Gas phase Chemistry of *N*-benzylbenzamides with silver(I) cation: Characterization of benzylsilver cation

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Supporting information

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Experimental Section

1. Chemicals

The *N*-benzylbenzamides were synthesized and purified according to previous reported procedures[9]. The structures were confirmed by ^{1}H and ^{13}C NMR spectroscopy and mass spectrometry. *N*-benzylbenzamide, ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.80 (d, 2H), 7.50 (t, 1H), 7.42 (t, 2H), 7.27-7.40 (m, 5H), 6.65 (b, 1H), 4,63 (d, 2H); 13C NMR (CDCl3, 125 MHz): δ 167.64, 138.43, 134.57, 313.75, 128.97, 128.78, 128.10, 127.79, 127.21, 44.31; HRMS calc for $C_{14}H_{14}NO^{+}$([Cmpd **1** + H]$^{+}$): 212.1075, found: 212.1079.

2. Mass Spectrometry

The CID experiments were performed in the positive-ion mode using a Varian 500-MS mass spectrometer equipped with an electrospray source and an ion trap analyzer. Dilute methanol solutions containing samples were introduced to the ion source with a syringe pump at a flow rate of 10 μL min-1 and relevant parameters were set as below: spray chamber temperature, 50 °C; drying gas temperature, 350 °C ; needle voltage, 5000V; capillary voltage, 80 V; spray shield voltage, 600V; RF loading, 85%; scan mode, standard. Nitrogen was used as nebulizing gas at a pressure of 35 psi and drying gas at a pressure of 15 psi. The CID mass spectra were obtained with helium as the collision gas at appropriate collision energy after isolation of the desired precursor ion. Data reported in the article was acquired through a Varian MS Workstation.

A TripleTOF®4600 system with a DuoSpray™ ion source operating was operated in the positive-ion mode for accurate mass spectrometric experiments. The APCI probe of the source was used for fully automatic mass calibration using the Calibrant Delivery System (CDS). A calibration solution matching polarity of ionization was injected during CDS and the mass axis of the TripleTOF® system was correspondingly calibrated in all scan functions used (MS or MS/MS). Solutions were

infused from the ESI source at 10 μl min^{-1} with the parameters: ion spray voltage floating , 5500 V; temperature, 550 °C; curtain gas, 25 psi, ion source gas, 40 psi. The CE was 40 eV, and the CES was 15 eV in the MS/MS experiments.

The accurate mass spectrometric experiments (data in Table S1) were operated in the positive-ion mode of a TripleTOF®4600 system with a DuoSpray™ ion source (AB SCIEX, Foster City, CA, USA). The APCI probe of the source was used for fully automatic mass calibration using the Calibrant Delivery System (CDS). A calibration solution matching polarity of ionization was injected during CDS and the mass axis of the TripleTOF®4600 system was correspondingly calibrated in all scan functions used (MS or MS/MS). Solutions were infused from the ESI source at 10 μl min^{-1} with the parameters: ion spray voltage floating , 5500 V; temperature, 550 °C; curtain gas, 25 psi, ion source gas, 40 psi. Nitrogen was used both as the curtain gas and ion source gas. The CE was 40 eV, and the CES was 15 eV in the MS/MS experiments.

All compounds were purified after synthesis and mixed with 1 equiv of silver nitrate aqueous solution in methanol. The mixtures were infused to the mass spectrometer at a final concentration of approximate 1 μg mL^{-1}, with a syringe pump at a flow rate of 180 μL h^{-1}. All product ion spectra involving Ag^{+} will be those of the ^{107}Ag isotope and no subsequent isotope identification will be made from now on.

3. Theoretical calculations

Theoretical calculations were performed using the Gaussian 03 package of programs. All structures were optimized by density functional theory (DFT) using the RB3LYP hybrid method: LANL2DZ basis set for silver while 6-311+G(*d,p*) basis set for the other atoms. No symmetry constraints were imposed on the optimizations. All optimized structures were subjected to vibrational frequency analysis to ensure they corresponded to either true minima (no imaginary frequencies) or transition states (1 imaginary frequency). The reaction pathways were traced forward and backward by the intrinsic reaction coordinate (IRC) method. Considering the existence of the weakly bonded interactions involved, a vibrational frequency scaling factor of 0.967 is applied to the B3LYP/6-311G+(*d,p*) harmonic vibrational frequencies, which refers the NIST database available on the Internet.[17] All optimized structures were subjected

to vibrational frequency analysis for zero-point energies (ZPE) correction to the temperature at 298.15 K. While the effect of basis set superposition error (BSSE) was analyzed by means of the counterpoise correction method. The energies discussed below are the Gibbs free energies.

Table of accurate masses, Figures of complexes studied and DFT potential surface

Table S1. Accurate masses of the product ions in the fragmentation of the [M + ^{107}Ag]$^+$ ion of Cmpd **1**.

Precursor ions	Product ions	formula	Calculated mass	Measured mass	Error (ppm)
318		$C_{14}H_{13}AgNO^+$	318.0048	318.0052	1.3
	210	$C_{14}H_{12}NO^+$	210.0919	210.0923	1.9
	197	$C_7H_6Ag^+$	196.9520	196.9521	0.5
	107	Ag+	106.9051	106.9045	-5.6
	105	$C_7H_5O^+$	105.0340	105.0339	-1.0
	91	$C_7H_7^+$	91.0548	91.0546	-2.2

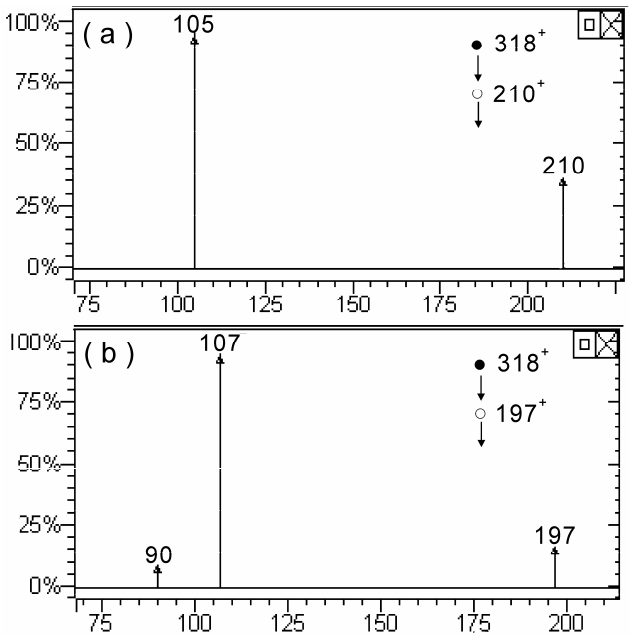


Figure S1. CID spectra of the ion at (a) *m/z* 210 and (b) *m/z* 197 derived from the fragmentation of argentinated *N*-benzylbenzamide.

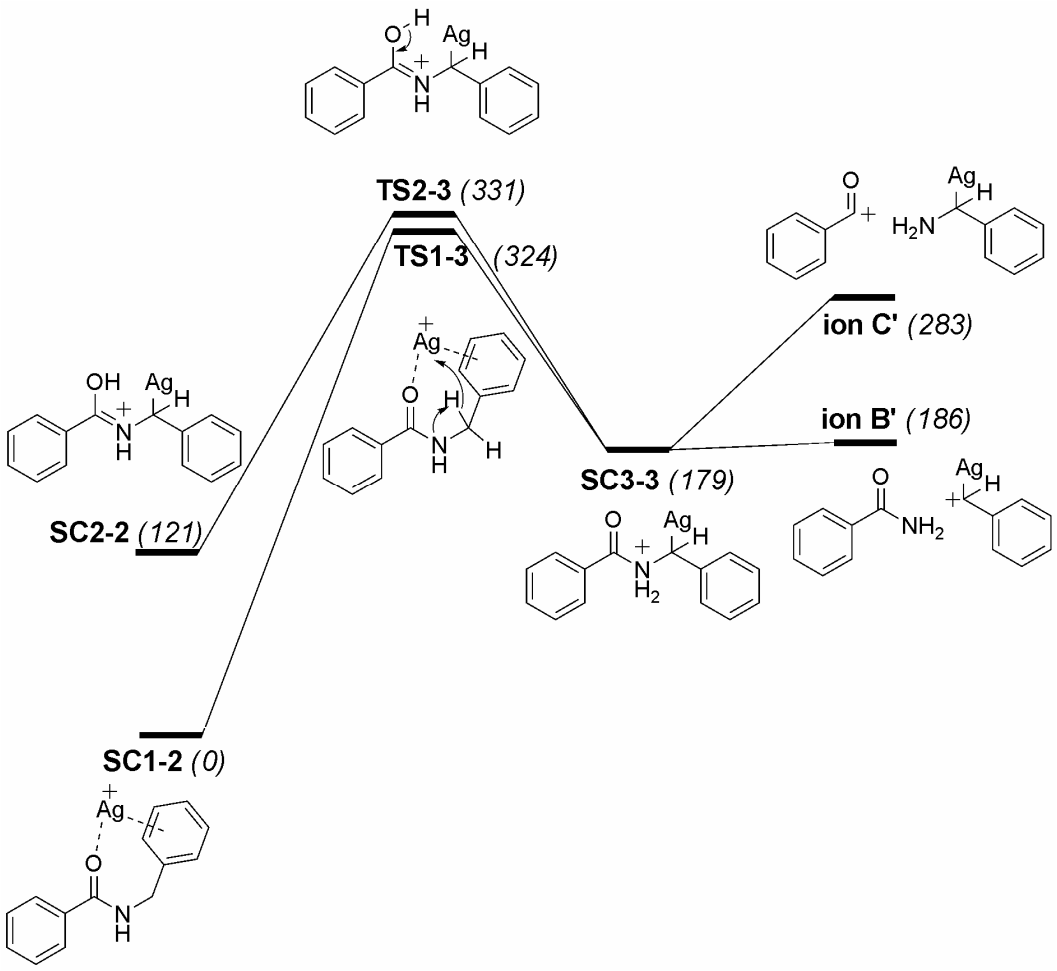
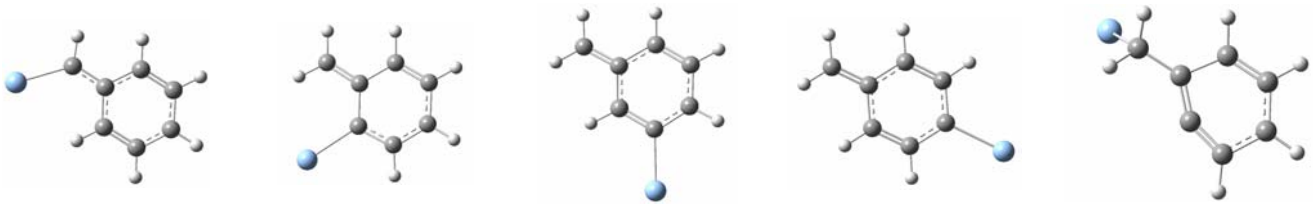


Figure S2. DFT potential energy surfaces of less possible pathways for formation of ion **B** and ion **C**. All energy values are in kJ mol^{-1}.



0 kJ mol^{-1}	25 kJ mol^{-1}	31 kJ mol^{-1}	22 kJ mol^{-1}	177 kJ mol^{-1}
Benzylsilver cation	2-methylphenyl-silver cation	3-methylphenyl-silver cation	4-methylphenyl-silver cation	Phenyl-2-yliummethyl silver

Figure S3. Gibbs free energies of different isomers of $C_7H_6Ag^+$ relative to benzylsilver cation using the theoretical calculation method described above.

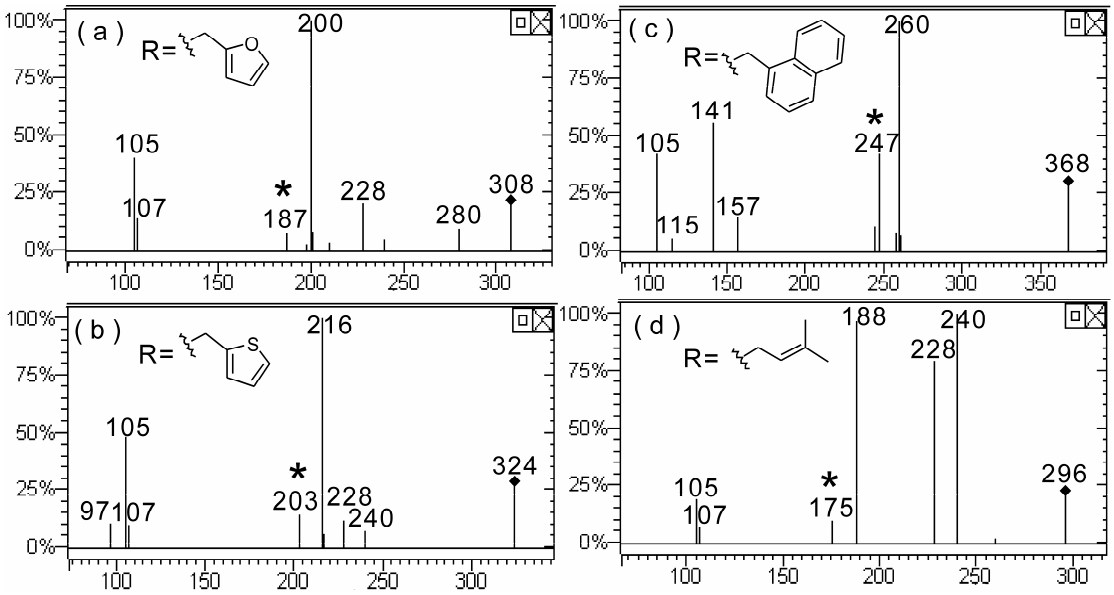
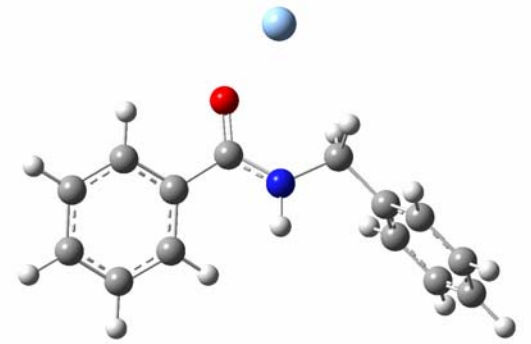


Figure S4. CID mass spectra of argentinated PhCONH-R, with R = (a) furylmehtyl, (b) thienylmethyl, (c) naphthylmethyl and (d) 3-methyl-2-butenyl.

Results of DFT calculations



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	-1.716010	-2.657995	-0.380793
3	6	0	-2.044208	-1.353082	0.016476
4	6	0	-3.358627	-1.056494	0.401540
5	6	0	-4.322945	-2.057070	0.415571
6	6	0	-3.989179	-3.354936	0.029323
7	1	0	-2.432725	-4.655464	-0.693903
8	1	0	-0.720508	-2.902010	-0.735182
9	1	0	-3.610574	-0.045802	0.694736
10	1	0	-5.334747	-1.825705	0.725809
11	1	0	-4.743559	-4.132792	0.035441
12	6	0	-1.042202	-0.258699	0.027365
13	8	0	-1.440360	0.933442	-0.079229
14	7	0	0.250576	-0.578374	0.156250
15	1	0	0.484690	-1.546105	0.326316
16	6	0	1.377785	0.365005	0.119364
17	1	0	1.343300	1.007596	1.007180
18	1	0	1.273899	0.993144	-0.773266
19	6	0	2.694969	-0.374415	0.075556
20	6	0	3.400766	-0.628812	1.255187
21	6	0	3.207722	-0.830235	-1.143928
22	6	0	4.602170	-1.334331	1.217021
23	1	0	3.017192	-0.271507	2.205685

24	6	0	4.407992	-1.535502	-1.181026
25	1	0	2.673783	-0.628645	-2.067387
26	6	0	5.105509	-1.788572	-0.000301
27	1	0	5.145413	-1.523597	2.135213
28	1	0	4.801698	-1.880458	-2.129778
29	1	0	6.041712	-2.333307	-0.030365
30	47	0	-0.680572	2.966613	-0.085582

Zero-point correction= 0.229623 (Hartree/Particle)
Thermal correction to Energy= 0.245616
Thermal correction to Enthalpy= 0.246560
Thermal correction to Gibbs Free Energy= 0.181218
Sum of electronic and zero-point Energies= -816.816527
Sum of electronic and thermal Energies= -816.800534
Sum of electronic and thermal Enthalpies= -816.799590
Sum of electronic and thermal Free Energies= -816.864932
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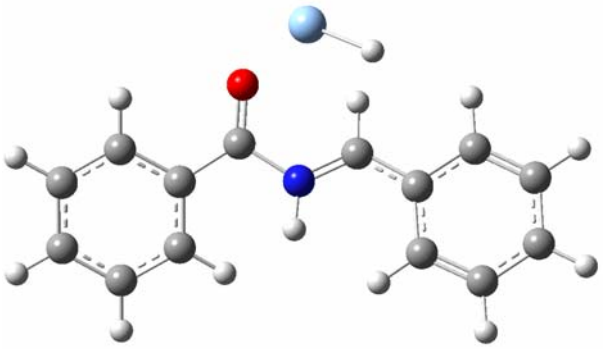
Counterpoise: BSSE energy = 0.000894306530

No imaginary vibrational frequency

TS1-1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.015570	-2.665509	-0.139005
2	6	0	2.760572	-2.116221	0.087005
3	6	0	2.613907	-0.722125	0.207993
4	6	0	3.746159	0.105909	0.111302
5	6	0	4.994719	-0.449796	-0.124981
6	6	0	5.130586	-1.833673	-0.252308
7	1	0	4.128280	-3.739681	-0.218099
8	1	0	1.919391	-2.789452	0.212543
9	1	0	3.627965	1.176409	0.219343

10	1	0	5.863579	0.191347	-0.208414
11	1	0	6.107553	-2.265999	-0.433657
12	6	0	1.326422	-0.071798	0.471295
13	8	0	1.171234	1.067637	0.858706
14	7	0	0.146259	-0.871569	0.207907
15	1	0	0.270663	-1.713761	-0.340952
16	6	0	-1.072620	-0.483071	0.543989
17	1	0	-1.918842	2.324548	-0.996360
18	1	0	-1.111855	0.414095	1.149875
19	6	0	-2.282306	-1.163725	0.233490
20	6	0	-2.343654	-2.328995	-0.568121
21	6	0	-3.474662	-0.634919	0.781717
22	6	0	-3.558680	-2.943664	-0.799019
23	1	0	-1.451179	-2.749951	-1.018361
24	6	0	-4.687638	-1.260580	0.548277
25	1	0	-3.432313	0.270650	1.375614
26	6	0	-4.729773	-2.411902	-0.240195
27	1	0	-3.609356	-3.833065	-1.414517
28	1	0	-5.598796	-0.853988	0.968522
29	1	0	-5.679294	-2.899339	-0.428841
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Zero-point correction= 0.222777 (Hartree/Particle)
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Thermal correction to Enthalpy= 0.240067
Thermal correction to Gibbs Free Energy= 0.174557
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Sum of electronic and thermal Enthalpies= -816.751805
Sum of electronic and thermal Free Energies= -816.817315
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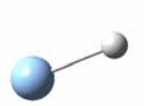
Counterpoise: BSSE energy = 0.002496431065
One imaginary vibrational frequency: -116.524

AgH



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

1	47	0	0.000000	0.000000	0.033886
2	1	0	0.000000	0.000000	-1.592624

Zero-point correction= 0.003762 (Hartree/Particle)
Thermal correction to Energy= 0.006125
Thermal correction to Enthalpy= 0.007069
Thermal correction to Gibbs Free Energy= -0.016144
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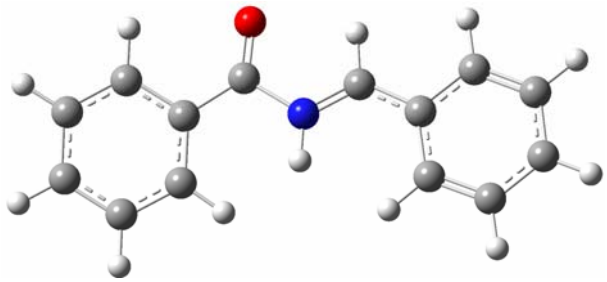
Sum of electronic and thermal Enthalpies= -146.337453
Sum of electronic and thermal Free Energies= -146.360665

No imaginary vibrational frequency

Ion A



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5	6	0	4.840982	-0.323391	0.177286
6	6	0	4.898945	1.065348	0.044942
7	1	0	3.777158	2.883399	-0.226744
8	1	0	1.616242	1.778270	-0.295160
9	1	0	3.555127	-2.048994	0.241964
10	1	0	5.751044	-0.895634	0.308648
11	1	0	5.856469	1.571899	0.073675
12	6	0	1.183807	-1.010550	-0.055560
13	8	0	1.075648	-2.204631	-0.105631
14	7	0	-0.073429	-0.225625	-0.015503
15	1	0	-0.019585	0.784580	0.026503
16	6	0	-1.237570	-0.827096	-0.034297
17	1	0	-1.162723	-1.911418	-0.080195

18	6	0	-2.524007	-0.220107	-0.001748
19	6	0	-2.734712	1.178827	0.057983
20	6	0	-3.639186	-1.090569	-0.032030
21	6	0	-4.020736	1.680368	0.086115
22	1	0	-1.900434	1.871321	0.082342
23	6	0	-4.926306	-0.577526	-0.003412
24	1	0	-3.479826	-2.162025	-0.077790
25	6	0	-5.115784	0.803559	0.055483
26	1	0	-4.186336	2.749450	0.131788
27	1	0	-5.778575	-1.244803	-0.026640
28	1	0	-6.121588	1.206906	0.077949

Zero-point correction= 0.218021 (Hartree/Particle)
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Thermal correction to Enthalpy= 0.231606
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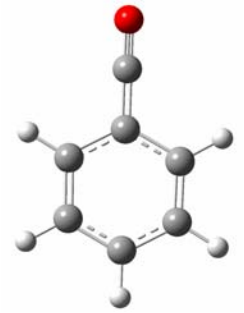
No imaginary vibrational frequency

Ion C



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6	6	0	2.194815	0.000130	0.000019
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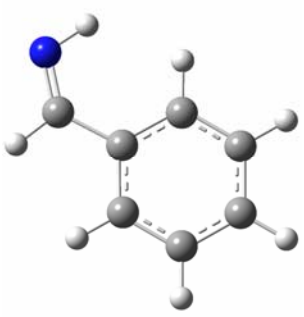
Sum of electronic and thermal Free Energies= -344.713191

No imaginary vibrational frequency



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5	6	0	0.000000	0.570165	0.000000
6	6	0	-1.033222	-0.377573	0.000000
7	6	0	1.325857	0.118290	0.000000
8	6	0	-0.745723	-1.736985	0.000000
9	1	0	-2.069081	-0.054930	0.000000
10	6	0	1.616965	-1.243637	0.000000
11	1	0	2.132475	0.844422	0.000000
12	6	0	0.580698	-2.174526	0.000000
13	1	0	-1.554338	-2.459100	0.000000
14	1	0	2.648424	-1.577134	0.000000

15	1	0	0.801906	-3.235822	0.000000

Zero-point correction= 0.117855 (Hartree/Particle)
Thermal correction to Energy= 0.124634
Thermal correction to Enthalpy= 0.125578
Thermal correction to Gibbs Free Energy= 0.086398
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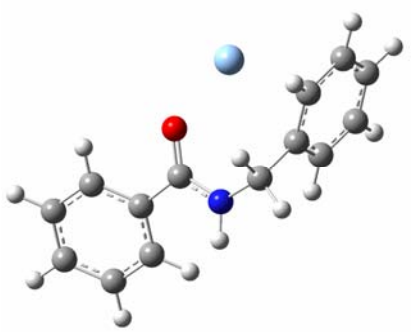
Sum of electronic and thermal Free Energies= -325.695334

No imaginary vibrational frequency

SC1-2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.745789	1.331693	-0.501983
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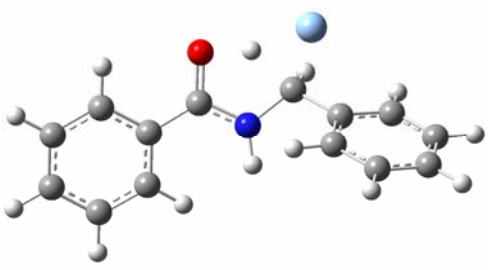
3	6	0	2.741562	0.133134	0.137761
4	6	0	3.422914	-1.079791	-0.031779
5	6	0	4.758390	-1.083311	-0.416615
6	6	0	5.421431	0.120739	-0.651923
7	1	0	5.254844	2.266951	-0.701042
8	1	0	2.900872	2.294241	-0.031381
9	1	0	2.898575	-2.008538	0.151801
10	1	0	5.282568	-2.024118	-0.533922
11	1	0	6.461306	0.116708	-0.956709
12	6	0	1.318924	0.075004	0.563039
13	8	0	0.655678	-0.973323	0.411508
14	7	0	0.779782	1.179042	1.132483
15	1	0	1.407979	1.933592	1.361390
16	6	0	-0.568458	1.233227	1.697930
17	1	0	-0.629756	2.160004	2.273029

18	1	0	-0.700245	0.410994	2.406284
19	6	0	-1.687560	1.208221	0.666087
20	6	0	-1.662409	2.030291	-0.462298
21	6	0	-2.809330	0.368902	0.867191
22	6	0	-2.718381	2.021621	-1.374635
23	1	0	-0.814315	2.684133	-0.630994
24	6	0	-3.864778	0.353315	-0.066114
25	1	0	-2.917960	-0.168026	1.807091
26	6	0	-3.813702	1.179214	-1.188443
27	1	0	-2.684680	2.678673	-2.235763
28	1	0	-4.733757	-0.267692	0.118869
29	1	0	-4.629778	1.178864	-1.900543
30	47	0	-1.488983	-1.428111	-0.151820

Zero-point correction= 0.230090 (Hartree/Particle)
Thermal correction to Energy= 0.245759
Thermal correction to Enthalpy= 0.246703
Thermal correction to Gibbs Free Energy= 0.184131
Sum of electronic and zero-point Energies= -816.834172
Sum of electronic and thermal Energies= -816.818503
Sum of electronic and thermal Enthalpies= -816.817559
Sum of electronic and thermal Free Energies= -816.880131
Counterpoise: corrected energy = -817.062888119177
Counterpoise: BSSE energy = 0.001374135768

No imaginary vibrational frequency

TS1-2

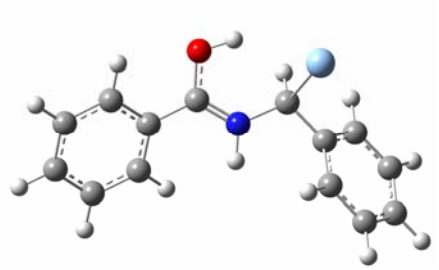


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.810405	1.755955	0.016624
2	6	0	3.502746	1.432447	-0.320384
3	6	0	3.053798	0.107900	-0.196248
4	6	0	3.935045	-0.888150	0.251300
5	6	0	5.240209	-0.555690	0.591471

6	6	0	5.677882	0.763802	0.476659
7	1	0	5.157548	2.776592	-0.087410
8	1	0	2.854670	2.211976	-0.705432
9	1	0	3.586441	-1.909980	0.328377
10	1	0	5.918123	-1.324608	0.941349
11	1	0	6.698131	1.019454	0.737565
12	6	0	1.682714	-0.276821	-0.533913
13	8	0	1.309355	-1.487158	-0.626613
14	7	0	0.698348	0.618496	-0.748837
15	1	0	0.817422	1.607217	-0.577707
16	6	0	-0.609735	0.048761	-1.027627
17	1	0	0.058176	-1.214717	-0.728756
18	1	0	-0.755397	-0.078064	-2.101884
19	6	0	-1.745490	0.854662	-0.422475
20	6	0	-1.732073	1.241735	0.934296
21	6	0	-2.830570	1.248755	-1.221337
22	6	0	-2.780121	1.989482	1.468319
23	1	0	-0.883977	0.984827	1.563203
24	6	0	-3.878773	1.989064	-0.677861
25	1	0	-2.845674	0.986222	-2.273966
26	6	0	-3.857647	2.361654	0.665145
27	1	0	-2.749907	2.286768	2.510007
28	1	0	-4.705801	2.288243	-1.310976
29	1	0	-4.669629	2.945625	1.081009
30	47	0	-1.843697	-1.647938	0.230969

Zero-point correction= 0.224103 (Hartree/Particle)
Thermal correction to Energy= 0.239710
Thermal correction to Enthalpy= 0.240654
Thermal correction to Gibbs Free Energy= 0.177016
Sum of electronic and zero-point Energies= -816.761100
Sum of electronic and thermal Energies= -816.745493
Sum of electronic and thermal Enthalpies= -816.744549
Sum of electronic and thermal Free Energies= -816.808187
Counterpoise: corrected energy = -816.984119507039
Counterpoise: BSSE energy = 0.001083302854
One imaginary vibrational frequency: -1477.72

SC2-2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.327579	2.104907	-0.229058
2	6	0	-3.072214	1.604845	0.084576
3	6	0	-2.884990	0.217748	0.225659
4	6	0	-3.977494	-0.653579	0.072856
5	6	0	-5.228800	-0.142055	-0.244380
6	6	0	-5.405126	1.232936	-0.398774
7	1	0	-4.472051	3.173763	-0.326221
8	1	0	-2.260105	2.302295	0.259255
9	1	0	-3.837357	-1.719700	0.192917
10	1	0	-6.067642	-0.815432	-0.370042
11	1	0	-6.384387	1.628334	-0.641204
12	6	0	-1.574988	-0.339349	0.531041
13	8	0	-1.533674	-1.562130	1.015073
14	7	0	-0.448139	0.310135	0.327650
15	1	0	-0.512600	1.209768	-0.137068
16	6	0	0.890199	-0.137768	0.673172
17	1	0	-0.622772	-1.919971	0.983045
18	1	0	0.920972	-0.396524	1.730934
19	6	0	1.922395	0.883366	0.323357
20	6	0	1.947345	1.512611	-0.932150
21	6	0	2.889368	1.238405	1.274489
22	6	0	2.902913	2.483333	-1.218012
23	1	0	1.241279	1.224924	-1.706333
24	6	0	3.853337	2.198376	0.979206
25	1	0	2.883150	0.768296	2.252379
26	6	0	3.861277	2.827043	-0.264744
27	1	0	2.909468	2.959814	-2.191259
28	1	0	4.592415	2.462309	1.726340
29	1	0	4.610322	3.575756	-0.492254
30	47	0	1.524081	-2.006648	-0.360810

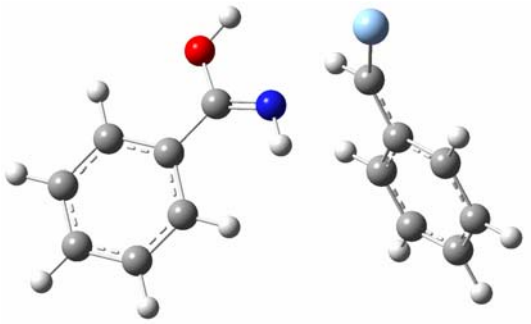
Zero-point correction= 0.229630 (Hartree/Particle)

Thermal correction to Energy= 0.245275

Thermal correction to Enthalpy=	0.246219
Thermal correction to Gibbs Free Energy=	0.183353
Sum of electronic and zero-point Energies=	-816.787659
Sum of electronic and thermal Energies=	-816.772014
Sum of electronic and thermal Enthalpies=	-816.771070
Sum of electronic and thermal Free Energies=	-816.833936

No imaginary vibrational frequency

TS2-2

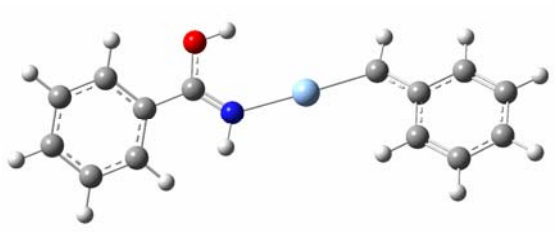


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.158136	1.438991	-1.261450
2	6	0	-2.949101	0.805845	-0.978508
3	6	0	-2.892032	-0.217877	-0.010741
4	6	0	-4.067048	-0.589451	0.673632
5	6	0	-5.274625	0.048045	0.385438
6	6	0	-5.324009	1.059750	-0.581434
7	1	0	-4.194094	2.226746	-2.005533
8	1	0	-2.053193	1.124999	-1.502763
9	1	0	-4.023557	-1.374199	1.417689
10	1	0	-6.175734	-0.245137	0.912099
11	1	0	-6.264290	1.552231	-0.804215
12	6	0	-1.624536	-0.902265	0.285346
13	8	0	-1.678405	-1.678644	1.410088
14	7	0	-0.503324	-0.850403	-0.373712
15	1	0	-0.521241	-0.281250	-1.220174
16	6	0	1.675585	-0.230529	0.832500
17	1	0	-0.863745	-2.209839	1.521240
18	1	0	1.070901	-0.380915	1.731404
19	6	0	1.941924	1.125428	0.513154
20	6	0	2.788997	1.471994	-0.583128
21	6	0	1.411029	2.180414	1.322624
22	6	0	3.086841	2.800187	-0.857142

23	1	0	3.209334	0.673601	-1.186451
24	6	0	1.720668	3.506197	1.048700
25	1	0	0.765828	1.929202	2.158695
26	6	0	2.554884	3.815086	-0.040836
27	1	0	3.734823	3.057679	-1.686773
28	1	0	1.323895	4.301165	1.669367
29	1	0	2.796339	4.851699	-0.251760
30	47	0	2.017077	-1.993934	-0.295882

Zero-point correction= 0.225191 (Hartree/Particle)
Thermal correction to Energy= 0.240872
Thermal correction to Enthalpy= 0.241816
Thermal correction to Gibbs Free Energy= 0.179323
Sum of electronic and zero-point Energies= -816.734813
Sum of electronic and thermal Energies= -816.719132
Sum of electronic and thermal Enthalpies= -816.718188
Sum of electronic and thermal Free Energies= -816.780681
Counterpoise: corrected energy = -816.958225960824
Counterpoise: BSSE energy = 0.001777848945
One imaginary vibrational frequency: -92.7392

SC3-2

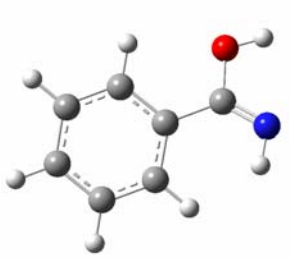


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.419049	1.783177	-0.455526
2	6	0	4.120577	1.291460	-0.465582
3	6	0	3.847976	0.009043	0.035219
4	6	0	4.898603	-0.777251	0.531531
5	6	0	6.194997	-0.275389	0.546278
6	6	0	6.457103	1.002387	0.054984
7	1	0	5.624776	2.769311	-0.853573
8	1	0	3.332778	1.899692	-0.896215
9	1	0	4.694260	-1.769451	0.910904
10	1	0	7.001054	-0.882917	0.939324
11	1	0	7.469491	1.388762	0.062728

12	6	0	2.472613	-0.518763	0.044611
13	8	0	2.405906	-1.845784	0.149349
14	7	0	1.389979	0.186128	-0.030292
15	1	0	1.584490	1.180995	-0.044024
16	6	0	-2.678732	-0.962908	-0.266487
17	1	0	1.484626	-2.132652	0.227792
18	1	0	-2.873908	-2.006324	-0.531124
19	6	0	-3.861397	-0.241938	-0.066198
20	6	0	-3.830667	1.141411	0.291178
21	6	0	-5.136345	-0.875684	-0.213724
22	6	0	-5.000739	1.843909	0.487295
23	1	0	-2.867245	1.624325	0.405553
24	6	0	-6.303117	-0.166376	-0.015410
25	1	0	-5.170076	-1.924904	-0.485144
26	6	0	-6.232250	1.189317	0.333949
27	1	0	-4.976966	2.891961	0.758549
28	1	0	-7.267081	-0.646915	-0.127151
29	1	0	-7.150543	1.745087	0.489571
30	47	0	-0.682314	-0.368680	-0.146652

Zero-point correction= 0.227387 (Hartree/Particle)
Thermal correction to Energy= 0.244001
Thermal correction to Enthalpy= 0.244945
Thermal correction to Gibbs Free Energy= 0.177672
Sum of electronic and zero-point Energies= -816.783508
Sum of electronic and thermal Energies= -816.766895
Sum of electronic and thermal Enthalpies= -816.765950
Sum of electronic and thermal Free Energies= -816.833223
Counterpoise: corrected energy = -817.009129693597
Counterpoise: BSSE energy = 0.001765524321

No imaginary vibrational frequency



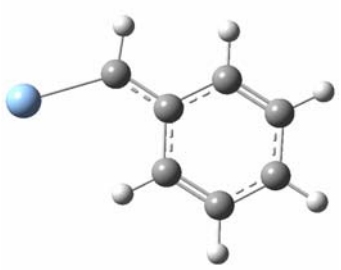
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.918207	1.176402	-0.106790
2	6	0	0.528437	1.220373	-0.113911
3	6	0	-0.222001	0.043076	-0.003013
4	6	0	0.448330	-1.182590	0.099245
5	6	0	1.840099	-1.223962	0.112471
6	6	0	2.578415	-0.046762	0.010114
7	1	0	2.486107	2.094986	-0.199465
8	1	0	0.029043	2.176405	-0.224103
9	1	0	-0.126888	-2.095745	0.173604
10	1	0	2.347847	-2.177711	0.200409
11	1	0	3.661982	-0.080794	0.016620
12	6	0	-1.709823	0.093832	0.012085
13	8	0	-2.271006	-1.118225	-0.234210
14	7	0	-2.476075	1.085783	0.226549
15	1	0	-1.958943	1.935867	0.431308
16	1	0	-3.228559	-0.989898	-0.171747

Zero-point correction= 0.123150 (Hartree/Particle)
Thermal correction to Energy= 0.130679
Thermal correction to Enthalpy= 0.131623
Thermal correction to Gibbs Free Energy= 0.090542
Sum of electronic and zero-point Energies= -400.926236
Sum of electronic and thermal Energies= -400.918707
Sum of electronic and thermal Enthalpies= -400.917763
Sum of electronic and thermal Free Energies= -400.958844

No imaginary vibrational frequency

Ion B



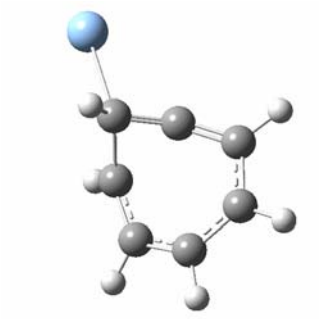
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.679650	-0.550932	-0.000048
2	6	0	2.608794	-1.460402	0.000042
3	6	0	1.317384	-0.984271	0.000041
4	6	0	1.059550	0.425229	0.000106

5	6	0	2.180270	1.323945	-0.000004
6	6	0	3.468838	0.836229	-0.000105
7	1	0	4.695488	-0.931234	-0.000128
8	1	0	2.805297	-2.525166	0.000084
9	1	0	0.474815	-1.665989	0.000110
10	1	0	1.995130	2.392013	-0.000017
11	1	0	4.314782	1.512173	-0.000188
12	6	0	-0.233727	0.930569	0.000254
13	1	0	-0.292989	2.020603	-0.000102
14	47	0	-2.095257	-0.083502	-0.000032

Zero-point correction= 0.102205 (Hartree/Particle)
Thermal correction to Energy= 0.109612
Thermal correction to Enthalpy= 0.110557
Thermal correction to Gibbs Free Energy= 0.068290
Sum of electronic and zero-point Energies= -415.795415
Sum of electronic and thermal Energies= -415.788008
Sum of electronic and thermal Enthalpies= -415.787063
Sum of electronic and thermal Free Energies= -415.829330

No imaginary vibrational frequency

TS3-2



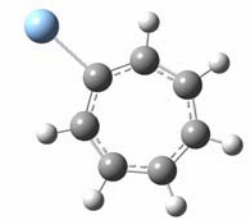
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.367563	-0.451050	0.165778
2	6	0	3.181050	0.919263	0.003040
3	6	0	1.925977	1.519072	-0.248780
4	6	0	0.889541	0.691716	-0.009850
5	6	0	1.001540	-1.146280	-0.243609
6	6	0	2.372122	-1.395157	-0.118798
7	1	0	4.381056	-0.806639	0.307300
8	1	0	4.036945	1.581040	0.078405
9	1	0	1.814399	2.571235	-0.479677

10	1	0	0.463534	-1.723061	-0.987023
11	1	0	2.710269	-2.370665	-0.460788
12	6	0	0.174956	-0.226259	0.653376
13	1	0	0.103225	-0.248504	1.741333
14	47	0	-1.935871	0.032527	-0.029925

Zero-point correction= 0.098937 (Hartree/Particle)
Thermal correction to Energy= 0.106331
Thermal correction to Enthalpy= 0.107276
Thermal correction to Gibbs Free Energy= 0.064929
Sum of electronic and zero-point Energies= -415.723889
Sum of electronic and thermal Energies= -415.716495
Sum of electronic and thermal Enthalpies= -415.715550
Sum of electronic and thermal Free Energies= -415.757897

One imaginary vibrational frequency: -500.133

Ion B’



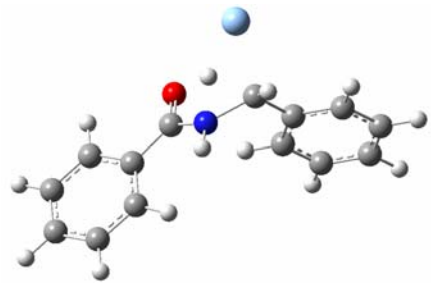
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.318388	0.695771	-0.000393
2	6	0	2.217428	1.557299	0.000406
3	6	0	0.852856	1.251965	0.000297
4	6	0	0.200219	0.000156	0.000258
5	6	0	2.217160	-1.557356	0.000159
6	6	0	3.318250	-0.696036	-0.000541
7	1	0	4.294031	1.173041	-0.000966
8	1	0	2.455930	2.617868	0.000837
9	1	0	0.208630	2.126232	0.000490
10	1	0	2.455451	-2.617975	0.000487
11	1	0	4.293812	-1.173487	-0.001127
12	6	0	0.852619	-1.251762	0.000632
13	1	0	0.208315	-2.125960	0.001205
14	47	0	-1.952717	0.000001	-0.000124

Zero-point correction= 0.108016 (Hartree/Particle)

Thermal correction to Energy=	0.115262
Thermal correction to Enthalpy=	0.116206
Thermal correction to Gibbs Free Energy=	0.074335
Sum of electronic and zero-point Energies=	-414.245129
Sum of electronic and thermal Energies=	-414.237884
Sum of electronic and thermal Enthalpies=	-414.236940
Sum of electronic and thermal Free Energies=	-414.278811

No imaginary vibrational frequency

TS1-3

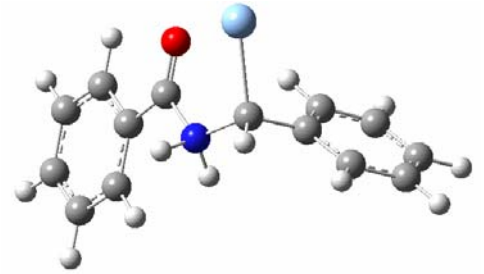


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.535410	1.405345	0.916974
2	6	0	3.188906	1.063042	0.938012
3	6	0	2.691599	0.109801	0.033086
4	6	0	3.559709	-0.478554	-0.902302
5	6	0	4.904534	-0.136916	-0.912085
6	6	0	5.393927	0.801932	-0.002168
7	1	0	4.913325	2.148404	1.608322
8	1	0	2.537872	1.580686	1.634334
9	1	0	3.165658	-1.201907	-1.604651
10	1	0	5.572914	-0.599417	-1.628010
11	1	0	6.443851	1.069910	-0.014186
12	6	0	1.279900	-0.301951	-0.011625
13	8	0	0.751536	-0.894251	-0.935917
14	7	0	0.494600	-0.055042	1.170198
15	1	0	0.947422	0.409906	1.952386
16	6	0	-1.031638	-0.073203	1.163115
17	1	0	-1.329352	-0.147390	2.203289
18	1	0	-0.138931	-1.142056	1.222843
19	6	0	-1.764989	0.987968	0.419174
20	6	0	-1.255532	1.655721	-0.702750
21	6	0	-3.033766	1.346989	0.909307
22	6	0	-1.995353	2.670368	-1.307524
23	1	0	-0.294162	1.392000	-1.120722

24	6	0	-3.769601	2.351111	0.293477
25	1	0	-3.438028	0.846398	1.783461
26	6	0	-3.251981	3.017357	-0.818396
27	1	0	-1.586893	3.184973	-2.169087
28	1	0	-4.741369	2.622874	0.688137
29	1	0	-3.824583	3.802704	-1.296831
30	47	0	-1.583169	-1.977486	-0.086406

Zero-point correction= 0.223517 (Hartree/Particle)
Thermal correction to Energy= 0.239163
Thermal correction to Enthalpy= 0.240107
Thermal correction to Gibbs Free Energy= 0.176488
Sum of electronic and zero-point Energies= -816.709521
Sum of electronic and thermal Energies= -816.693875
Sum of electronic and thermal Enthalpies= -816.692931
Sum of electronic and thermal Free Energies= -816.756549
Counterpoise: corrected energy = -817.040792094776
Counterpoise: BSSE energy = 0.001384897169
One imaginary vibrational frequency: -1624.26

SC3-3

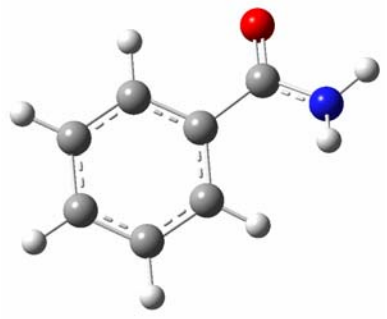


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.481966	1.206247	1.071859
2	6	0	3.157349	0.790741	1.076007
3	6	0	2.675349	-0.032681	0.040552
4	6	0	3.546394	-0.428821	-0.993667
5	6	0	4.866093	-0.005141	-0.990942
6	6	0	5.334864	0.811649	0.040024
7	1	0	4.850438	1.837296	1.870943
8	1	0	2.528646	1.113516	1.897789
9	1	0	3.170709	-1.064201	-1.785440
10	1	0	5.531500	-0.309631	-1.789302
11	1	0	6.367050	1.141657	0.040601

12	6	0	1.304832	-0.537717	-0.037779
13	8	0	0.843119	-1.281007	-0.845127
14	7	0	0.351382	-0.046864	1.117028
15	1	0	0.576502	0.938648	1.293891
16	6	0	-1.164146	-0.174683	0.960977
17	1	0	-1.525827	-0.276485	1.982202
18	1	0	0.634899	-0.572218	1.948996
19	6	0	-1.723378	1.057623	0.326537
20	6	0	-1.275546	1.538846	-0.915242
21	6	0	-2.736517	1.767399	0.990506
22	6	0	-1.811220	2.702509	-1.461373
23	1	0	-0.531003	0.989579	-1.481400
24	6	0	-3.286869	2.917112	0.430711
25	1	0	-3.098835	1.414766	1.950891
26	6	0	-2.821407	3.393201	-0.793670
27	1	0	-1.452382	3.058900	-2.419948
28	1	0	-4.072345	3.446573	0.957145
29	1	0	-3.245462	4.291097	-1.226761
30	47	0	-1.749470	-2.031300	-0.058825

Zero-point correction= 0.229775 (Hartree/Particle)
Thermal correction to Energy= 0.245642
Thermal correction to Enthalpy= 0.246586
Thermal correction to Gibbs Free Energy= 0.181267
Sum of electronic and zero-point Energies= -816.763465
Sum of electronic and thermal Energies= -816.747598
Sum of electronic and thermal Enthalpies= -816.746654
Sum of electronic and thermal Free Energies= -816.811973

No imaginary vibrational frequency



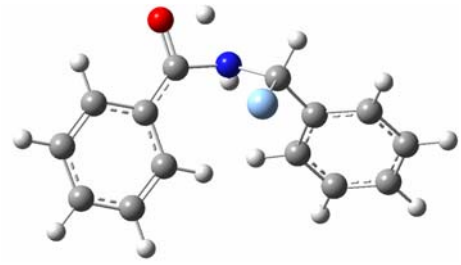
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.516491	-1.205596	0.127331
2	6	0	-0.219613	-0.024685	-0.016677
3	6	0	0.458879	1.191824	-0.157201
4	6	0	1.851508	1.226521	-0.139868
5	6	0	2.577146	0.047671	0.022348
6	6	0	1.906625	-1.168591	0.154661
7	1	0	-0.021377	-2.141591	0.213777
8	1	0	-0.090532	2.112930	-0.316276
9	1	0	2.368852	2.171376	-0.261717
10	1	0	3.660891	0.075837	0.038126
11	1	0	2.468460	-2.087878	0.275066
12	6	0	-1.718689	-0.136696	-0.037501
13	8	0	-2.285066	-1.181225	-0.314810
14	7	0	-2.419043	1.007915	0.252917
15	1	0	-3.419722	0.909346	0.334654
16	1	0	-1.986830	1.771682	0.745872

Zero-point correction= 0.122858 (Hartree/Particle)
Thermal correction to Energy= 0.130657
Thermal correction to Enthalpy= 0.131601
Thermal correction to Gibbs Free Energy= 0.090308
Sum of electronic and zero-point Energies= -400.947400
Sum of electronic and thermal Energies= -400.939601
Sum of electronic and thermal Enthalpies= -400.938657
Sum of electronic and thermal Free Energies= -400.979950

No imaginary vibrational frequency

TS2-3

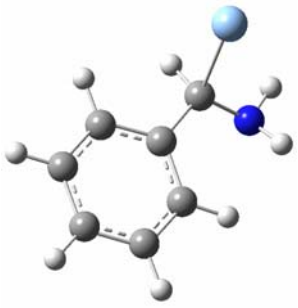


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.494104	1.922029	-1.390192
2	6	0	-1.650305	1.341750	-0.457908
3	6	0	-2.191224	0.528359	0.561640

4	6	0	-3.585203	0.304165	0.623485
5	6	0	-4.416279	0.888228	-0.318030
6	6	0	-3.872969	1.695480	-1.321652
7	1	0	-2.086049	2.551555	-2.171162
8	1	0	-0.583386	1.510397	-0.519881
9	1	0	-3.991271	-0.317411	1.411686
10	1	0	-5.485401	0.722425	-0.272724
11	1	0	-4.527278	2.152921	-2.054791
12	6	0	-1.372295	-0.044067	1.588439
13	8	0	-1.773615	-0.694564	2.589621
14	7	0	0.066451	0.027778	1.805768
15	1	0	0.374757	0.973714	2.051042
16	6	0	1.036350	-0.644755	0.883411
17	1	0	-0.550138	-0.656494	2.836422
18	1	0	1.417955	-1.507473	1.424027
19	6	0	2.155662	0.237067	0.448622
20	6	0	2.058033	1.633342	0.349077
21	6	0	3.393660	-0.359036	0.144285
22	6	0	3.155443	2.405646	-0.034081
23	1	0	1.129775	2.152888	0.568288
24	6	0	4.481482	0.408959	-0.245122
25	1	0	3.502170	-1.436170	0.224138
26	6	0	4.368628	1.798534	-0.338520
27	1	0	3.055900	3.483137	-0.093777
28	1	0	5.425840	-0.074370	-0.466432
29	1	0	5.219682	2.397316	-0.638946
30	47	0	0.094041	-1.686906	-0.821616

Zero-point correction= 0.224596 (Hartree/Particle)
Thermal correction to Energy= 0.240083
Thermal correction to Enthalpy= 0.241028
Thermal correction to Gibbs Free Energy= 0.178302
Sum of electronic and zero-point Energies= -816.707604
Sum of electronic and thermal Energies= -816.692116
Sum of electronic and thermal Enthalpies= -816.691172
Sum of electronic and thermal Free Energies= -816.753897

One imaginary vibrational frequency: -1790.8

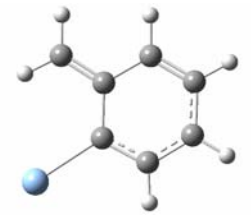


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.577160	2.279617	0.581921
2	1	0	0.517433	2.585453	-0.380247
3	6	0	0.341457	0.887378	0.771917
4	1	0	0.578850	0.605952	1.794279
5	1	0	1.464103	2.577944	0.964511
6	6	0	-0.991012	0.380724	0.362265
7	6	0	-1.819111	1.070754	-0.536116
8	6	0	-1.480929	-0.814878	0.920315
9	6	0	-3.074009	0.571021	-0.881611
10	1	0	-1.496952	2.012561	-0.963961
11	6	0	-2.732512	-1.307511	0.582317
12	1	0	-0.857986	-1.364706	1.619430
13	6	0	-3.538336	-0.620072	-0.330608
14	1	0	-3.694070	1.123261	-1.579540
15	1	0	-3.085524	-2.229609	1.031158
16	1	0	-4.514513	-1.006436	-0.599981
17	47	0	1.847133	-0.452473	-0.240212

Zero-point correction= 0.129937 (Hartree/Particle)
Thermal correction to Energy= 0.138983
Thermal correction to Enthalpy= 0.139927
Thermal correction to Gibbs Free Energy= 0.093578
Sum of electronic and zero-point Energies= -472.022846
Sum of electronic and thermal Energies= -472.013800
Sum of electronic and thermal Enthalpies= -472.012856
Sum of electronic and thermal Free Energies= -472.059205

No imaginary vibrational frequency

2-methylphenylsilver cation

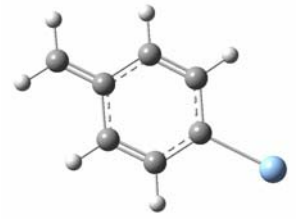


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.419638	-1.521951	0.000635
2	6	0	3.260494	-0.388139	-0.000283
3	6	0	2.687890	0.852361	-0.000891
4	6	0	1.244612	0.988364	-0.000239
5	6	0	0.384958	-0.187332	0.000126
6	6	0	1.021294	-1.421974	0.000195
7	1	0	2.873246	-2.508473	0.001744
8	1	0	4.336266	-0.509197	-0.000462
9	1	0	3.298197	1.748781	-0.001959
10	1	0	0.448543	-2.341091	0.000305
11	47	0	-1.752697	-0.113457	-0.000116
12	6	0	0.718383	2.246710	0.000906
13	1	0	-0.354664	2.405669	0.001988
14	1	0	1.351573	3.128542	0.001147

Zero-point correction= 0.101695 (Hartree/Particle)
Thermal correction to Energy= 0.109358
Thermal correction to Enthalpy= 0.110302
Thermal correction to Gibbs Free Energy= 0.067804
Sum of electronic and zero-point Energies= -415.786055
Sum of electronic and thermal Energies= -415.778392
Sum of electronic and thermal Enthalpies= -415.777447
Sum of electronic and thermal Free Energies= -415.819946

No imaginary vibrational frequency

4-methylphenylsilver cation

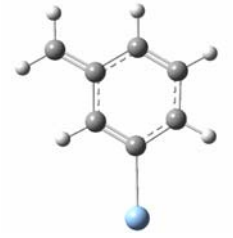


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.819978	1.225457	0.000081
2	6	0	2.189902	1.239209	0.000019
3	6	0	2.927941	-0.000010	-0.000079
4	6	0	2.189863	-1.239213	-0.000026
5	6	0	0.819948	-1.225414	0.000059
6	6	0	0.095895	0.000039	0.000051
7	1	0	0.286485	2.167827	0.000153
8	1	0	2.738969	2.175111	0.000042
9	1	0	2.738915	-2.175125	-0.000099
10	1	0	0.286415	-2.167762	0.000097
11	6	0	4.290830	-0.000031	-0.000141
12	1	0	4.857051	0.925703	-0.000170
13	1	0	4.857024	-0.925783	0.000825
14	47	0	-2.037681	-0.000004	-0.000013

Zero-point correction= 0.101723 (Hartree/Particle)
Thermal correction to Energy= 0.109396
Thermal correction to Enthalpy= 0.110340
Thermal correction to Gibbs Free Energy= 0.067766
Sum of electronic and zero-point Energies= -415.786991
Sum of electronic and thermal Energies= -415.779318
Sum of electronic and thermal Enthalpies= -415.778373
Sum of electronic and thermal Free Energies= -415.820948

No imaginary vibrational frequency

3-methylphenylsilver cation



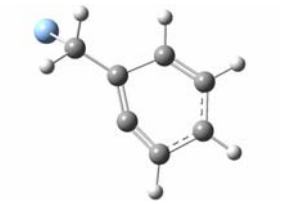
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.707980	1.493143	0.000055
2	6	0	-2.095803	1.769655	-0.000045
3	6	0	-2.990411	0.734111	-0.000009

4	6	0	-2.494052	-0.618596	-0.000043
5	6	0	-1.065435	-0.851763	0.000060
6	6	0	-0.157094	0.188270	0.000048
7	1	0	-0.039977	2.348487	0.000248
8	1	0	-2.436414	2.798005	-0.000090
9	1	0	-4.060301	0.908676	-0.000040
10	6	0	-3.361968	-1.671912	-0.000065
11	1	0	-3.006770	-2.697636	0.000224
12	1	0	-4.437145	-1.522083	0.000151
13	1	0	-0.739926	-1.886644	0.000030
14	47	0	1.956532	-0.132048	-0.000011

Zero-point correction= 0.101486 (Hartree/Particle)
Thermal correction to Energy= 0.109235
Thermal correction to Enthalpy= 0.110179
Thermal correction to Gibbs Free Energy= 0.067571
Sum of electronic and zero-point Energies= -415.783545
Sum of electronic and thermal Energies= -415.775795
Sum of electronic and thermal Enthalpies= -415.774851
Sum of electronic and thermal Free Energies= -415.817460

No imaginary vibrational frequency

Phenyl-2-yliummethyl silver cation



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.715628	-0.092766	-0.438524
2	6	0	3.035106	1.120665	-0.297024
3	6	0	1.729810	1.170594	0.157341
4	6	0	0.945177	-0.007136	0.526964
5	6	0	1.809212	-0.983642	0.244575
6	6	0	3.055415	-1.305273	-0.091918
7	1	0	4.693880	-0.167682	-0.899522
8	1	0	3.545871	2.048117	-0.525881
9	1	0	1.251697	2.113021	0.413434
10	1	0	3.469358	-2.287193	-0.280706

11	6	0	-0.346508	0.040221	1.196255
12	1	0	-0.506691	0.986784	1.705510
13	1	0	-0.519079	-0.806406	1.856296
14	47	0	-2.034002	-0.032822	-0.213939

Zero-point correction= 0.097941 (Hartree/Particle)
Thermal correction to Energy= 0.106208
Thermal correction to Enthalpy= 0.107152
Thermal correction to Gibbs Free Energy= 0.062504
Sum of electronic and zero-point Energies= -415.726265
Sum of electronic and thermal Energies= -415.717998
Sum of electronic and thermal Enthalpies= -415.717054
Sum of electronic and thermal Free Energies= -415.761702

No imaginary vibrational frequency