

Prepared April 10, 2000

## SUPPORTING INFORMATION

For article entitled "Interfacial Electronic Structure in Thiolate Self-assembled Monolayers: Implication for Molecular Electronics" by T. Vondrak, H. Wang, P. Winget, C. J. Cramer, and X.-Y. Zhu

CONTENTS: Absolute energies ( $E_h$ ), geometries, and, for all stationary points, vibrational frequencies ( $\text{cm}^{-1}$ ) and orbital energies ( $E_h$ ).

$\text{C}_6\text{H}_5\text{SCu}$  (neutral)

B3LYP/pVDZ geometry:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-.057773	.772826	.000000
2	6	-.272997	2.165090	.000000
3	6	.804208	3.052984	.000000
4	6	2.120066	2.579371	.000000
5	6	2.343676	1.199820	.000000
6	6	1.269830	.307227	.000000
7	16	-1.504750	-.280204	.000000
8	29	-.698872	-2.274950	.000000
9	1	-1.295618	2.548099	.000000
10	1	.609605	4.128595	.000000
11	1	1.461953	-.770012	.000000
12	1	2.960503	3.276516	.000000
13	1	3.364787	.809706	.000000

Energies:

B3LYP/pVDZ: -2270.21052565

B3LYP/pVDZ+//B3LYP/pVDZ: -2270.24560851

## Frequencies:

	1	2	3
	A"	A'	A"
Frequencies --	31.6023	88.2483	174.8211
Red. masses --	6.3540	11.6960	4.9606
Frc consts --	.0037	.0537	.0893
IR Inten --	4.1460	5.0877	.0069
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	4	5	6
	A'	A'	A"
Frequencies --	246.3673	399.0421	411.8689
Red. masses --	6.3790	12.2785	2.9170
Frc consts --	.2281	1.1519	.2915
IR Inten --	4.0900	2.4474	.0000
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	7	8	9
	A'	A"	A'
Frequencies --	427.0256	480.9171	628.4023
Red. masses --	15.5771	3.1827	6.4031
Frc consts --	1.6736	.4337	1.4898
IR Inten --	4.7782	5.8386	.1039
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	10	11	12
	A'	A"	A"
Frequencies --	700.5127	702.1566	746.7415
Red. masses --	6.6950	2.0562	1.6374
Frc consts --	1.9357	.5973	.5380
IR Inten --	22.1678	12.8581	29.3228
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	13	14	15
	A"	A"	A"
Frequencies --	836.9935	899.7115	971.1080
Red. masses --	1.2602	1.3796	1.3557
Frc consts --	.5201	.6580	.7533
IR Inten --	.8327	.2194	.1940
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

	16	17	18
	A''	A'	A'
Frequencies --	997.6626	1006.2591	1046.4090
Red. masses --	1.2809	6.0706	2.8621
Frc consts --	.7511	3.6216	1.8464
IR Inten --	.0059	1.9022	16.2453
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	19	20	21
	A'	A'	A'
Frequencies --	1094.2766	1105.6249	1166.4712
Red. masses --	1.5713	2.7061	1.0754
Frc consts --	1.1086	1.9490	.8622
IR Inten --	6.5936	43.6001	.5965
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	22	23	24
	A'	A'	A'
Frequencies --	1193.1704	1306.9297	1344.6289
Red. masses --	1.1203	1.7889	3.0721
Frc consts --	.9397	1.8003	3.2726
IR Inten --	1.2339	6.4158	.1318
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	25	26	27
	A'	A'	A'
Frequencies --	1462.9280	1496.1318	1614.1873
Red. masses --	2.3021	2.1478	5.8052
Frc consts --	2.9028	2.8325	8.9120
IR Inten --	6.9517	45.9870	3.4377
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	28	29	30
	A'	A'	A'
Frequencies --	1634.3627	3140.1523	3166.9271
Red. masses --	5.8684	1.0876	1.0850
Frc consts --	9.2356	6.3188	6.4115
IR Inten --	55.8621	17.9321	1.2151
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	31	32	33
	A'	A'	A'
Frequencies --	3175.3417	3188.3471	3198.1335
Red. masses --	1.0909	1.0932	1.0987
Frc consts --	6.4808	6.5473	6.6209
IR Inten --	18.6953	18.9453	19.0949
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

## Orbital energies:

Alpha	occ. eigenvalues	--	-323.06320	-88.86283	-38.86560	-34.08357	-34.08347
Alpha	occ. eigenvalues	--	-34.08260	-10.21831	-10.19107	-10.19043	-10.18917
Alpha	occ. eigenvalues	--	-10.18624	-10.18476	-7.92276	-5.88647	-5.88265
Alpha	occ. eigenvalues	--	-5.87848	-4.32662	-2.82501	-2.81966	-2.81756
Alpha	occ. eigenvalues	--	-.85760	-.76888	-.74610	-.67667	-.60497
Alpha	occ. eigenvalues	--	-.58037	-.50731	-.45377	-.45001	-.41989
Alpha	occ. eigenvalues	--	-.40267	-.37361	-.34841	-.34308	-.32507
Alpha	occ. eigenvalues	--	-.32183	-.30681	-.30642	-.30305	-.28042
Alpha	occ. eigenvalues	--	-.25585	-.25463	-.20313		
Alpha	virt. eigenvalues	--	-.11298	-.02472	-.02384	-.01234	-.00236
Alpha	virt. eigenvalues	--	.00779	.00848	.01365	.02694	.03641
Alpha	virt. eigenvalues	--	.04454	.05831	.06155	.06372	.07377
Alpha	virt. eigenvalues	--	.08308	.09110	.09730	.09748	.09929
Alpha	virt. eigenvalues	--	.10475	.10742	.11315	.11420	.11502
Alpha	virt. eigenvalues	--	.12109	.12835	.13196	.13774	.14799
Alpha	virt. eigenvalues	--	.15780	.16032	.16834	.17546	.17663
Alpha	virt. eigenvalues	--	.18848	.19394	.19908	.20757	.21807
Alpha	virt. eigenvalues	--	.23558	.23676	.24318	.24344	.25112
Alpha	virt. eigenvalues	--	.25873	.26016	.26826	.27043	.27384
Alpha	virt. eigenvalues	--	.27972	.28605	.29098	.30877	.31316
Alpha	virt. eigenvalues	--	.31903	.32348	.32729	.33251	.33912
Alpha	virt. eigenvalues	--	.34428	.35513	.38075	.39396	.39799
Alpha	virt. eigenvalues	--	.41385	.41639	.43314	.43953	.44264
Alpha	virt. eigenvalues	--	.44396	.45897	.46566	.47293	.48436
Alpha	virt. eigenvalues	--	.49024	.52496	.52950	.53948	.54540
Alpha	virt. eigenvalues	--	.54874	.56198	.56794	.57048	.58088
Alpha	virt. eigenvalues	--	.59146	.59796	.60387	.61534	.62492
Alpha	virt. eigenvalues	--	.62776	.64086	.64662	.64968	.66544
Alpha	virt. eigenvalues	--	.66992	.68629	.70765	.73740	.74091
Alpha	virt. eigenvalues	--	.74828	.75125	.75333	.76988	.77027
Alpha	virt. eigenvalues	--	.78224	.78585	.79077	.79769	.82746
Alpha	virt. eigenvalues	--	.83067	.84207	.86335	.89949	.91427
Alpha	virt. eigenvalues	--	.94558	.96767	.96852	.99316	1.00410
Alpha	virt. eigenvalues	--	1.02849	1.06515	1.07469	1.09517	1.11199
Alpha	virt. eigenvalues	--	1.13155	1.21495	1.22862	1.23665	1.25632
Alpha	virt. eigenvalues	--	1.26133	1.28005	1.28036	1.29512	1.30920
Alpha	virt. eigenvalues	--	1.32787	1.34439	1.35670	1.36667	1.39758
Alpha	virt. eigenvalues	--	1.41276	1.42734	1.43739	1.45207	1.45763
Alpha	virt. eigenvalues	--	1.47170	1.48218	1.49258	1.51841	1.52949
Alpha	virt. eigenvalues	--	1.55019	1.56965	1.58473	1.60953	1.63584
Alpha	virt. eigenvalues	--	1.64735	1.65270	1.68691	1.70797	1.72248
Alpha	virt. eigenvalues	--	1.73728	1.74826	1.77240	1.77763	1.78028
Alpha	virt. eigenvalues	--	1.83625	1.83644	1.84490	1.87509	1.89299
Alpha	virt. eigenvalues	--	1.92082	1.93326	1.98158	1.98720	2.00388
Alpha	virt. eigenvalues	--	2.01429	2.02762	2.08440	2.08536	2.09782
Alpha	virt. eigenvalues	--	2.14591	2.15052	2.31607	2.32726	2.37206
Alpha	virt. eigenvalues	--	2.46780	2.49492	2.50968	2.59925	2.63810

Alpha virt. eigenvalues -- 2.69454 2.77209 2.81379 2.85130 2.89106  
 Alpha virt. eigenvalues -- 3.01058 3.08759 3.27090 3.45583 4.22625

**C<sub>6</sub>H<sub>5</sub>SCu** (<sup>1</sup>2A'' radical cation at neutral geometry)

B3LYP/pVDZ+//B3LYP/pVDZ: -2269.9758162

**C<sub>6</sub>H<sub>5</sub>SCu** (<sup>1</sup>2A' radical anion at neutral geometry)

B3LYP/pVDZ+//B3LYP/pVDZ: -2270.2931925

**nC<sub>3</sub>H<sub>7</sub>SCu** (neutral)

B3LYP/pVDZ geometry:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.346057	2.860076	0.000000
2	6	-0.908754	2.329596	0.000000
3	6	-0.852299	0.800077	0.000000
4	16	0.921346	0.236406	0.000000
5	29	0.742457	-1.894690	0.000000
6	1	-0.366443	2.709686	0.883359
7	1	-0.366443	2.709686	-0.883359
8	1	-1.365767	0.404066	-0.890926
9	1	-1.365767	0.404066	0.890926
10	1	-2.363195	3.962120	0.000000
11	1	-2.901257	2.517701	0.890046
12	1	-2.901257	2.517701	-0.890046

Energies:

B3LYP/pVDZ: -2157.08544545

B3LYP/pVDZ+//B3LYP/pVDZ: -2157.1204261

## Frequencies:

	1	2	3
	A''	A'	A''
Frequencies --	41.0504	95.3152	112.5776
Red. masses --	2.1599	6.9408	2.5140
Frc consts --	0.0021	0.0372	0.0188
IR Inten --	1.4369	4.5603	1.3377
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000
	4	5	6
	A'	A''	A'
Frequencies --	225.6863	245.8048	326.5631
Red. masses --	3.9940	1.0936	3.8899
Frc consts --	0.1199	0.0389	0.2444
IR Inten --	0.4219	0.0026	3.3273
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000
	7	8	9
	A'	A'	A''
Frequencies --	417.2881	717.9913	750.4927
Red. masses --	15.3813	4.4621	1.0844
Frc consts --	1.5780	1.3553	0.3598
IR Inten --	4.7977	8.6665	2.9171
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000
	10	11	12
	A''	A'	A''
Frequencies --	853.7262	902.9477	1036.5067
Red. masses --	1.1950	1.9462	1.1509
Frc consts --	0.5131	0.9349	0.7285
IR Inten --	0.0161	2.1595	1.7613
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000
	13	14	15
	A'	A'	A'
Frequencies --	1046.3247	1096.4479	1228.7425
Red. masses --	2.6379	2.0359	1.2564
Frc consts --	1.7015	1.4420	1.1176
IR Inten --	0.0355	9.5509	38.8131
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

	16	17	18
	A"	A"	A'
Frequencies --	1229.6581	1308.3014	1351.2404
Red. masses --	1.4258	1.1053	1.4416
Frc consts --	1.2703	1.1147	1.5508
IR Inten --	0.2263	0.1096	1.7258
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000
	19	20	21
	A'	A'	A'
Frequencies --	1393.9451	1458.6913	1465.4836
Red. masses --	1.2554	1.0844	1.0621
Frc consts --	1.4372	1.3594	1.3439
IR Inten --	1.6340	4.9237	0.2062
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000
	22	23	24
	A"	A'	A'
Frequencies --	1468.6618	1480.6242	3020.2669
Red. masses --	1.0375	1.0845	1.0364
Frc consts --	1.3185	1.4008	5.5704
IR Inten --	6.3424	2.6772	29.2151
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000
	25	26	27
	A'	A'	A"
Frequencies --	3026.6634	3036.1605	3056.7867
Red. masses --	1.0590	1.0572	1.1021
Frc consts --	5.7160	5.7417	6.0674
IR Inten --	10.0697	48.2867	0.5781
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000
	28	29	30
	A"	A'	A"
Frequencies --	3082.9316	3096.5340	3097.4866
Red. masses --	1.1065	1.1012	1.1058
Frc consts --	6.1962	6.2212	6.2508
IR Inten --	0.0527	36.9599	69.3586
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

## Orbital energies:

Alpha occ. eigenvalues --	-323.05257	-88.84768	-38.85571	-34.07384	-34.07345
Alpha occ. eigenvalues --	-34.07243	-10.20268	-10.18097	-10.17675	-7.90729
Alpha occ. eigenvalues --	-5.87089	-5.86788	-5.86250	-4.31583	-2.81469
Alpha occ. eigenvalues --	-2.80847	-2.80626	-0.79245	-0.71342	-0.62228
Alpha occ. eigenvalues --	-0.57228	-0.46200	-0.41857	-0.40277	-0.39056
Alpha occ. eigenvalues --	-0.34531	-0.33261	-0.33064	-0.31311	-0.30763

Alpha occ. eigenvalues --	-0.29502	-0.29496	-0.28734	-0.24214	-0.20852
Alpha virt. eigenvalues --	-0.10374	-0.01896	-0.00306	-0.00273	0.00919
Alpha virt. eigenvalues --	0.01988	0.02278	0.02681	0.04817	0.05239
Alpha virt. eigenvalues --	0.05719	0.06231	0.06905	0.07313	0.08783
Alpha virt. eigenvalues --	0.10323	0.10421	0.10608	0.11615	0.11881
Alpha virt. eigenvalues --	0.12209	0.12490	0.13652	0.13792	0.14366
Alpha virt. eigenvalues --	0.15304	0.16080	0.17032	0.17087	0.18910
Alpha virt. eigenvalues --	0.19172	0.19790	0.20567	0.21792	0.21817
Alpha virt. eigenvalues --	0.23036	0.23247	0.25887	0.26252	0.26506
Alpha virt. eigenvalues --	0.27485	0.27787	0.28492	0.29650	0.32948
Alpha virt. eigenvalues --	0.34682	0.34916	0.35169	0.36097	0.36484
Alpha virt. eigenvalues --	0.36764	0.37092	0.37984	0.38518	0.40140
Alpha virt. eigenvalues --	0.40228	0.40673	0.42999	0.44992	0.45838
Alpha virt. eigenvalues --	0.46428	0.46515	0.47375	0.48377	0.49957
Alpha virt. eigenvalues --	0.50612	0.51022	0.51792	0.53795	0.54040
Alpha virt. eigenvalues --	0.55167	0.56703	0.57952	0.60773	0.64108
Alpha virt. eigenvalues --	0.64809	0.65642	0.66754	0.67154	0.68160
Alpha virt. eigenvalues --	0.68332	0.70505	0.72869	0.73463	0.75761
Alpha virt. eigenvalues --	0.75781	0.79758	0.80264	0.80916	0.85829
Alpha virt. eigenvalues --	0.87965	0.89334	0.92195	0.94098	0.98313
Alpha virt. eigenvalues --	0.99422	1.02600	1.02892	1.03329	1.05717
Alpha virt. eigenvalues --	1.08553	1.11020	1.11277	1.12681	1.16625
Alpha virt. eigenvalues --	1.21029	1.24355	1.24827	1.28104	1.29114
Alpha virt. eigenvalues --	1.30471	1.31257	1.39626	1.41426	1.41758
Alpha virt. eigenvalues --	1.44654	1.55720	1.58655	1.59671	1.62241
Alpha virt. eigenvalues --	1.62929	1.67180	1.70048	1.71053	1.72863
Alpha virt. eigenvalues --	1.78695	1.78705	1.80115	1.80947	1.86010
Alpha virt. eigenvalues --	1.88624	1.89278	1.95040	1.96767	1.96806
Alpha virt. eigenvalues --	2.02208	2.03686	2.05346	2.08159	2.11218
Alpha virt. eigenvalues --	2.13528	2.19774	2.28360	2.34720	2.35421
Alpha virt. eigenvalues --	2.36278	2.43130	2.44995	2.52148	2.53569
Alpha virt. eigenvalues --	2.58595	2.61371	2.74510	2.76660	2.83224
Alpha virt. eigenvalues --	2.84423	2.95543			

$nC_3H_7SCu$  ( $1^2A'$  radical cation at neutral geometry)

B3LYP/pVDZ+//B3LYP/pVDZ: -2156.8317801

$nC_3H_7SCu$  ( $1^2A'$  radical anion at neutral geometry)

B3LYP/pVDZ+//B3LYP/pVDZ: -2157.1581114



**C<sub>6</sub>H<sub>5</sub>SLi** (neutral)

B3LYP/pVDZ geometry:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	.000000	-.226818	-.062525
2	6	.000000	-1.257228	-1.019836
3	6	.000000	-.952653	-2.381403
4	6	.000000	.379994	-2.811252
5	6	.000000	1.403421	-1.859609
6	6	.000000	1.107100	-.492834
7	16	.000000	-.678979	1.679214
8	6	.000000	.818550	2.703014
9	1	.000000	-2.300044	-.691575
10	1	.000000	-1.764076	-3.114198
11	3	.000000	-.176948	4.439225
12	1	.000000	.616086	-3.877700
13	1	.000000	2.448553	-2.181067
14	1	.000000	1.910413	.246129
15	1	-.899093	1.424693	2.489988
16	1	.899093	1.424693	2.489988

Energies:

B3LYP/pVDZ: -676.684945342

B3LYP/pVDZ+//B3LYP/pVDZ: -637.446479537

Frequencies:

	1	2	3
	A"	A'	A"
Frequencies --	10.3164	56.0394	77.6608
Red. masses --	7.1551	7.0294	3.2767
Frc consts --	.0004	.0130	.0116
IR Inten --	54.6585	93.0209	12.9326
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	4	5	6
	A"	A'	A'
Frequencies --	177.0394	180.1959	315.1437
Red. masses --	4.8551	4.5884	5.5105
Frc consts --	.0897	.0878	.3224
IR Inten --	.9677	28.2228	4.2840
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

	7	8	9
	A"	A'	A"
Frequencies --	413.5965	431.4953	474.4085
Red. masses --	2.9311	9.5585	2.7895
Frc consts --	.2954	1.0486	.3699
IR Inten --	.0925	23.9544	.1734
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	10	11	12
	A"	A'	A'
Frequencies --	562.5364	626.1419	633.9288
Red. masses --	1.2254	6.4250	4.2069
Frc consts --	.2285	1.4841	.9961
IR Inten --	70.2545	.9870	46.6347
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	13	14	15
	A'	A'	A"
Frequencies --	662.8206	694.3561	709.9852
Red. masses --	9.5912	6.7474	2.1515
Frc consts --	2.4827	1.9167	.6390
IR Inten --	60.5071	8.5754	15.2794
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	16	17	18
	A"	A"	A"
Frequencies --	754.3278	852.4457	909.7361
Red. masses --	1.5798	1.2507	1.3842
Frc consts --	.5296	.5355	.6750
IR Inten --	28.1074	.0351	.9910
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	19	20	21
	A'	A"	A"
Frequencies --	953.0230	977.9736	997.8191
Red. masses --	1.3190	1.3546	1.2678
Frc consts --	.7058	.7633	.7437
IR Inten --	1.8715	.0012	.1766
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	22	23	24
	A'	A"	A'
Frequencies --	1007.9480	1031.6184	1045.1419
Red. masses --	6.1262	1.0814	2.6465
Frc consts --	3.6671	.6781	1.7032
IR Inten --	.9465	2.6100	13.7697
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

	25	26	27
	A'	A'	A'
Frequencies --	1092.2591	1095.2778	1165.7890
Red. masses --	2.8016	1.5306	1.0804
Frc consts --	1.9693	1.0818	.8651
IR Inten --	20.9338	5.2132	.5063
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	28	29	30
	A'	A'	A'
Frequencies --	1188.2493	1313.2886	1354.7810
Red. masses --	1.1364	1.5666	4.1341
Frc consts --	.9453	1.5920	4.4706
IR Inten --	.2686	4.5118	2.2249
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	31	32	33
	A'	A'	A'
Frequencies --	1400.2749	1465.2559	1499.8957
Red. masses --	1.0861	2.2906	2.1219
Frc consts --	1.2547	2.8975	2.8126
IR Inten --	31.5795	8.3774	36.3276
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	34	35	36
	A'	A'	A'
Frequencies --	1621.1938	1635.0780	3001.3662
Red. masses --	5.9431	5.7528	1.0519
Frc consts --	9.2031	9.0616	5.5827
IR Inten --	2.9572	56.2798	28.5224
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	37	38	39
	A''	A'	A'
Frequencies --	3062.3895	3158.5644	3165.5430
Red. masses --	1.1082	1.0838	1.0873
Frc consts --	6.1235	6.3706	6.4194
IR Inten --	19.2920	4.7770	4.5634
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
	40	41	42
	A'	A'	A'
Frequencies --	3176.8187	3190.1902	3195.9492
Red. masses --	1.0928	1.0936	1.0962
Frc consts --	6.4982	6.5574	6.5970
IR Inten --	28.2043	21.6129	22.2152
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

## Orbital energies:

Alpha occ. eigenvalues	--	-88.81180	-10.20256	-10.18376	-10.18294	-10.17823
Alpha occ. eigenvalues	--	-10.17454	-10.17028	-7.87350	-5.83775	-5.83098
Alpha occ. eigenvalues	--	-5.83091	-2.04417	-.84472	-.75055	-.73548
Alpha occ. eigenvalues	--	-.64871	-.59338	-.56506	-.49494	-.44079
Alpha occ. eigenvalues	--	-.43939	-.40931	-.38023	-.36078	-.33370
Alpha occ. eigenvalues	--	-.31541	-.26943	-.24493	-.22416	-.18350
Alpha virt. eigenvalues	--	-.06410	-.01842	-.01777	-.00274	.00024
Alpha virt. eigenvalues	--	.00229	.00649	.01334	.01863	.02169
Alpha virt. eigenvalues	--	.02580	.03725	.04845	.05092	.06474
Alpha virt. eigenvalues	--	.06623	.07301	.08665	.08984	.09454
Alpha virt. eigenvalues	--	.09664	.10416	.10663	.10889	.11194
Alpha virt. eigenvalues	--	.11867	.11982	.12417	.12427	.13034
Alpha virt. eigenvalues	--	.14400	.15085	.15440	.15944	.16450
Alpha virt. eigenvalues	--	.16546	.17900	.18203	.18839	.19787
Alpha virt. eigenvalues	--	.20813	.22371	.23022	.23876	.24916
Alpha virt. eigenvalues	--	.25198	.25369	.25512	.26348	.27494
Alpha virt. eigenvalues	--	.27765	.28300	.29888	.30434	.31718
Alpha virt. eigenvalues	--	.32285	.32325	.32737	.33108	.33949
Alpha virt. eigenvalues	--	.34489	.35097	.37617	.39513	.41184
Alpha virt. eigenvalues	--	.43323	.43976	.44181	.44799	.44952
Alpha virt. eigenvalues	--	.45564	.46314	.47689	.47900	.49501
Alpha virt. eigenvalues	--	.51703	.51763	.52516	.53861	.55473
Alpha virt. eigenvalues	--	.56334	.57125	.57700	.59216	.59690
Alpha virt. eigenvalues	--	.60365	.60480	.61030	.61908	.62708
Alpha virt. eigenvalues	--	.63662	.64627	.64723	.65335	.66136
Alpha virt. eigenvalues	--	.67358	.69286	.69522	.72790	.73936
Alpha virt. eigenvalues	--	.75699	.75976	.76237	.76383	.76542
Alpha virt. eigenvalues	--	.78306	.78843	.79060	.80263	.81864
Alpha virt. eigenvalues	--	.82738	.83779	.84486	.85784	.86006
Alpha virt. eigenvalues	--	.92380	.93415	.93846	.94935	.99586
Alpha virt. eigenvalues	--	.99621	1.00309	1.07728	1.08611	1.10815
Alpha virt. eigenvalues	--	1.11946	1.13299	1.16077	1.23467	1.24304
Alpha virt. eigenvalues	--	1.28039	1.30489	1.31174	1.33629	1.34178
Alpha virt. eigenvalues	--	1.35202	1.37560	1.39208	1.41893	1.42057
Alpha virt. eigenvalues	--	1.45079	1.47144	1.48192	1.48399	1.48628
Alpha virt. eigenvalues	--	1.49194	1.50222	1.52681	1.55395	1.56149
Alpha virt. eigenvalues	--	1.59279	1.64719	1.65236	1.65511	1.68533
Alpha virt. eigenvalues	--	1.69580	1.71931	1.73105	1.73537	1.76699
Alpha virt. eigenvalues	--	1.77607	1.78732	1.79881	1.84219	1.85007
Alpha virt. eigenvalues	--	1.85336	1.89084	1.89401	1.92941	1.94876
Alpha virt. eigenvalues	--	1.98757	1.99241	2.00265	2.02181	2.03264
Alpha virt. eigenvalues	--	2.08771	2.09180	2.10358	2.15295	2.15731
Alpha virt. eigenvalues	--	2.32636	2.33412	2.37247	2.47442	2.50758
Alpha virt. eigenvalues	--	2.51549	2.60086	2.63717	2.71238	2.78330
Alpha virt. eigenvalues	--	2.81869	2.83962	2.90675	3.01394	3.10248
Alpha virt. eigenvalues	--	3.26807	3.45492	4.20370		

**C<sub>6</sub>H<sub>5</sub>SLi** (<sup>1</sup>2A' radical anion at neutral geometry)

B3LYP/pVDZ+//B3LYP/pVDZ: -637.475836

**C<sub>6</sub>H<sub>5</sub>SLi** (<sup>1</sup>2A'' radical anion at neutral geometry)

B3LYP/pVDZ+//B3LYP/pVDZ: -637.442135462

**1a**

Geometry:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	-1.565496	-.384372	.000000
2	16	0	.000000	1.217098	.000000
3	29	0	.959462	-.806493	.000000
4	6	0	.346561	3.043618	.000000
5	6	0	1.845210	3.339730	.000000
6	6	0	2.138555	4.843848	.000000
7	1	0	-.138348	3.469451	.892726
8	1	0	-.138348	3.469451	-.892726
9	1	0	2.304871	2.864687	-.883846
10	1	0	2.304871	2.864687	.883846
11	1	0	1.712478	5.337466	.889901
12	1	0	1.712478	5.337466	-.889901
13	1	0	3.223871	5.035624	.000000
14	29	0	-.668580	-2.782086	.000000

B3LYP/pVDZ energy: -5437.78876

Orbital energies:

Alpha	occ. eigenvalues	--	-322.99750	-322.99743	-322.98328	-88.83487	-38.79998
Alpha	occ. eigenvalues	--	-38.79990	-38.78565	-34.01850	-34.01839	-34.01747
Alpha	occ. eigenvalues	--	-34.01740	-34.01709	-34.01705	-34.00460	-34.00362
Alpha	occ. eigenvalues	--	-34.00189	-10.20769	-10.18586	-10.18021	-7.89758
Alpha	occ. eigenvalues	--	-5.86200	-5.85696	-5.85337	-4.25981	-4.25968
Alpha	occ. eigenvalues	--	-4.24253	-2.75818	-2.75726	-2.75468	-2.75423
Alpha	occ. eigenvalues	--	-2.75164	-2.75150	-2.74009	-2.73751	-2.73341
Alpha	occ. eigenvalues	--	-.79244	-.71271	-.62444	-.57495	-.46248
Alpha	occ. eigenvalues	--	-.42446	-.40301	-.39071	-.34887	-.34292

Alpha occ. eigenvalues --	-.33140	-.28624	-.27579	-.27141	-.26238
Alpha occ. eigenvalues --	-.25363	-.24932	-.24509	-.24080	-.23787
Alpha occ. eigenvalues --	-.23690	-.22747	-.22579	-.22495	-.22317
Alpha occ. eigenvalues --	-.22260	-.20256	-.19448	-.19346	
Alpha virt. eigenvalues --	-.06959	-.05342	-.00439	.04680	.05072
Alpha virt. eigenvalues --	.07582	.08296	.09717	.10400	.10784
Alpha virt. eigenvalues --	.11386	.11835	.13734	.14354	.15291
Alpha virt. eigenvalues --	.15668	.16160	.17418	.21367	.23342
Alpha virt. eigenvalues --	.27382	.29975	.35089	.36284	.41034
Alpha virt. eigenvalues --	.41052	.43868	.44712	.46233	.56193
Alpha virt. eigenvalues --	.56422	.59205	.59350	.59704	.62878
Alpha virt. eigenvalues --	.64139	.64758	.65587	.66664	.66979
Alpha virt. eigenvalues --	.67912	.70008	.70367	.75601	.77810
Alpha virt. eigenvalues --	.80209	.80919	.86137	.90875	.93214
Alpha virt. eigenvalues --	.95429	.99231	1.01805	1.02794	1.03888
Alpha virt. eigenvalues --	1.05338	1.11962	1.14098	1.16709	1.17986
Alpha virt. eigenvalues --	1.20658	1.20931	1.21941	1.22102	1.24634
Alpha virt. eigenvalues --	1.31438	1.39390	1.42230	1.42629	1.46061
Alpha virt. eigenvalues --	1.48604	1.49706	1.53266	1.59742	1.60631
Alpha virt. eigenvalues --	1.60981	1.62282	1.63708	1.64634	1.68052
Alpha virt. eigenvalues --	1.68328	1.69466	1.71738	1.72317	1.78463
Alpha virt. eigenvalues --	1.83726	1.85619	1.89857	1.93447	2.03641
Alpha virt. eigenvalues --	2.07672	2.12887	2.18428	2.25067	2.25563
Alpha virt. eigenvalues --	2.27601	2.40283	2.40537	2.42928	2.52788
Alpha virt. eigenvalues --	2.56495	2.63257	2.65266		

## 1b

Geometry:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	-0.182943	-0.647710	1.280000
2	16	0	-0.182943	1.193519	0.000000
3	29	0	-0.182943	-0.647710	-1.280000
4	6	0	-0.182943	3.051586	0.000000
5	6	0	1.216672	3.661802	0.000000
6	6	0	1.182332	5.194249	0.000000
7	1	0	-0.755054	3.363415	-0.888423
8	1	0	-0.755054	3.363415	0.888423
9	1	0	1.767924	3.294277	-0.882566
10	1	0	1.767924	3.294277	0.882566
11	1	0	0.659915	5.585859	0.889614
12	1	0	0.659915	5.585859	-0.889614
13	1	0	2.201147	5.614594	0.000000
14	29	0	-0.182943	-2.864710	0.000000

B3LYP/pVDZ energy: -5437.78912

Orbital energies:

Alpha	occ. eigenvalues	--	-322.99748	-322.99745	-322.98349	-88.83567	-38.79995
Alpha	occ. eigenvalues	--	-38.79991	-38.78585	-34.01845	-34.01841	-34.01740
Alpha	occ. eigenvalues	--	-34.01739	-34.01709	-34.01708	-34.00480	-34.00382
Alpha	occ. eigenvalues	--	-34.00211	-10.20793	-10.18282	-10.17904	-7.89826
Alpha	occ. eigenvalues	--	-5.86266	-5.85760	-5.85413	-4.25977	-4.25966
Alpha	occ. eigenvalues	--	-4.24276	-2.75812	-2.75720	-2.75460	-2.75415
Alpha	occ. eigenvalues	--	-2.75164	-2.75155	-2.74031	-2.73774	-2.73366
Alpha	occ. eigenvalues	--	-0.79104	-0.71276	-0.62441	-0.57379	-0.46159
Alpha	occ. eigenvalues	--	-0.42391	-0.40122	-0.39121	-0.34824	-0.34147
Alpha	occ. eigenvalues	--	-0.33034	-0.28563	-0.27585	-0.27153	-0.26228
Alpha	occ. eigenvalues	--	-0.25369	-0.24934	-0.24505	-0.24088	-0.23787
Alpha	occ. eigenvalues	--	-0.23693	-0.22768	-0.22601	-0.22516	-0.22321
Alpha	occ. eigenvalues	--	-0.22281	-0.20219	-0.19586	-0.19365	
Alpha	virt. eigenvalues	--	-0.06950	-0.05394	-0.00455	0.04547	0.05182
Alpha	virt. eigenvalues	--	0.07732	0.08350	0.09609	0.10620	0.10747
Alpha	virt. eigenvalues	--	0.11387	0.11485	0.14014	0.14167	0.15038
Alpha	virt. eigenvalues	--	0.15961	0.16318	0.16727	0.22695	0.24324
Alpha	virt. eigenvalues	--	0.27195	0.28443	0.34960	0.36134	0.41155
Alpha	virt. eigenvalues	--	0.41210	0.42933	0.44602	0.46166	0.55927
Alpha	virt. eigenvalues	--	0.57648	0.58426	0.59693	0.60335	0.62635
Alpha	virt. eigenvalues	--	0.64680	0.64707	0.65795	0.66877	0.66893

Alpha virt. eigenvalues --	0.67816	0.69894	0.71172	0.76228	0.78381
Alpha virt. eigenvalues --	0.78690	0.80224	0.85700	0.90785	0.92937
Alpha virt. eigenvalues --	0.96781	0.99237	1.00588	1.01847	1.05197
Alpha virt. eigenvalues --	1.05598	1.10016	1.14455	1.15554	1.17934
Alpha virt. eigenvalues --	1.20754	1.21604	1.21875	1.22055	1.24995
Alpha virt. eigenvalues --	1.31779	1.42313	1.42382	1.43102	1.43768
Alpha virt. eigenvalues --	1.48537	1.49044	1.51780	1.58356	1.60871
Alpha virt. eigenvalues --	1.60964	1.63373	1.63514	1.64287	1.68475
Alpha virt. eigenvalues --	1.68848	1.70531	1.71464	1.72025	1.78126
Alpha virt. eigenvalues --	1.83412	1.85202	1.92417	1.93755	2.03975
Alpha virt. eigenvalues --	2.07135	2.13575	2.17745	2.24784	2.25380
Alpha virt. eigenvalues --	2.27645	2.40420	2.40532	2.42604	2.52860
Alpha virt. eigenvalues --	2.56725	2.63609	2.65941		

## 1c

Geometry:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	1.914582	-.716187	.000000
2	16	0	.000000	.765502	.000000
3	29	0	-.230459	-1.276446	1.279986
4	6	0	-.501992	2.594642	.000000
5	6	0	-2.016923	2.790066	.000000
6	6	0	-2.417860	4.269371	.000000
7	1	0	-.038215	3.046985	-.891396
8	1	0	-.038215	3.046985	.891396
9	1	0	-2.445974	2.284180	.882540
10	1	0	-2.445974	2.284180	-.882540
11	1	0	-2.026475	4.791606	-.889617
12	1	0	-2.026475	4.791606	.889617
13	1	0	-3.514270	4.385227	.000000
14	29	0	-.230459	-1.276446	-1.279986

B3LYP/pVDZ energy: -5437.76533

Orbital energies:

Alpha occ. eigenvalues --	-322.98170	-322.98168	-322.98145	-88.85147	-38.78352
Alpha occ. eigenvalues --	-38.78350	-38.78325	-34.00219	-34.00216	-34.00191
Alpha occ. eigenvalues --	-34.00169	-34.00167	-34.00141	-33.99996	-33.99995
Alpha occ. eigenvalues --	-33.99972	-10.19934	-10.18474	-10.17883	-7.91185
Alpha occ. eigenvalues --	-5.87556	-5.86966	-5.86965	-4.24417	-4.24403
Alpha occ. eigenvalues --	-4.24389	-2.74275	-2.74146	-2.74134	-2.73891



Alpha occ. eigenvalues --	-2.73881	-2.73835	-2.73659	-2.73644	-2.73633
Alpha occ. eigenvalues --	-.78871	-.71115	-.62800	-.57469	-.46032
Alpha occ. eigenvalues --	-.42339	-.40032	-.38917	-.34871	-.34135
Alpha occ. eigenvalues --	-.33017	-.27721	-.27665	-.26228	-.24790
Alpha occ. eigenvalues --	-.24780	-.23995	-.23728	-.23080	-.23077
Alpha occ. eigenvalues --	-.22522	-.22513	-.22325	-.22321	-.22301
Alpha occ. eigenvalues --	-.21320	-.19792	-.19739	-.16105	
Alpha virt. eigenvalues --	-.06801	-.06773	-.01023	.06219	.07205
Alpha virt. eigenvalues --	.07293	.07893	.08193	.08269	.10454
Alpha virt. eigenvalues --	.11091	.11665	.12681	.15223	.16062
Alpha virt. eigenvalues --	.16301	.17685	.19059	.22656	.23520
Alpha virt. eigenvalues --	.24621	.25325	.36022	.36111	.40487
Alpha virt. eigenvalues --	.41138	.43836	.45057	.45141	.55736
Alpha virt. eigenvalues --	.57535	.57669	.59371	.60647	.63523
Alpha virt. eigenvalues --	.64463	.65295	.65887	.66747	.67527
Alpha virt. eigenvalues --	.68431	.70301	.73749	.74172	.74822
Alpha virt. eigenvalues --	.78065	.80279	.87755	.89403	.94451
Alpha virt. eigenvalues --	.95178	1.00896	1.02636	1.04231	1.04530
Alpha virt. eigenvalues --	1.08589	1.08594	1.15332	1.15661	1.19497
Alpha virt. eigenvalues --	1.19684	1.20391	1.20812	1.22040	1.31276
Alpha virt. eigenvalues --	1.35614	1.36643	1.42332	1.44368	1.47973
Alpha virt. eigenvalues --	1.49419	1.49930	1.51253	1.59309	1.60558
Alpha virt. eigenvalues --	1.61089	1.62380	1.64130	1.68122	1.68263
Alpha virt. eigenvalues --	1.69623	1.70511	1.71799	1.73821	1.77449
Alpha virt. eigenvalues --	1.82638	1.85081	1.90662	1.93324	2.03414
Alpha virt. eigenvalues --	2.07557	2.12943	2.18072	2.25182	2.25253
Alpha virt. eigenvalues --	2.27512	2.40409	2.40536	2.42688	2.52729
Alpha virt. eigenvalues --	2.56472	2.63672	2.65649		

## 2a

Geometry:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	.000000	1.280000	1.212083
2	16	0	.000000	.000000	-.636416
3	29	0	.000000	-1.280000	1.212083
4	6	0	.000000	.000000	-2.425322
5	6	0	.000000	-1.212869	-3.133170
6	6	0	.000000	-1.206889	-4.529794
7	6	0	.000000	1.212869	-3.133170
8	6	0	.000000	1.206889	-4.529794
9	6	0	.000000	.000000	-5.236310
10	1	0	.000000	-2.156790	-2.584829
11	1	0	.000000	-2.157602	-5.069104
12	1	0	.000000	2.156790	-2.584829
13	1	0	.000000	2.157602	-5.069104
14	1	0	.000000	.000000	-6.328307
15	29	0	.000000	.000000	3.429083

B3LYP/pVDZ energy: -5550.91238

Orbital energies:

Alpha	occ. eigenvalues	--	-323.00756	-323.00752	-322.99192	-88.85000	-38.80990
Alpha	occ. eigenvalues	--	-38.80986	-38.79425	-34.02841	-34.02837	-34.02733
Alpha	occ. eigenvalues	--	-34.02732	-34.02710	-34.02709	-34.01320	-34.01223
Alpha	occ. eigenvalues	--	-34.01051	-10.21537	-10.18633	-10.18631	-10.18451
Alpha	occ. eigenvalues	--	-10.18451	-10.18177	-7.91308	-5.87736	-5.87207
Alpha	occ. eigenvalues	--	-5.86931	-4.26999	-4.26988	-4.25127	-2.76840
Alpha	occ. eigenvalues	--	-2.76748	-2.76474	-2.76430	-2.76198	-2.76189
Alpha	occ. eigenvalues	--	-2.74885	-2.74626	-2.74216	-.85169	-.76284
Alpha	occ. eigenvalues	--	-.74023	-.67311	-.59912	-.57666	-.50362
Alpha	occ. eigenvalues	--	-.44835	-.44613	-.41447	-.41003	-.36760
Alpha	occ. eigenvalues	--	-.34637	-.34043	-.29926	-.29476	-.28550
Alpha	occ. eigenvalues	--	-.27288	-.26522	-.25901	-.25843	-.25507
Alpha	occ. eigenvalues	--	-.25133	-.24805	-.24790	-.24731	-.23626
Alpha	occ. eigenvalues	--	-.23409	-.23382	-.23290	-.23160	-.21430
Alpha	occ. eigenvalues	--	-.20350	-.19319			
Alpha	virt. eigenvalues	--	-.07815	-.06039	-.01064	-.00408	-.00071
Alpha	virt. eigenvalues	--	.04494	.05301	.07260	.08368	.09840
Alpha	virt. eigenvalues	--	.10433	.11133	.11147	.12999	.13656
Alpha	virt. eigenvalues	--	.14412	.15448	.15977	.17026	.23977
Alpha	virt. eigenvalues	--	.24610	.29028	.29586	.30737	.33336

Alpha virt. eigenvalues --	.35394	.35404	.42378	.43338	.46872
Alpha virt. eigenvalues --	.47693	.50688	.50765	.51108	.51954
Alpha virt. eigenvalues --	.52264	.52677	.53045	.56309	.57477
Alpha virt. eigenvalues --	.57992	.59399	.60811	.64596	.64598
Alpha virt. eigenvalues --	.64709	.66635	.66675	.70591	.71560
Alpha virt. eigenvalues --	.73343	.76690	.79892	.84572	.85616
Alpha virt. eigenvalues --	.88672	.89512	.89553	.92799	.92902
Alpha virt. eigenvalues --	.93003	.97119	1.00297	1.00459	1.00861
Alpha virt. eigenvalues --	1.01255	1.01753	1.04024	1.04640	1.04687
Alpha virt. eigenvalues --	1.06063	1.07662	1.08818	1.10281	1.16380
Alpha virt. eigenvalues --	1.17026	1.17858	1.21013	1.21142	1.24551
Alpha virt. eigenvalues --	1.28292	1.30335	1.37212	1.42981	1.43922
Alpha virt. eigenvalues --	1.47357	1.47780	1.49592	1.51339	1.52557
Alpha virt. eigenvalues --	1.53558	1.56253	1.58257	1.61313	1.61446
Alpha virt. eigenvalues --	1.65441	1.65548	1.67584	1.68277	1.71139
Alpha virt. eigenvalues --	1.75235	1.78341	1.78425	1.79441	1.84427
Alpha virt. eigenvalues --	1.84781	1.86414	1.86622	1.90536	1.94972
Alpha virt. eigenvalues --	1.97944	1.99581	2.01545	2.11011	2.19478
Alpha virt. eigenvalues --	2.21847	2.33419	2.37620	2.42601	2.42683
Alpha virt. eigenvalues --	2.51724	2.62250	2.69635	2.74290	2.77835
Alpha virt. eigenvalues --	2.89609	3.50466			

## 2b

Geometry:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	-1.280000	.000000	1.217702
2	16	0	.000000	.000000	-.640163
3	29	0	1.280000	.000000	1.217702
4	6	0	.000000	.000000	-2.436430
5	6	0	.000000	1.212969	-3.143980
6	6	0	.000000	1.208848	-4.541031
7	6	0	.000000	-1.212969	-3.143980
8	6	0	.000000	-1.208848	-4.541031
9	6	0	.000000	.000000	-5.244576
10	1	0	.000000	2.153826	-2.591030
11	1	0	.000000	2.158108	-5.082679
12	1	0	.000000	-2.153826	-2.591030
13	1	0	.000000	-2.158108	-5.082679
14	1	0	.000000	.000000	-6.336885
15	29	0	.000000	.000000	3.434702

B3LYP/pVDZ energy: -5550.91205

## Orbital energies:

Alpha	occ. eigenvalues	--	-323.00303	-323.00300	-322.98887	-88.84531	-38.80534
Alpha	occ. eigenvalues	--	-38.80531	-38.79119	-34.02386	-34.02381	-34.02281
Alpha	occ. eigenvalues	--	-34.02280	-34.02250	-34.02249	-34.01011	-34.00915
Alpha	occ. eigenvalues	--	-34.00748	-10.21433	-10.18914	-10.18905	-10.18800
Alpha	occ. eigenvalues	--	-10.18755	-10.18755	-7.90810	-5.87253	-5.86746
Alpha	occ. eigenvalues	--	-5.86384	-4.26549	-4.26537	-4.24827	-2.76383
Alpha	occ. eigenvalues	--	-2.76291	-2.76036	-2.75992	-2.75745	-2.75736
Alpha	occ. eigenvalues	--	-2.74582	-2.74323	-2.73923	-.85387	-.76282
Alpha	occ. eigenvalues	--	-.74290	-.67151	-.60105	-.57800	-.50552
Alpha	occ. eigenvalues	--	-.44919	-.44790	-.41665	-.40972	-.37100
Alpha	occ. eigenvalues	--	-.34738	-.34194	-.30698	-.28150	-.27849
Alpha	occ. eigenvalues	--	-.26851	-.25957	-.25847	-.25267	-.25096
Alpha	occ. eigenvalues	--	-.25059	-.24708	-.24366	-.24240	-.23316
Alpha	occ. eigenvalues	--	-.23176	-.23074	-.22850	-.22724	-.20574
Alpha	occ. eigenvalues	--	-.20127	-.20063			
Alpha	virt. eigenvalues	--	-.07680	-.05880	-.00625	-.00342	-.00306
Alpha	virt. eigenvalues	--	.04017	.05120	.08139	.08182	.10246
Alpha	virt. eigenvalues	--	.10365	.10740	.11181	.13377	.14022
Alpha	virt. eigenvalues	--	.14633	.15460	.15624	.15945	.25819
Alpha	virt. eigenvalues	--	.28373	.28615	.29047	.29968	.30042
Alpha	virt. eigenvalues	--	.35233	.36078	.41078	.41706	.46973
Alpha	virt. eigenvalues	--	.47539	.48422	.50614	.51214	.51301
Alpha	virt. eigenvalues	--	.52031	.52446	.52658	.52813	.57949
Alpha	virt. eigenvalues	--	.58914	.60863	.61590	.63958	.64610
Alpha	virt. eigenvalues	--	.64870	.66038	.69081	.70120	.70484
Alpha	virt. eigenvalues	--	.73522	.77684	.78806	.85521	.85636
Alpha	virt. eigenvalues	--	.88467	.89407	.89554	.92545	.92614
Alpha	virt. eigenvalues	--	.93824	.97185	.99913	1.00152	1.00878
Alpha	virt. eigenvalues	--	1.01224	1.01448	1.01487	1.04553	1.04642
Alpha	virt. eigenvalues	--	1.05157	1.07419	1.10395	1.10678	1.17309
Alpha	virt. eigenvalues	--	1.17689	1.18529	1.19976	1.21392	1.24416
Alpha	virt. eigenvalues	--	1.27908	1.29667	1.37077	1.42665	1.44495
Alpha	virt. eigenvalues	--	1.47543	1.48098	1.48538	1.49414	1.51585
Alpha	virt. eigenvalues	--	1.52882	1.58743	1.59000	1.60989	1.61150
Alpha	virt. eigenvalues	--	1.64226	1.65326	1.68037	1.68044	1.70689
Alpha	virt. eigenvalues	--	1.74635	1.76330	1.78045	1.79273	1.84056
Alpha	virt. eigenvalues	--	1.84331	1.85564	1.86377	1.90801	1.93418
Alpha	virt. eigenvalues	--	1.97798	1.99181	1.99337	2.10579	2.19176
Alpha	virt. eigenvalues	--	2.21731	2.32290	2.37358	2.42209	2.42403
Alpha	virt. eigenvalues	--	2.50657	2.62195	2.69433	2.73822	2.77551
Alpha	virt. eigenvalues	--	2.89440	3.50260			

2c

Geometry:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	1.411413	-1.760985	.000000
2	16	0	.000000	.245509	.000000
3	29	0	-.804337	-1.686533	1.279986
4	6	0	.078583	2.069217	.000000
5	6	0	-1.102654	2.828500	.000000
6	6	0	-1.041507	4.224004	.000000
7	6	0	1.318626	2.727374	.000000
8	6	0	1.373522	4.123692	.000000
9	6	0	.195513	4.877321	.000000
10	1	0	-2.068911	2.319867	.000000
11	1	0	-1.967489	4.804856	.000000
12	1	0	2.238882	2.139800	.000000
13	1	0	2.344603	4.625492	.000000
14	1	0	.240968	5.968677	.000000
15	29	0	-.804337	-1.686533	-1.279986

B3LYP/pVDZ energy: -5550.88757

Orbital energies:

Alpha	occ. eigenvalues	--	-322.98757	-322.98678	-322.98676	-88.85846	-38.78923
Alpha	occ. eigenvalues	--	-38.78848	-38.78845	-34.00792	-34.00744	-34.00715
Alpha	occ. eigenvalues	--	-34.00711	-34.00669	-34.00667	-34.00565	-34.00492
Alpha	occ. eigenvalues	--	-34.00491	-10.20700	-10.18855	-10.18849	-10.18726
Alpha	occ. eigenvalues	--	-10.18711	-10.18670	-7.91893	-5.88278	-5.87683
Alpha	occ. eigenvalues	--	-5.87646	-4.25010	-4.24932	-4.24921	-2.74840
Alpha	occ. eigenvalues	--	-2.74707	-2.74666	-2.74490	-2.74423	-2.74384
Alpha	occ. eigenvalues	--	-2.74242	-2.74166	-2.74155	-.85217	-.76015
Alpha	occ. eigenvalues	--	-.74209	-.67259	-.60018	-.57827	-.50520
Alpha	occ. eigenvalues	--	-.44858	-.44667	-.41622	-.40835	-.36878
Alpha	occ. eigenvalues	--	-.34722	-.34129	-.29808	-.28254	-.26832
Alpha	occ. eigenvalues	--	-.25669	-.25333	-.25013	-.24620	-.24610
Alpha	occ. eigenvalues	--	-.24327	-.23637	-.23499	-.23114	-.23043
Alpha	occ. eigenvalues	--	-.22893	-.22865	-.22836	-.21867	-.20552
Alpha	occ. eigenvalues	--	-.19718	-.17003			
Alpha	virt. eigenvalues	--	-.07578	-.07453	-.01194	-.00304	.00018
Alpha	virt. eigenvalues	--	.06221	.06797	.07159	.07796	.08293
Alpha	virt. eigenvalues	--	.08529	.10686	.11441	.12079	.14714
Alpha	virt. eigenvalues	--	.14740	.15706	.17651	.19542	.21813
Alpha	virt. eigenvalues	--	.24787	.28601	.28702	.29862	.30452

Alpha virt. eigenvalues --	.36426	.36582	.41322	.42756	.46955
Alpha virt. eigenvalues --	.47176	.49884	.50181	.51169	.51612
Alpha virt. eigenvalues --	.52004	.52095	.52677	.54205	.57519
Alpha virt. eigenvalues --	.58859	.60049	.62674	.63771	.64586
Alpha virt. eigenvalues --	.65975	.66142	.68790	.71226	.71952
Alpha virt. eigenvalues --	.73072	.73547	.79251	.84463	.84966
Alpha virt. eigenvalues --	.88289	.89325	.89393	.91302	.92689
Alpha virt. eigenvalues --	.92825	.99036	1.00936	1.01042	1.01366
Alpha virt. eigenvalues --	1.01431	1.01782	1.04436	1.04531	1.05375
Alpha virt. eigenvalues --	1.07456	1.07822	1.08781	1.13446	1.15120
Alpha virt. eigenvalues --	1.17149	1.17957	1.19119	1.19180	1.27559
Alpha virt. eigenvalues --	1.30122	1.35788	1.36571	1.39935	1.47501
Alpha virt. eigenvalues --	1.47608	1.49199	1.49449	1.50715	1.51483
Alpha virt. eigenvalues --	1.52736	1.56833	1.59114	1.61035	1.63686
Alpha virt. eigenvalues --	1.64960	1.65223	1.68071	1.69221	1.71958
Alpha virt. eigenvalues --	1.75805	1.77072	1.78000	1.79309	1.84174
Alpha virt. eigenvalues --	1.84421	1.85855	1.86204	1.90360	1.94352
Alpha virt. eigenvalues --	1.97742	1.99166	2.00394	2.09556	2.19263
Alpha virt. eigenvalues --	2.21501	2.31848	2.37292	2.42337	2.42389
Alpha virt. eigenvalues --	2.50986	2.62159	2.69302	2.73795	2.77022
Alpha virt. eigenvalues --	2.89432	3.49407			