HyperChem log start -- Mon Oct 28 14:21:01 2019.

Geometry optimization, SemiEmpirical, molecule = Анилин.hin.

PM3

PolakRibiere optimizer

Convergence limit = 0.0100000 Iteration limit = 50

Accelerate convergence = YES

Optimization algorithm = Polak-Ribiere

Criterion of RMS gradient = 0.1000 kcal/(A mol) Maximum cycles = 210

RHF Calculation:

Singlet state calculation

Number of electrons = 36

Number of Double Occupied Levels = 18

Charge on the System = 0

Total Orbitals = 35

Starting PM3 calculation with 35 orbitals

E=0.0000 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=1 Diff=6834.19990]

E=0.0000 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=2 Diff=35.34632]

E=0.0000 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=3 Diff=6.18747]

E=0.0000 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=4 Diff=1.40873]

E=0.0000 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=5 Diff=0.11620]

E=0.0000 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=6 Diff=0.00266]

E=-1471.8729 kcal/mol Grad=17.921 Conv=NO(0 cycles 1 points) [Iter=1 Diff=3.69839]

E=-1471.8729 kcal/mol Grad=17.921 Conv=NO(0 cycles 1 points) [Iter=2 Diff=0.48965]

E=-1471.8729 kcal/mol Grad=17.921 Conv=NO(0 cycles 1 points) [Iter=3 Diff=0.10927]

E=-1471.8729 kcal/mol Grad=17.921 Conv=NO(0 cycles 1 points) [Iter=4 Diff=0.04581]

E=-1471.8729 kcal/mol Grad=17.921 Conv=NO(0 cycles 1 points) [Iter=5 Diff=0.00380]

E=-1469.9789 kcal/mol Grad=24.371 Conv=NO(0 cycles 2 points) [Iter=1 Diff=1.20666]

E=-1469.9789 kcal/mol Grad=24.371 Conv=NO(0 cycles 2 points) [Iter=2 Diff=0.16645]

E=-1469.9789 kcal/mol Grad=24.371 Conv=NO(0 cycles 2 points) [Iter=3 Diff=0.03662]

E=-1469.9789 kcal/mol Grad=24.371 Conv=NO(0 cycles 2 points) [Iter=4 Diff=0.01442]

E=-1469.9789 kcal/mol Grad=24.371 Conv=NO(0 cycles 2 points) [Iter=5 Diff=0.00111]

E=-1474.6005 kcal/mol Grad=6.782 Conv=NO(1 cycles 3 points) [Iter=1 Diff=0.04577]

E=-1474.6005 kcal/mol Grad=6.782 Conv=NO(1 cycles 3 points) [Iter=2 Diff=0.00589]

E=-1475.3118 kcal/mol Grad=4.870 Conv=NO(1 cycles 4 points) [Iter=1 Diff=0.04592]

E=-1475.3118 kcal/mol Grad=4.870 Conv=NO(1 cycles 4 points) [Iter=2 Diff=0.00605]

E=-1475.6460 kcal/mol Grad=5.633 Conv=NO(1 cycles 5 points) [Iter=1 Diff=0.18287]

E=-1475.6460 kcal/mol Grad=5.633 Conv=NO(1 cycles 5 points) [Iter=2 Diff=0.02394]

E=-1475.6460 kcal/mol Grad=5.633 Conv=NO(1 cycles 5 points) [Iter=3 Diff=0.00478]

E=-1475.1892 kcal/mol Grad=11.607 Conv=NO(1 cycles 6 points) [Iter=1 Diff=0.11810]

E=-1475.1892 kcal/mol Grad=11.607 Conv=NO(1 cycles 6 points) [Iter=2 Diff=0.01528]

E=-1475.1892 kcal/mol Grad=11.607 Conv=NO(1 cycles 6 points) [Iter=3 Diff=0.00300]

E=-1475.6748 kcal/mol Grad=6.543 Conv=NO(2 cycles 7 points) [Iter=1 Diff=0.45309]

E=-1475.6748 kcal/mol Grad=6.543 Conv=NO(2 cycles 7 points) [Iter=2 Diff=0.05804]

E=-1475.6748 kcal/mol Grad=6.543 Conv=NO(2 cycles 7 points) [Iter=3 Diff=0.00940]

E=-1476.6640 kcal/mol Grad=5.088 Conv=NO(2 cycles 8 points) [Iter=1 Diff=0.01515]

E=-1476.6640 kcal/mol Grad=5.088 Conv=NO(2 cycles 8 points) [Iter=2 Diff=0.00191]

E=-1476.7214 kcal/mol Grad=3.953 Conv=NO(3 cycles 9 points) [Iter=1 Diff=0.21713]

E=-1476.7214 kcal/mol Grad=3.953 Conv=NO(3 cycles 9 points) [Iter=2 Diff=0.02506]

E=-1476.7214 kcal/mol Grad=3.953 Conv=NO(3 cycles 9 points) [Iter=3 Diff=0.00419]

E=-1476.7724 kcal/mol Grad=6.859 Conv=NO(3 cycles 10 points) [Iter=1 Diff=0.04887]

E=-1476.7724 kcal/mol Grad=6.859 Conv=NO(3 cycles 10 points) [Iter=2 Diff=0.00563]

E=-1476.9869 kcal/mol Grad=3.137 Conv=NO(4 cycles 11 points) [Iter=1 Diff=0.07848]

E=-1476.9869 kcal/mol Grad=3.137 Conv=NO(4 cycles 11 points) [Iter=2 Diff=0.00843]

E=-1477.1690 kcal/mol Grad=4.109 Conv=NO(4 cycles 12 points) [Iter=1 Diff=0.00568]

E=-1477.1985 kcal/mol Grad=2.857 Conv=NO(5 cycles 13 points) [Iter=1 Diff=0.07526]

E=-1477.1985 kcal/mol Grad=2.857 Conv=NO(5 cycles 13 points) [Iter=2 Diff=0.01037]

E=-1477.1985 kcal/mol Grad=2.857 Conv=NO(5 cycles 13 points) [Iter=3 Diff=0.00207]

E=-1477.3417 kcal/mol Grad=2.674 Conv=NO(5 cycles 14 points) [Iter=1 Diff=0.00442]

E=-1477.3583 kcal/mol Grad=1.885 Conv=NO(6 cycles 15 points) [Iter=1 Diff=0.05580]

E=-1477.3583 kcal/mol Grad=1.885 Conv=NO(6 cycles 15 points) [Iter=2 Diff=0.00641]

E=-1477.3711 kcal/mol Grad=2.773 Conv=NO(6 cycles 16 points) [Iter=1 Diff=0.01226]

E=-1477.3711 kcal/mol Grad=2.773 Conv=NO(6 cycles 16 points) [Iter=2 Diff=0.00140]

E=-1477.4128 kcal/mol Grad=1.195 Conv=NO(7 cycles 17 points) [Iter=1 Diff=0.01692]

E=-1477.4128 kcal/mol Grad=1.195 Conv=NO(7 cycles 17 points) [Iter=2 Diff=0.00200]

E=-1477.4281 kcal/mol Grad=1.731 Conv=NO(7 cycles 18 points) [Iter=1 Diff=0.00263]

E=-1477.4394 kcal/mol Grad=0.929 Conv=NO(8 cycles 19 points) [Iter=1 Diff=0.00488]

E=-1477.4633 kcal/mol Grad=0.638 Conv=NO(8 cycles 20 points) [Iter=1 Diff=0.00001]

E=-1477.4635 kcal/mol Grad=0.592 Conv=NO(9 cycles 21 points) [Iter=1 Diff=0.00639]

E=-1477.4567 kcal/mol Grad=1.266 Conv=NO(9 cycles 22 points) [Iter=1 Diff=0.00212]

E=-1477.4677 kcal/mol Grad=0.302 Conv=NO(10 cycles 23 points) [Iter=1 Diff=0.00036]

E=-1477.4696 kcal/mol Grad=0.135 Conv=NO(10 cycles 24 points) [Iter=1 Diff=0.00044]

E=-1477.4688 kcal/mol Grad=0.310 Conv=NO(10 cycles 25 points) [Iter=1 Diff=0.00021]

E=-1477.4696 kcal/mol Grad=0.143 Conv=NO(11 cycles 26 points) [Iter=1 Diff=0.00039]

E=-1477.4699 kcal/mol Grad=0.307 Conv=NO(11 cycles 27 points) [Iter=1 Diff=0.00005]

E=-1477.4701 kcal/mol Grad=0.163 Conv=NO(12 cycles 28 points) [Iter=1 Diff=0.00018]

E=-1477.4708 kcal/mol Grad=0.104 Conv=NO(12 cycles 29 points) [Iter=1 Diff=0.00000]

E=-1477.4708 kcal/mol Grad=0.103 Conv=NO(13 cycles 30 points) [Iter=1 Diff=0.00015]

E=-1477.4708 kcal/mol Grad=0.154 Conv=NO(13 cycles 31 points) [Iter=1 Diff=0.00003]

E=-1477.4710 kcal/mol Grad=0.056 Conv=YES(14 cycles 32 points) [Iter=1 Diff=0.00000]

Eigenvalues(a.u.) and Eigenvectors

Mol. Orbital	1	2	3	4	5	6
Symmetry:	1 A1	2 A1	1 B2	3 A1	2 B2	4 A1
Eigenvalue	-39.36561	-31.92184	-29.49517	-25.81795	-21.59082	-20.65103
S C 1	-0.41178	-0.39820	0.00000	0.19493	0.00000	0.41134
Px C 1	-0.04943	0.15035	-0.10281	0.22202	0.18461	0.01511
Py C 1	-0.02854	0.08681	0.17808	0.12818	-0.31975	0.00873
Pz C 1	-0.00000	-0.00000	0.00000	0.00000	-0.00000	0.00000
S C 2	-0.37262	-0.07312	0.43469	0.30274	-0.29316	-0.11362
Px C 2	-0.07379	0.10317	0.05033	0.02288	0.17875	-0.04091
Py C 2	0.05389	0.10697	0.07590	-0.05910	0.12432	-0.32718

Pz	C	2	0.00000	0.00000	0.00000	-0.00000	-0.00000	-0.00000
S	C	3	-0.35665	0.25996	0.42217	-0.07776	0.32963	-0.18878
Px	C	3	0.00346	0.08756	-0.09838	-0.20920	0.14061	0.24828
Py	C	3	0.09156	-0.03155	-0.00454	-0.03447	0.08899	-0.11785
Pz	C	3	0.00000	-0.00000	-0.00000	-0.00000	-0.00000	0.00000
S	C	4	-0.35126	0.38587	-0.00000	-0.40352	0.00000	0.29963
Px	C	4	0.07986	-0.03467	-0.09388	-0.04963	-0.16019	0.04174
Py	C	4	0.04611	-0.02002	0.16261	-0.02865	0.27747	0.02410
Pz	C	4	0.00000	-0.00000	-0.00000	0.00000	-0.00000	-0.00000
S	C	5	-0.35665	0.25996	-0.42217	-0.07776	-0.32963	-0.18878
Px	C	5	0.08102	0.01645	0.05312	-0.13446	-0.14738	0.02208
Py	C	5	-0.04278	0.09160	0.08293	-0.16394	-0.07728	0.27395
Pz	C	5	-0.00000	0.00000	-0.00000	-0.00000	-0.00000	0.00000
S	C	6	-0.37262	-0.07312	-0.43469	0.30274	0.29316	-0.11362
Px	C	6	0.00977	0.14423	-0.09090	-0.03975	-0.19704	-0.30380
Py	C	6	-0.09084	0.03586	-0.00564	0.04936	-0.09264	0.12816
Pz	C	6	-0.00000	-0.00000	0.00000	0.00000	-0.00000	0.00000
S	N	7	-0.19748	-0.53852	0.00000	-0.49228	-0.00000	-0.16640
Px	N	7	-0.05194	-0.07071	-0.02832	0.07147	0.09301	0.22480
Py	N	7	-0.02998	-0.04082	0.04904	0.04126	-0.16110	0.12979
Pz	N	7	0.00000	0.00000	0.00000	0.00000	-0.00000	0.00000
S	H	8	-0.12514	-0.05491	0.19421	0.10305	-0.19239	-0.14072
S	H	9	-0.11662	0.10083	0.18825	-0.05532	0.20636	-0.16059
S	H	10	-0.11377	0.15316	-0.00000	-0.21451	-0.00000	0.16869
S	H	11	-0.11662	0.10083	-0.18825	-0.05532	-0.20636	-0.16059
S	H	12	-0.12514	-0.05491	-0.19421	0.10305	0.19239	-0.14072
S	H	13	-0.08850	-0.23124	-0.03609	-0.23907	0.11798	-0.17042
S	H	14	-0.08850	-0.23124	0.03609	-0.23907	-0.11798	-0.17042

Mol. Orbital	7	8	9	10	11	12
Symmetry:	5 A1	3 B2	6 A1	4 B2	7 A1	5 B2
Eigenvalue	-18.07642	-16.98074	-15.84449	-14.89497	-14.60723	-14.43118

S	C	1	-0.09094	0.00000	0.11984	-0.00000	-0.18947	0.00000
Px	C	1	0.29361	-0.13995	-0.32230	-0.14798	-0.25187	0.03809
Py	C	1	0.16952	0.24239	-0.18608	0.25630	-0.14542	-0.06597
Pz	C	1	-0.00000	-0.00000	0.00000	0.00000	0.00000	-0.00000
S	C	2	-0.02554	-0.10714	-0.16534	0.10691	0.09712	-0.03320
Px	C	2	0.26822	-0.12527	0.19971	-0.04287	-0.17178	-0.41729
Py	C	2	-0.12399	-0.25770	0.04439	-0.25991	0.24200	0.08551
Pz	C	2	-0.00000	-0.00000	0.00000	0.00000	0.00000	-0.00000
S	C	3	-0.00035	0.05193	0.20820	-0.00878	-0.08421	-0.07964
Px	C	3	-0.00663	0.34108	-0.04058	0.21289	0.06929	0.14303
Py	C	3	-0.30738	0.04715	-0.01954	-0.15740	-0.32078	0.34654
Pz	C	3	-0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000
S	C	4	-0.01565	-0.00000	-0.16925	0.00000	0.18400	-0.00000
Px	C	4	-0.27473	-0.17561	-0.30031	-0.13821	-0.22613	0.02102
Py	C	4	-0.15862	0.30417	-0.17338	0.23938	-0.13056	-0.03642
Pz	C	4	0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000
S	C	5	-0.00035	-0.05193	0.20820	0.00878	-0.08421	0.07964
Px	C	5	-0.26951	-0.21137	-0.03721	0.02987	-0.24315	-0.37162
Py	C	5	0.14795	-0.27180	-0.02537	-0.26307	0.22040	0.04940
Pz	C	5	-0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000
S	C	6	-0.02554	0.10714	-0.16534	-0.10691	0.09712	0.03320
Px	C	6	0.02673	0.28581	0.13829	0.24652	0.12369	0.13459
Py	C	6	0.29428	-0.02037	0.15076	-0.09283	-0.26977	0.40414
Pz	C	6	-0.00000	0.00000	0.00000	0.00000	0.00000	-0.00000
S	N	7	0.09077	-0.00000	0.08372	0.00000	0.01190	0.00000
Px	N	7	-0.31403	-0.21394	0.37781	0.23662	0.14211	0.08880
Py	N	7	-0.18130	0.37055	0.21813	-0.40983	0.08204	-0.15380
Pz	N	7	-0.00000	-0.00000	0.00000	-0.00000	0.00000	-0.00000
S	H	8	-0.19905	-0.05844	-0.20527	-0.03427	0.25933	0.28996
S	H	9	-0.20581	0.05944	0.09489	-0.12516	-0.29579	0.22877
S	H	10	-0.21711	0.00000	-0.33732	-0.00000	-0.09977	0.00000

S H 11	-0.20581	-0.05944	0.09489	0.12516	-0.29579	-0.22877
S H 12	-0.19905	0.05844	-0.20527	0.03427	0.25933	-0.28996
S H 13	0.17335	-0.29297	-0.16690	0.37174	-0.05640	0.12082
S H 14	0.17335	0.29297	-0.16690	-0.37174	-0.05640	-0.12082

Mol. Orbital	13	14	15	16	17	18
Symmetry:	1 B1	8 A1	6 B2	2 B1	1 A2	3 B1
Eigenvalue	-13.39364	-12.61557	-12.18265	-10.91622	-9.60960	-8.06728

S C 1	0.00000	-0.02147	0.00000	0.00000	0.00000	-0.00000
Px C 1	-0.00000	-0.12273	-0.17777	-0.00000	-0.00000	0.00000
Py C 1	-0.00000	-0.07086	0.30791	-0.00000	-0.00000	0.00000
Pz C 1	-0.50996	-0.00000	-0.00000	-0.38303	-0.00000	-0.28039
S C 2	-0.00000	0.04972	-0.02273	-0.00000	0.00000	0.00000
Px C 2	-0.00000	0.29922	0.12626	0.00000	0.00000	0.00000
Py C 2	0.00000	0.14315	-0.28624	0.00000	0.00000	0.00000
Pz C 2	-0.39719	-0.00000	-0.00000	0.00517	-0.51175	-0.36166
S C 3	0.00000	-0.05995	0.01708	-0.00000	-0.00000	-0.00000
Px C 3	0.00000	-0.32452	-0.17267	-0.00000	-0.00000	-0.00000
Py C 3	-0.00000	-0.14860	0.29669	-0.00000	-0.00000	-0.00000
Pz C 3	-0.33629	-0.00000	-0.00000	0.34284	-0.48797	0.12496
S C 4	-0.00000	0.04473	-0.00000	0.00000	-0.00000	0.00000
Px C 4	-0.00000	0.37462	0.18142	0.00000	-0.00000	0.00000
Py C 4	-0.00000	0.21629	-0.31422	0.00000	0.00000	-0.00000
Pz C 4	-0.31195	-0.00000	-0.00000	0.49550	0.00000	0.43470
S C 5	0.00000	-0.05995	-0.01708	-0.00000	0.00000	-0.00000
Px C 5	0.00000	-0.29095	-0.17060	-0.00000	0.00000	0.00000
Py C 5	0.00000	-0.20674	0.29788	-0.00000	-0.00000	-0.00000
Pz C 5	-0.33629	-0.00000	0.00000	0.34284	0.48797	0.12496
S C 6	-0.00000	0.04972	0.02273	0.00000	-0.00000	0.00000
Px C 6	-0.00000	0.27358	0.18476	0.00000	-0.00000	0.00000
Py C 6	-0.00000	0.18755	-0.25247	0.00000	0.00000	-0.00000

Pz	C	6	-0.39719	-0.00000	-0.00000	0.00517	0.51175	-0.36166
S	N	7	-0.00000	0.08638	-0.00000	-0.00000	0.00000	0.00000
Px	N	7	0.00000	0.14143	0.02768	0.00000	0.00000	0.00000
Py	N	7	0.00000	0.08165	-0.04794	0.00000	-0.00000	-0.00000
Pz	N	7	-0.31770	-0.00000	-0.00000	-0.61044	-0.00000	0.66301
S	H	8	0.00000	-0.13845	-0.25539	-0.00000	-0.00000	0.00000
S	H	9	0.00000	-0.17082	0.28601	-0.00000	-0.00000	-0.00000
S	H	10	-0.00000	0.40749	-0.00000	0.00000	0.00000	0.00000
S	H	11	0.00000	-0.17082	-0.28601	-0.00000	0.00000	-0.00000
S	H	12	0.00000	-0.13845	0.25539	-0.00000	0.00000	0.00000
S	H	13	0.00000	-0.05692	0.07677	0.00000	-0.00000	-0.00000
S	H	14	0.00000	-0.05692	-0.07677	0.00000	-0.00000	-0.00000

Mol. Orbital	19	20	21	22	23	24
Symmetry:	2 A2	4 B1	9 A1	5 B1	10 A1	7 B2
Eigenvalue	0.61514	0.70745	1.91582	3.06938	3.47741	3.65437

S	C	1	-0.00000	-0.00000	0.31206	-0.00000	-0.32904	-0.00000
Px	C	1	-0.00000	-0.00000	-0.24817	-0.00000	-0.23285	0.16996
Py	C	1	0.00000	-0.00000	-0.14328	0.00000	-0.13444	-0.29438
Pz	C	1	-0.00000	0.59604	-0.00000	0.39918	-0.00000	0.00000
S	C	2	-0.00000	-0.00000	-0.12186	0.00000	0.40446	0.38405
Px	C	2	-0.00000	-0.00000	-0.01949	-0.00000	-0.08898	0.10334
Py	C	2	-0.00000	-0.00000	0.09598	-0.00000	-0.08686	0.01478
Pz	C	2	0.48797	-0.24683	-0.00000	-0.38793	0.00000	-0.00000
S	C	3	-0.00000	0.00000	0.06187	0.00000	-0.16766	-0.34665
Px	C	3	-0.00000	0.00000	-0.07198	0.00000	0.03821	0.13961
Py	C	3	0.00000	0.00000	-0.01781	-0.00000	0.03752	0.03832
Pz	C	3	-0.51175	-0.28623	0.00000	0.41452	-0.00000	0.00000
S	C	4	0.00000	-0.00000	0.00446	0.00000	0.15652	-0.00000
Px	C	4	-0.00000	0.00000	-0.00715	0.00000	-0.00804	-0.10535
Py	C	4	-0.00000	-0.00000	-0.00413	-0.00000	-0.00464	0.18247

Pz	C	4	-0.00000	0.53864	-0.00000	-0.42199	0.00000	-0.00000
S	C	5	-0.00000	0.00000	0.06187	-0.00000	-0.16766	0.34665
Px	C	5	-0.00000	0.00000	-0.05141	0.00000	0.05159	-0.10299
Py	C	5	-0.00000	0.00000	-0.05343	0.00000	0.01433	-0.10174
Pz	C	5	0.51175	-0.28623	0.00000	0.41452	-0.00000	0.00000
S	C	6	0.00000	-0.00000	-0.12186	0.00000	0.40446	-0.38405
Px	C	6	0.00000	0.00000	0.07338	-0.00000	-0.11971	-0.06447
Py	C	6	-0.00000	0.00000	-0.06487	0.00000	-0.03362	-0.08211
Pz	C	6	-0.48797	-0.24683	-0.00000	-0.38793	0.00000	-0.00000
S	N	7	0.00000	-0.00000	-0.59830	-0.00000	-0.09802	-0.00000
Px	N	7	-0.00000	0.00000	-0.03493	0.00000	0.08154	0.05193
Py	N	7	0.00000	0.00000	-0.02017	0.00000	0.04708	-0.08995
Pz	N	7	0.00000	-0.26248	0.00000	-0.13397	0.00000	-0.00000
S	H	8	0.00000	-0.00000	-0.02327	-0.00000	-0.37757	-0.22023
S	H	9	-0.00000	-0.00000	-0.04944	-0.00000	0.11243	0.23297
S	H	10	-0.00000	-0.00000	0.01518	-0.00000	-0.13223	0.00000
S	H	11	0.00000	-0.00000	-0.04944	0.00000	0.11243	-0.23297
S	H	12	-0.00000	0.00000	-0.02327	-0.00000	-0.37757	0.22023
S	H	13	0.00000	0.00000	0.43994	0.00000	0.11926	-0.11111
S	H	14	-0.00000	0.00000	0.43994	0.00000	0.11926	0.11111

Mol. Orbital	25	26	27	28	29	30
Symmetry:	11 A1	12 A1	8 B2	13 A1	9 B2	14 A1
Eigenvalue	3.68521	3.96175	4.13872	4.70486	4.74532	5.24760

S	C	1	-0.19777	-0.19014	-0.00000	0.27840	-0.00000	-0.18127
Px	C	1	-0.10055	-0.07306	-0.06182	-0.00973	0.20622	-0.07384
Py	C	1	-0.05805	-0.04218	0.10708	-0.00562	-0.35718	-0.04263
Pz	C	1	-0.00000	-0.00000	-0.00000	0.00000	-0.00000	0.00000
S	C	2	0.07803	-0.02730	0.14454	-0.00084	0.11150	-0.13942
Px	C	2	-0.13964	0.07347	-0.22789	-0.28925	-0.11154	-0.24675
Py	C	2	-0.17346	-0.18100	0.23657	0.20716	-0.28589	-0.35767

Pz	C	2	0.00000	0.00000	0.00000	-0.00000	0.00000	-0.00000
S	C	3	0.37353	-0.12253	0.09203	-0.00812	0.25038	0.11571
Px	C	3	0.17617	0.01833	-0.04548	-0.12561	0.10094	-0.46339
Py	C	3	0.00264	-0.27463	0.28449	-0.04193	0.04793	-0.03276
Pz	C	3	-0.00000	-0.00000	0.00000	0.00000	-0.00000	-0.00000
S	C	4	-0.47090	-0.28544	0.00000	-0.07926	0.00000	0.25418
Px	C	4	0.10621	-0.22849	-0.06575	-0.32213	0.17699	-0.04460
Py	C	4	0.06132	-0.13192	0.11388	-0.18598	-0.30656	-0.02575
Pz	C	4	-0.00000	0.00000	-0.00000	-0.00000	0.00000	0.00000
S	C	5	0.37353	-0.12253	-0.09203	-0.00812	-0.25038	0.11571
Px	C	5	0.09037	-0.22867	-0.22363	-0.09912	-0.09198	-0.26007
Py	C	5	0.15125	0.15319	0.18164	-0.08781	-0.06346	-0.38493
Pz	C	5	0.00000	-0.00000	0.00000	0.00000	-0.00000	-0.00000
S	C	6	0.07803	-0.02730	-0.14454	-0.00084	-0.11150	-0.13942
Px	C	6	-0.22004	-0.12002	-0.09093	0.03478	0.30336	-0.43312
Py	C	6	-0.03420	0.15412	0.31565	-0.35407	-0.04635	-0.03486
Pz	C	6	0.00000	0.00000	-0.00000	-0.00000	0.00000	0.00000
S	N	7	-0.00647	-0.05645	-0.00000	0.06806	-0.00000	0.02096
Px	N	7	0.03024	0.12290	-0.04145	-0.30084	0.17567	0.00142
Py	N	7	0.01746	0.07096	0.07179	-0.17369	-0.30426	0.00082
Pz	N	7	0.00000	0.00000	0.00000	-0.00000	0.00000	-0.00000
S	H	8	-0.08462	0.15586	-0.38811	-0.28401	-0.02891	0.05143
S	H	9	-0.29553	0.34614	-0.32606	0.03689	-0.18727	-0.03425
S	H	10	0.25888	0.46733	-0.00000	0.37545	-0.00000	-0.09580
S	H	11	-0.29553	0.34614	0.32606	0.03689	0.18727	-0.03425
S	H	12	-0.08462	0.15586	0.38811	-0.28401	0.02891	0.05143
S	H	13	0.02058	0.09043	0.05533	-0.17183	-0.26998	-0.01533
S	H	14	0.02058	0.09043	-0.05533	-0.17183	0.26998	-0.01533

Mol. Orbital	31	32	33	34	35
Symmetry:	10 B2	11 B2	15 A1	12 B2	16 A1
Eigenvalue	5.41992	5.85160	5.95862	6.58099	6.66610

S	C 1	-0.00000	-0.00000	0.11772	-0.00000	-0.02340
Px	C 1	-0.00699	0.12792	-0.23622	-0.19790	0.46285
Py	C 1	0.01210	-0.22157	-0.13638	0.34278	0.26723
Pz	C 1	0.00000	-0.00000	0.00000	-0.00000	-0.00000
S	C 2	-0.00419	0.14049	-0.02839	0.00238	-0.07642
Px	C 2	0.36794	0.12460	-0.08217	0.17876	-0.25759
Py	C 2	-0.07538	-0.06492	-0.02241	0.32828	0.16662
Pz	C 2	-0.00000	0.00000	-0.00000	0.00000	0.00000
S	C 3	-0.09141	0.06323	0.06954	0.00587	0.06881
Px	C 3	-0.01119	0.27997	0.07771	0.38518	-0.02333
Py	C 3	0.41019	0.06232	-0.35967	-0.01032	-0.21529
Pz	C 3	0.00000	-0.00000	0.00000	-0.00000	-0.00000
S	C 4	-0.00000	0.00000	-0.09551	0.00000	-0.05110
Px	C 4	-0.13416	0.16958	0.42851	0.19679	0.16761
Py	C 4	0.23237	-0.29372	0.24740	-0.34085	0.09677
Pz	C 4	0.00000	0.00000	0.00000	-0.00000	0.00000
S	C 5	0.09141	-0.06323	0.06954	-0.00587	0.06881
Px	C 5	-0.34964	-0.19395	-0.27263	-0.18365	-0.19812
Py	C 5	0.21479	-0.21130	0.24714	-0.33874	0.08744
Pz	C 5	0.00000	-0.00000	0.00000	0.00000	-0.00000
S	C 6	0.00419	-0.14049	-0.02839	-0.00238	-0.07642
Px	C 6	-0.11868	-0.00607	-0.06049	-0.37368	0.01551
Py	C 6	-0.35633	-0.14037	-0.05995	0.00933	-0.30639
Pz	C 6	-0.00000	0.00000	-0.00000	0.00000	0.00000
S	N 7	-0.00000	0.00000	-0.00535	-0.00000	0.04714
Px	N 7	0.04834	-0.27555	-0.32899	0.12884	0.42718
Py	N 7	-0.08373	0.47727	-0.18994	-0.22316	0.24663
Pz	N 7	-0.00000	0.00000	-0.00000	-0.00000	-0.00000
S	H 8	0.26420	0.03871	-0.01939	-0.01052	-0.15650
S	H 9	-0.26048	-0.07154	0.21094	0.00311	0.10040
S	H 10	-0.00000	0.00000	-0.29937	0.00000	-0.09648

S H 11	0.26048	0.07154	0.21094	-0.00311	0.10040
S H 12	-0.26420	-0.03871	-0.01939	0.01052	-0.15650
S H 13	-0.06134	0.35432	-0.13691	-0.15054	0.15263
S H 14	0.06134	-0.35432	-0.13691	0.15054	0.15263

Density Matrix

	S C 1 Px	C 1 Py	C 1 Pz	C 1 S	C 2 Px	C 2
S C 1	1.18863	-0.00998	-0.00576	-0.00000	0.31574	0.00520
Px C 1	-0.00998	0.92470	-0.01663	0.00000	-0.01743	0.11582
Py C 1	-0.00576	-0.01663	0.94390	0.00000	0.43733	0.00517
Pz C 1	-0.00000	0.00000	0.00000	0.97078	0.00000	-0.00000
S C 2	0.31574	-0.01743	0.43733	0.00000	1.17613	-0.04170
Px C 2	0.00520	0.11582	0.00517	-0.00000	-0.04170	0.98248
Py C 2	-0.48644	0.01987	-0.65278	-0.00000	0.03572	-0.01280
Pz C 2	-0.00000	0.00000	0.00000	0.60395	-0.00000	0.00000
S C 3	-0.01448	0.00674	-0.02109	-0.00000	0.29769	0.41304
Px C 3	0.02927	-0.00643	0.02871	-0.00000	-0.40071	-0.47642
Py C 3	0.01849	-0.01916	0.01645	0.00000	-0.24901	-0.34463
Pz C 3	-0.00000	-0.00000	0.00000	0.01027	-0.00000	-0.00000
S C 4	-0.03821	-0.02313	-0.01335	0.00000	-0.01011	-0.02397
Px C 4	0.02443	0.00242	0.03070	0.00000	0.02343	0.02732
Py C 4	0.01410	0.03070	-0.03302	0.00000	-0.01128	-0.02439
Pz C 4	0.00000	0.00000	-0.00000	-0.30519	0.00000	0.00000
S C 5	-0.01448	-0.01489	0.01638	-0.00000	-0.03282	-0.02468
Px C 5	0.03065	0.01486	-0.03145	0.00000	0.01740	0.00359
Py C 5	0.01611	0.01642	-0.00484	-0.00000	-0.01736	-0.02954
Pz C 5	0.00000	-0.00000	0.00000	0.01027	-0.00000	-0.00000
S C 6	0.31574	0.37002	-0.23376	0.00000	-0.02156	0.00109
Px C 6	-0.41867	-0.44979	0.34642	0.00000	0.03136	0.00416

Py	C	6	0.24773	0.33172	-0.08717	0.00000	-0.01684	0.01391
Pz	C	6	-0.00000	-0.00000	-0.00000	0.60395	0.00000	-0.00000
S	N	7	0.25804	-0.39390	-0.22742	0.00000	-0.05574	0.03885
Px	N	7	0.39963	-0.48490	-0.34217	0.00000	-0.01586	-0.00720
Py	N	7	0.23073	-0.34217	-0.08979	0.00000	-0.03255	0.00371
Pz	N	7	-0.00000	0.00000	0.00000	0.41986	0.00000	-0.00000
S	H	8	-0.03413	-0.01543	-0.07455	0.00000	0.58950	-0.67549
S	H	9	0.04166	-0.00503	0.05801	-0.00000	-0.04517	-0.05463
S	H	10	0.00582	0.00734	0.00424	0.00000	0.03795	0.05171
S	H	11	0.04166	0.04772	-0.03336	0.00000	0.00488	0.00566
S	H	12	-0.03413	-0.07228	0.02391	0.00000	0.03112	0.00078
S	H	13	-0.02407	0.08454	0.03756	-0.00000	0.05367	-0.02139
S	H	14	-0.02407	0.07480	0.05443	-0.00000	-0.00674	-0.01863

			Py	C	2	Pz	C	2	S	C	3
Px	C	3	Py	C	3	Pz	C	3			
S	C	1	-0.48644	-0.00000	-0.01448	0.02927	0.01849	-0.00000			
Px	C	1	0.01987	0.00000	0.00674	-0.00643	-0.01916	-0.00000			
Py	C	1	-0.65278	0.00000	-0.02109	0.02871	0.01645	0.00000			
Pz	C	1	-0.00000	0.60395	-0.00000	-0.00000	0.00000	0.01027			
S	C	2	0.03572	-0.00000	0.29769	-0.40071	-0.24901	-0.00000			
Px	C	2	-0.01280	0.00000	0.41304	-0.47642	-0.34463	-0.00000			
Py	C	2	0.93142	-0.00000	0.21098	-0.32308	-0.07062	-0.00000			
Pz	C	2	-0.00000	1.10095	0.00000	-0.00000	-0.00000	0.67974			
S	C	3	0.21098	0.00000	1.17357	0.00485	0.04951	0.00000			
Px	C	3	-0.32308	-0.00000	0.00485	0.93255	-0.00360	-0.00000			
Py	C	3	-0.07062	-0.00000	0.04951	-0.00360	0.97470	-0.00000			
Pz	C	3	-0.00000	0.67974	0.00000	-0.00000	-0.00000	0.96872			
S	C	4	-0.01295	-0.00000	0.29398	0.39318	-0.24658	0.00000			
Px	C	4	0.02703	-0.00000	-0.41257	-0.47235	0.34627	0.00000			
Py	C	4	-0.00289	0.00000	0.21870	0.33202	-0.08069	-0.00000			
Pz	C	4	0.00000	-0.06150	0.00000	-0.00000	-0.00000	0.65820			

S C 5	0.01011	-0.00000	-0.01159	-0.02045	0.01463	-0.00000
Px C 5	-0.02482	0.00000	0.00244	0.00164	0.01263	-0.00000
Py C 5	-0.02823	0.00000	-0.02502	-0.03901	0.01687	-0.00000
Pz C 5	0.00000	-0.31913	-0.00000	-0.00000	0.00000	0.01626
S C 6	0.03558	0.00000	-0.03282	-0.00634	0.02375	0.00000
Px C 6	-0.04174	-0.00000	-0.00358	-0.04381	0.00255	-0.00000
Py C 6	0.02023	0.00000	-0.02643	-0.00218	0.01917	0.00000
Pz C 6	-0.00000	0.05341	0.00000	0.00000	-0.00000	-0.31913
S N 7	0.04599	-0.00000	0.02268	-0.03473	-0.02139	-0.00000
Px N 7	0.04984	0.00000	0.01877	-0.02723	-0.01777	0.00000
Py N 7	0.01622	-0.00000	0.01583	-0.02122	-0.01052	0.00000
Pz N 7	-0.00000	-0.23352	-0.00000	0.00000	0.00000	-0.03919
S H 8	0.39705	0.00000	-0.03783	0.04600	0.03047	0.00000
S H 9	-0.02228	0.00000	0.59150	0.00009	0.78559	-0.00000
S H 10	0.02775	-0.00000	-0.04192	-0.04850	0.03410	-0.00000
S H 11	-0.00169	0.00000	0.03810	0.05023	-0.03099	0.00000
S H 12	-0.05369	0.00000	0.00864	-0.00274	-0.00692	-0.00000
S H 13	-0.06231	0.00000	-0.01515	0.02144	0.01406	0.00000
S H 14	0.02104	0.00000	-0.00260	0.00791	0.00214	0.00000

S C 4 Px C 4 Py C 4 Pz C 4 S C 5 Px C 5

S C 1	-0.03821	0.02443	0.01410	0.00000	-0.01448	0.03065
Px C 1	-0.02313	0.00242	0.03070	0.00000	-0.01489	0.01486
Py C 1	-0.01335	0.03070	-0.03302	-0.00000	0.01638	-0.03145
Pz C 1	0.00000	0.00000	0.00000	-0.30519	-0.00000	0.00000
S C 2	-0.01011	0.02343	-0.01128	0.00000	-0.03282	0.01740
Px C 2	-0.02397	0.02732	-0.02439	0.00000	-0.02468	0.00359
Py C 2	-0.01295	0.02703	-0.00289	0.00000	0.01011	-0.02482
Pz C 2	-0.00000	-0.00000	0.00000	-0.06150	-0.00000	0.00000
S C 3	0.29398	-0.41257	0.21870	0.00000	-0.01159	0.00244
Px C 3	0.39318	-0.47235	0.33202	-0.00000	-0.02045	0.00164

Py	C	3	-0.24658	0.34627	-0.08069	-0.00000	0.01463	0.01263
Pz	C	3	0.00000	0.00000	-0.00000	0.65820	-0.00000	-0.00000
S	C	4	1.17927	0.04275	0.02468	0.00000	0.29398	-0.01695
Px	C	4	0.04275	0.97339	0.01803	0.00000	-0.01688	0.11510
Py	C	4	0.02468	0.01803	0.95258	-0.00000	-0.46665	0.00710
Pz	C	4	0.00000	0.00000	-0.00000	1.06359	-0.00000	0.00000
S	C	5	0.29398	-0.01688	-0.46665	-0.00000	1.17357	0.04530
Px	C	5	-0.01695	0.11510	0.00710	0.00000	0.04530	0.96105
Py	C	5	0.46379	-0.00715	-0.66814	-0.00000	-0.02055	-0.02005
Pz	C	5	0.00000	0.00000	-0.00000	0.65820	-0.00000	0.00000
S	C	6	-0.01011	0.00194	0.02593	0.00000	0.29769	-0.41601
Px	C	6	-0.02320	0.00580	0.03945	0.00000	0.38924	-0.46120
Py	C	6	-0.01429	-0.01197	0.01863	-0.00000	0.25222	-0.35341
Pz	C	6	0.00000	-0.00000	-0.00000	-0.06150	-0.00000	0.00000
S	N	7	0.00162	-0.00005	-0.00003	0.00000	0.02268	-0.03589
Px	N	7	0.00584	-0.00536	-0.00085	-0.00000	0.02310	-0.03158
Py	N	7	0.00337	-0.00085	-0.00438	-0.00000	0.00834	-0.01526
Pz	N	7	0.00000	-0.00000	-0.00000	0.16969	-0.00000	0.00000
S	H	8	0.03682	-0.05182	0.02851	-0.00000	0.00864	-0.00736
S	H	9	-0.04167	0.05399	-0.02806	-0.00000	0.03810	-0.00173
S	H	10	0.59304	0.67891	0.39197	-0.00000	-0.04192	0.00528
S	H	11	-0.04167	0.00270	0.06079	0.00000	0.59150	0.68039
S	H	12	0.03682	-0.00122	-0.05913	-0.00000	-0.03783	0.04938
S	H	13	-0.00024	0.00131	-0.00399	-0.00000	-0.00260	0.00581
S	H	14	-0.00024	-0.00279	0.00313	-0.00000	-0.01515	0.02290

	Py	C	5	Pz	C	5	S	C	6	Px	C	6	Py	C	6	Pz	C	6
S	C	1	0.01611	0.00000	0.31574	-0.41867	0.24773	-0.00000										
Px	C	1	0.01642	-0.00000	0.37002	-0.44979	0.33172	-0.00000										
Py	C	1	-0.00484	0.00000	-0.23376	0.34642	-0.08717	-0.00000										
Pz	C	1	-0.00000	0.01027	0.00000	0.00000	0.00000	0.60395										

S C 2	-0.01736	-0.00000	-0.02156	0.03136	-0.01684	0.00000
Px C 2	-0.02954	-0.00000	0.00109	0.00416	0.01391	-0.00000
Py C 2	-0.02823	0.00000	0.03558	-0.04174	0.02023	-0.00000
Pz C 2	0.00000	-0.31913	0.00000	-0.00000	0.00000	0.05341
S C 3	-0.02502	-0.00000	-0.03282	-0.00358	-0.02643	0.00000
Px C 3	-0.03901	-0.00000	-0.00634	-0.04381	-0.00218	0.00000
Py C 3	0.01687	0.00000	0.02375	0.00255	0.01917	-0.00000
Pz C 3	-0.00000	0.01626	0.00000	-0.00000	0.00000	-0.31913
S C 4	0.46379	0.00000	-0.01011	-0.02320	-0.01429	0.00000
Px C 4	-0.00715	0.00000	0.00194	0.00580	-0.01197	-0.00000
Py C 4	-0.66814	-0.00000	0.02593	0.03945	0.01863	-0.00000
Pz C 4	-0.00000	0.65820	0.00000	0.00000	-0.00000	-0.06150
S C 5	-0.02055	-0.00000	0.29769	0.38924	0.25222	-0.00000
Px C 5	-0.02005	0.00000	-0.41601	-0.46120	-0.35341	0.00000
Py C 5	0.94620	-0.00000	-0.22251	-0.33187	-0.08584	0.00000
Pz C 5	-0.00000	0.96872	-0.00000	0.00000	0.00000	0.67974
S C 6	-0.22251	-0.00000	1.17613	0.01009	-0.05398	-0.00000
Px C 6	-0.33187	0.00000	0.01009	0.93311	0.01571	0.00000
Py C 6	-0.08584	0.00000	-0.05398	0.01571	0.98080	0.00000
Pz C 6	0.00000	0.67974	-0.00000	0.00000	0.00000	1.10095
S N 7	-0.01938	-0.00000	-0.05574	0.05925	0.01064	-0.00000
Px N 7	-0.01872	-0.00000	-0.03612	0.03356	-0.01982	-0.00000
Py N 7	-0.00617	0.00000	0.00254	0.02631	-0.02453	0.00000
Pz N 7	0.00000	-0.03919	0.00000	-0.00000	-0.00000	-0.23352
S H 8	0.00109	-0.00000	0.03112	-0.04611	0.02752	-0.00000
S H 9	0.05900	0.00000	0.00488	0.00137	0.00574	-0.00000
S H 10	-0.05905	0.00000	0.03795	0.04988	0.03091	-0.00000
S H 11	-0.39272	0.00000	-0.04517	-0.04661	-0.03617	0.00000
S H 12	0.02460	0.00000	0.58950	0.00612	-0.78352	0.00000
S H 13	0.00579	0.00000	-0.00674	0.00890	-0.02665	0.00000
S H 14	0.01154	-0.00000	0.05367	-0.06466	0.01263	0.00000

	S N 7	Px N 7	Py N 7	Pz N 7	S H 8	S H 9
S C 1	0.25804	0.39963	0.23073	-0.00000	-0.03413	0.04166
Px C 1	-0.39390	-0.48490	-0.34217	0.00000	-0.01543	-0.00503
Py C 1	-0.22742	-0.34217	-0.08979	0.00000	-0.07455	0.05801
Pz C 1	0.00000	0.00000	0.00000	0.41986	0.00000	-0.00000
S C 2	-0.05574	-0.01586	-0.03255	0.00000	0.58950	-0.04517
Px C 2	0.03885	-0.00720	0.00371	-0.00000	-0.67549	-0.05463
Py C 2	0.04599	0.04984	0.01622	-0.00000	0.39705	-0.02228
Pz C 2	-0.00000	0.00000	-0.00000	-0.23352	0.00000	0.00000
S C 3	0.02268	0.01877	0.01583	-0.00000	-0.03783	0.59150
Px C 3	-0.03473	-0.02723	-0.02122	0.00000	0.04600	0.00009
Py C 3	-0.02139	-0.01777	-0.01052	0.00000	0.03047	0.78559
Pz C 3	-0.00000	0.00000	0.00000	-0.03919	0.00000	-0.00000
S C 4	0.00162	0.00584	0.00337	0.00000	0.03682	-0.04167
Px C 4	-0.00005	-0.00536	-0.00085	-0.00000	-0.05182	0.05399
Py C 4	-0.00003	-0.00085	-0.00438	-0.00000	0.02851	-0.02806
Pz C 4	0.00000	-0.00000	-0.00000	0.16969	-0.00000	-0.00000
S C 5	0.02268	0.02310	0.00834	-0.00000	0.00864	0.03810
Px C 5	-0.03589	-0.03158	-0.01526	0.00000	-0.00736	-0.00173
Py C 5	-0.01938	-0.01872	-0.00617	0.00000	0.00109	0.05900
Pz C 5	-0.00000	-0.00000	0.00000	-0.03919	-0.00000	0.00000
S C 6	-0.05574	-0.03612	0.00254	0.00000	0.03112	0.00488
Px C 6	0.05925	0.03356	0.02631	-0.00000	-0.04611	0.00137
Py C 6	0.01064	-0.01982	-0.02453	-0.00000	0.02752	0.00574
Pz C 6	-0.00000	-0.00000	0.00000	-0.23352	-0.00000	-0.00000
S N 7	1.24377	-0.01445	-0.00834	0.00000	-0.03431	-0.01266
Px N 7	-0.01445	0.92950	-0.01697	-0.00000	-0.02397	-0.01416
Py N 7	-0.00834	-0.01697	0.94909	-0.00000	-0.01236	-0.00707
Pz N 7	0.00000	-0.00000	-0.00000	1.82631	0.00000	0.00000
S H 8	-0.03431	-0.02397	-0.01236	0.00000	0.89179	-0.02930
S H 9	-0.01266	-0.01416	-0.00707	0.00000	-0.02930	0.90402

S H 10	0.00716	0.00372	0.00215	-0.00000	-0.01970	-0.02787
S H 11	-0.01266	-0.01321	-0.00873	-0.00000	0.00684	-0.02141
S H 12	-0.03431	-0.02269	-0.01458	0.00000	-0.02268	0.00684
S H 13	0.56846	0.01495	-0.80190	-0.00000	0.01247	0.01139
S H 14	0.56846	-0.68699	0.41390	-0.00000	0.05205	-0.00143

	S H 10	S H 11	S H 12	S H 13	S H 14
S C 1	0.00582	0.04166	-0.03413	-0.02407	-0.02407
Px C 1	0.00734	0.04772	-0.07228	0.08454	0.07480
Py C 1	0.00424	-0.03336	0.02391	0.03756	0.05443
Pz C 1	0.00000	0.00000	0.00000	-0.00000	-0.00000
S C 2	0.03795	0.00488	0.03112	0.05367	-0.00674
Px C 2	0.05171	0.00566	0.00078	-0.02139	-0.01863
Py C 2	0.02775	-0.00169	-0.05369	-0.06231	0.02104
Pz C 2	-0.00000	0.00000	0.00000	0.00000	0.00000
S C 3	-0.04192	0.03810	0.00864	-0.01515	-0.00260
Px C 3	-0.04850	0.05023	-0.00274	0.02144	0.00791
Py C 3	0.03410	-0.03099	-0.00692	0.01406	0.00214
Pz C 3	-0.00000	0.00000	-0.00000	0.00000	0.00000
S C 4	0.59304	-0.04167	0.03682	-0.00024	-0.00024
Px C 4	0.67891	0.00270	-0.00122	0.00131	-0.00279
Py C 4	0.39197	0.06079	-0.05913	-0.00399	0.00313
Pz C 4	-0.00000	0.00000	-0.00000	-0.00000	-0.00000
S C 5	-0.04192	0.59150	-0.03783	-0.00260	-0.01515
Px C 5	0.00528	0.68039	0.04938	0.00581	0.02290
Py C 5	-0.05905	-0.39272	0.02460	0.00579	0.01154
Pz C 5	0.00000	0.00000	0.00000	0.00000	-0.00000
S C 6	0.03795	-0.04517	0.58950	-0.00674	0.05367
Px C 6	0.04988	-0.04661	0.00612	0.00890	-0.06466
Py C 6	0.03091	-0.03617	-0.78352	-0.02665	0.01263
Pz C 6	-0.00000	0.00000	0.00000	0.00000	0.00000

S	N	7	0.00716	-0.01266	-0.03431	0.56846	0.56846
Px	N	7	0.00372	-0.01321	-0.02269	0.01495	-0.68699
Py	N	7	0.00215	-0.00873	-0.01458	-0.80190	0.41390
Pz	N	7	-0.00000	-0.00000	0.00000	-0.00000	-0.00000
S	H	8	-0.01970	0.00684	-0.02268	0.01247	0.05205
S	H	9	-0.02787	-0.02141	0.00684	0.01139	-0.00143
S	H	10	0.89559	-0.02787	-0.01970	-0.00343	-0.00343
S	H	11	-0.02787	0.90402	-0.02930	-0.00143	0.01139
S	H	12	-0.01970	-0.02930	0.89179	0.05205	0.01247
S	H	13	-0.00343	-0.00143	0.05205	0.94313	-0.09581
S	H	14	-0.00343	0.01139	0.01247	-0.09581	0.94313

ENERGIES AND GRADIENT

Total Energy = -22612.9927700 (kcal/mol)

Total Energy = -36.036093336 (a.u.)

Binding Energy = -1477.4709650 (kcal/mol)

Isolated Atomic Energy = -21135.5218050 (kcal/mol)

Electronic Energy = -97316.0724398 (kcal/mol)

Core-Core Interaction = 74703.0796699 (kcal/mol)

Heat of Formation = 25.5830350 (kcal/mol)

Gradient = 0.0568472 (kcal/mol/Ang)

MOLECULAR POINT GROUP

C2V

EIGENVALUES(eV)

Symmetry:	1 A1	2 A1	1 B2	3 A1	2 B2
Eigenvalue:	-39.365614	-31.921836	-29.495170	-25.817955	-21.590818

Symmetry:	4 A1	5 A1	3 B2	6 A1	4 B2
Eigenvalue:	-20.651034	-18.076422	-16.980739	-15.844487	-14.894967

Symmetry: 7 A1 5 B2 1 B1 8 A1 6 B2

Eigenvalue: -14.607227 -14.431180 -13.393639 -12.615574 -12.182648

Symmetry: 2 B1 1 A2 3 B1 2 A2 4 B1

Eigenvalue: -10.916223 -9.609596 -8.067279 0.615139 0.707451

Symmetry: 9 A1 5 B1 10 A1 7 B2 11 A1

Eigenvalue: 1.915824 3.069378 3.477410 3.654370 3.685206

Symmetry: 12 A1 8 B2 13 A1 9 B2 14 A1

Eigenvalue: 3.961752 4.138724 4.704861 4.745324 5.247596

Symmetry: 10 B2 11 B2 15 A1 12 B2 16 A1

Eigenvalue: 5.419919 5.851598 5.958624 6.580990 6.666104

ATOMIC ORBITAL ELECTRON POPULATIONS

AO: 1 S C 1 Px C 1 Py C 1 Pz C 2 S C

1.188629 0.924699 0.943897 0.970777 1.176135

AO: 2 Px C 2 Py C 2 Pz C 3 S C 3 Px C

0.982477 0.931424 1.100946 1.173570 0.932548

AO: 3 Py C 3 Pz C 4 S C 4 Px C 4 Py C

0.974701 0.968718 1.179275 0.973391 0.952575

AO: 4 Pz C 5 S C 5 Px C 5 Py C 5 Pz C

1.063587 1.173570 0.961049 0.946200 0.968718

AO: 6 S C 6 Px C 6 Py C 6 Pz C 7 S N

1.176135 0.933106 0.980795 1.100946 1.243766

AO:	7 Px N	7 Py N	7 Pz N	8 S H	9 S H
	0.929501	0.949092	1.826309	0.891787	0.904023

AO:	10 S H	11 S H	12 S H	13 S H	14 S H
	0.895590	0.904023	0.891787	0.943127	0.943127

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom)			Mass
			x	y	z	
1	6	-0.028002	-1.74270	-0.43495	-0.00000	12.01100
2	6	-0.190982	-1.74106	0.97072	0.00000	12.01100
3	6	-0.049537	-0.53335	1.65337	0.00000	12.01100
4	6	-0.168827	0.67276	0.95962	0.00000	12.01100
5	6	-0.049537	0.67051	-0.43177	-0.00000	12.01100
6	6	-0.190982	-0.52454	-1.13636	-0.00000	12.01100
7	7	0.051332	-2.95554	-1.13518	0.00000	14.00700
8	1	0.108213	-2.68320	1.53058	0.00000	1.00800
9	1	0.095977	-0.53147	2.74823	0.00000	1.00800
10	1	0.104410	1.62036	1.50672	-0.00000	1.00800
11	1	0.095977	1.61963	-0.97758	-0.00000	1.00800
12	1	0.108213	-0.51076	-2.23221	0.00000	1.00800
13	1	0.056873	-2.95650	-2.12283	-0.00000	1.00800
14	1	0.056873	-3.81135	-0.64219	-0.00000	1.00800

ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	-0.00477	-0.00276	-0.00000
2	6	-0.14842	0.10805	0.00000
3	6	0.08931	-0.00779	-0.00000

4	6	0.05843	0.03375	0.00000
5	6	0.03791	0.08124	0.00000
6	6	0.01935	-0.18254	-0.00000
7	7	0.05833	0.03368	-0.00000
8	1	-0.05789	-0.05125	-0.00000
9	1	-0.01847	-0.04701	-0.00000
10	1	0.12235	0.07064	-0.00000
11	1	-0.04994	0.00750	0.00000
12	1	-0.07333	-0.02451	0.00000
13	1	0.00954	-0.05449	0.00000
14	1	-0.04242	0.03551	0.00000

Dipole (Debyes)	x	y	z	Total
Point-Chg.	-1.189	-0.686	0.000	1.373
sp Hybrid	-0.169	-0.098	-0.000	0.195
pd Hybrid	0.000	0.000	0.000	0.000
Sum	-1.358	-0.784	-0.000	1.568

HyperChem log stop -- Mon Oct 28 14:21:40 2019.