Electronic Supplementary Material (ESI) for ChemComm.

Gas-Phase Synthesis and Reactivity of Cu^+/Benzyne Complexes

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Contents

Mass spectrometry

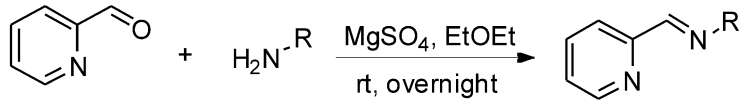
The general ESI experimental conditions were described as follows: The experiments were performed on a Varian 500-MS ion trap mass spectrometer equipped with an ESI interface. Nitrogen gas was used as the nebulizing gas and the drying gas. A solution containing the analytes (10 μg mL^{-1}) was infused to the mass spectrometer with a syringe pump at a flow rate of 10 μL min^{-1}. ESI in positive ion mode was performed using the following settings: spray chamber temperature 50 °C, nebulizer gas pressure 35 psi, drying gas pressure 12 psi, drying gas temperature 350 °C, needle voltage 5000 V, spray shield voltage 600 V, capillary voltage 80 V, RF loading 85%, scan mass range 50-800 *m/z*. The CID mass spectra were obtained with helium as the collision gas after isolation of the desired precursor ion. All the CID mass spectra presented in this study are single isotope mass spectra with the ^{63}Cu.

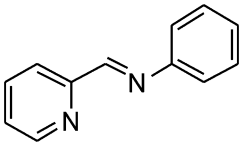
Materials

The benzoic acids, 1,10-phenanthroline, 2,2-bipyridine, 2-(aminomethyl)pyridine, *N,N,N′,N′*-tetramethylethylenediamine were all commercial products, and were used without further treatment. $Cu(CH_3COO)_2$ and CuI were used as the source of Cu^{2+} and Cu^{+}, respectively. *N*-(pyridin-2-ylmethyl)aniline, *N*-benzyl-*N,N′,N′*-trimethylethylenediamine, *N*-(2-methylphenyl)-*N,N′,N′*-trimethylethylenediamine, *N*-(pyridin-2-ylmethylene)methanamine, 1-phenyl-*N*-(pyridin-2-ylmethylene)methanamine, and 2-methyl-*N*-(pyridin-2-ylmethylene)aniline were synthesized and purified following modified reported procedures. Their structures were confirmed via ^{1}H and ^{13}C NMR spectroscopy and mass spectrometry.

1. The *N*-(pyridin-2-ylmethylene)aniline, *N*-(pyridin-2-ylmethylene)methanamine, 1-phenyl-*N*-(pyridin-2-ylmethylene)methanamine, and 2-methyl-*N*-(pyridin-2-ylmethylene)aniline were synthesized with the corresponding picolinaldehyde and amines. The compounds after synthesis were

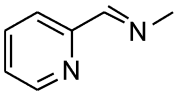
purified and the structures were confirmed by ^{1}H and ^{13}C NMR spectroscopy and mass spectrometry.





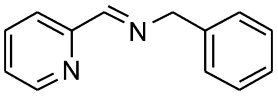
N-(pyridin-2-ylmethylene)aniline:

^{1}H NMR (500MHz, $CDCl_3$): δ (ppm) = 7.14–8.60 (m, 10H); ^{13}C NMR (125MHz, $CDCl_3$): δ (ppm)=160.7, 154.6, 151.1, 149.8, 136.8, 129.4, 126.8, 125.2, 122.0, 121.2.



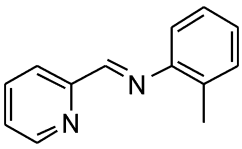
N-(pyridin-2-ylmethylene)methanamine:

^{1}H NMR (500MHz, $CDCl_3$): δ (ppm) = 7.22–8.57 (m, 5H), 3.50 (s, 3H); ^{13}C NMR (125MHz, $CDCl_3$): δ (ppm)= 163.6, 154.7, 149.6, 136.8, 124.9, 121.2, 48.3.



1-phenyl-*N*-(pyridin-2-ylmethylene)methanamine:

^{1}H NMR (500MHz, $CDCl_3$): δ (ppm) = 7.29–8.68 (m, 10H), 4.91 (s, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ (ppm)= 163.0, 154.7, 149.6, 138.9, 136.8, 128.8, 128.4, 127.4, 125.1, 121.6, 65.1.

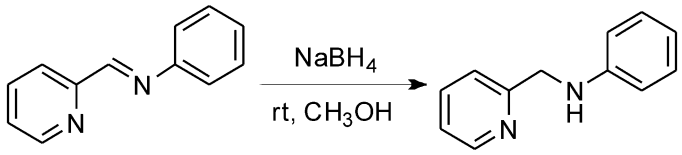


2-methyl-*N*-(pyridin-2-ylmethylene)aniline:

^{1}H NMR (500MHz, $CDCl_3$): δ (ppm) = 7.04–8.74 (m, 9H), 2.43 (s, 3H); ^{13}C NMR (125MHz, $CDCl_3$): δ (ppm)= 160.1, 155.1, 150.3, 149.8, 136.8, 132.5, 130.6, 127.0, 126.6, 125.3, 121.9, 117.8, 18.1.

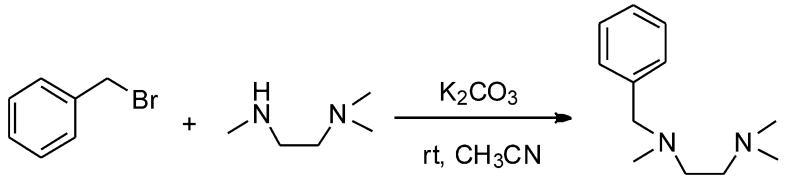
2. The *N*-(pyridin-2-ylmethyl)aniline was synthesized by reducing the

N-(pyridin-2-ylmethylene)aniline using $NaBH_4$. The compounds after synthesis were purified and the structures were confirmed by ^{1}H and ^{13}C NMR spectroscopy and mass spectrometry.



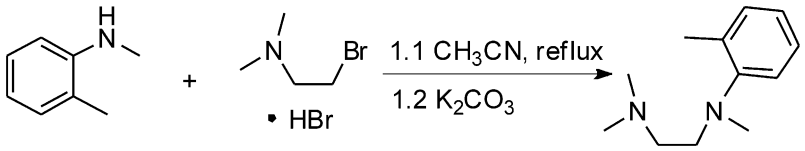
N-(pyridin-2-ylmethyl)aniline: ^{1}H NMR (500MHz, $CDCl_3$): δ (ppm) = 6.68–8.60 (m, 9H), 4.48 (s, 2H), 4.15 (s, 1H); ^{13}C NMR (125MHz, $CDCl_3$): δ (ppm)= 158.7, 149.3, 148.0, 136.8, 129.4, 122.2, 121.7, 117.7, 113.2, 49.4.

3. The *N*-benzyl-*N,N′,N′*-trimethylethylenediamine was synthesized with the benzyl bromide and *N,N,N′*-trimethylethylenediamine. The compounds after synthesis were purified and the structures were confirmed by ^{1}H and ^{13}C NMR spectroscopy and mass spectrometry.



N-benzyl-*N,N′,N′*-trimethylethylenediamine: ^{1}H NMR (500MHz, $CDCl_3$): δ (ppm) = 7.15–7.25 (m, 5H), 3.45 (s, 2H), 2.41-2.44 (m, 2H), 2.35-2.38 (m, 2H), 2.17 (s, 3H), 2.14 (s, 6); ^{13}C NMR (125MHz, $CDCl_3$): δ (ppm)= 139.2, 129.4, 128.4, 127.2, 63.2, 57.7, 55.4, 46.1, 42.8.

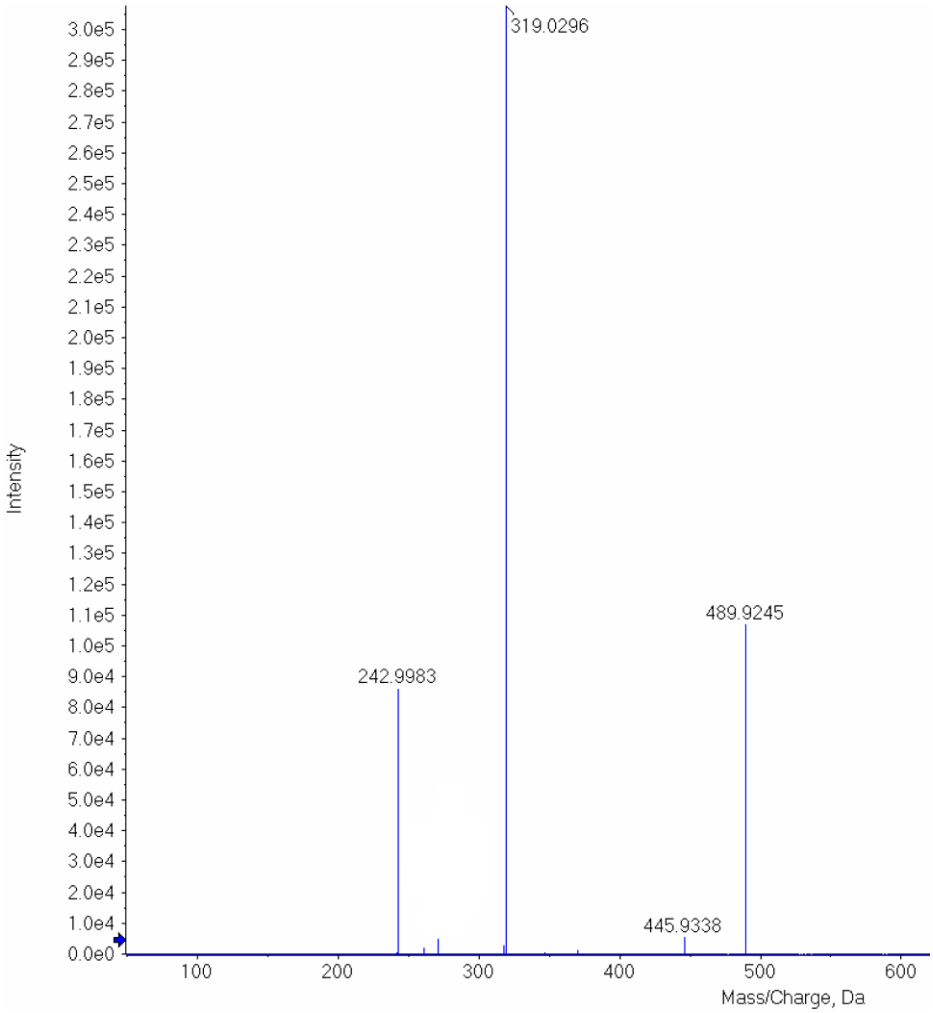
4. The *N*-(2-methylphenyl)-*N,N′,N′*-trimethylethylenediamine was synthesized with the (2-bromoethyl)dimethylamine hydrobromide and *N,2*-dimethylaniline. The compounds after synthesis were purified and the structures were confirmed by ^{1}H and ^{13}C NMR spectroscopy and mass spectrometry.



N-(2-methylphenyl)-*N,N′,N′*-trimethylethylenediamine: ^{1}H NMR (500MHz, $CDCl_3$): δ (ppm) = 6.89–7.19 (m, 4H), 3.03 (t, 2H), 2.61 (s, 3H), 2.51 (t, 2H), 2.26 (s, 6H), 2.23 (s, 3H); ^{13}C NMR (125MHz, $CDCl_3$): δ (ppm)= 151.9, 133.5, 131.4, 126.7, 123.4, 120.2, 56.9, 53.7, 45.3, 42.8, 18.5.

Computational methods

All the calculations were performed with the Gaussian 09 software package. Molecular geometries of the complexes were optimized at the B3LYP level of density functional theory. The SDD basis set with Stuttgart potentials was used to describe Cu and I. The 6-31+G(d,p) basis set was used for C, H, O, and N. Frequency calculations at the same level of theory have also been performed to identify all stationary points as minima (no imaginary frequency) or transition states (one imaginary frequency). The relative free energies at 298.15 K were used to generate the energy profile. The minima connected by a given transition structure were confirmed by intrinsic reaction coordinate (IRC) calculations.



Ion	Elemental composition	Measured mass	Calculated mass	Error (ppm)
A1	$C_{19}H_{12}CuIN_2O_2^+$	489.9245	489.9234	2.2
A2	$C_{18}H_{12}CuIN_2^+$	445.9338	445.9336	0.4
A3	$C_{18}H_{12}CuN_2^+$	319.0296	319.0291	1.6
A4	$C_{12}H_8CuN_2^+$	242.9983	242.9978	2.1

Figure S1. CID mass spectrum of the [1,10-phenanthroline ··Cu ··2-iodobenzoic acid]$^+$ ion (**A1**, *m/z* 489) acquired on the Q-TOF mass spectrometer with the exact mass measured for each ion.

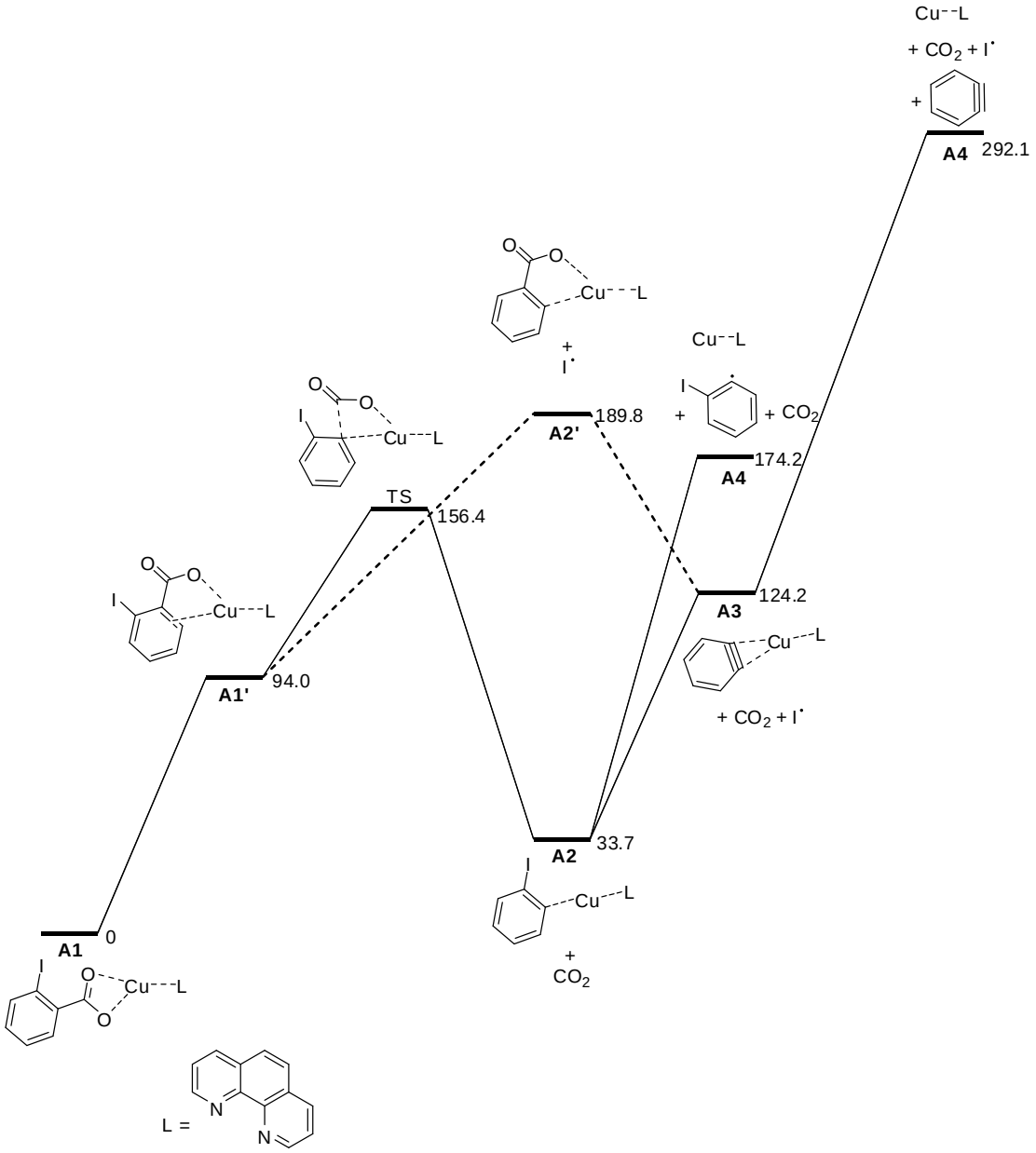


Figure S2. Energy profile calculated for the copper-mediated fragmentation reaction of the ternary complex consisting of 2-iodobenzoic acid, Cu^{2+}, and 1,10-phenanthroline. The energy barrier for radical loss is not included. The relative free energies in the gas phase are given in kJ mol^{-1}.

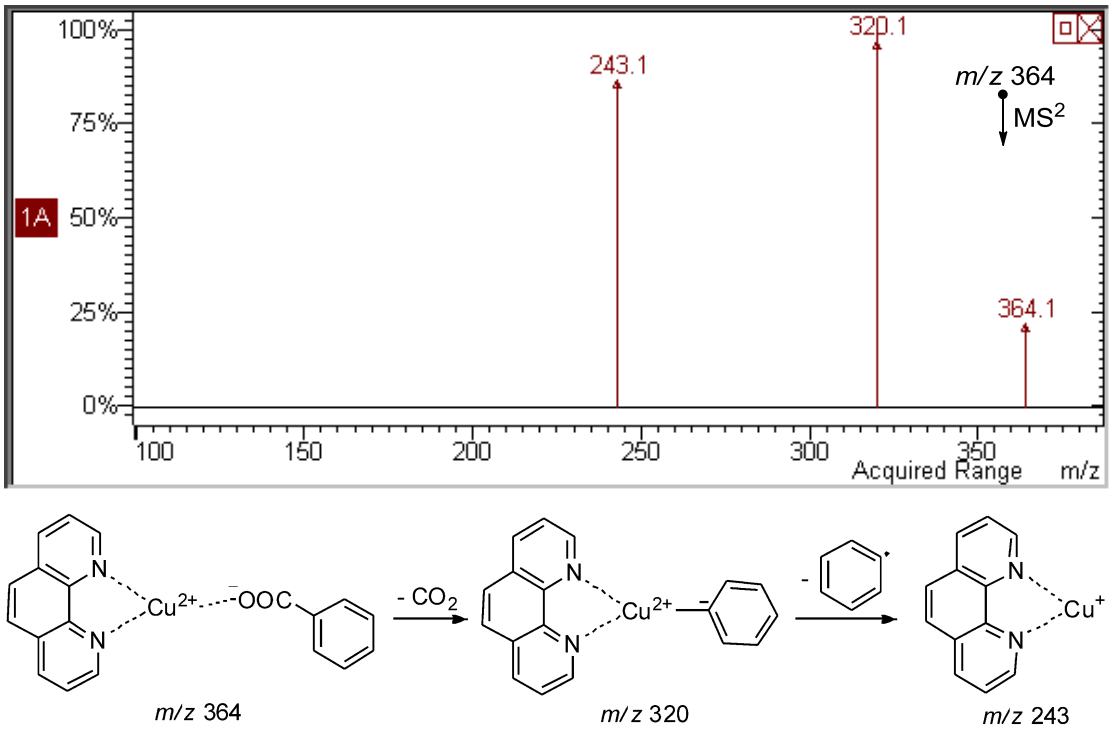


Figure S3. CID mass spectrum of the [1,10-phenanthroline ··Cu ··benzoic acid]$^{+}$ ion (*m/z* 364).

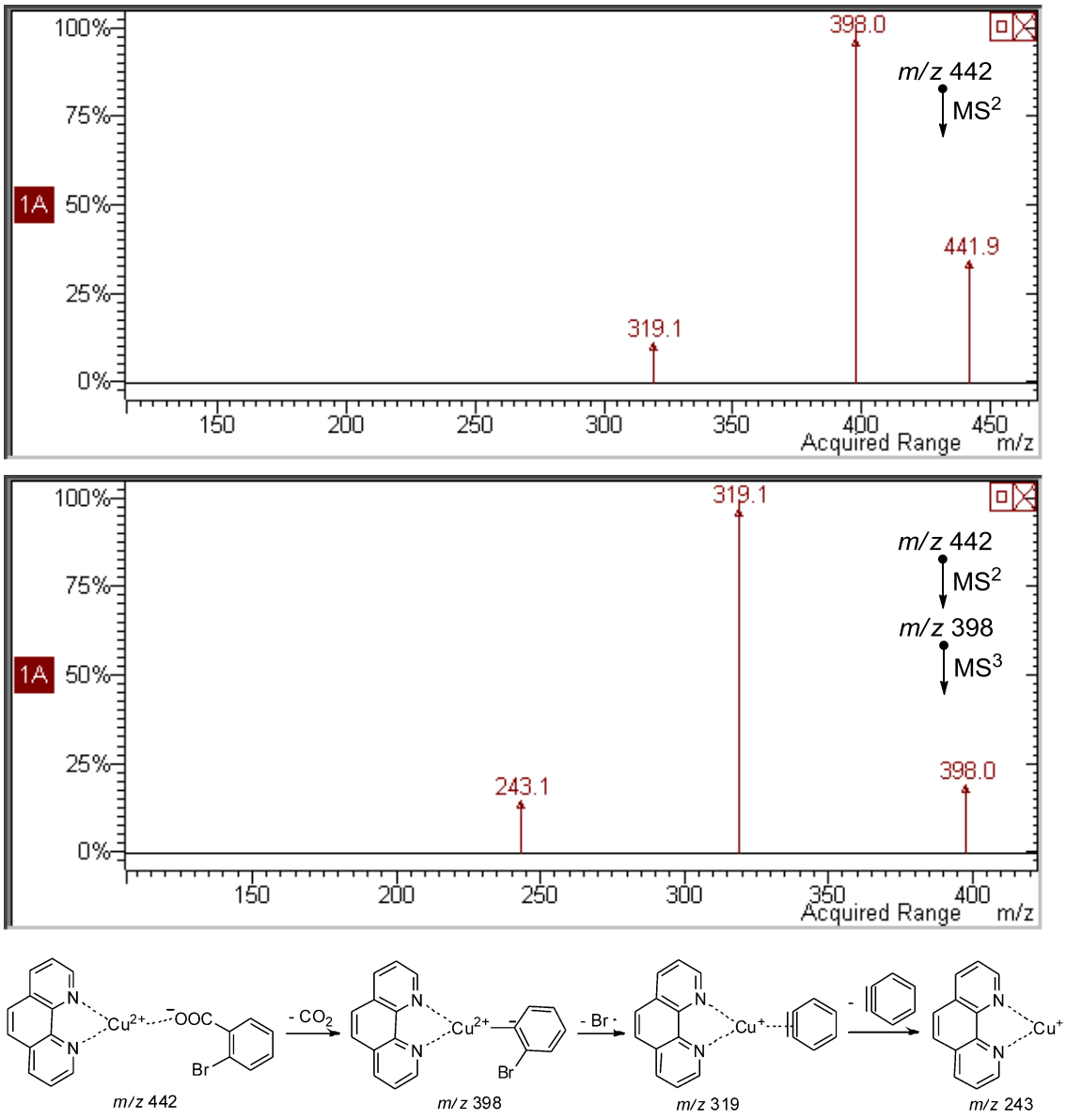


Figure S4. CID mass spectra of the [1,10-phenanthroline ··Cu ··2-bromobenzoic acid]$^{+}$ ion (*m/z* 442).

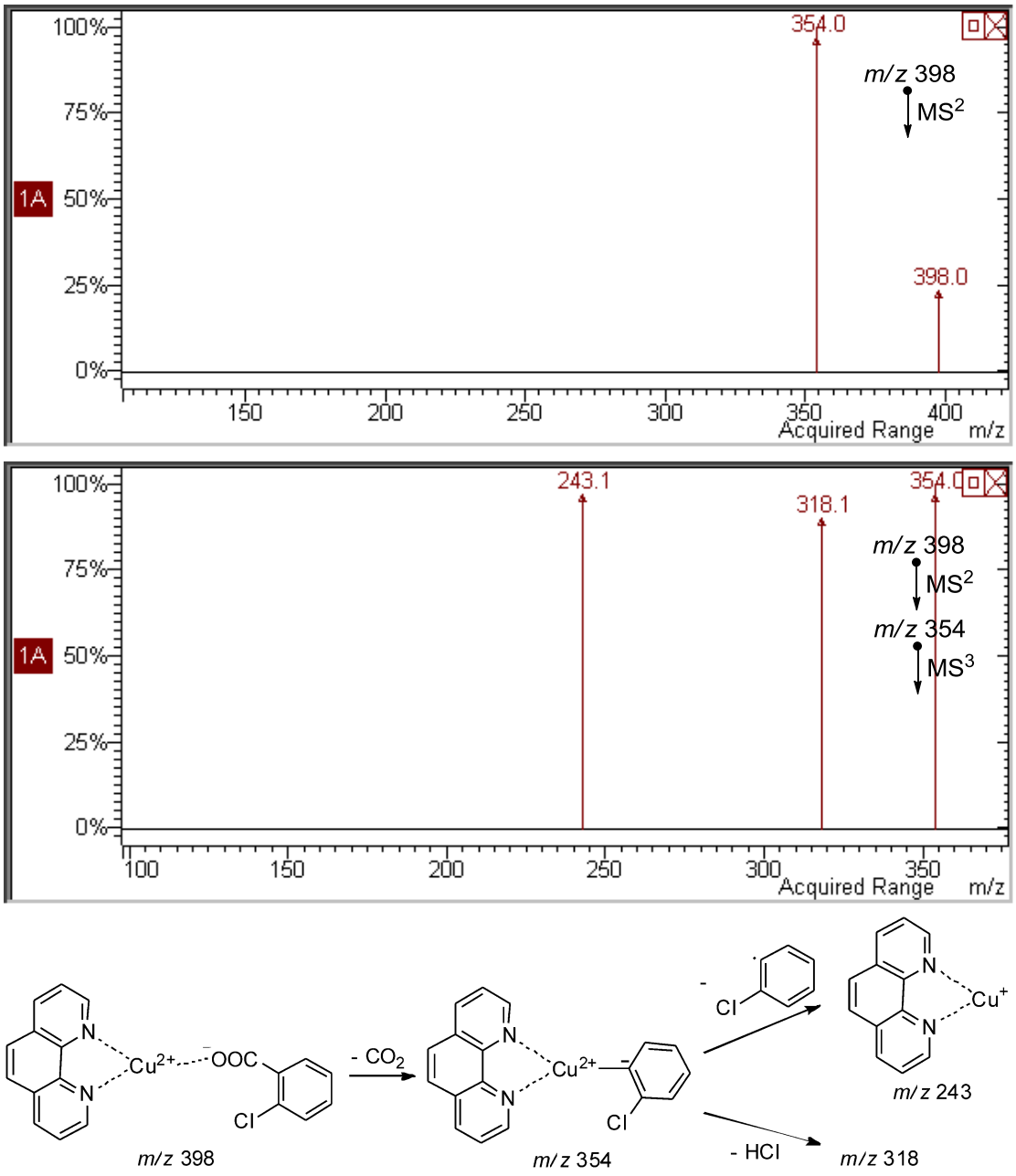


Figure S5. CID mass spectra of the [1,10-phenanthroline ··Cu ··2-chlorobenzoic acid]$^{+}$ ion (*m/z* 398).

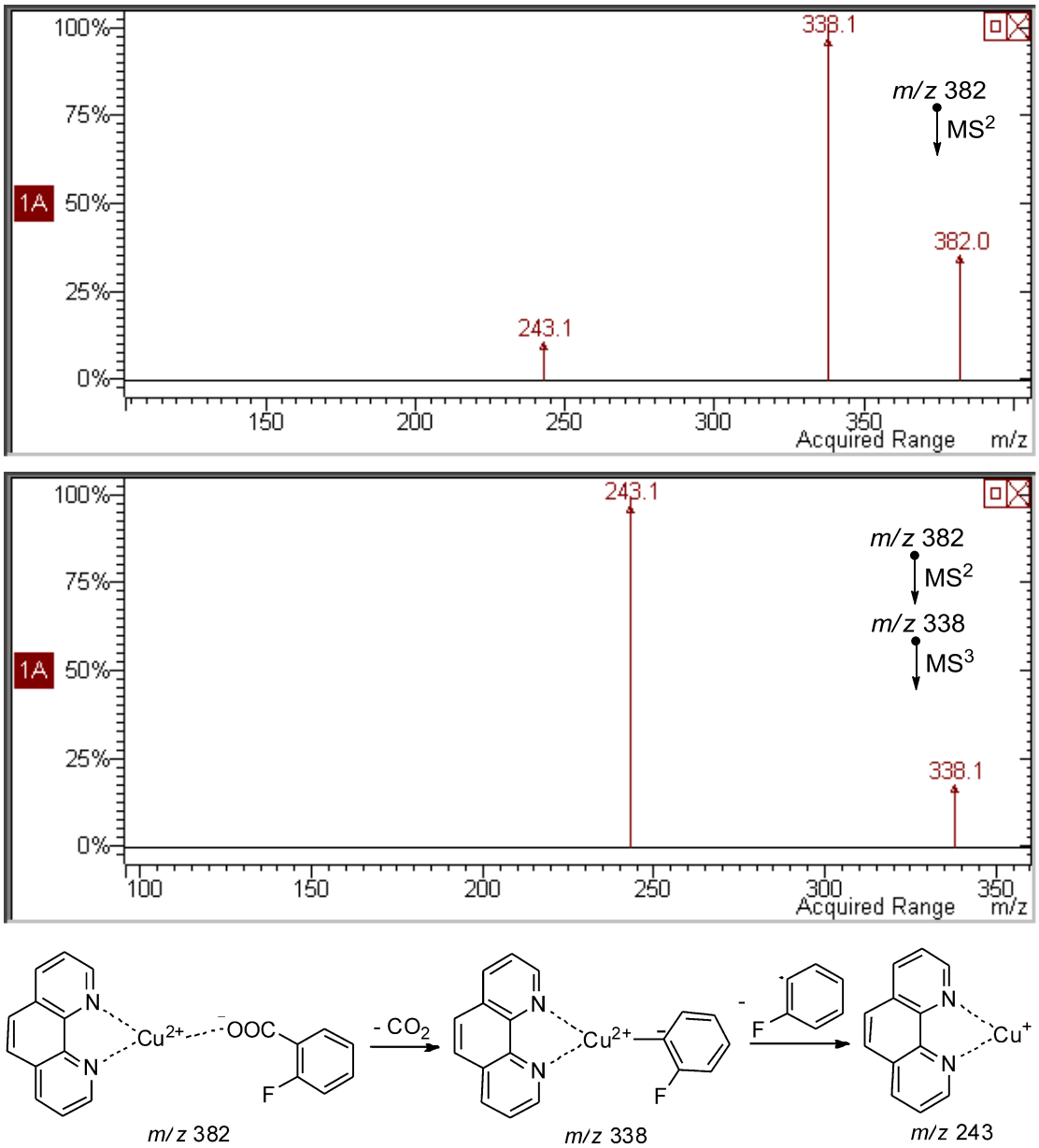


Figure S6. CID mass spectra of the [1,10-phenanthroline ··Cu ··2-fluorobenzoic acid]$^{+}$ ion (*m/z* 382).

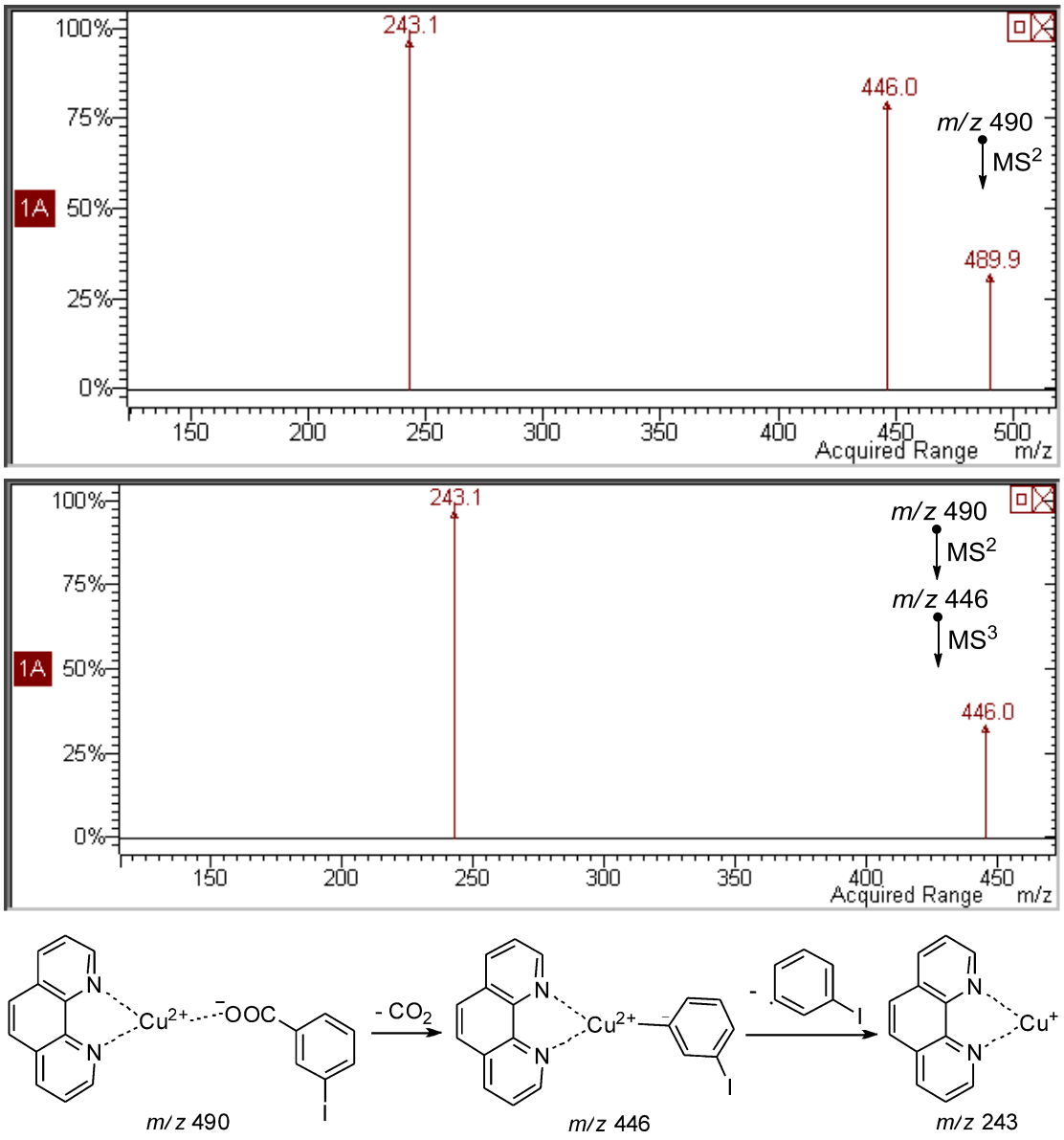


Figure S7. CID mass spectra of the [1,10-phenanthroline···Cu···3-iodobenzoic acid]$^{+}$ ion (*m/z* 490).

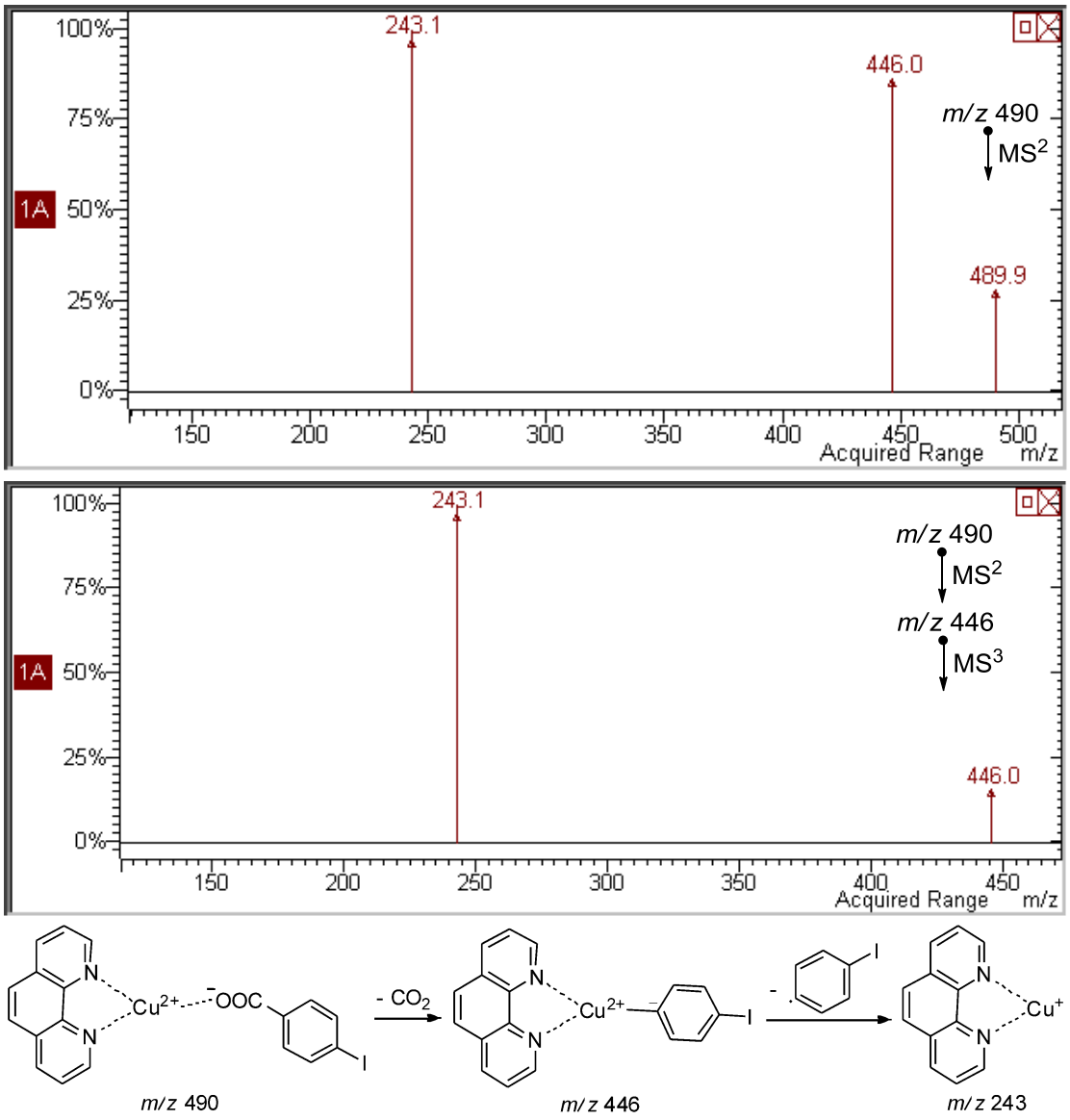


Figure S8. CID mass spectra of the [1,10-phenanthroline···Cu···4-iodobenzoic acid]$^{+}$ ion (*m/z* 490).

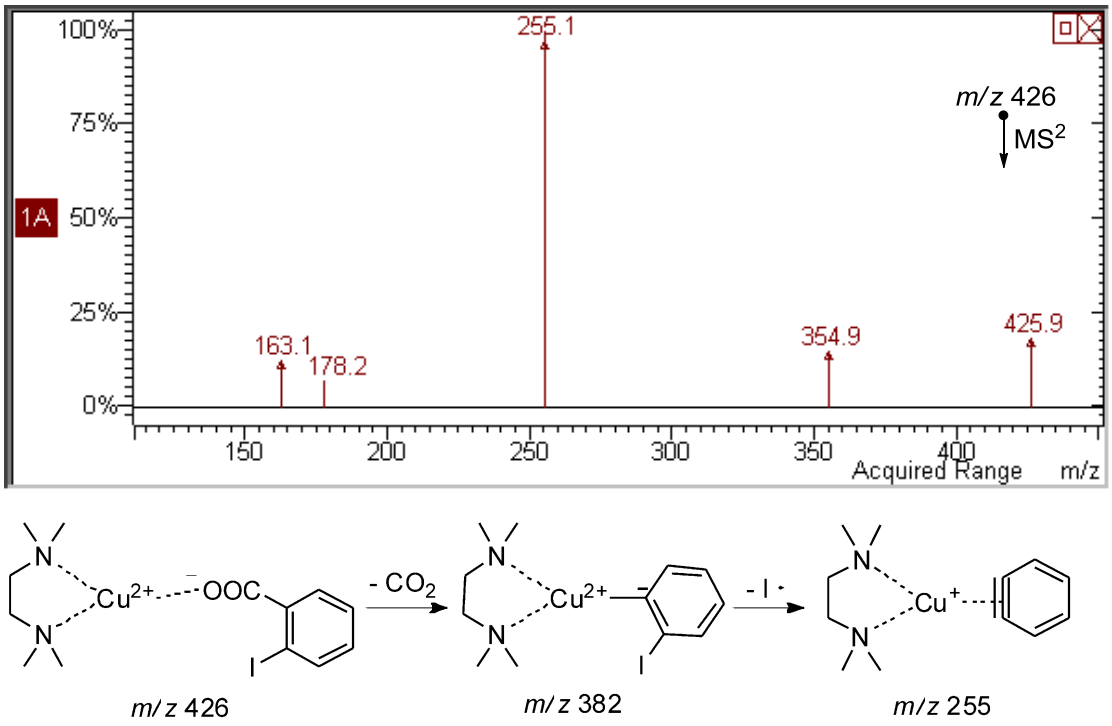


Figure S9. CID mass spectrum of the [TMEDA ··Cu ··2-iodobenzoic acid]$^{+}$ ion (*m/z* 426).

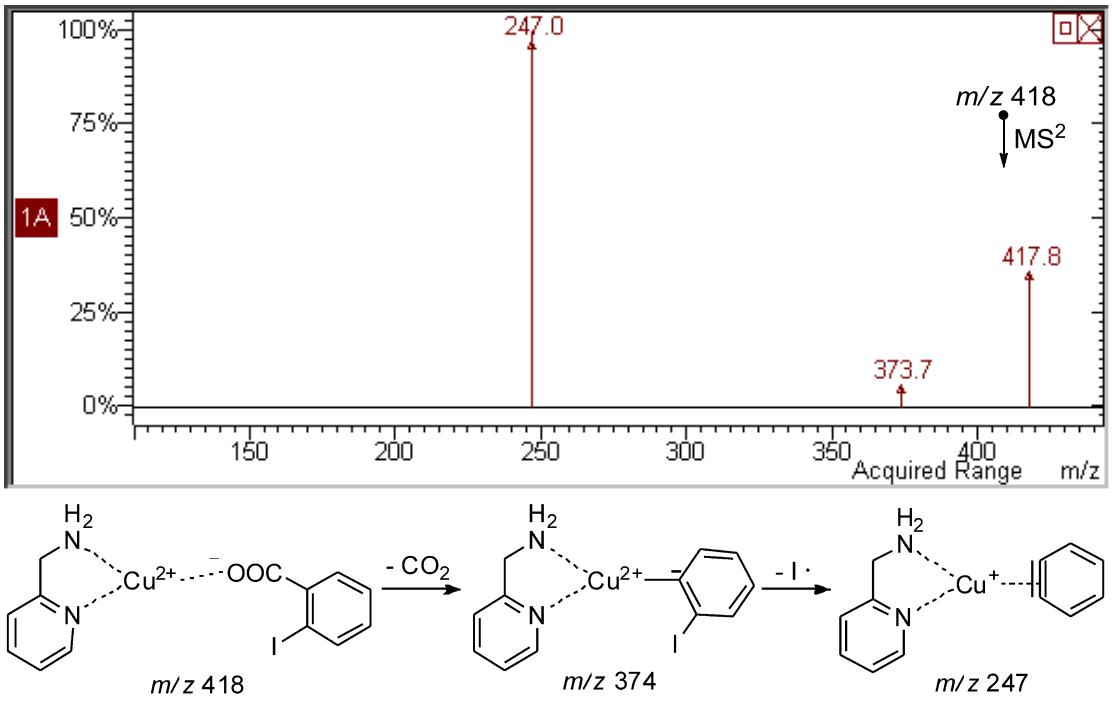


Figure S10. CID mass spectrum of the [2-AMP ··Cu ··2-iodobenzoic acid]$^{+}$ ion (*m/z* 418).

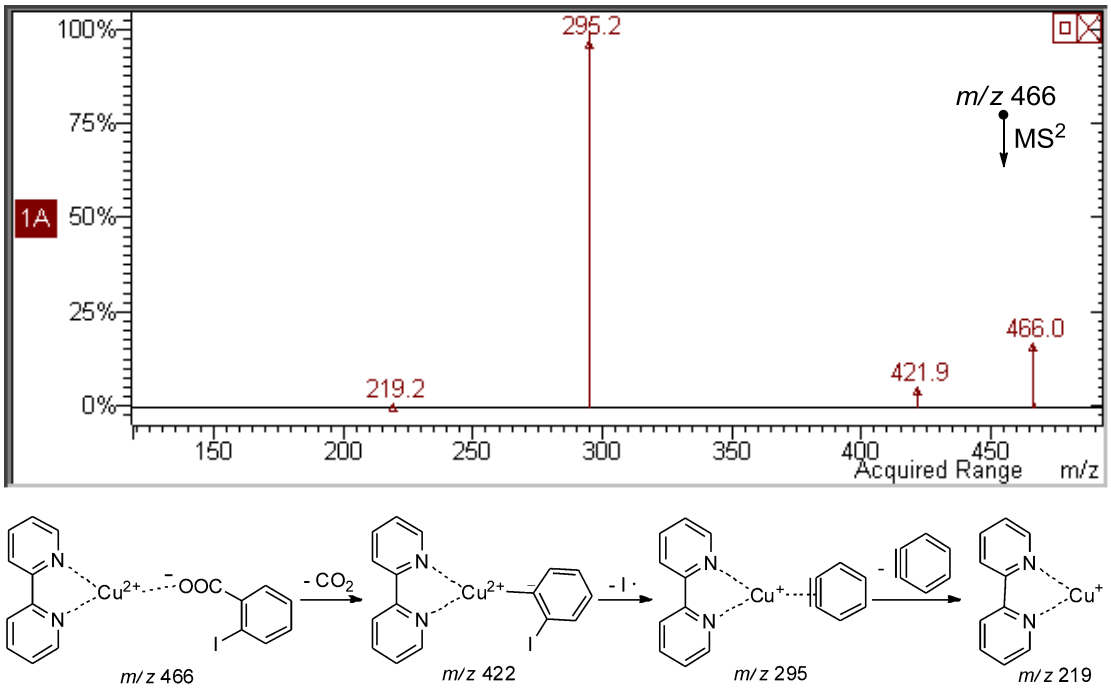


Figure S11. CID mass spectrum of the [2,2-bipyridine··Cu··2-iodobenzoic acid]$^{+}$ ion (*m/z* 466).

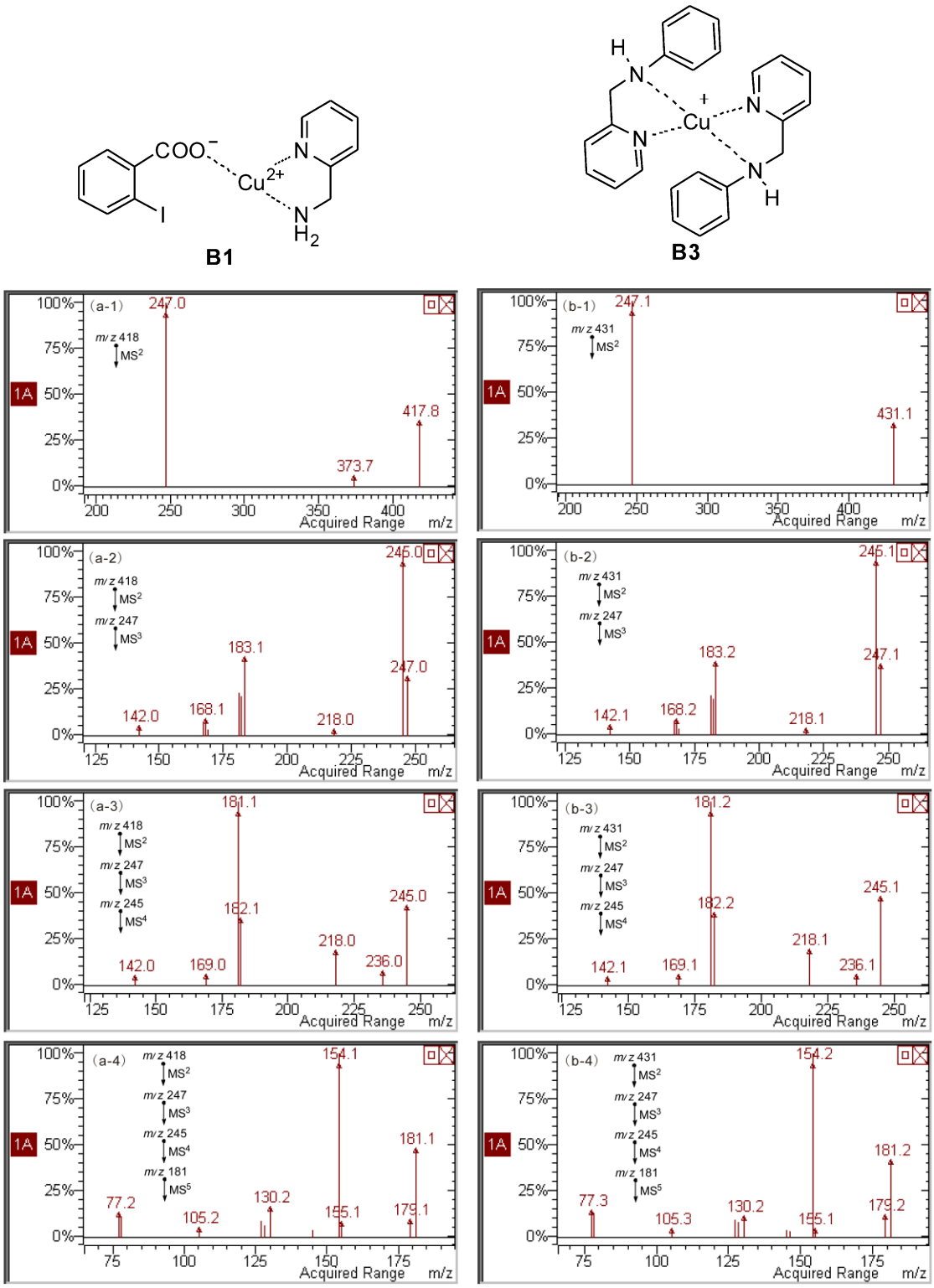


Figure S12. A comparision of the multi-stage mass spectra of complex ions **B1** and **B3** generated via ESI. a-1, a-2, a-3, and a-4 are the MS^2, MS^3, MS^4, and MS^5 mass spectra of complex ion **B1**, respectively. b-1, b-2, b-3, and b-4 are the MS^2, MS^3, MS^4, and MS^5 mass spectra of complex ion **B3**, respectively.

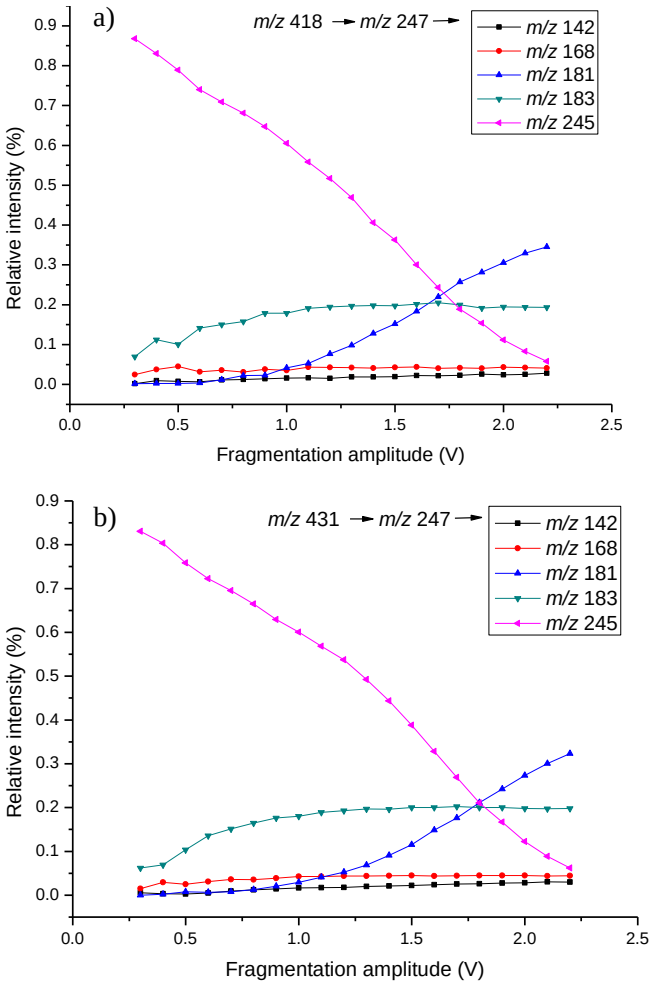


Figure S13. Energy resolved mass spectra of fragmentation of ion at *m/z* 247 generated from a) **B1** (*m/z* 418), and b) **B3** (*m/z* 431).

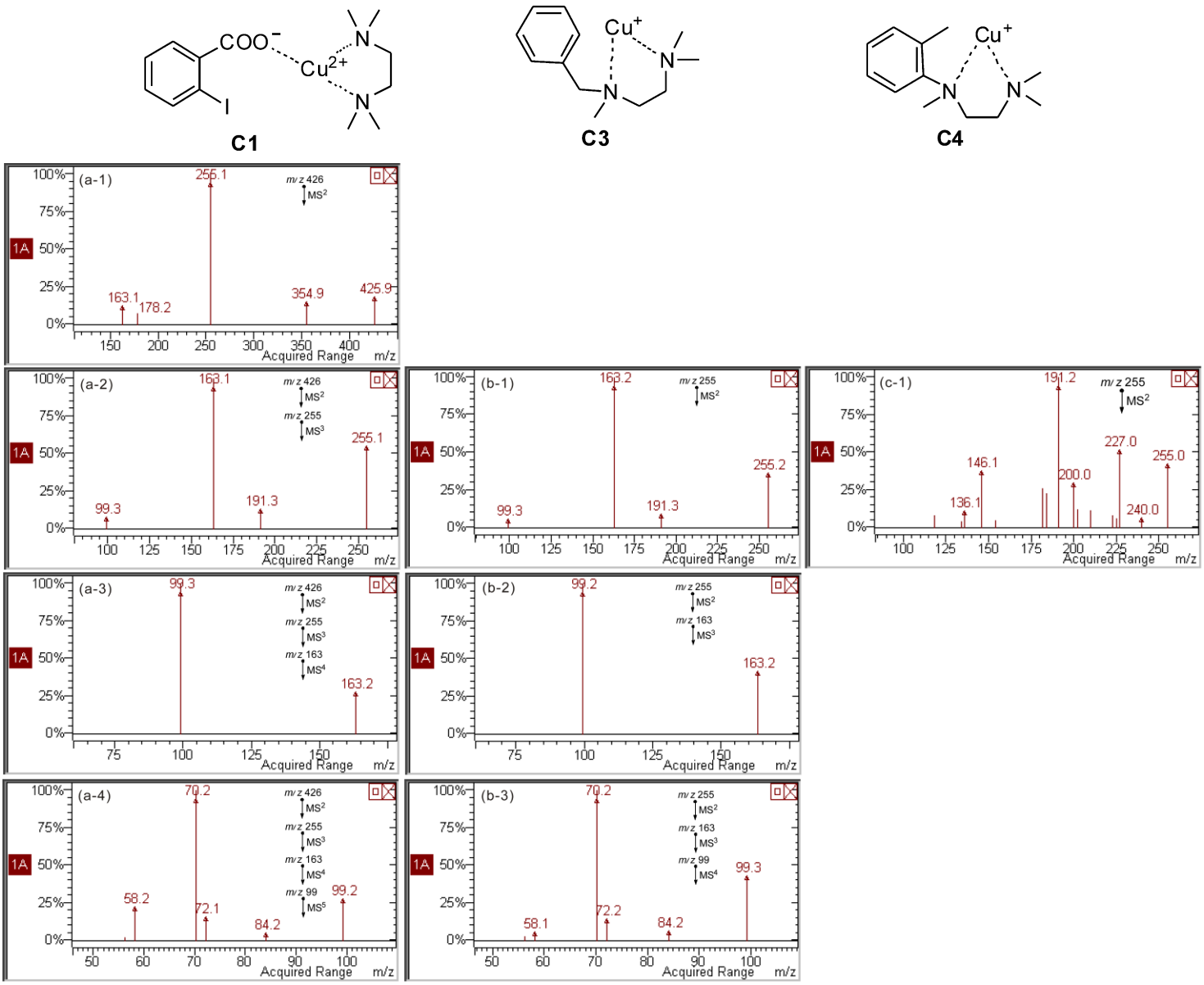


Figure S14. A comparision of the multi-stage mass spectra of complex ions **C1**, **C3** and **C4** generated via ESI. a-1, a-2, a-3, and a-4 are the MS^2, MS^3, MS^4, and MS^5 mass spectra of complex ion **C1**, respectively. b-1, b-2, and b-3 are the MS^2, MS^3, and MS^4 mass spectra of complex ion **C3**, respectively. c-1 is the MS^2 mass spectrum of complex ion **C4**.

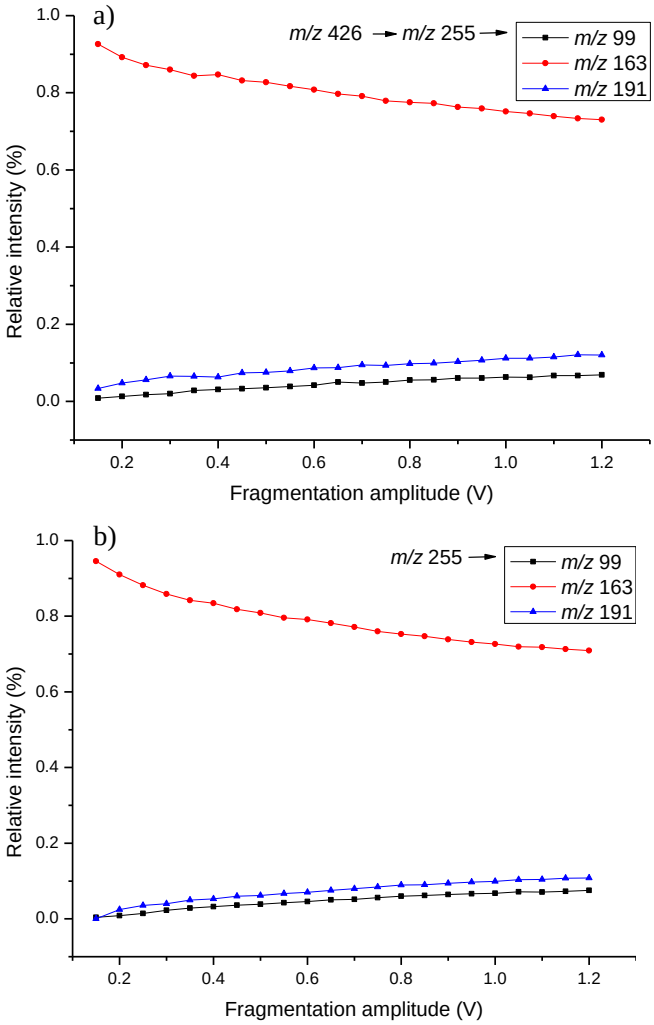


Figure S15. Energy resolved mass spectra of fragmentation of a) ion at *m/z* 255 generated from **C1** (*m/z* 426), and b) **C3** (*m/z* 255).

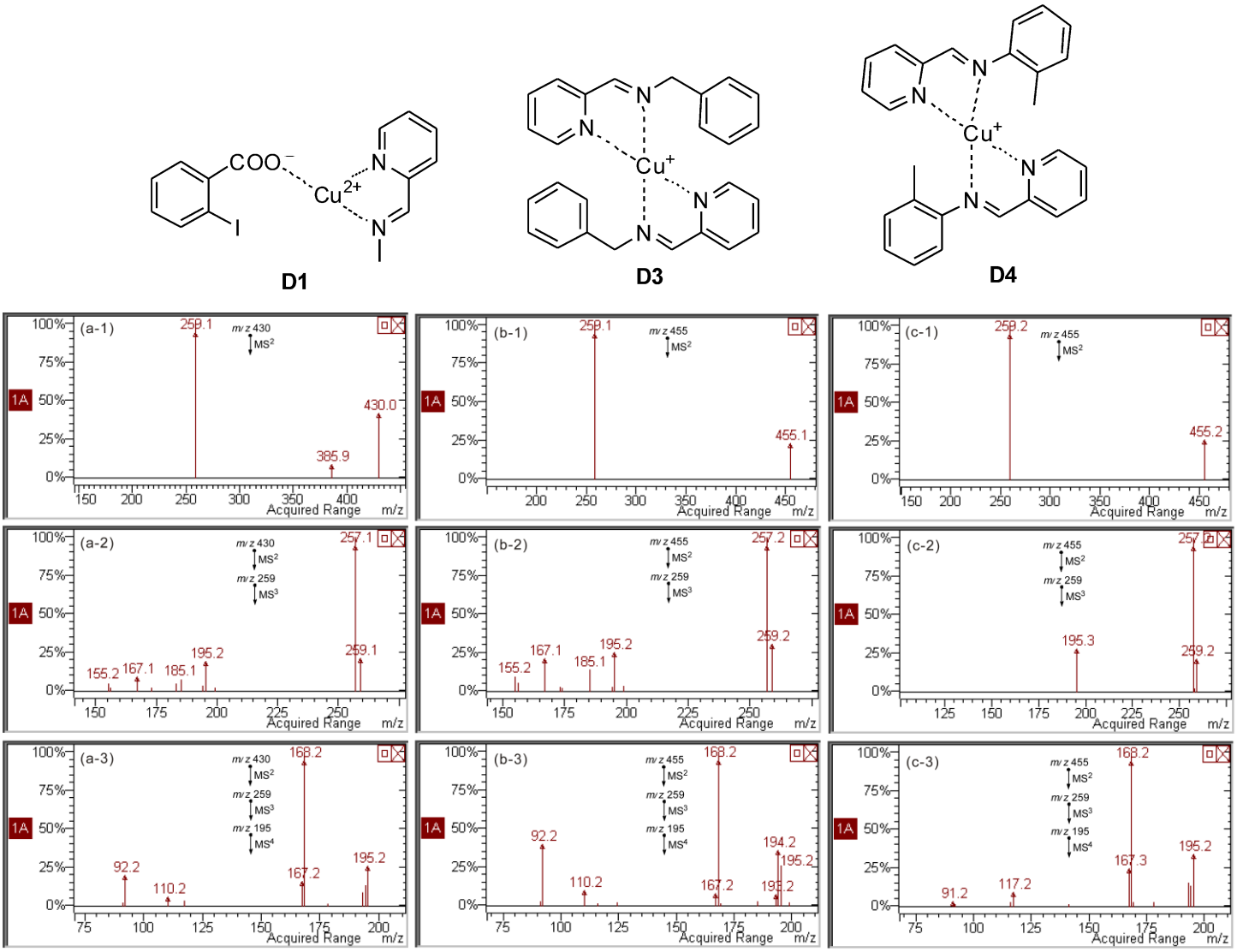


Figure S16. A comparision of the multi-stage mass spectra of complex ions **D1**, **D3** and **D4** generated via ESI. a-1, a-2, and a-3 are the MS^2, MS^3 and MS^4 mass spectra of complex ion **D1**, respectively. b-1, b-2, and b-3 are the MS^2, MS^3, and MS^4 mass spectra of complex ion **D3**, respectively. c-1, c-2, and c-3 are the MS^2, MS^3, and MS^4 mass spectra of complex ion **D4**, respectively.

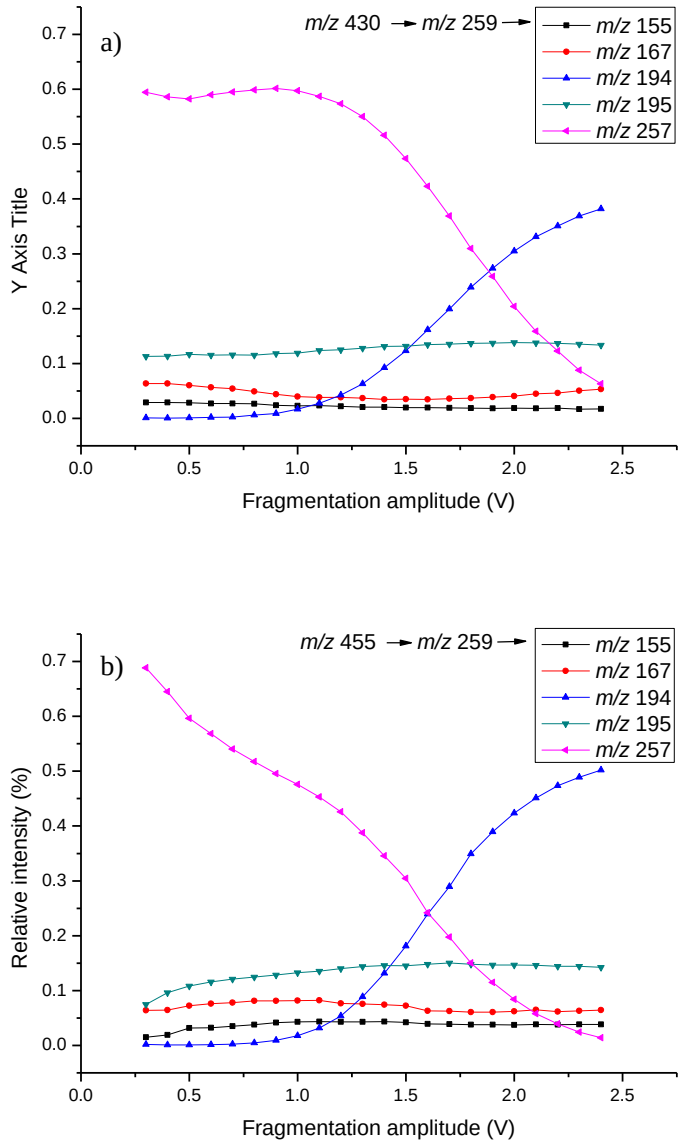
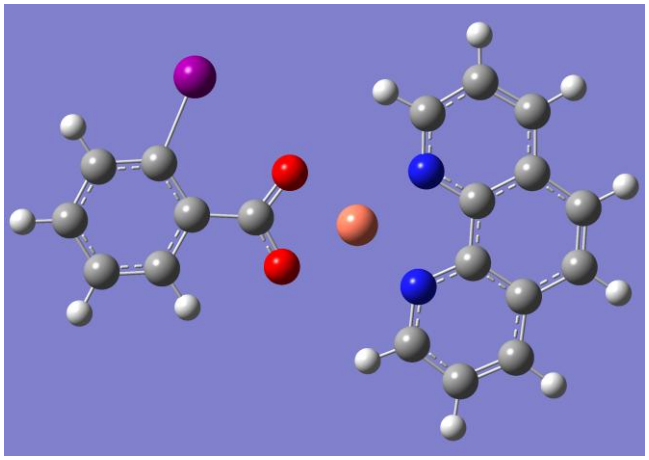


Figure S17. Energy resolved mass spectra of fragmentation of ion at *m/z* 259 generated from a) **D1** (*m/z* 430), and b) **D3** (*m/z* 455).

A1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	5.046155	0.953450	0.000003
4	6	0	3.692512	0.553186	-0.000014
5	6	0	2.918416	2.745711	-0.000155
6	6	0	6.065576	-0.061496	0.000085
7	6	0	3.353219	-0.841260	0.000043
8	6	0	4.369403	-1.820620	0.000119
9	6	0	5.741676	-1.389721	0.000141
10	6	0	3.949841	-3.173498	0.000167
11	1	0	4.691415	-3.967283	0.000226
12	6	0	2.598662	-3.474971	0.000137
13	6	0	1.653667	-2.430312	0.000061
14	1	0	7.106402	0.247491	0.000101
15	1	0	4.405466	4.308852	-0.000201
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17	1	0	2.060289	3.410942	-0.000212
18	1	0	6.523302	-2.143274	0.000201
19	1	0	2.253402	-4.502778	0.000172
20	1	0	0.584620	-2.621136	0.000037
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23	6	0	-5.217202	0.924259	0.000150
24	6	0	-2.825702	1.357582	0.000055
25	6	0	-5.472362	2.297207	0.000243
26	1	0	-6.045185	0.224577	0.000149
27	6	0	-3.110064	2.741385	0.000145
28	6	0	-4.416146	3.212075	0.000240

29	1	0	-6.501020	2.645263	0.000317
30	1	0	-2.275104	3.432776	0.000140
31	1	0	-4.610595	4.279508	0.000311
32	6	0	-1.399068	0.994236	-0.000028
33	8	0	-0.960473	-0.212589	-0.000028
34	8	0	-0.484253	1.906246	-0.000083
35	7	0	2.029550	-1.153363	0.000016
36	7	0	2.660349	1.439878	-0.000090
37	53	0	-3.716058	-1.689422	-0.000098

Zero-point correction= 0.268601 (Hartree/Particle)
Thermal correction to Energy= 0.288899
Thermal correction to Enthalpy= 0.289843
Thermal correction to Gibbs Free Energy= 0.215564
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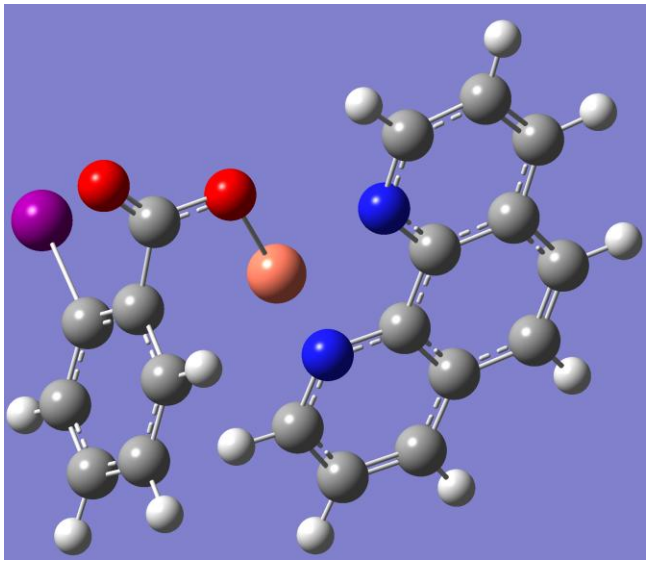
Sum of electronic and thermal Energies= -1199.607873
Sum of electronic and thermal Enthalpies= -1199.606929
Sum of electronic and thermal Free Energies= -1199.681207

A1’



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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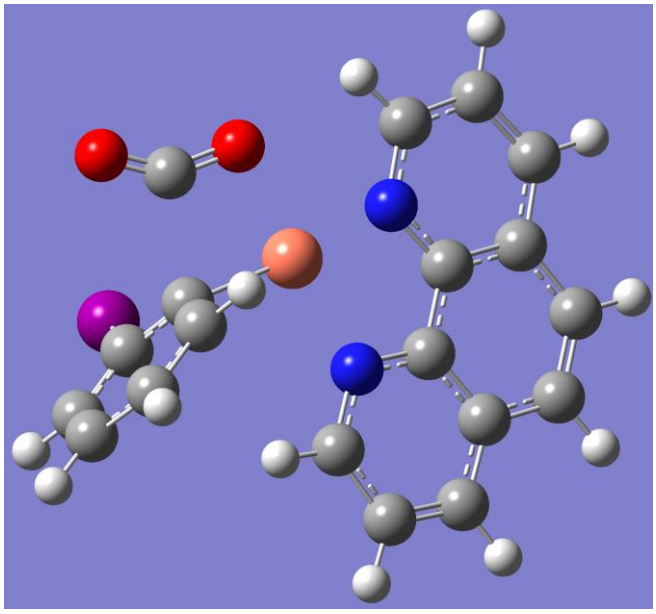
3	6	0	4.295140	0.925906	-0.365341
4	6	0	2.980608	0.515781	-0.055403

5	6	0	2.290302	2.682059	0.446045
6	6	0	5.247264	-0.069260	-0.777590
7	6	0	2.604537	-0.865195	-0.153596
8	6	0	3.558081	-1.823723	-0.564451
9	6	0	4.893158	-1.385933	-0.872864
10	6	0	3.123350	-3.167792	-0.646688
11	1	0	3.819093	-3.941593	-0.958392
12	6	0	1.814041	-3.484487	-0.330215
13	6	0	0.931770	-2.465043	0.070678
14	1	0	6.259235	0.244003	-1.015477
15	1	0	3.766461	4.245233	0.253887
16	1	0	5.569963	2.679704	-0.471330
17	1	0	1.471115	3.321313	0.762697
18	1	0	5.621445	-2.127336	-1.186818
19	1	0	1.453804	-4.505565	-0.386183
20	1	0	-0.099646	-2.683369	0.325408
21	29	0	0.269426	0.426352	0.686119
22	6	0	-2.633297	-0.603820	0.166535
23	6	0	-2.920005	-1.967583	0.252297
24	6	0	-2.073471	0.077469	1.274790
25	6	0	-2.655598	-2.667654	1.436846
26	1	0	-3.369153	-2.481914	-0.590519
27	6	0	-1.789001	-0.660251	2.454790
28	6	0	-2.077691	-2.020973	2.535076
29	1	0	-2.914078	-3.720879	1.498776
30	1	0	-1.395700	-0.130922	3.318894
31	1	0	-1.883549	-2.564513	3.454193
32	6	0	-1.927935	1.598000	1.342254
33	8	0	-2.855013	2.329235	1.603335
34	8	0	-0.677271	1.965679	1.125907
35	7	0	1.315009	-1.190529	0.158688
36	7	0	2.018371	1.385873	0.339669
37	53	0	-3.095451	0.432387	-1.641075

Zero-point correction= 0.267321 (Hartree/Particle)
Thermal correction to Energy= 0.288167
Thermal correction to Enthalpy= 0.289111
Thermal correction to Gibbs Free Energy= 0.212773
Sum of electronic and zero-point Energies= -1199.590866
Sum of electronic and thermal Energies= -1199.570021
Sum of electronic and thermal Enthalpies= -1199.569077
Sum of electronic and thermal Free Energies= -1199.645414

TS



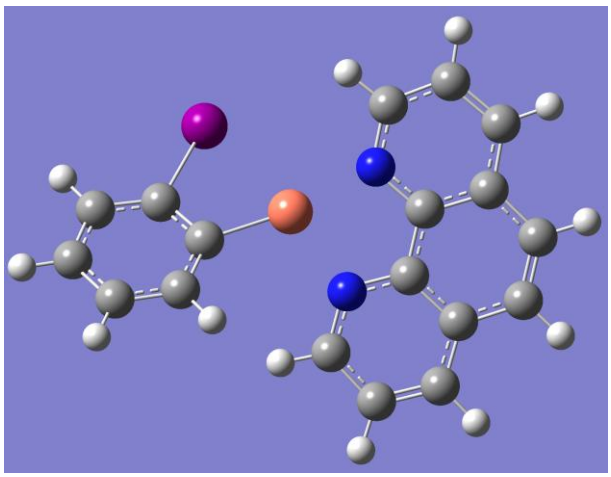
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.266401	3.533127	0.254625
2	6	0	-2.607989	3.383560	-0.047559
3	6	0	-3.172406	2.086924	-0.104698
4	6	0	-2.307681	0.999508	0.155589
5	6	0	-0.480201	2.391031	0.497593
6	6	0	-4.552829	1.819939	-0.406158
7	6	0	-2.815079	-0.343499	0.119179
8	6	0	-4.175780	-0.581105	-0.177172
9	6	0	-5.034028	0.541680	-0.441229
10	6	0	-4.600674	-1.931816	-0.191692
11	1	0	-5.637336	-2.167652	-0.414682
12	6	0	-3.692255	-2.939980	0.078530
13	6	0	-2.353729	-2.607074	0.363625
14	1	0	-5.211679	2.659265	-0.606835
15	1	0	-0.807742	4.514257	0.306177
16	1	0	-3.231659	4.251794	-0.240387
17	1	0	0.575291	2.472216	0.734466
18	1	0	-6.078870	0.355276	-0.670090
19	1	0	-3.991472	-3.982154	0.074691
20	1	0	-1.610797	-3.368706	0.579903
21	29	0	-0.060585	-0.632746	0.730865
22	6	0	2.583733	0.472101	-0.018295
23	6	0	3.580725	1.431407	0.137184
24	6	0	1.880790	-0.064537	1.076895

25	6	0	3.882932	1.886047	1.429075
26	1	0	4.121032	1.822348	-0.718331
27	6	0	2.197339	0.433238	2.364625
28	6	0	3.189056	1.397830	2.541896
29	1	0	4.668501	2.624867	1.558899
30	1	0	1.680371	0.036322	3.235880
31	1	0	3.432069	1.756460	3.537371
32	6	0	1.928084	-2.116112	1.169710
33	8	0	3.043162	-2.483725	1.242721
34	8	0	0.729488	-2.428458	1.133551
35	7	0	-1.933877	-1.344292	0.381266
36	7	0	-0.987714	1.161666	0.448028
37	53	0	2.094671	-0.203819	-2.003731

Zero-point correction= 0.264876 (Hartree/Particle)
Thermal correction to Energy= 0.285797
Thermal correction to Enthalpy= 0.286741
Thermal correction to Gibbs Free Energy= 0.211385
Sum of electronic and zero-point Energies= -1199.568142
Sum of electronic and thermal Energies= -1199.547221
Sum of electronic and thermal Enthalpies= -1199.546276
Sum of electronic and thermal Free Energies= -1199.621632

one imaginary frequency, -366.6

A2

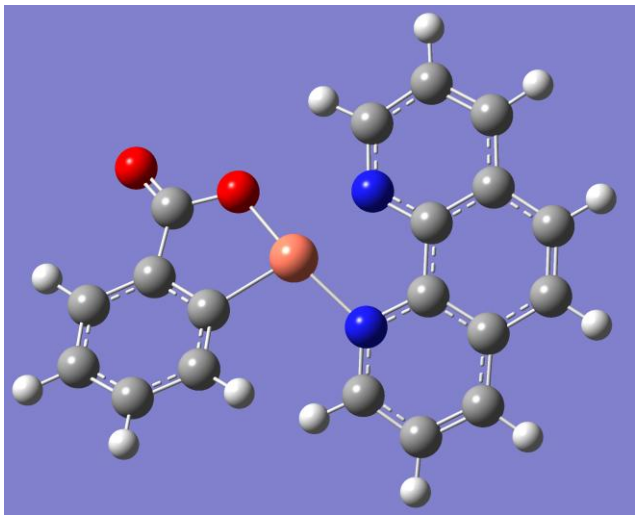


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.507752	-3.242571	0.940262
2	6	0	-3.725818	-2.637733	0.687791
3	6	0	-3.766797	-1.272561	0.317337
4	6	0	-2.530405	-0.591213	0.230887
5	6	0	-1.326561	-2.487407	0.820782
6	6	0	-4.979687	-0.557993	0.025881
7	6	0	-2.503284	0.798292	-0.139571
8	6	0	-3.710106	1.474863	-0.433918
9	6	0	-4.952378	0.758256	-0.336891
10	6	0	-3.608739	2.834152	-0.815732
11	1	0	-4.508445	3.394961	-1.052459
12	6	0	-2.364941	3.434395	-0.889240
13	6	0	-1.216830	2.683672	-0.570716
14	1	0	-5.924366	-1.088591	0.095666
15	1	0	-2.445750	-4.286833	1.225418
16	1	0	-4.650952	-3.201122	0.769474
17	1	0	-0.354778	-2.935193	1.004108
18	1	0	-5.874953	1.285329	-0.560306
19	1	0	-2.257080	4.471679	-1.186290
20	1	0	-0.224692	3.120822	-0.616295
21	29	0	0.220868	0.097020	0.315815
22	6	0	2.962933	0.437133	0.105286
23	6	0	4.264821	0.912901	0.192263
24	6	0	1.833605	1.127211	0.519657
25	6	0	4.432595	2.192402	0.738902
26	1	0	5.116352	0.330758	-0.142603
27	6	0	2.033572	2.404249	1.067047
28	6	0	3.328143	2.928610	1.178260
29	1	0	5.433035	2.606382	0.821836
30	1	0	1.191108	2.988163	1.429973
31	1	0	3.474649	3.913481	1.612005
32	7	0	-1.288919	1.407964	-0.200858
33	7	0	-1.336593	-1.199768	0.477601
34	53	0	2.509907	-1.548127	-0.685398

Zero-point correction= 0.252660 (Hartree/Particle)
Thermal correction to Energy= 0.270786
Thermal correction to Enthalpy= 0.271730
Thermal correction to Gibbs Free Energy= 0.202811
Sum of electronic and zero-point Energies= -1011.018341
Sum of electronic and thermal Energies= -1011.000214
Sum of electronic and thermal Enthalpies= -1010.999270
Sum of electronic and thermal Free Energies= -1011.068190

A2’

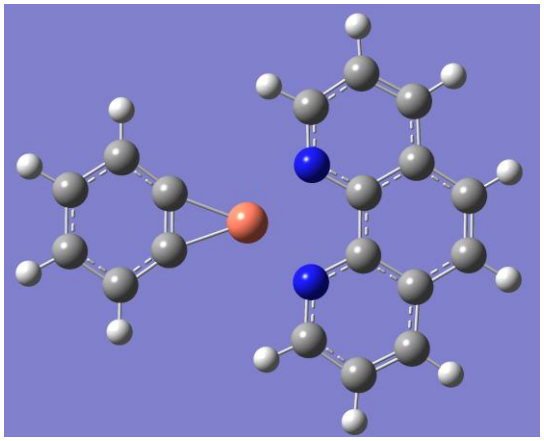


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.363465	3.485128	-0.572539
2	6	0	-2.682069	3.129621	-0.352772
3	6	0	-3.004681	1.776211	-0.098829
4	6	0	-1.933394	0.855202	-0.058926
5	6	0	-0.356474	2.506748	-0.494976
6	6	0	-4.344107	1.286212	0.090013
7	6	0	-2.203696	-0.539939	0.096287
8	6	0	-3.525344	-1.006494	0.256027
9	6	0	-4.594556	-0.045913	0.266508
10	6	0	-3.692334	-2.408875	0.373695
11	1	0	-4.687855	-2.823932	0.502583
12	6	0	-2.587241	-3.239780	0.312462
13	6	0	-1.303306	-2.682901	0.137137
14	1	0	-5.161515	2.000548	0.078756
15	1	0	-1.085925	4.507872	-0.801662
16	1	0	-3.470834	3.875289	-0.393742
17	1	0	0.680921	2.763583	-0.667466
18	1	0	-5.612598	-0.398572	0.400457
19	1	0	-2.690484	-4.316297	0.390917
20	1	0	-0.405572	-3.290193	0.069250
21	29	0	0.591069	-0.328972	-0.075788
22	6	0	2.346964	0.484221	0.185368
23	6	0	2.611595	1.744303	0.701619
24	6	0	3.360741	-0.417237	-0.119725
25	6	0	3.963907	2.120698	0.819570
26	1	0	1.842320	2.427317	1.041528

27	6	0	4.698749	-0.034696	-0.008292
28	6	0	4.994610	1.251397	0.449358
29	1	0	4.198226	3.104166	1.217440
30	1	0	5.475645	-0.754523	-0.252850
31	1	0	6.027581	1.569210	0.548954
32	6	0	2.878020	-1.786550	-0.425058
33	8	0	3.522554	-2.764023	-0.723603
34	8	0	1.534564	-1.863345	-0.282407
35	7	0	-1.131491	-1.368720	0.037632
36	7	0	-0.624420	1.230224	-0.213317

Zero-point correction=	0.267435 (Hartree/Particle)
Thermal correction to Energy=	0.285473
Thermal correction to Enthalpy=	0.286417
Thermal correction to Gibbs Free Energy=	0.221094
Sum of electronic and zero-point Energies=	-1188.150382
Sum of electronic and thermal Energies=	-1188.132344
Sum of electronic and thermal Enthalpies=	-1188.131400
Sum of electronic and thermal Free Energies=	-1188.196723

A3

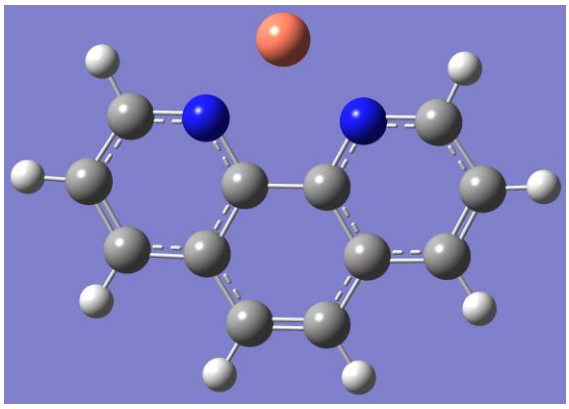


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.627002	-3.460863	-0.000057
2	6	0	-2.861777	-2.837732	0.000430
3	6	0	-2.932541	-1.424293	0.000458
4	6	0	-1.707209	-0.718905	-0.000006

5	6	0	-0.458219	-2.676663	-0.000503
6	6	0	-4.163883	-0.682263	0.000902
7	6	0	-1.706950	0.719104	-0.000049
8	6	0	-2.932028	1.424933	0.000351
9	6	0	-4.163638	0.683349	0.000847
10	6	0	-2.860749	2.838347	0.000218
11	1	0	-3.775701	3.423838	0.000510
12	6	0	-1.625747	3.461027	-0.000296
13	6	0	-0.457248	2.676401	-0.000649
14	1	0	-5.100754	-1.230969	0.001273
15	1	0	-1.542207	-4.541834	-0.000106
16	1	0	-3.776941	-3.422891	0.000779
17	1	0	0.524346	-3.136050	-0.000895
18	1	0	-5.100311	1.232392	0.001171
19	1	0	-1.540560	4.541967	-0.000424
20	1	0	0.525483	3.135432	-0.001044
21	29	0	0.996638	-0.000431	-0.000811
22	6	0	2.816210	0.649128	-0.000218
23	6	0	3.946491	1.463222	0.000957
24	6	0	2.816407	-0.649630	-0.000510
25	6	0	5.131720	0.705259	0.001452
26	1	0	3.952981	2.546898	0.001344
27	6	0	3.946937	-1.463375	-0.000122
28	6	0	5.131935	-0.705050	0.000903
29	1	0	6.084124	1.228534	0.002294
30	1	0	3.953749	-2.547048	-0.000458
31	1	0	6.084500	-1.228033	0.001333
32	7	0	-0.496004	1.344792	-0.000520
33	7	0	-0.496489	-1.345035	-0.000465

Zero-point correction= 0.251800 (Hartree/Particle)
Thermal correction to Energy= 0.267821
Thermal correction to Enthalpy= 0.268766
Thermal correction to Gibbs Free Energy= 0.207421
Sum of electronic and zero-point Energies= -999.577147
Sum of electronic and thermal Energies= -999.561125
Sum of electronic and thermal Enthalpies= -999.560181
Sum of electronic and thermal Free Energies= -999.621526

A4



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.489801	-0.324991	-0.000003
2	6	0	2.834384	-1.540617	-0.000010
3	6	0	1.419370	-1.579192	-0.000010
4	6	0	0.726939	-0.341660	-0.000002
5	6	0	2.728389	0.857087	0.000005
6	6	0	0.681467	-2.810890	-0.000018
7	6	0	-0.726939	-0.341660	-0.000002
8	6	0	-1.419370	-1.579192	-0.000010
9	6	0	-0.681467	-2.810889	-0.000018
10	6	0	-2.834384	-1.540617	-0.000010
11	1	0	-3.393683	-2.471785	-0.000016
12	6	0	-3.489801	-0.324992	-0.000002
13	6	0	-2.728389	0.857087	0.000005
14	1	0	1.233371	-3.745855	-0.000024
15	1	0	4.572417	-0.264696	-0.000003
16	1	0	3.393683	-2.471785	-0.000016
17	1	0	3.212311	1.828485	0.000011
18	1	0	-1.233371	-3.745854	-0.000023
19	1	0	-4.572417	-0.264696	-0.000002
20	1	0	-3.212311	1.828485	0.000011
21	29	0	0.000000	2.285430	0.000015
22	7	0	-1.395948	0.850956	0.000005
23	7	0	1.395948	0.850956	0.000005

Zero-point correction= 0.173252 (Hartree/Particle)
Thermal correction to Energy= 0.184039
Thermal correction to Enthalpy= 0.184983
Thermal correction to Gibbs Free Energy= 0.136100
Sum of electronic and zero-point Energies= -768.639712

Sum of electronic and thermal Energies=	-768.628925
Sum of electronic and thermal Enthalpies=	-768.627981
Sum of electronic and thermal Free Energies=	-768.676864

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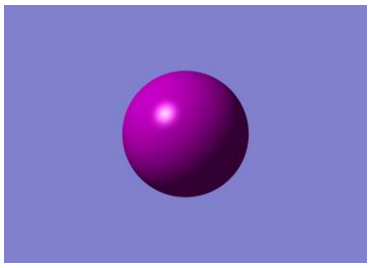

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	53	0	0.000000	0.000000	0.000000

Zero-point correction=	0.000000 (Hartree/Particle)
Thermal correction to Energy=	0.001416
Thermal correction to Enthalpy=	0.002360
Thermal correction to Gibbs Free Energy=	-0.017503
Sum of electronic and zero-point Energies=	-11.394690
Sum of electronic and thermal Energies=	-11.393274
Sum of electronic and thermal Enthalpies=	-11.392330
Sum of electronic and thermal Free Energies=	-11.412193

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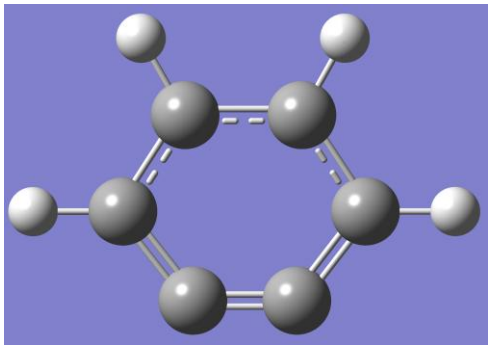
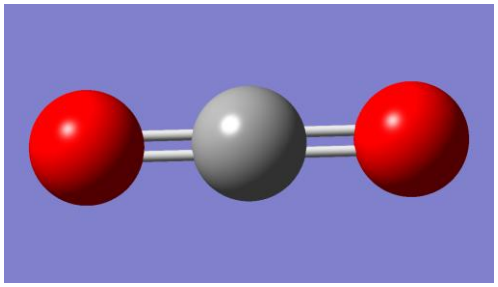


Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.626277	-1.238337	-0.000011
2	6	0	1.463402	-0.133740	0.000007
3	6	0	-0.626249	-1.238335	-0.000010
4	6	0	0.704282	1.059518	0.000004
5	1	0	2.547600	-0.135588	0.000001
6	6	0	-1.463404	-0.133765	0.000007
7	6	0	-0.704303	1.059506	0.000002
8	1	0	1.230425	2.011080	0.000001
9	1	0	-2.547601	-0.135635	0.000002
10	1	0	-1.230462	2.011059	-0.000002

Zero-point correction= 0.075064 (Hartree/Particle)
Thermal correction to Energy= 0.079572
Thermal correction to Enthalpy= 0.080516
Thermal correction to Gibbs Free Energy= 0.047679
Sum of electronic and zero-point Energies= -230.853308
Sum of electronic and thermal Energies= -230.848800
Sum of electronic and thermal Enthalpies= -230.847856
Sum of electronic and thermal Free Energies= -230.880693

CO_2

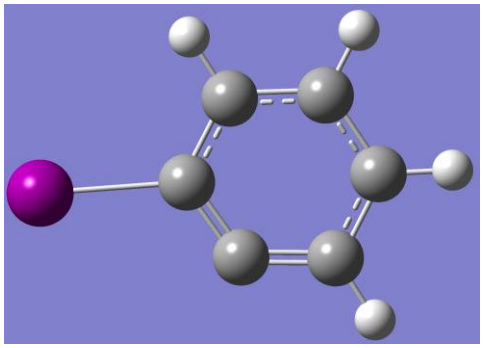


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.000011
2	8	0	0.000000	0.000000	1.169366
3	8	0	0.000000	0.000000	-1.169358

Zero-point correction= 0.011565 (Hartree/Particle)
Thermal correction to Energy= 0.014202

Thermal correction to Enthalpy=	0.015146
Thermal correction to Gibbs Free Energy=	-0.009804
Sum of electronic and zero-point Energies=	-188.578828
Sum of electronic and thermal Energies=	-188.576191
Sum of electronic and thermal Enthalpies=	-188.575246
Sum of electronic and thermal Free Energies=	-188.600197

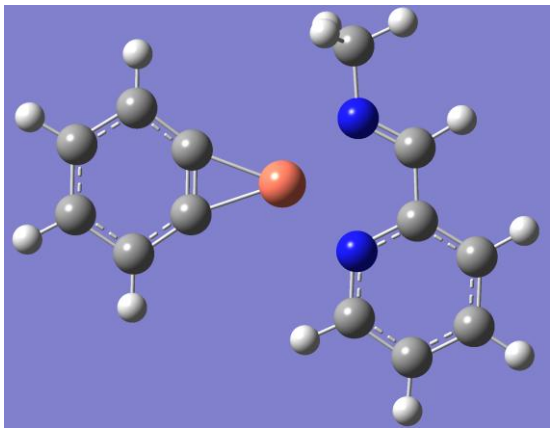
Iodobenzene radical



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.579193	-0.000593	0.000044
2	6	0	1.297105	1.204960	0.000141
3	6	0	1.287781	-1.169167	0.000045
4	6	0	2.696221	1.156504	0.000234
5	1	0	0.776128	2.157493	0.000144
6	6	0	2.662796	-1.274754	0.000133
7	6	0	3.379481	-0.065201	0.000230
8	1	0	3.256192	2.087130	0.000309
9	1	0	3.171988	-2.233995	0.000128
10	1	0	4.465997	-0.083608	0.000302
11	53	0	-1.567656	-0.019576	-0.000110

Zero-point correction=	0.076870 (Hartree/Particle)
Thermal correction to Energy=	0.082791
Thermal correction to Enthalpy=	0.083735
Thermal correction to Gibbs Free Energy=	0.044396
Sum of electronic and zero-point Energies=	-242.305309
Sum of electronic and thermal Energies=	-242.299387
Sum of electronic and thermal Enthalpies=	-242.298443
Sum of electronic and thermal Free Energies=	-242.337782

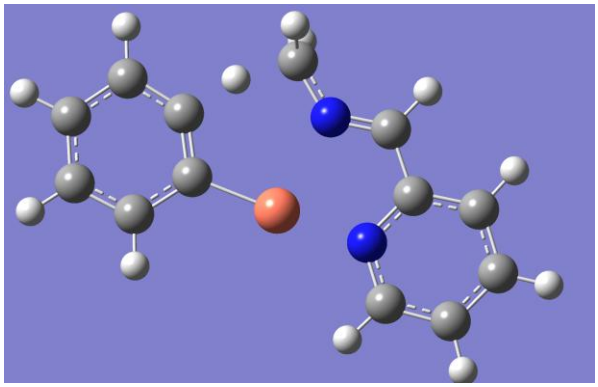
D2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.200829	-2.286605	-0.000007
2	6	0	-4.202531	-1.319275	0.000006
3	6	0	-2.487571	0.361859	0.000013
4	6	0	-1.862153	-1.877559	-0.000009
5	1	0	-3.438227	-3.344742	-0.000018
6	1	0	-5.249094	-1.606476	0.000007
7	1	0	-1.051957	-2.598610	-0.000019
8	29	0	0.317729	0.260045	0.000001
9	6	0	3.557131	0.838704	0.000027
10	6	0	1.881821	-0.878171	-0.000006
11	6	0	4.483400	-0.219983	0.000014
12	1	0	3.862544	1.878309	0.000046
13	6	0	2.742228	-1.974617	-0.000020
14	6	0	4.090807	-1.575049	-0.000010
15	1	0	5.543824	0.017498	0.000023
16	1	0	2.447565	-3.017436	-0.000038
17	1	0	4.860249	-2.342395	-0.000020
18	7	0	-0.740426	1.973206	-0.000001
19	7	0	-1.514103	-0.585742	0.000001
20	6	0	-3.840748	0.032840	0.000016
21	1	0	-4.593323	0.814780	0.000026
22	6	0	-2.003281	1.751760	0.000010
23	1	0	-2.733419	2.565022	0.000011
24	6	0	2.246698	0.367456	0.000013
25	1	0	0.411806	3.473758	-0.883388
26	6	0	-0.218720	3.336933	-0.000039
27	1	0	-1.020289	4.082612	-0.000950
28	1	0	0.410386	3.474379	0.884231

Zero-point correction=	0.219461 (Hartree/Particle)
Thermal correction to Energy=	0.234011
Thermal correction to Enthalpy=	0.234955
Thermal correction to Gibbs Free Energy=	0.176917
Sum of electronic and zero-point Energies=	-809.029615
Sum of electronic and thermal Energies=	-809.015065
Sum of electronic and thermal Enthalpies=	-809.014121
Sum of electronic and thermal Free Energies=	-809.072159

HT-TS



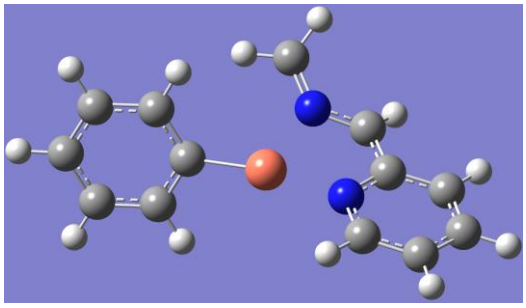
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.119713	-1.491334	-0.000013
2	6	0	4.689507	-0.221377	0.000120
3	6	0	2.465461	0.696220	0.000117
4	6	0	2.724570	-1.609704	-0.000074
5	1	0	4.732994	-2.385811	-0.000069
6	1	0	5.767355	-0.095720	0.000171
7	1	0	2.247654	-2.584388	-0.000178
8	29	0	-0.076798	-0.550437	-0.000062
9	6	0	-3.964954	0.983122	0.000004
10	6	0	-1.978278	-0.490395	-0.000085
11	6	0	-4.785219	-0.155174	-0.000095
12	1	0	-4.375114	1.987075	0.000076
13	6	0	-2.834953	-1.625989	-0.000180
14	6	0	-4.221090	-1.437366	-0.000184
15	1	0	-5.864061	-0.029384	-0.000099

16	1	0	-2.433542	-2.633713	-0.000251
17	1	0	-4.873189	-2.306343	-0.000260
18	7	0	0.275113	1.654885	0.000116
19	7	0	1.911919	-0.544734	-0.000011
20	6	0	3.845495	0.894363	0.000187
21	1	0	4.250443	1.901511	0.000290
22	6	0	1.538225	1.842461	0.000182
23	1	0	1.976486	2.843898	0.000289
24	6	0	-2.609210	0.694166	-0.000002
25	1	0	-1.846647	1.729282	0.000097
26	6	0	-0.777478	2.525214	0.000138
27	1	0	-0.967643	3.069944	0.926797
28	1	0	-0.967581	3.070032	-0.926484

Zero-point correction= 0.213981 (Hartree/Particle)
Thermal correction to Energy= 0.227832
Thermal correction to Enthalpy= 0.228777
Thermal correction to Gibbs Free Energy= 0.172667
Sum of electronic and zero-point Energies= -808.989996
Sum of electronic and thermal Energies= -808.976145
Sum of electronic and thermal Enthalpies= -808.975201
Sum of electronic and thermal Free Energies= -809.031311

one imaginary frequency, -280.18

HT-01

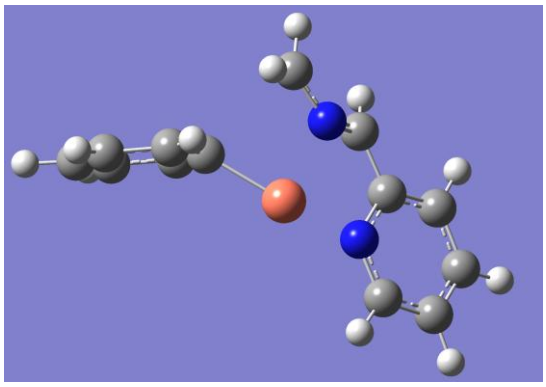


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.893261	-1.711848	0.409360
2	6	0	4.588279	-0.632824	-0.149145
3	6	0	2.500819	0.564169	-0.276905
4	6	0	2.510129	-1.614302	0.568936

5	1	0	4.404140	-2.624017	0.696480
6	1	0	5.660996	-0.689571	-0.303410
7	1	0	1.929414	-2.445659	0.956453
8	29	0	-0.139115	-0.225428	0.209717
9	6	0	-4.215162	0.152996	0.904363
10	6	0	-2.008916	-0.197462	-0.041916
11	6	0	-4.773630	-0.616542	-0.123202
12	1	0	-4.848412	0.571528	1.681496
13	6	0	-2.576690	-0.926610	-1.100949
14	6	0	-3.958176	-1.156726	-1.121905
15	1	0	-5.847375	-0.776059	-0.155773
16	1	0	-1.961553	-1.331388	-1.900524
17	1	0	-4.393263	-1.741785	-1.927181
18	7	0	0.434732	1.758978	-0.179142
19	7	0	1.823314	-0.513846	0.227176
20	6	0	3.888782	0.516020	-0.502655
21	1	0	4.397343	1.375911	-0.926164
22	6	0	1.712390	1.728325	-0.558070
23	1	0	2.102584	2.530517	-1.179163
24	6	0	-2.835334	0.387422	0.929387
25	1	0	-2.421338	0.992786	1.735313
26	6	0	-0.314677	2.772277	0.123864
27	1	0	0.131072	3.717705	0.430202
28	1	0	-1.392056	2.652154	0.107264

Zero-point correction= 0.217922 (Hartree/Particle)
Thermal correction to Energy= 0.232488
Thermal correction to Enthalpy= 0.233433
Thermal correction to Gibbs Free Energy= 0.174628
Sum of electronic and zero-point Energies= -808.999761
Sum of electronic and thermal Energies= -808.985195
Sum of electronic and thermal Enthalpies= -808.984251
Sum of electronic and thermal Free Energies= -809.043055

BT-TS1

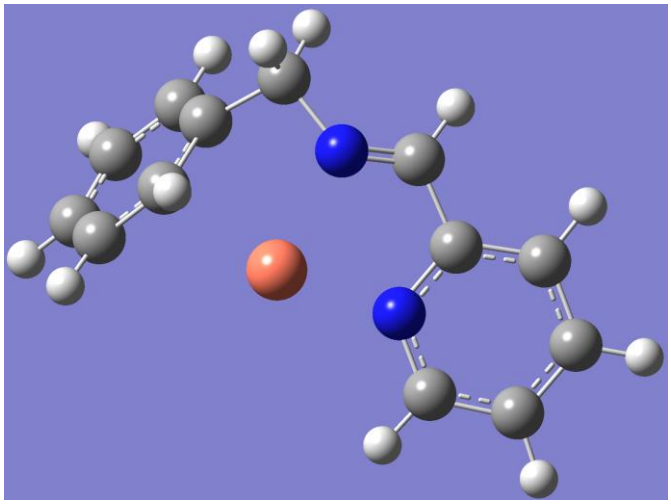


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.020303	-1.517829	-0.022946
2	6	0	-4.477661	-0.369688	0.633012
3	6	0	-2.299440	0.613247	0.315071
4	6	0	-2.697099	-1.559714	-0.457966
5	1	0	-4.666154	-2.374686	-0.178605
6	1	0	-5.499204	-0.312508	0.995218
7	1	0	-2.293466	-2.446413	-0.936607
8	29	0	0.142868	-0.305966	-0.677458
9	6	0	3.333064	-0.629416	1.732051
10	6	0	1.956280	0.121688	-0.107549
11	6	0	4.376494	-0.863355	0.830444
12	1	0	3.465136	-0.835135	2.790136
13	6	0	3.026403	-0.036364	-1.006589
14	6	0	4.226099	-0.573071	-0.533623
15	1	0	5.324316	-1.248890	1.194076
16	1	0	2.924036	0.213154	-2.059864
17	1	0	5.045598	-0.751465	-1.223707
18	7	0	-0.310761	1.624232	-0.399666
19	7	0	-1.845067	-0.535074	-0.287964
20	6	0	-3.609757	0.703244	0.809634
21	1	0	-3.937371	1.614994	1.298519
22	6	0	-1.323835	1.685226	0.439660
23	1	0	-1.372073	2.405136	1.257074
24	6	0	2.123613	-0.096628	1.270106
25	1	0	1.324207	0.121857	1.975079
26	6	0	0.775924	2.401117	-0.473865
27	1	0	1.469611	2.241471	-1.283367
28	1	0	0.824297	3.350642	0.067071

Zero-point correction=	0.217026 (Hartree/Particle)
Thermal correction to Energy=	0.231007
Thermal correction to Enthalpy=	0.231951
Thermal correction to Gibbs Free Energy=	0.174730
Sum of electronic and zero-point Energies=	-808.977202
Sum of electronic and thermal Energies=	-808.963221
Sum of electronic and thermal Enthalpies=	-808.962276
Sum of electronic and thermal Free Energies=	-809.019498

one imaginary frequency, -380.86

P3

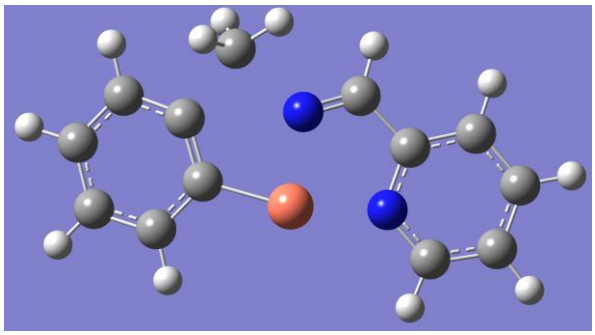


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.055270	-1.230010	0.406209
2	6	0	-4.435879	0.100784	0.565565
3	6	0	-2.154352	0.737999	0.137983
4	6	0	-2.716306	-1.520552	0.131861
5	1	0	-4.770805	-2.038871	0.505342
6	1	0	-5.466029	0.360152	0.787768
7	1	0	-2.378628	-2.546530	0.028356
8	29	0	0.175625	-0.721796	-0.499750
9	6	0	3.641079	-0.060712	1.486915
10	6	0	2.218551	0.954416	-0.197388
11	6	0	3.651309	-1.269474	0.791548
12	1	0	4.185733	0.028967	2.421958
13	6	0	2.255301	-0.269982	-0.931484

14	6	0	2.972127	-1.373330	-0.429737
15	1	0	4.203939	-2.118742	1.180102
16	1	0	1.906698	-0.288410	-1.968036
17	1	0	3.036028	-2.285187	-1.015950
18	7	0	-0.032904	1.376524	-0.658576
19	7	0	-1.780992	-0.567069	0.003174
20	6	0	-3.466915	1.099815	0.436780
21	1	0	-3.724910	2.147788	0.553036
22	6	0	-1.073686	1.744870	-0.019188
23	1	0	-1.192845	2.724765	0.455303
24	6	0	2.913915	1.040979	1.005134
25	1	0	2.888822	1.962164	1.580631
26	6	0	1.269033	2.050456	-0.670980
27	1	0	1.490605	2.352141	-1.701267
28	1	0	1.312093	2.936110	-0.025981

Zero-point correction= 0.221696 (Hartree/Particle)
Thermal correction to Energy= 0.235242
Thermal correction to Enthalpy= 0.236186
Thermal correction to Gibbs Free Energy= 0.180350
Sum of electronic and zero-point Energies= -809.082507
Sum of electronic and thermal Energies= -809.068962
Sum of electronic and thermal Enthalpies= -809.068018
Sum of electronic and thermal Free Energies= -809.123853

MT-TS



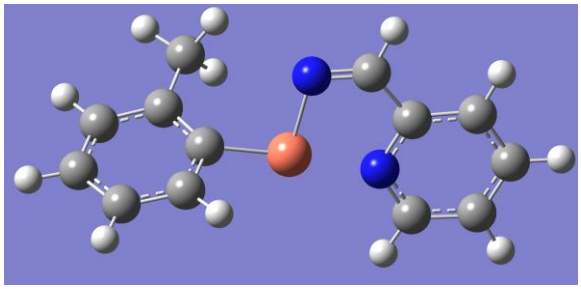
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.310145	-1.097585	-0.208567
2	6	0	4.599917	0.240972	-0.466442

3	6	0	2.274289	0.742387	-0.135701
4	6	0	2.989483	-1.463977	0.066661
5	1	0	5.084611	-1.856352	-0.227591
6	1	0	5.613887	0.553669	-0.694396
7	1	0	2.721052	-2.498314	0.255899
8	29	0	0.017041	-0.740806	0.352381
9	6	0	-3.729618	0.996607	-0.298843
10	6	0	-1.860430	-0.498573	0.117737
11	6	0	-4.560203	-0.109435	-0.502823
12	1	0	-4.115225	2.010449	-0.370114
13	6	0	-2.702224	-1.619088	-0.091059
14	6	0	-4.049932	-1.408216	-0.397151
15	1	0	-5.609254	0.049051	-0.734932
16	1	0	-2.325870	-2.634498	-0.021989
17	1	0	-4.701634	-2.263413	-0.551145
18	7	0	0.043064	1.242519	0.511971
19	7	0	1.991859	-0.569992	0.100536
20	6	0	3.564253	1.180170	-0.430843
21	1	0	3.754274	2.231044	-0.623445
22	6	0	1.132325	1.675036	-0.024136
23	1	0	1.256831	2.696748	-0.382731
24	6	0	-2.400834	0.732054	0.012634
25	6	0	-1.520131	2.330193	0.314414
26	1	0	-2.146606	2.516761	1.191476
27	1	0	-0.680266	3.018268	0.551618
28	1	0	-1.872690	2.749010	-0.634522

Zero-point correction= 0.214405 (Hartree/Particle)
Thermal correction to Energy= 0.228684
Thermal correction to Enthalpy= 0.229629
Thermal correction to Gibbs Free Energy= 0.172744
Sum of electronic and zero-point Energies= -808.898106
Sum of electronic and thermal Energies= -808.883827
Sum of electronic and thermal Enthalpies= -808.882883
Sum of electronic and thermal Free Energies= -808.939767

one imaginary frequency, -681.04

MT-01

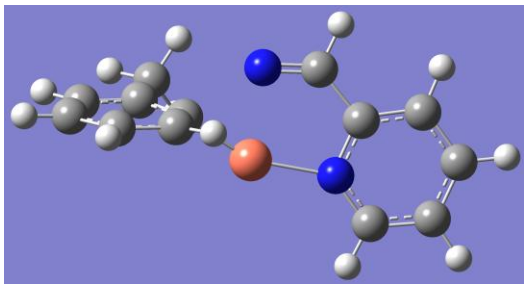


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.113284	-1.207694	-0.883845
2	6	0	4.703806	-0.192425	-0.132804
3	6	0	2.508097	0.559604	0.470951
4	6	0	2.718922	-1.295102	-0.924990
5	1	0	4.712856	-1.925062	-1.433081
6	1	0	5.784291	-0.101274	-0.083482
7	1	0	2.217064	-2.068600	-1.498191
8	29	0	-0.033686	-0.214465	-0.042613
9	6	0	-4.025821	0.372819	-0.679917
10	6	0	-1.872789	-0.135011	0.169104
11	6	0	-4.539894	-0.725538	0.019442
12	1	0	-4.686856	0.979412	-1.293351
13	6	0	-2.365610	-1.173877	0.967024
14	6	0	-3.720163	-1.503551	0.842219
15	1	0	-5.599524	-0.952103	-0.051587
16	1	0	-1.728607	-1.734845	1.645541
17	1	0	-4.125305	-2.338699	1.404989
18	7	0	0.260646	1.331632	1.094071
19	7	0	1.939064	-0.430790	-0.262669
20	6	0	3.887705	0.711080	0.558688
21	1	0	4.312650	1.513655	1.152608
22	6	0	1.527298	1.446114	1.147072
23	1	0	1.921721	2.281956	1.742486
24	6	0	-2.673157	0.738134	-0.586060
25	6	0	-2.135601	1.970244	-1.270869
26	1	0	-1.622182	2.618127	-0.553261
27	1	0	-1.419321	1.712012	-2.059722
28	1	0	-2.944338	2.540255	-1.733072

Zero-point correction= 0.217629 (Hartree/Particle)
Thermal correction to Energy= 0.232388
Thermal correction to Enthalpy= 0.233332

Thermal correction to Gibbs Free Energy=	0.173891
Sum of electronic and zero-point Energies=	-809.003217
Sum of electronic and thermal Energies=	-808.988458
Sum of electronic and thermal Enthalpies=	-808.987514
Sum of electronic and thermal Free Energies=	-809.046955

BT-TS2



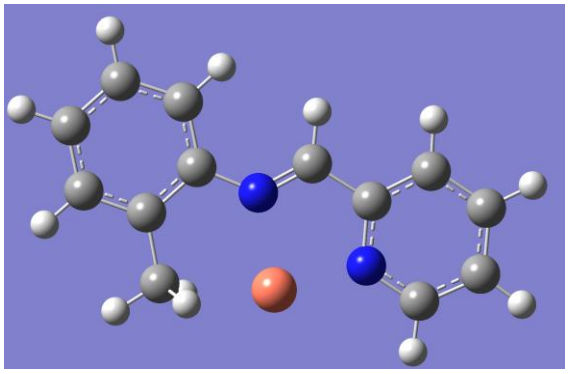
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.287509	-0.800701	-0.744605
2	6	0	4.603459	0.063058	0.302901
3	6	0	2.254672	0.473076	0.598318
4	6	0	2.945054	-0.992667	-1.081114
5	1	0	5.059953	-1.320915	-1.300100
6	1	0	5.637759	0.231316	0.585851
7	1	0	2.653415	-1.653207	-1.891099
8	29	0	-0.002745	-0.366302	-0.463320
9	6	0	-3.933680	0.404205	-0.490757
10	6	0	-1.719168	-0.081071	0.189540
11	6	0	-4.373527	-0.734646	0.194719
12	1	0	-4.650188	1.018618	-1.028966
13	6	0	-2.129081	-1.171891	0.969082
14	6	0	-3.480311	-1.523616	0.926982
15	1	0	-5.428990	-0.988363	0.181777
16	1	0	-1.426561	-1.735680	1.574655
17	1	0	-3.828382	-2.389818	1.480558
18	7	0	-0.164470	1.024369	1.084283
19	7	0	1.956582	-0.369216	-0.425267
20	6	0	3.570330	0.714198	0.986053
21	1	0	3.779610	1.395143	1.804698
22	6	0	1.097341	1.140149	1.263628

23	1	0	1.374502	1.882678	2.027911
24	6	0	-2.588903	0.802748	-0.475951
25	6	0	-2.133009	2.091644	-1.107977
26	1	0	-1.727420	2.760629	-0.340613
27	1	0	-1.347166	1.933277	-1.854269
28	1	0	-2.965837	2.596086	-1.602133

Zero-point correction= 0.217224 (Hartree/Particle)
Thermal correction to Energy= 0.231352
Thermal correction to Enthalpy= 0.232296
Thermal correction to Gibbs Free Energy= 0.174674
Sum of electronic and zero-point Energies= -808.994425
Sum of electronic and thermal Energies= -808.980297
Sum of electronic and thermal Enthalpies= -808.979353
Sum of electronic and thermal Free Energies= -809.036975

one imaginary frequency, -221.15

MT-02



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.533878	0.074207	-0.000097
2	6	0	-4.260243	1.439732	0.000619
3	6	0	-1.907544	0.909711	0.000439
4	6	0	-3.463711	-0.826216	-0.000510
5	1	0	-5.551391	-0.300688	-0.000332
6	1	0	-5.066128	2.166649	0.000954
7	1	0	-3.637226	-1.897210	-0.001049
8	29	0	-0.471153	-1.450387	-0.000927
9	7	0	-2.184998	-0.425921	-0.000252

10	6	0	-2.927887	1.862325	0.000902
11	1	0	-2.678152	2.918673	0.001465
12	6	0	-0.487735	1.321712	0.000714
13	1	0	-0.282646	2.394556	0.001488
14	7	0	0.425524	0.416961	0.000147
15	6	0	1.818916	0.571786	0.000099
16	6	0	2.477696	1.813489	-0.000885
17	6	0	2.562441	-0.636146	0.000840
18	6	0	3.867909	1.865115	-0.001040
19	1	0	1.909311	2.738141	-0.001668
20	6	0	3.957441	-0.558696	0.000658
21	6	0	4.608880	0.677998	-0.000260
22	1	0	4.373557	2.825293	-0.001831
23	1	0	4.544339	-1.472567	0.001240
24	1	0	5.693654	0.714559	-0.000415
25	6	0	1.875939	-1.989233	0.002045
26	1	0	1.273338	-2.154390	0.919990
27	1	0	1.272217	-2.155472	-0.915187
28	1	0	2.599560	-2.808292	0.001821

Zero-point correction= 0.220307 (Hartree/Particle)
Thermal correction to Energy= 0.234267
Thermal correction to Enthalpy= 0.235211
Thermal correction to Gibbs Free Energy= 0.178155
Sum of electronic and zero-point Energies= -809.086791
Sum of electronic and thermal Energies= -809.072831
Sum of electronic and thermal Enthalpies= -809.071886
Sum of electronic and thermal Free Energies= -809.128943