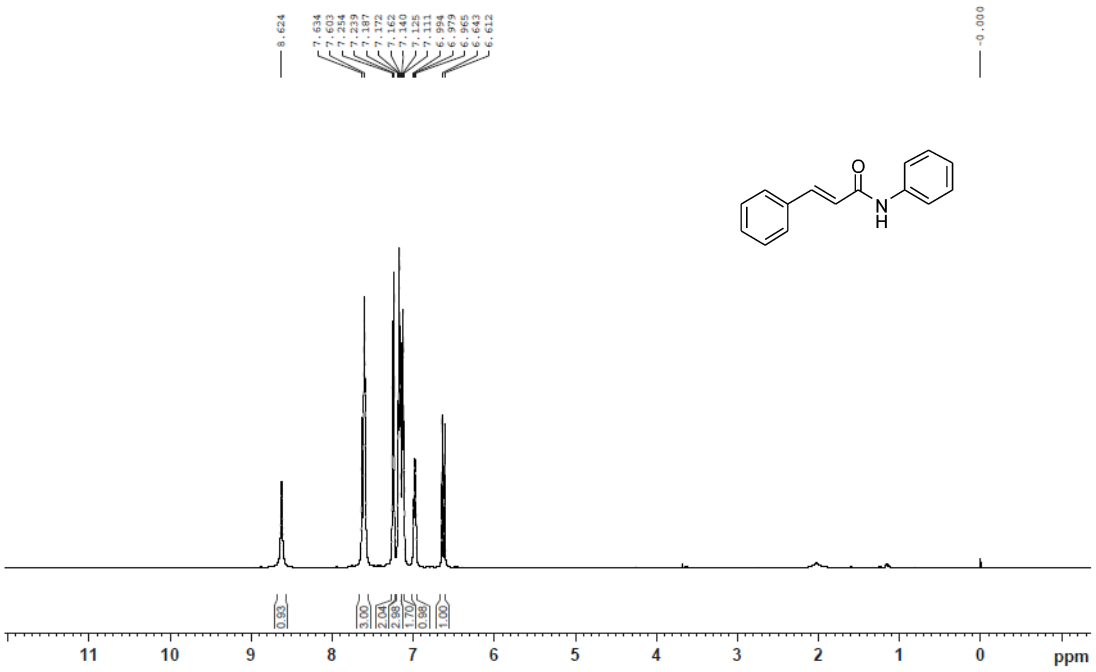


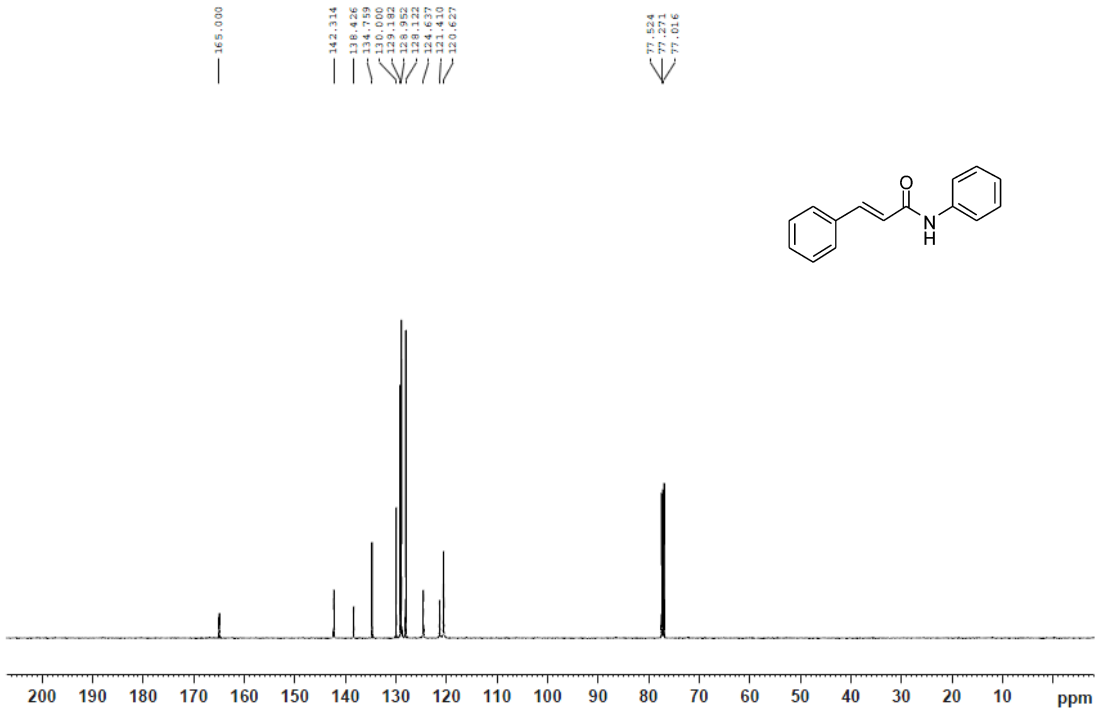
Scheme S3 Proposed mechanism to explain the formations of ions at *m/z* 183, 182, 147 and 146 from $[M + D]^+$ ion of compound **1**



Scheme S4 Proposed mechanism to explain the formations of ions at *m/z* 183 and 182 from $[M + D]^+$ ion of compound **1**

■ ^{1}H NMR, ^{13}C NMR spectra of *N*-phenylcinnamide (compound **1**)





■ Cartesian coordinates, total energies, zero point energy corrections and the number of imaginary frequencies of all structures discussed in the text.

MH-1 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.099787	-1.188881	-0.408554
2	6	0	3.184688	-0.166657	-0.068836
3	6	0	3.689153	1.088456	0.345051
4	6	0	5.056774	1.304864	0.414634
5	6	0	5.949337	0.278305	0.074683
6	6	0	5.469942	-0.968066	-0.336676
7	1	0	3.721817	-2.156523	-0.728043
8	1	0	3.009908	1.892628	0.610876
9	1	0	5.437133	2.270483	0.732734
10	1	0	7.019436	0.454533	0.131513
11	1	0	6.163090	-1.760812	-0.599375
12	6	0	1.777225	-0.462862	-0.162393
13	6	0	0.728183	0.364959	0.124506
14	1	0	1.532974	-1.467787	-0.501155
15	1	0	0.879228	1.381542	0.472666
16	6	0	-0.623210	-0.062655	-0.015050
17	8	0	-0.861377	-1.296863	-0.418657
18	7	0	-1.644515	0.755571	0.251979
19	6	0	-3.037932	0.408823	0.143993
20	6	0	-3.858582	1.152384	-0.709777
21	6	0	-3.553436	-0.648242	0.906307
22	6	0	-5.210928	0.827896	-0.802092
23	1	0	-3.441952	1.966118	-1.296281
24	6	0	-4.906513	-0.973482	0.787799
25	1	0	-2.918854	-1.177931	1.611962
26	6	0	-5.732973	-0.237035	-0.061997
27	1	0	-5.855249	1.402872	-1.459632
28	1	0	-5.313890	-1.788758	1.377271
29	1	0	-6.786159	-0.486940	-0.143040
30	1	0	-1.411181	1.711662	0.499048
31	1	0	-1.822770	-1.462012	-0.512730

Zero-point correction= 0.255707 (Hartree/Particle)
Thermal correction to Energy= 0.270052

Thermal correction to Enthalpy=	0.270996
Thermal correction to Gibbs Free Energy=	0.212325
Sum of electronic and zero-point Energies=	-709.524046
Sum of electronic and thermal Energies=	-709.509701
Sum of electronic and thermal Enthalpies=	-709.508757
Sum of electronic and thermal Free Energies=	-709.567428

no imaginary vibrational frequency

TS1 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.959523	0.720826	0.577590
2	6	0	-2.774973	0.168432	0.028960
3	6	0	-2.812760	-1.147724	-0.498231
4	6	0	-3.990742	-1.874871	-0.472854
5	6	0	-5.153103	-1.309812	0.075030
6	6	0	-5.137110	-0.013238	0.599673
7	1	0	-3.937513	1.728952	0.982581
8	1	0	-1.919092	-1.592241	-0.924590
9	1	0	-4.016935	-2.881754	-0.877015
10	1	0	-6.073568	-1.886047	0.090770
11	1	0	-6.039939	0.416617	1.021166
12	6	0	-1.593696	0.975399	0.036369
13	6	0	-0.339314	0.650835	-0.439151
14	1	0	-1.699590	1.970211	0.467870
15	1	0	-0.106253	-0.313154	-0.876458
16	6	0	0.694872	1.593219	-0.363352
17	8	0	0.723117	2.774632	0.101303
18	7	0	2.083214	1.408297	-0.826355
19	6	0	2.864581	0.296229	-0.293397
20	6	0	3.420903	-0.637753	-1.165840
21	6	0	3.053415	0.210817	1.087450
22	6	0	4.185436	-1.681476	-0.641506
23	1	0	3.271901	-0.552854	-2.239912
24	6	0	3.809479	-0.842572	1.598533
25	1	0	2.632006	0.960429	1.751716
26	6	0	4.375748	-1.786398	0.737159
27	1	0	4.630854	-2.408562	-1.313098
28	1	0	3.965873	-0.917770	2.669965
29	1	0	4.971189	-2.599139	1.141047
30	1	0	2.144981	1.446956	-1.848593
31	1	0	1.949375	2.641759	-0.269993

Zero-point correction=	0.250634 (Hartree/Particle)
Thermal correction to Energy=	0.264739
Thermal correction to Enthalpy=	0.265683
Thermal correction to Gibbs Free Energy=	0.206931
Sum of electronic and zero-point Energies=	-709.456389
Sum of electronic and thermal Energies=	-709.442284
Sum of electronic and thermal Enthalpies=	-709.441340
Sum of electronic and thermal Free Energies=	-709.500093

one imaginary vibrational frequency, -1786.09

MH-2 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.871082	0.728272	0.641064
2	6	0	-2.685034	0.224363	0.059954
3	6	0	-2.695662	-1.079117	-0.489697
4	6	0	-3.851750	-1.843304	-0.456474
5	6	0	-5.019358	-1.326302	0.123288
6	6	0	-5.028044	-0.041161	0.671718
7	1	0	-3.871735	1.728557	1.065952
8	1	0	-1.797558	-1.490559	-0.940291
9	1	0	-3.853877	-2.842964	-0.879550
10	1	0	-5.921909	-1.929908	0.145789
11	1	0	-5.933314	0.355719	1.119891
12	6	0	-1.521152	1.072464	0.059419
13	6	0	-0.280056	0.805600	-0.452636
14	1	0	-1.648745	2.050365	0.522103
15	1	0	-0.031019	-0.137109	-0.926043
16	6	0	0.732300	1.806348	-0.346638
17	8	0	0.784540	2.899302	0.140162
18	7	0	2.125042	1.351658	-1.047485
19	6	0	2.817902	0.220371	-0.395664
20	6	0	2.959548	-0.979926	-1.086001
21	6	0	3.291892	0.396538	0.903066
22	6	0	3.603718	-2.042593	-0.449104
23	1	0	2.593117	-1.090213	-2.104294
24	6	0	3.934160	-0.674475	1.523458
25	1	0	3.166682	1.344245	1.419741
26	6	0	4.088832	-1.889817	0.850727
27	1	0	3.730575	-2.983402	-0.974935
28	1	0	4.315407	-0.555711	2.532530

29	1	0	4.592705	-2.717427	1.339786
30	1	0	1.957570	1.141855	-2.037998
31	1	0	2.693203	2.206968	-1.010469

Zero-point correction= 0.255711 (Hartree/Particle)
Thermal correction to Energy= 0.270280
Thermal correction to Enthalpy= 0.271224
Thermal correction to Gibbs Free Energy= 0.210899
Sum of electronic and zero-point Energies= -709.502171
Sum of electronic and thermal Energies= -709.487602
Sum of electronic and thermal Enthalpies= -709.486657
Sum of electronic and thermal Free Energies= -709.546982

no imaginary vibrational frequency

INC-1 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.871830	-1.274153	-0.000385
2	6	0	2.679175	-0.506754	-0.000048
3	6	0	2.767641	0.909668	0.000477
4	6	0	4.007341	1.525076	0.000650
5	6	0	5.177653	0.748761	0.000255
6	6	0	5.110207	-0.648726	-0.000274
7	1	0	3.808731	-2.359012	-0.000716
8	1	0	1.864858	1.512565	0.000783
9	1	0	4.077346	2.608039	0.001105
10	1	0	6.146141	1.240291	0.000369
11	1	0	6.020092	-1.239825	-0.000575
12	6	0	1.434414	-1.205721	-0.000293
13	6	0	0.171224	-0.634976	-0.000221
14	1	0	1.501275	-2.292707	-0.000467
15	1	0	-0.033938	0.446895	-0.000364
16	6	0	-0.922168	-1.458906	-0.000239
17	8	0	-1.773205	-2.228965	0.000763
18	7	0	-1.259102	2.116300	-0.000955
19	6	0	-2.387758	1.264616	-0.000526
20	6	0	-2.924024	0.799916	1.213650
21	6	0	-2.924614	0.799108	-1.214114
22	6	0	-3.994408	-0.093250	1.207429
23	1	0	-2.518264	1.160845	2.156216
24	6	0	-3.994949	-0.094080	-1.206740
25	1	0	-2.519297	1.159360	-2.157127

26	6	0	-4.531321	-0.549780	0.000632
27	1	0	-4.411679	-0.430968	2.151535
28	1	0	-4.412656	-0.432488	-2.150407
29	1	0	-5.366950	-1.242223	0.001047
30	1	0	-1.198833	2.701323	0.828060
31	1	0	-1.198924	2.700737	-0.830392

Zero-point correction=	0.252676 (Hartree/Particle)
Thermal correction to Energy=	0.268254
Thermal correction to Enthalpy=	0.269199
Thermal correction to Gibbs Free Energy=	0.207509
Sum of electronic and zero-point Energies=	-709.485906
Sum of electronic and thermal Energies=	-709.470328
Sum of electronic and thermal Enthalpies=	-709.469383
Sum of electronic and thermal Free Energies=	-709.531073

no imaginary vibrational frequency

product ion a (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.277396	-1.301846	0.000014
2	6	0	-0.404929	-0.177701	0.000029
3	6	0	-0.961728	1.131674	0.000010
4	6	0	-2.333292	1.299569	-0.000024
5	6	0	-3.177681	0.174988	-0.000039
6	6	0	-2.650987	-1.122886	-0.000020
7	1	0	-0.857129	-2.303836	0.000029
8	1	0	-0.317093	2.004994	0.000022
9	1	0	-2.760208	2.297032	-0.000039
10	1	0	-4.254560	0.316666	-0.000066
11	1	0	-3.314180	-1.981488	-0.000031
12	6	0	0.990585	-0.429865	0.000060
13	6	0	2.012223	0.518658	0.000051
14	1	0	1.287972	-1.477286	0.000079
15	1	0	1.857321	1.594348	0.000071
16	6	0	3.314697	0.114980	0.000066
17	8	0	4.411116	-0.211981	-0.000118

Zero-point correction=	0.133118 (Hartree/Particle)
Thermal correction to Energy=	0.141471
Thermal correction to Enthalpy=	0.142415
Thermal correction to Gibbs Free Energy=	0.099241

Sum of electronic and zero-point Energies=	-421.977796
Sum of electronic and thermal Energies=	-421.969444
Sum of electronic and thermal Enthalpies=	-421.968500
Sum of electronic and thermal Free Energies=	-422.011674

no imaginary vibrational frequency

aniline

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.171829	1.202609	0.003362
2	6	0	-1.881699	0.000000	0.008429
3	6	0	-1.171827	-1.202610	0.003362
4	6	0	0.221250	-1.208252	-0.005255
5	6	0	0.938733	0.000001	-0.010131
6	6	0	0.221250	1.208252	-0.005254
7	1	0	-1.705690	2.149759	0.008754
8	1	0	-2.967660	-0.000003	0.016965
9	1	0	-1.705690	-2.149758	0.008752
10	1	0	0.763352	-2.151730	-0.013704
11	1	0	0.763347	2.151733	-0.013701
12	7	0	2.337428	-0.000002	-0.078806
13	1	0	2.777539	0.834907	0.288730
14	1	0	2.777537	-0.834898	0.288759

Zero-point correction=	0.117389 (Hartree/Particle)
Thermal correction to Energy=	0.123173
Thermal correction to Enthalpy=	0.124117
Thermal correction to Gibbs Free Energy=	0.088238
Sum of electronic and zero-point Energies=	-287.484372
Sum of electronic and thermal Energies=	-287.478588
Sum of electronic and thermal Enthalpies=	-287.477644
Sum of electronic and thermal Free Energies=	-287.513523

no imaginary vibrational frequency

TS2 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.749637	-0.246241	-0.282719
2	6	0	-2.381163	0.087269	-0.155179

3	6	0	-1.439808	-0.952763	0.021761
4	6	0	-1.857941	-2.272801	0.085285
5	6	0	-3.221763	-2.583033	-0.020240
6	6	0	-4.166381	-1.569603	-0.205218
7	1	0	-4.479032	0.545476	-0.432409
8	1	0	-0.381059	-0.719589	0.065434
9	1	0	-1.129567	-3.068932	0.205155
10	1	0	-3.543975	-3.618943	0.030672
11	1	0	-5.219744	-1.814689	-0.295567
12	6	0	-2.013115	1.476411	-0.231001
13	6	0	-0.781453	2.032011	0.041923
14	1	0	-2.828627	2.135688	-0.532136
15	1	0	0.487067	1.389629	0.764446
16	6	0	-0.517519	3.332556	-0.108830
17	8	0	-0.088912	4.409193	-0.176962
18	7	0	1.429194	0.999842	1.364392
19	6	0	2.261845	0.056525	0.601085
20	6	0	2.438607	-1.242041	1.072992
21	6	0	2.834523	0.489717	-0.593555
22	6	0	3.216050	-2.129752	0.326213
23	1	0	1.992437	-1.559153	2.012915
24	6	0	3.612487	-0.406405	-1.326800
25	1	0	2.684047	1.506206	-0.946884
26	6	0	3.802634	-1.712741	-0.869436
27	1	0	3.367983	-3.141919	0.687461
28	1	0	4.069538	-0.080852	-2.255811
29	1	0	4.411055	-2.403956	-1.443999
30	1	0	1.964240	1.831632	1.637525
31	1	0	1.088377	0.572313	2.230464

Zero-point correction= 0.249887 (Hartree/Particle)
Thermal correction to Energy= 0.264940
Thermal correction to Enthalpy= 0.265884
Thermal correction to Gibbs Free Energy= 0.203303
Sum of electronic and zero-point Energies= -709.466628
Sum of electronic and thermal Energies= -709.451575
Sum of electronic and thermal Enthalpies= -709.450630
Sum of electronic and thermal Free Energies= -709.513211

one imaginary vibrational frequency, -190.327

product ion b (Compound **1**)

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

1	6	0	1.227164	-1.213017	0.001659
2	6	0	1.920680	-0.000217	0.005706
3	6	0	1.228323	1.212551	0.001675
4	6	0	-0.167823	1.223851	-0.005529
5	6	0	-0.826310	0.000340	-0.010179
6	6	0	-0.168490	-1.224144	-0.005505
7	1	0	1.767513	-2.153884	0.000607
8	1	0	3.005913	-0.000702	0.008736
9	1	0	1.768811	2.153320	0.000648
10	1	0	-0.711678	2.165402	-0.008069
11	1	0	-0.713012	-2.165190	-0.008144
12	7	0	-2.326019	0.000128	0.007720
13	1	0	-2.704495	-0.091068	0.961276
14	1	0	-2.703332	0.870692	-0.387934
15	1	0	-2.708853	-0.775650	-0.548128

Zero-point correction= 0.131854 (Hartree/Particle)
Thermal correction to Energy= 0.138110
Thermal correction to Enthalpy= 0.139054
Thermal correction to Gibbs Free Energy= 0.100843
Sum of electronic and zero-point Energies= -287.823992
Sum of electronic and thermal Energies= -287.817736
Sum of electronic and thermal Enthalpies= -287.816792
Sum of electronic and thermal Free Energies= -287.855003

no imaginary vibrational frequency

PhCH=C=C=O (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.468052	-1.284197	-0.000005
2	6	0	0.425295	-0.339281	-0.000033
3	6	0	0.748276	1.032290	-0.000022
4	6	0	2.075706	1.440685	0.000020
5	6	0	3.104185	0.489916	0.000036
6	6	0	2.798412	-0.872967	0.000009
7	1	0	1.225123	-2.344385	-0.000011
8	1	0	-0.062130	1.755284	-0.000035
9	1	0	2.316735	2.500102	0.000048
10	1	0	4.141617	0.813340	0.000073
11	1	0	3.595446	-1.611123	0.000009
12	6	0	-0.959333	-0.795533	0.000002

13	6	0	-2.037234	0.006537	-0.000212
14	1	0	-1.077810	-1.884610	0.000266
15	6	0	-3.332068	0.051653	0.000050
16	8	0	-4.485841	0.299596	0.000072

Zero-point correction= 0.120370 (Hartree/Particle)
Thermal correction to Energy= 0.128621
Thermal correction to Enthalpy= 0.129565
Thermal correction to Gibbs Free Energy= 0.086424
Sum of electronic and zero-point Energies= -421.606392
Sum of electronic and thermal Energies= -421.598140
Sum of electronic and thermal Enthalpies= -421.597196
Sum of electronic and thermal Free Energies= -421.640338

no imaginary vibrational frequency

TS3 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.864401	-0.524522	1.286497
2	6	0	-3.110390	-0.087460	0.165509
3	6	0	-3.787454	0.203318	-1.048811
4	6	0	-5.162114	0.067483	-1.126583
5	6	0	-5.889666	-0.364159	-0.005061
6	6	0	-5.241790	-0.661529	1.199091
7	1	0	-3.352062	-0.748674	2.218278
8	1	0	-3.231578	0.529385	-1.922100
9	1	0	-5.679049	0.289715	-2.054446
10	1	0	-6.968153	-0.471145	-0.075952
11	1	0	-5.813085	-0.995474	2.058945
12	6	0	-1.699209	0.030314	0.318247
13	6	0	-0.776515	0.573846	-0.587315
14	1	0	-1.306363	-0.266565	1.291702
15	1	0	-1.032585	0.696795	-1.639734
16	6	0	0.683577	0.664546	-0.252442
17	8	0	0.866215	1.849400	0.188020
18	7	0	1.592044	-0.283872	-0.410689
19	6	0	3.001935	-0.246467	-0.158990
20	6	0	3.716034	-1.412061	-0.458925
21	6	0	3.647047	0.882589	0.357299
22	6	0	5.090497	-1.450323	-0.242281
23	1	0	3.203796	-2.284003	-0.860830
24	6	0	5.024993	0.825432	0.566436

25	1	0	3.091320	1.781610	0.588564
26	6	0	5.748744	-0.330879	0.271004
27	1	0	5.643932	-2.354405	-0.475700
28	1	0	5.532825	1.697847	0.965834
29	1	0	6.820545	-0.360344	0.439973
30	1	0	1.252256	-1.163612	-0.782845
31	1	0	-0.523554	1.820004	-0.083069

Zero-point correction=	0.249765 (Hartree/Particle)
Thermal correction to Energy=	0.263965
Thermal correction to Enthalpy=	0.264909
Thermal correction to Gibbs Free Energy=	0.206164
Sum of electronic and zero-point Energies=	-709.448987
Sum of electronic and thermal Energies=	-709.434787
Sum of electronic and thermal Enthalpies=	-709.433843
Sum of electronic and thermal Free Energies=	-709.492589

one imaginary vibrational frequency, -1612.22

MH-3 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.058038	-1.231128	-0.154339
2	6	0	-3.150389	-0.154231	0.117237
3	6	0	-3.635165	1.192940	0.050140
4	6	0	-4.954015	1.436545	-0.268638
5	6	0	-5.821776	0.357698	-0.531856
6	6	0	-5.376472	-0.972345	-0.475256
7	1	0	-3.690869	-2.252168	-0.104311
8	1	0	-2.963893	2.020569	0.253420
9	1	0	-5.327798	2.453769	-0.320040
10	1	0	-6.858494	0.561800	-0.784933
11	1	0	-6.063326	-1.786131	-0.682081
12	6	0	-1.834926	-0.481282	0.434748
13	6	0	-0.715304	0.415193	0.765567
14	1	0	-1.559093	-1.536659	0.457740
15	1	0	-0.805746	1.413530	0.325382
16	6	0	0.640316	-0.287770	0.466997
17	8	0	0.682713	-1.505775	0.387738
18	7	0	1.685103	0.570835	0.358605
19	6	0	3.045993	0.285127	0.061930
20	6	0	3.900033	1.388847	-0.083708
21	6	0	3.542314	-1.018762	-0.077809

22	6	0	5.248538	1.192443	-0.361204
23	1	0	3.509649	2.399160	0.023856
24	6	0	4.896447	-1.196227	-0.358204
25	1	0	2.882648	-1.867865	0.031864
26	6	0	5.753113	-0.102922	-0.500847
27	1	0	5.903605	2.051491	-0.468784
28	1	0	5.282552	-2.205480	-0.465196
29	1	0	6.804955	-0.257756	-0.719935
30	1	0	1.480452	1.556565	0.468394
31	1	0	-0.736075	0.554783	1.863928

Zero-point correction=	0.254091 (Hartree/Particle)
Thermal correction to Energy=	0.268633
Thermal correction to Enthalpy=	0.269577
Thermal correction to Gibbs Free Energy=	0.209897
Sum of electronic and zero-point Energies=	-709.493130
Sum of electronic and thermal Energies=	-709.478588
Sum of electronic and thermal Enthalpies=	-709.477644
Sum of electronic and thermal Free Energies=	-709.537323

no imaginary vibrational frequency

INC-2 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.902452	0.425890	-1.216509
2	6	0	2.307407	0.971974	-0.057975
3	6	0	2.510977	0.313815	1.179746
4	6	0	3.271444	-0.849214	1.244491
5	6	0	3.834527	-1.386606	0.081531
6	6	0	3.653353	-0.743459	-1.147557
7	1	0	2.775424	0.933290	-2.169589
8	1	0	2.107729	0.738066	2.094772
9	1	0	3.433643	-1.335103	2.201847
10	1	0	4.426992	-2.294895	0.136115
11	1	0	4.103911	-1.151219	-2.047177
12	6	0	1.517345	2.205117	-0.184269
13	6	0	0.746741	2.780369	0.762999
14	1	0	1.542609	2.667525	-1.170711
15	1	0	0.689614	2.412264	1.784939
16	6	0	0.138272	-0.954488	-0.196227
17	8	0	0.666869	-1.966330	-0.360290
18	7	0	-0.653390	0.024642	-0.019458

19	6	0	-2.113394	-0.103851	-0.022394
20	6	0	-2.844000	1.015694	-0.411516
21	6	0	-2.713149	-1.300344	0.361137
22	6	0	-4.236207	0.924926	-0.411217
23	1	0	-2.345994	1.932854	-0.711364
24	6	0	-4.106091	-1.373306	0.341560
25	1	0	-2.122070	-2.154143	0.680737
26	6	0	-4.865543	-0.265315	-0.040865
27	1	0	-4.824913	1.787533	-0.706472
28	1	0	-4.593849	-2.296633	0.636801
29	1	0	-5.948891	-0.328819	-0.047128
30	1	0	-0.236468	0.981711	0.083775
31	1	0	0.206236	3.698488	0.554377

Zero-point correction= 0.250856 (Hartree/Particle)
Thermal correction to Energy= 0.266534
Thermal correction to Enthalpy= 0.267479
Thermal correction to Gibbs Free Energy= 0.204851
Sum of electronic and zero-point Energies= -709.465297
Sum of electronic and thermal Energies= -709.449619
Sum of electronic and thermal Enthalpies= -709.448674
Sum of electronic and thermal Free Energies= -709.511302

no imaginary vibrational frequency

product ion e (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.409877	-0.000146	-0.067028
2	8	0	-3.176001	0.001017	-0.916420
3	7	0	-1.512922	-0.001246	0.833320
4	6	0	-0.087268	-0.000550	0.396341
5	6	0	0.540743	-1.229645	0.208713
6	6	0	0.539912	1.229138	0.209827
7	6	0	1.882734	-1.214913	-0.172522
8	1	0	0.010104	-2.163742	0.363743
9	6	0	1.881908	1.215669	-0.171443
10	1	0	0.008687	2.162752	0.365757
11	6	0	2.546637	0.000684	-0.361920
12	1	0	2.404765	-2.154382	-0.321675
13	1	0	2.403328	2.155605	-0.319789
14	1	0	3.589853	0.001184	-0.661687
15	1	0	-1.787008	-0.002251	1.819963

Zero-point correction=	0.115606 (Hartree/Particle)
Thermal correction to Energy=	0.123106
Thermal correction to Enthalpy=	0.124050
Thermal correction to Gibbs Free Energy=	0.082379
Sum of electronic and zero-point Energies=	-399.920855
Sum of electronic and thermal Energies=	-399.913356
Sum of electronic and thermal Enthalpies=	-399.912412
Sum of electronic and thermal Free Energies=	-399.954082

no imaginary vibrational frequency

styrene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.406504	-1.281400	0.000006
2	6	0	-0.515181	-0.220540	-0.000171
3	6	0	-0.008915	1.092408	-0.000249
4	6	0	1.362147	1.329628	-0.000081
5	6	0	2.265308	0.261889	0.000147
6	6	0	1.780914	-1.046109	0.000179
7	1	0	0.035070	-2.303878	0.000031
8	1	0	-0.694157	1.935175	-0.000496
9	1	0	1.730280	2.352368	-0.000154
10	1	0	3.335430	0.450578	0.000269
11	1	0	2.472125	-1.884876	0.000331
12	6	0	-1.954717	-0.529332	-0.000285
13	6	0	-2.977325	0.335006	0.000389
14	1	0	-2.186288	-1.594703	-0.000970
15	1	0	-2.840501	1.413054	0.001172
16	1	0	-4.004369	-0.017009	0.000197

Zero-point correction=	0.133736 (Hartree/Particle)
Thermal correction to Energy=	0.140506
Thermal correction to Enthalpy=	0.141451
Thermal correction to Gibbs Free Energy=	0.102259
Sum of electronic and zero-point Energies=	-309.514523
Sum of electronic and thermal Energies=	-309.507753
Sum of electronic and thermal Enthalpies=	-309.506808
Sum of electronic and thermal Free Energies=	-309.546000

no imaginary vibrational frequency

TS4 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.663010	-0.846156	-0.977390
2	6	0	-2.736044	-0.785887	0.087820
3	6	0	-3.057668	-0.014187	1.229169
4	6	0	-4.258115	0.677895	1.289994
5	6	0	-5.162204	0.612329	0.220180
6	6	0	-4.865169	-0.151255	-0.911915
7	1	0	-3.429830	-1.445803	-1.853621
8	1	0	-2.375459	0.023801	2.073122
9	1	0	-4.503088	1.262237	2.171418
10	1	0	-6.102909	1.152086	0.276538
11	1	0	-5.570759	-0.205659	-1.734806
12	6	0	-1.504179	-1.530422	-0.035008
13	6	0	-0.404531	-1.508798	0.791074
14	1	0	-1.429389	-2.144983	-0.933319
15	1	0	-0.446571	-1.039047	1.772665
16	6	0	0.724097	1.522139	-0.786238
17	8	0	0.237255	2.484715	-1.200178
18	7	0	1.161142	0.444506	-0.323214
19	6	0	2.585308	0.164310	-0.117048
20	6	0	3.112385	-0.988449	-0.694818
21	6	0	3.350671	1.028775	0.663493
22	6	0	4.460074	-1.279319	-0.479100
23	1	0	2.493387	-1.633829	-1.309987
24	6	0	4.699150	0.726892	0.857890
25	1	0	2.906384	1.909061	1.118786
26	6	0	5.251197	-0.423813	0.291261
27	1	0	4.890250	-2.172311	-0.921284
28	1	0	5.312683	1.390572	1.458749
29	1	0	6.299659	-0.654897	0.450613
30	1	0	0.378817	-0.379676	0.050653
31	1	0	0.359012	-2.275135	0.668222

Zero-point correction=	0.246264 (Hartree/Particle)
Thermal correction to Energy=	0.261543
Thermal correction to Enthalpy=	0.262487
Thermal correction to Gibbs Free Energy=	0.198152
Sum of electronic and zero-point Energies=	-709.466267
Sum of electronic and thermal Energies=	-709.450989
Sum of electronic and thermal Enthalpies=	-709.450044
Sum of electronic and thermal Free Energies=	-709.514379

one imaginary vibrational frequency, -510.454

product ion f (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.509525	-1.313478	-0.000161
2	6	0	-0.452239	-0.246399	-0.000389
3	6	0	0.014679	1.110728	-0.000447
4	6	0	1.367884	1.372290	-0.000003
5	6	0	2.286634	0.303647	0.000316
6	6	0	1.861093	-1.036011	0.000229
7	1	0	0.156931	-2.341149	-0.000236
8	1	0	-0.695915	1.929554	-0.000828
9	1	0	1.729934	2.394934	0.000009
10	1	0	3.351163	0.522027	0.000591
11	1	0	2.590290	-1.839087	0.000447
12	6	0	-1.802062	-0.581065	-0.000393
13	6	0	-2.975118	0.305614	0.000308
14	1	0	-2.031272	-1.647931	-0.000685
15	1	0	-2.755546	1.372722	-0.003800
16	1	0	-3.600399	0.061500	0.874082
17	1	0	-3.607556	0.055482	-0.866332

Zero-point correction= 0.145676 (Hartree/Particle)
Thermal correction to Energy= 0.152845
Thermal correction to Enthalpy= 0.153789
Thermal correction to Gibbs Free Energy= 0.114346
Sum of electronic and zero-point Energies= -309.850731
Sum of electronic and thermal Energies= -309.843562
Sum of electronic and thermal Enthalpies= -309.842618
Sum of electronic and thermal Free Energies= -309.882062

no imaginary vibrational frequency

phenyl isocyanate

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.539194	-0.073949	-0.000168
2	8	0	3.656583	0.301064	-0.001628
3	7	0	1.448479	-0.595671	0.002039

4	6	0	0.091865	-0.255850	0.000603
5	6	0	-0.849241	-1.292114	0.000057
6	6	0	-0.336041	1.080110	0.000882
7	6	0	-2.210182	-0.991280	-0.000737
8	1	0	-0.500899	-2.319831	0.000208
9	6	0	-1.698980	1.367962	0.000067
10	1	0	0.398956	1.880209	0.001725
11	6	0	-2.641187	0.336633	-0.000813
12	1	0	-2.935606	-1.800058	-0.001287
13	1	0	-2.024481	2.404638	0.000179
14	1	0	-3.702556	0.567148	-0.001419

Zero-point correction=	0.104075 (Hartree/Particle)
Thermal correction to Energy=	0.111175
Thermal correction to Enthalpy=	0.112119
Thermal correction to Gibbs Free Energy=	0.071683
Sum of electronic and zero-point Energies=	-399.628441
Sum of electronic and thermal Energies=	-399.621341
Sum of electronic and thermal Enthalpies=	-399.620396
Sum of electronic and thermal Free Energies=	-399.660832

no imaginary vibrational frequency

TS5 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.185685	-1.181037	-0.059451
2	6	0	3.222913	-0.159555	0.054039
3	6	0	3.634427	1.186677	0.028005
4	6	0	4.979094	1.498417	-0.123097
5	6	0	5.929722	0.475073	-0.242559
6	6	0	5.531690	-0.863167	-0.212837
7	1	0	3.872743	-2.221421	-0.032655
8	1	0	2.911222	1.993721	0.109986
9	1	0	5.292479	2.537123	-0.153488
10	1	0	6.979547	0.725895	-0.360094
11	1	0	6.266957	-1.655642	-0.307820
12	6	0	1.816963	-0.577468	0.211529
13	6	0	0.657645	0.246111	0.233942
14	1	0	1.587191	-1.623833	-0.005159
15	1	0	1.495698	-0.476629	1.359445
16	6	0	-0.680348	-0.396157	0.186311
17	8	0	-0.794457	-1.615397	0.131994

18	7	0	-1.699758	0.523070	0.187603
19	6	0	-3.076158	0.293129	0.045854
20	6	0	-3.907416	1.432066	0.013108
21	6	0	-3.629933	-0.999141	-0.060620
22	6	0	-5.278506	1.282341	-0.125256
23	1	0	-3.472735	2.426173	0.094956
24	6	0	-5.008176	-1.125549	-0.201497
25	1	0	-2.989151	-1.868501	-0.029720
26	6	0	-5.835014	0.001176	-0.234398
27	1	0	-5.916047	2.160247	-0.149426
28	1	0	-5.440737	-2.117679	-0.283401
29	1	0	-6.908770	-0.115401	-0.342704
30	1	0	-1.441888	1.500202	0.271085
31	1	0	0.761919	1.319938	0.381379

Zero-point correction= 0.250397 (Hartree/Particle)
Thermal correction to Energy= 0.264637
Thermal correction to Enthalpy= 0.265582
Thermal correction to Gibbs Free Energy= 0.207000
Sum of electronic and zero-point Energies= -709.452719
Sum of electronic and thermal Energies= -709.438478
Sum of electronic and thermal Enthalpies= -709.437534
Sum of electronic and thermal Free Energies= -709.496116

one imaginary vibrational frequency, -672.333

MH-4 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.492293	-1.104368	-0.308265
2	6	0	2.579862	-0.288862	0.437650
3	6	0	2.540538	1.121219	0.192278
4	6	0	3.387284	1.676261	-0.749349
5	6	0	4.272355	0.855725	-1.465380
6	6	0	4.324730	-0.533187	-1.247864
7	1	0	3.528874	-2.173871	-0.118192
8	1	0	1.833458	1.728038	0.746969
9	1	0	3.368440	2.745369	-0.933103
10	1	0	4.932415	1.301947	-2.204143
11	1	0	5.019678	-1.147066	-1.811052
12	6	0	2.113616	-0.821364	1.866321
13	6	0	1.138372	-1.068311	0.838480
14	1	0	2.731776	-1.630902	2.239865

15	1	0	1.901036	-0.013843	2.560280
16	6	0	-0.111735	-0.209779	0.786943
17	8	0	-0.150207	0.863000	1.379920
18	7	0	-1.117974	-0.773083	0.068851
19	6	0	-2.448473	-0.310560	-0.108446
20	6	0	-3.299110	-1.129698	-0.867319
21	6	0	-2.919216	0.896089	0.430276
22	6	0	-4.615476	-0.743518	-1.092834
23	1	0	-2.930271	-2.066814	-1.280238
24	6	0	-4.242883	1.265424	0.194927
25	1	0	-2.264167	1.523142	1.017918
26	6	0	-5.093441	0.457322	-0.561475
27	1	0	-5.267288	-1.381355	-1.681728
28	1	0	-4.609616	2.198567	0.611768
29	1	0	-6.121747	0.758680	-0.734962
30	1	0	-0.925888	-1.663046	-0.374708
31	1	0	1.118476	-2.045636	0.364347

Zero-point correction=	0.254874 (Hartree/Particle)
Thermal correction to Energy=	0.268982
Thermal correction to Enthalpy=	0.269926
Thermal correction to Gibbs Free Energy=	0.212416
Sum of electronic and zero-point Energies=	-709.477307
Sum of electronic and thermal Energies=	-709.463199
Sum of electronic and thermal Enthalpies=	-709.462255
Sum of electronic and thermal Free Energies=	-709.519765

no imaginary vibrational frequency

TS6 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.188157	-1.197597	0.078620
2	6	0	3.228330	-0.141257	0.133223
3	6	0	3.668139	1.213170	0.023285
4	6	0	5.009070	1.479955	-0.179255
5	6	0	5.936931	0.427901	-0.259629
6	6	0	5.524641	-0.905136	-0.129043
7	1	0	3.855817	-2.225683	0.189927
8	1	0	2.953464	2.027325	0.083627
9	1	0	5.344227	2.507050	-0.279870
10	1	0	6.987515	0.652170	-0.417317
11	1	0	6.250617	-1.709327	-0.186491

12	6	0	1.747564	-0.539554	0.155307
13	6	0	0.659589	0.282087	0.192054
14	1	0	1.560449	-1.609584	0.106544
15	1	0	2.533804	-0.282899	1.190836
16	6	0	-0.680001	-0.362073	0.098493
17	8	0	-0.791858	-1.581790	0.028578
18	7	0	-1.712112	0.540780	0.098920
19	6	0	-3.095695	0.292508	0.016626
20	6	0	-3.942762	1.416205	0.051082
21	6	0	-3.638390	-1.000626	-0.097611
22	6	0	-5.318719	1.251715	-0.029056
23	1	0	-3.518675	2.414503	0.139917
24	6	0	-5.021420	-1.143983	-0.176583
25	1	0	-2.985210	-1.860818	-0.122594
26	6	0	-5.865247	-0.031359	-0.143488
27	1	0	-5.965940	2.122798	-0.002423
28	1	0	-5.442286	-2.140905	-0.264995
29	1	0	-6.941276	-0.160409	-0.205832
30	1	0	-1.464426	1.520790	0.164052
31	1	0	0.750444	1.362120	0.279397

Zero-point correction=	0.249277 (Hartree/Particle)
Thermal correction to Energy=	0.263552
Thermal correction to Enthalpy=	0.264496
Thermal correction to Gibbs Free Energy=	0.206127
Sum of electronic and zero-point Energies=	-709.431751
Sum of electronic and thermal Energies=	-709.417477
Sum of electronic and thermal Enthalpies=	-709.416532
Sum of electronic and thermal Free Energies=	-709.474902

one imaginary vibrational frequency, -792.159

TS7 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.124094	-1.038419	-0.663324
2	6	0	3.137943	-0.183169	-0.127715
3	6	0	3.538153	0.937363	0.632503
4	6	0	4.886334	1.205455	0.827879
5	6	0	5.855146	0.356091	0.277833
6	6	0	5.471731	-0.767661	-0.463462
7	1	0	3.825498	-1.910054	-1.240347
8	1	0	2.788824	1.574114	1.096195

9	1	0	5.188504	2.061790	1.422492
10	1	0	6.908606	0.560856	0.443066
11	1	0	6.225139	-1.428807	-0.879619
12	6	0	1.721531	-0.473656	-0.357454
13	6	0	0.708882	0.505152	-0.418915
14	1	0	1.537191	-1.346834	-1.009633
15	1	0	0.882745	1.570003	-0.551828
16	6	0	-0.598053	-0.066859	-0.082937
17	8	0	-0.565912	-1.216227	0.438714
18	7	0	-1.711439	0.635776	-0.364139
19	6	0	-3.060814	0.288722	-0.156281
20	6	0	-4.015860	1.276760	-0.464441
21	6	0	-3.458908	-0.964887	0.344303
22	6	0	-5.362068	1.021530	-0.249178
23	1	0	-3.698794	2.239610	-0.859182
24	6	0	-4.813988	-1.197340	0.559334
25	1	0	-2.724079	-1.730438	0.550572
26	6	0	-5.765927	-0.216463	0.266471
27	1	0	-6.097827	1.784361	-0.482286
28	1	0	-5.129082	-2.160446	0.948035
29	1	0	-6.820194	-0.417351	0.428830
30	1	0	-1.567633	1.526458	-0.829696
31	1	0	0.979300	-1.139589	0.454962

Zero-point correction=	0.248928 (Hartree/Particle)
Thermal correction to Energy=	0.262789
Thermal correction to Enthalpy=	0.263734
Thermal correction to Gibbs Free Energy=	0.206464
Sum of electronic and zero-point Energies=	-709.442195
Sum of electronic and thermal Energies=	-709.428334
Sum of electronic and thermal Enthalpies=	-709.427390
Sum of electronic and thermal Free Energies=	-709.484660

one imaginary vibrational frequency, -1298.66

TS8 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.061754	0.611261	0.814013
2	6	0	3.165053	-0.618729	0.025322
3	6	0	4.402703	-1.004742	-0.528535
4	6	0	5.446546	-0.094274	-0.496856

5	6	0	5.309952	1.177467	0.120169
6	6	0	4.152705	1.527278	0.789728
7	1	0	2.574023	0.511791	1.791501
8	1	0	4.489046	-1.932775	-1.085077
9	1	0	6.382585	-0.340517	-0.989182
10	1	0	6.159972	1.853014	0.121316
11	1	0	4.107495	2.440278	1.375647
12	6	0	1.892090	-1.154726	-0.263860
13	6	0	0.876626	-0.171401	-0.365536
14	1	0	1.657382	-2.214241	-0.330587
15	1	0	1.717733	0.769496	0.403521
16	6	0	-0.532565	-0.612243	-0.083023
17	8	0	-0.725104	-1.728939	0.385656
18	7	0	-1.484370	0.321238	-0.377084
19	6	0	-2.882603	0.250841	-0.176229
20	6	0	-3.625810	1.397466	-0.503824
21	6	0	-3.527220	-0.892753	0.323097
22	6	0	-5.004650	1.404765	-0.331879
23	1	0	-3.122165	2.280699	-0.892397
24	6	0	-4.910415	-0.864613	0.491794
25	1	0	-2.953926	-1.775377	0.568079
26	6	0	-5.653786	0.272283	0.168889
27	1	0	-5.572162	2.293975	-0.588449
28	1	0	-5.410348	-1.747791	0.877864
29	1	0	-6.730988	0.276889	0.303053
30	1	0	-1.162467	1.193866	-0.778067
31	1	0	1.032957	0.606263	-1.122514

Zero-point correction=	0.248443 (Hartree/Particle)
Thermal correction to Energy=	0.262373
Thermal correction to Enthalpy=	0.263317
Thermal correction to Gibbs Free Energy=	0.205838
Sum of electronic and zero-point Energies=	-709.420334
Sum of electronic and thermal Energies=	-709.406404
Sum of electronic and thermal Enthalpies=	-709.405460
Sum of electronic and thermal Free Energies=	-709.462939

one imaginary vibrational frequency, -1592.14

MH-5 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.138425	-1.219565	0.000194

2	6	0	3.140966	-0.234761	0.000141
3	6	0	3.562242	1.204572	0.000070
4	6	0	5.025438	1.475780	-0.000247
5	6	0	5.940744	0.471120	-0.000220
6	6	0	5.486828	-0.880733	0.000037
7	1	0	3.849777	-2.266171	0.000317
8	1	0	3.115775	1.723725	0.865532
9	1	0	5.336823	2.516762	-0.000400
10	1	0	7.005360	0.679359	-0.000390
11	1	0	6.224860	-1.678786	0.000095
12	6	0	1.769030	-0.637982	0.000181
13	6	0	0.681636	0.178515	0.000030
14	1	0	1.563141	-1.706545	0.000278
15	1	0	3.115206	1.723916	-0.864943
16	6	0	-0.673201	-0.436396	0.000023
17	8	0	-0.831825	-1.650944	0.000125
18	7	0	-1.686001	0.498523	-0.000174
19	6	0	-3.073527	0.288429	-0.000087
20	6	0	-3.657491	-0.994001	-0.000284
21	6	0	-3.890096	1.437410	0.000163
22	6	0	-5.045231	-1.100531	-0.000220
23	1	0	-3.027866	-1.871906	-0.000469
24	6	0	-5.271157	1.309186	0.000222
25	1	0	-3.435245	2.425986	0.000322
26	6	0	-5.856845	0.037172	0.000033
27	1	0	-5.496919	-2.087808	-0.000379
28	1	0	-5.893510	2.198608	0.000419
29	1	0	-6.937702	-0.063442	0.000079
30	1	0	-1.407336	1.472242	-0.000320
31	1	0	0.777684	1.262665	-0.000144

Zero-point correction= 0.253507 (Hartree/Particle)
Thermal correction to Energy= 0.268171
Thermal correction to Enthalpy= 0.269115
Thermal correction to Gibbs Free Energy= 0.209762
Sum of electronic and zero-point Energies= -709.479870
Sum of electronic and thermal Energies= -709.465206
Sum of electronic and thermal Enthalpies= -709.464262
Sum of electronic and thermal Free Energies= -709.523615

no imaginary vibrational frequency

TS9 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.148393	-1.149907	-0.427992
2	6	0	3.176898	-0.270025	0.188682
3	6	0	3.639227	1.067675	0.545575
4	6	0	4.967915	1.459856	0.306419
5	6	0	5.848262	0.576644	-0.300547
6	6	0	5.439834	-0.731531	-0.654216
7	1	0	3.822716	-2.142820	-0.722147
8	1	0	3.602326	-0.148628	1.339893
9	1	0	5.287319	2.453935	0.600787
10	1	0	6.872121	0.884493	-0.490851
11	1	0	6.151049	-1.406358	-1.120235
12	6	0	1.753519	-0.667541	0.222317
13	6	0	0.706764	0.161594	0.101298
14	1	0	1.540702	-1.730207	0.319836
15	1	0	2.937423	1.730679	1.042916
16	6	0	-0.673809	-0.431248	0.139517
17	8	0	-0.833347	-1.632303	0.325247
18	7	0	-1.667142	0.489131	-0.046738
19	6	0	-3.068952	0.291420	-0.061573
20	6	0	-3.669106	-0.960645	0.141491
21	6	0	-3.864126	1.425688	-0.291027
22	6	0	-5.060071	-1.054482	0.110610
23	1	0	-3.055127	-1.832141	0.317652
24	6	0	-5.249680	1.312536	-0.319057
25	1	0	-3.395745	2.395702	-0.448540
26	6	0	-5.855153	0.069552	-0.117767
27	1	0	-5.523877	-2.023794	0.268052
28	1	0	-5.855484	2.195695	-0.498155
29	1	0	-6.936854	-0.020253	-0.139053
30	1	0	-1.379595	1.446878	-0.203158
31	1	0	0.830302	1.233800	-0.044200

Zero-point correction= 0.250285 (Hartree/Particle)
Thermal correction to Energy= 0.264564
Thermal correction to Enthalpy= 0.265508
Thermal correction to Gibbs Free Energy= 0.206840
Sum of electronic and zero-point Energies= -709.441812
Sum of electronic and thermal Energies= -709.427533
Sum of electronic and thermal Enthalpies= -709.426589
Sum of electronic and thermal Free Energies= -709.485257

one imaginary vibrational frequency, -849.003

TS10 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.368798	1.222003	0.049542
2	6	0	2.511570	-0.202205	0.246085
3	6	0	3.840173	-0.768888	0.109828
4	6	0	4.872658	-0.006773	-0.394010
5	6	0	4.658537	1.349278	-0.701294
6	6	0	3.412809	1.956481	-0.483222
7	1	0	1.415107	1.685862	0.276189
8	1	0	3.991037	-1.820532	0.339812
9	1	0	5.853448	-0.447511	-0.540546
10	1	0	5.479039	1.940984	-1.096822
11	1	0	3.282819	3.013878	-0.690467
12	6	0	1.459321	-0.998110	1.014549
13	6	0	0.883904	-1.983524	-0.008423
14	1	0	1.691778	-1.279531	2.043763
15	1	0	1.983061	-0.736521	-0.770959
16	6	0	-0.300295	-1.264059	0.116117
17	8	0	0.158430	-0.297653	0.970634
18	7	0	-1.536663	-1.301541	-0.373811
19	6	0	-2.634355	-0.407644	-0.200135
20	6	0	-3.734881	-0.598175	-1.045427
21	6	0	-2.649600	0.601396	0.770637
22	6	0	-4.850381	0.225412	-0.924598
23	1	0	-3.718455	-1.384852	-1.796498
24	6	0	-3.774170	1.419670	0.874907
25	1	0	-1.812624	0.742096	1.441828
26	6	0	-4.873767	1.239889	0.034449
27	1	0	-5.700158	0.072110	-1.582448
28	1	0	-3.788574	2.200364	1.629428
29	1	0	-5.743773	1.881900	0.128666
30	1	0	-1.715058	-2.090114	-0.986264
31	1	0	1.129626	-2.994617	-0.298112

Zero-point correction=	0.249566 (Hartree/Particle)
Thermal correction to Energy=	0.263108
Thermal correction to Enthalpy=	0.264053
Thermal correction to Gibbs Free Energy=	0.207267
Sum of electronic and zero-point Energies=	-709.392679
Sum of electronic and thermal Energies=	-709.379137

Sum of electronic and thermal Enthalpies= -709.378193
Sum of electronic and thermal Free Energies= -709.434978

one imaginary vibrational frequency, -804.799

product ion g (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.208774	-0.236804	-0.051523
2	6	0	1.925394	1.198613	-0.179495
3	6	0	0.690521	1.690216	-0.019436
4	6	0	-0.473616	0.808465	0.358092
5	6	0	-0.230166	-0.654593	0.141490
6	7	0	1.032559	-1.072971	0.105298
7	6	0	-1.850187	1.277763	-0.001107
8	6	0	-2.857310	0.395138	-0.191301
9	6	0	-2.591055	-1.016346	-0.139434
10	6	0	-1.328681	-1.537008	0.029482
11	8	0	3.285525	-0.773887	-0.095430
12	1	0	1.240437	-2.070342	0.058090
13	1	0	2.778403	1.826412	-0.412298
14	1	0	0.496441	2.756391	-0.098853
15	1	0	-0.517600	0.864060	1.475310
16	1	0	-2.022716	2.350322	-0.006609
17	1	0	-3.868254	0.735634	-0.387723
18	1	0	-3.421676	-1.704285	-0.273339
19	1	0	-1.159191	-2.608956	-0.008841

Zero-point correction= 0.151748 (Hartree/Particle)
Thermal correction to Energy= 0.159938
Thermal correction to Enthalpy= 0.160882
Thermal correction to Gibbs Free Energy= 0.118564
Sum of electronic and zero-point Energies= -477.323269
Sum of electronic and thermal Energies= -477.315080
Sum of electronic and thermal Enthalpies= -477.314135
Sum of electronic and thermal Free Energies= -477.356454

no imaginary vibrational frequency

benzene

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

1	6	0	-0.580129	1.270257	0.000001
2	6	0	-1.390460	0.132760	-0.000175
3	6	0	-0.810207	-1.137542	0.000108
4	6	0	0.580184	-1.270234	-0.000034
5	6	0	1.390456	-0.132816	-0.000105
6	6	0	0.810158	1.137574	0.000125
7	1	0	-1.031694	2.259134	0.000031
8	1	0	-2.472583	0.236321	0.000042
9	1	0	-1.440545	-2.023209	0.000272
10	1	0	1.031613	-2.259173	0.000115
11	1	0	2.472593	-0.236225	-0.000166
12	1	0	1.440609	2.023161	0.000182

Zero-point correction= 0.100738 (Hartree/Particle)
Thermal correction to Energy= 0.105124
Thermal correction to Enthalpy= 0.106068
Thermal correction to Gibbs Free Energy= 0.073276
Sum of electronic and zero-point Energies= -232.147907
Sum of electronic and thermal Energies= -232.143520
Sum of electronic and thermal Enthalpies= -232.142576
Sum of electronic and thermal Free Energies= -232.175368

no imaginary vibrational frequency

TS11 (Compound **1**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.328929	-1.517485	0.590705
2	6	0	-2.027753	-0.133661	0.472524
3	6	0	-3.016773	0.742683	-0.049830
4	6	0	-4.253541	0.248041	-0.430551
5	6	0	-4.533269	-1.120212	-0.296416
6	6	0	-3.571997	-2.001701	0.215284
7	1	0	-1.577563	-2.192759	0.991127
8	1	0	-2.811933	1.803369	-0.155296
9	1	0	-5.008150	0.919511	-0.827130
10	1	0	-5.507809	-1.499173	-0.590015
11	1	0	-3.800774	-3.057364	0.318907
12	6	0	-0.745167	0.315972	0.897117
13	6	0	-0.333806	1.764751	1.038407
14	1	0	-0.111016	-0.417754	1.386402
15	1	0	-1.150996	2.480764	1.142334

16	6	0	0.372310	1.921994	-0.297661
17	8	0	0.469278	2.854083	-1.032299
18	7	0	0.708381	0.536065	-0.684409
19	6	0	1.984766	-0.042175	-0.373528
20	6	0	2.318472	-1.257541	-0.986712
21	6	0	2.857653	0.556438	0.543607
22	6	0	3.528174	-1.872674	-0.676819
23	1	0	1.637666	-1.714226	-1.700845
24	6	0	4.064533	-0.072580	0.846157
25	1	0	2.629958	1.520677	0.988648
26	6	0	4.401885	-1.285880	0.242763
27	1	0	3.789667	-2.809821	-1.158103
28	1	0	4.748578	0.398068	1.545309
29	1	0	5.346031	-1.766087	0.478940
30	1	0	0.450930	0.365681	-1.660105
31	1	0	0.353177	1.908175	1.878789

Zero-point correction= 0.253837 (Hartree/Particle)
Thermal correction to Energy= 0.267594
Thermal correction to Enthalpy= 0.268538
Thermal correction to Gibbs Free Energy= 0.210799
Sum of electronic and zero-point Energies= -709.470652
Sum of electronic and thermal Energies= -709.456896
Sum of electronic and thermal Enthalpies= -709.455952
Sum of electronic and thermal Free Energies= -709.513690

one imaginary vibrational frequency, -192.526