The Diels-Alder Cyclization of Ketenimines

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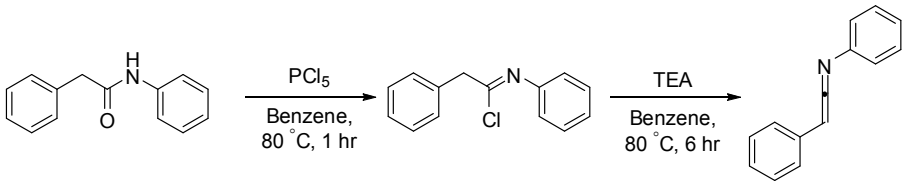
Contents:

General:

Unless otherwise stated, all reactions were carried out under strictly anhydrous, air-free conditions under nitrogen. All solvents and acid chlorides were dried and distilled by standard methods. ^{1}H and ^{13}C NMR spectra were acquired on a 400 MHz NMR and ^{19}F spectra were taken on a 300 MHz NMR in $CDCl_3$ or DMSO-D_6. The ^{1}H (400 MHz), 13C (101 MHz),and ^{19}F (282 MHz) chemical shifts are given in parts per million (δ) with respect to an internal tetramethylsilane (TMS, δ 0.00 ppm) standard, $CFCl_3$, or with the solvent reference relative to TMS employed as an internal standard. NMR data are reported in the following format: chemical shift (multiplicity, integration, coupling constants [Hz]). Diastereoselectivity was determined by ^{1}H and ^{19}F NMR. All measurements were recorded at 25 °C unless otherwise stated.

Synthesis of ketenimines:

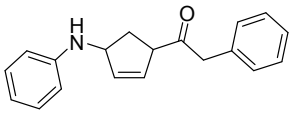
Synthetic preparation of ketenimines was based on a procedure by McCarthy et al.[i] To a dry 100 mL round bottom flask equipped with a stir bar was added a suitable amide (4.25 mmol). Benzene (20 mL) was added to the flask and the amide then dissolved. Next, PCl_5 (0.89 g, 4.30 mmol) was added to the reaction mixture, and the reaction was refluxed for 1 h at 80 °C. Upon addition of PCl_5, the solution quickly turned red or yellow. The solvent was evaporated and the crude mixture was placed under high vacuum for 1 h (to remove phosphorus oxychloride byproduct). Benzene (20 mL) was added to dissolve the residue, followed by triethylamine (0.60 mL, 4.30 mmol). The reaction was refluxed for 6 h; after reflux, the solvent was removed and pentane was added to the crude mixture. The solids were filtered off, and the filtrate was collected and concentrated. Ketenimine formation was verified by IR (2005-2015 cm^{-1}). Titration of the filtrate with ethyl acetate was performed using ^{1}H NMR to determine the concentration of the ketenimine (ketenimines were found to be more stable when stored in solution).



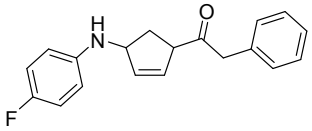
Optimized Cycloaddition Procedure:

To a dry 10 mL round bottom flask equipped with a stir bar was added $CuClO_4 \cdot (MeCN)_4$ (16.3 mg, 0.05 mmol), and PPh_3 (26.2 mg, 0.1 mmol). Under a nitrogen atmosphere, 0.5 mL CH_2Cl_2 was added and the solution was cooled to 0 °C. A solution of ketenimine (96.6 mg, 0.5 mmol) in 0.5 mL CH_2Cl_2 was added slowly, followed by a cyclopentadiene (0.2 mL, 3.84 mmol). Then the reaction was allowed to warm to 25 °C overnight. The solvents were removed and the crude mixture purified by column chromatography, eluting with a mixture of EtOAc and hexanes to give 83.2 mg of 2-phenyl-1-(4-(phenylamino)cyclopent-2-enyl)ethanone (60% yield).

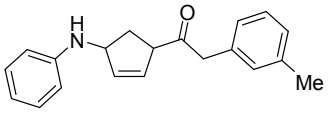
Compound Characterization:



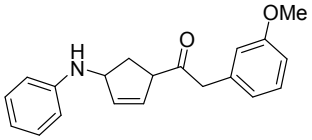
2-phenyl-1-(4-(phenylamino)cyclopent-2-enyl)ethanone: clear oil: % yield = 60; ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.20–7.00 (m, 7H), 6.68 (m, 3H), 6.02 (dt, J = 5.5 Hz, 2.1 Hz, 1H), 5.84 (d, J = 5.5 Hz, 1H), 4.59 (s, 1H), 3.80 (s, 3H), 2.44 (dt, J = 13.7 Hz, 7.7 Hz, 1H), 1.93 (dt, J = 13.7 Hz, 3.5 Hz, 1H); ^{13}C NMR (CDCl3) 208.6, 147.6, 135.5, 134.0, 131.2, 129.8, 129.6, 129.1, 127.5, 117.9, 114.0, 59.0, 56.5, 49.4, 33.99; IR 1712 (cm^{-1}, CaF_2, CH_2Cl_2); HRMS (EI) calc for $C_{19}H_{19}NO^+$: 277.1466, found 277.1463.



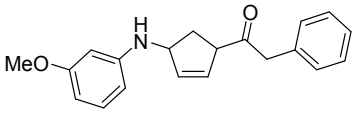
1-(4-(4-fluorophenylamino)cyclopent-2-enyl)-2-phenylethanone: clear oil: % yield = 65 %; ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.35-7.18 (m, 5H), 6.87 (t, 2H), 6.57 (dd, 2H), 5.99 (m, 1H), 5.82 (m, 1H), 4.49 (m, 1H), 3.80 (m, 3H), 2.37 (dt, J =13.4 Hz, 8.38 Hz, 1H), 1.88 (dt, J = 13.8 Hz, 3.7 Hz, 1H), 1.6 (br, 1H); ^{13}C NMR ($CDCl_3$) (@25 ºC) δ 208.5, 156.1 (d, J = 239.2 Hz),143.8, 135.2, 133.7, 131.2, 129.6, 128.9, 127.3, 115.8 (d, J = 22.1 Hz), 114.8 (d, J = 7.0 Hz), 59.6, 56.3, 49.3, 33.4; ^{19}F NMR ($CDCl_3$) δ –128.1 (m); IR 1712 (cm^{-1}, CaF_2, CH_2Cl_2); HRMS (EI) calc for $C_{19}H_{18}FNO^+$: 295.1372, found 295.1373.



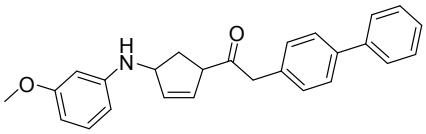
1-(4-(phenylamino)cyclopent-2-enyl)-2-m-tolylethanone: yellow oil; % yield = 45, ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.23–6.90 (m, 6H), 6.75-6.60 (m, 3H), 6.03 (dt, J = 5.6 Hz, 2.0 Hz 1H), 5.87 (ddd, J = 5.6 Hz, 2.4 Hz, 1.4Hz, 1H), 4.58 (s, 1H), 3.90 (br, 1H), 3.75 (m 3H), 2.50-2.40 (ddd, J = 16.6 Hz, 8.3 Hz, 7.9 Hz 1H), 2.33 (s, 3H), 1.95-1.85 (dt, J = 13.6 Hz, 3.9 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 208.5, 147.3, 138.4, 135.1, 133.5, 130.9, 130.2, 129.2, 128.6, 127.9, 126.5, 117.6, 113.6, 55.6, 56.1, 49.0, 33.6, 21.3; IR 1712 (cm^{-1}, CaF_2, CH_2Cl_2); HRMS (EI) calc for $C_{20}H_{20}NO^{+}$: 291.1623, found 291.1626.



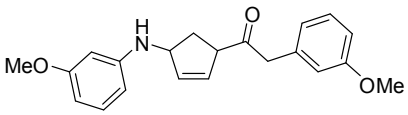
2-(3-methoxyphenyl)-1-(4-(phenylamino)cyclopent-2-enyl)ethanone: yellow oil; % yield = 62, ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.40–6.5 (m, 9H), 6.00 (dt, J = 5.5 Hz, 2.1 Hz, 1H), 5.83 (d, J = 5.5 Hz, 1H), 4.56 (s, 1H), 4.00-3.90 (br, 1H), 3.75-3.80 (m, 5H), 2.50-2.35 (m, 1H), 1.95-1.85 (dt, J = 13.7 Hz, 4.0 Hz, 1H); ^{13}C NMR (CDCl3)^{13}C NMR ($CDCl_3$) δ 208.2, 159.9, 147.4, 135.3, 135.2, 130.9, 129.8, 129.3, 121.9, 117.7, 115.2, 113.7, 112.7, 58.8, 56.2, 55.2, 49.2, 33.7; IR 1712 (cm^{-1}, CaF_2, CH_2Cl_2); HRMS (EI) calc for $C_{20}H_{20}NO_2^{+}$: 307.1572, found 307.1570.



1-(4-(3-methoxyphenylamino)cyclopent-2-enyl)-2-phenylethanone: yellow oil; % yield = 63; ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.60–7.00 (m, 6H), 6.30-6.15 (m, 3H), 6.03 (m, 1H), 5.87 (m, 1H), 4.57 (br, 1H), 4.00-3.90 (br, 1H), 3.80 (s, 2H), 3.78 (s, 3H), 2.47 (dt, J = 13.6 Hz, 8.2 Hz, 1H), 1.94 (dt, J = 13.6 Hz, 3.9 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 208.3, 160.7, 148.6, 135.1, 133.6, 130.8, 129.9, 129.5, 128.7, 127.1, 106.6, 102.7, 99.9, 58.6, 56.1, 55.0, 49.1, 33.6; IR 1712 (cm^{-1}, CaF_2, CH_2Cl_2); HRMS (EI) calc for $C_{20}H_{20}NO_2^{+}$ 307.1572, found 307.1569.



2-(biphenyl-4-yl)-1-(4-(3-methoxyphenylamino)cyclopent-2-enyl)ethanone: yellow oil; % yield = 38, ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.60–7.20 (m, 11H), 6.35-6.15 (m, 3H), 6.03 (dt, J = 5.6 Hz, 1.9 Hz 1H), 5.87 (d, J = 5.7 Hz, 1H), 4.56 (s, 1H), 3.96 (br, 1H), 3.77 (m 5H), 2.50-2.35 (dt, J = 13.6 Hz, 7.8 Hz 1H), 1.95-1.85 (dt, J = 13.3 Hz, 4.1 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 208.3, 160.9, 160.0, 135.3, 135.2, 131.0, 130.1, 129.9, 129.6, 129.4, 122.0, 115.3, 112.7, 106.8, 102.9, 100.1, 99.7, 58.6, 56.1, 55.1, 49.2, 33.8; IR 1713 (cm^{-1}, CaF_2, CH_2Cl_2); HRMS (EI) calc for $C_{26}H_{25}NO_2^+$: 383.1885, found 383.1881.

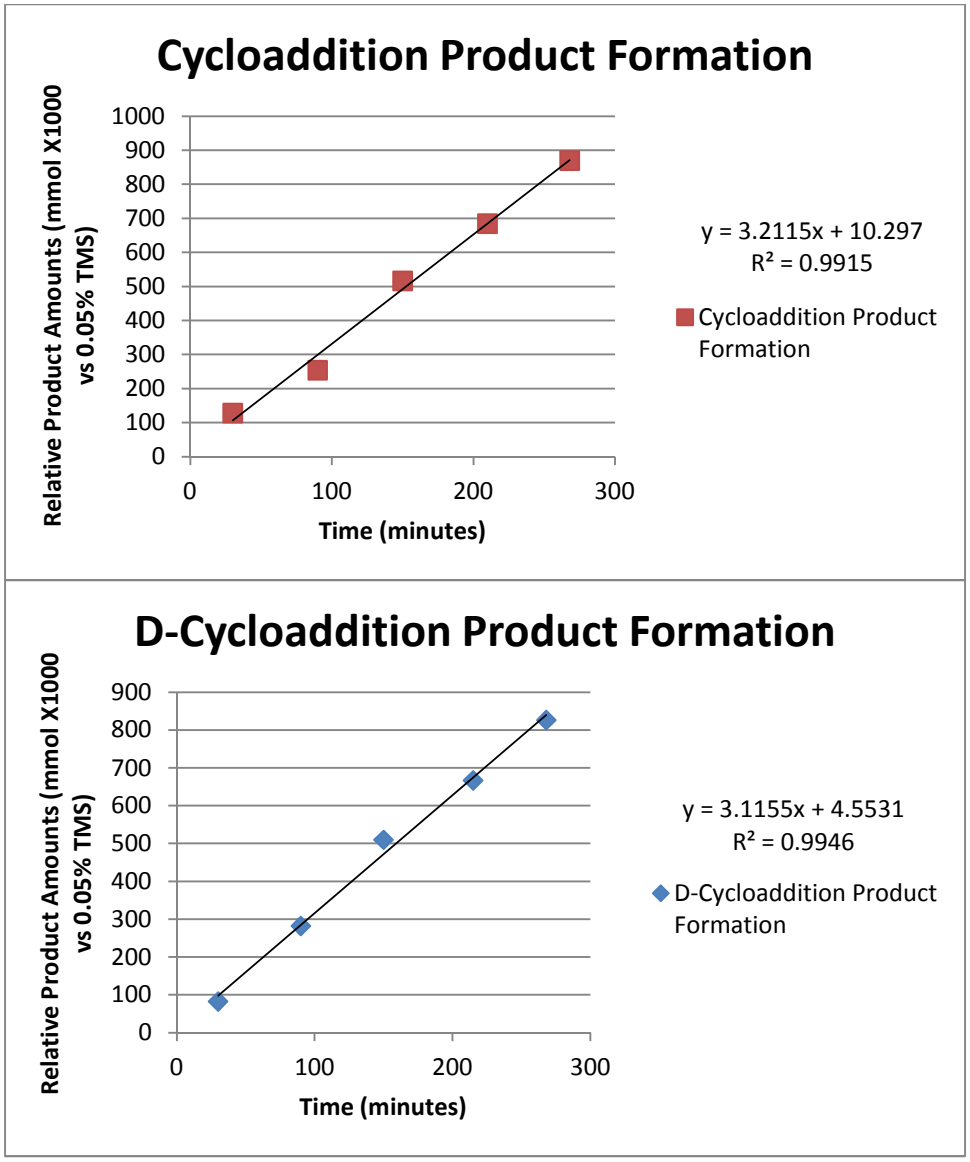


2-(3-methoxyphenyl)-1-(4-(3-methoxyphenylamino)cyclopent-2-enyl)ethanone: yellow oil; % yield = 73, ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.30–7.20 (m, 1H), 7.00 (t, 1H), 6.81 (dd, 1H), 6.78 (d, 1H), 6.73 (s, 1H), 6.26 (td, 2H), 6.19 (t, 1H), 6.00 (dt, J = 5.50 Hz, 2.24 Hz, 1H), 5.82 (m, 1H), 4.54 (s, 1H), 3.90-3.70 (m, 10H), 2.42 (dt, J = 14.0 Hz, 8.0 Hz, 1H), 1.89 (dt, J = 13.60 Hz, 4.0 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 208.2, 160.8, 159.8, 148.6, 135.1, 135.1, 130.9, 129.9, 129.7, 121.8, 115.1, 112.7, 106.6, 102.7, 99.5, 58.6, 56.1, 55.2, 55.0, 49.1, 33.6; IR 1713 (cm^{-1}, CaF_2, CH_2Cl_2); HRMS (EI) calc for $C_{21}H_{23}NO_2^+$: 337.1677, found 337.1680.

Procedure for rate studies:

To a dry NMR tube equipped with a small stir bar was added $CuClO_4{\cdot}(MeCN)_4$ (5.4 mg, 0.0166 mmol), PPh_3 (10.4 mg, 0.0166 mmol). Under a nitrogen atmosphere, 0.5 mL CH_2Cl_2 was added. A solution of ketenimine (0.166 mmol) in 0.5 mL CH_2Cl_2 was added slowly, followed by a cyclopentadiene (0.2 mL, 3.84 mmol). The stir bar was removed, and the tube inverted several times to obtain a homogenous solution. The reaction was allowed to react for 1 hr before the reaction was monitored once an hour for several hours. Kinetic isotope effects were measured by ^{1}H NMR in $CDCl_3$. The proton peak from the methoxy group appears near 3.7 and was used to monitor the rate of product formation against an internal standard (TMS, tetramethylsilane).

Rate plots:


Cycloaddition Product Formation
Relative Product Amounts (mmol X1000 vs 0.05% TMS)
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900
800
700
600
500
400
300
200
100
0
0
100
200
300
Time (minutes)
y = 3.2115x + 10.297
R² = 0.9915
Cycloaddition Product Formation

D-Cycloaddition Product Formation
Relative Product Amounts (mmol X1000 vs 0.05% TMS)
900
800
700
600
500
400
300
200
100
0
0
100
200
300
Time (minutes)
y = 3.1155x + 4.5531
R² = 0.9946
D-Cycloaddition Product Formation

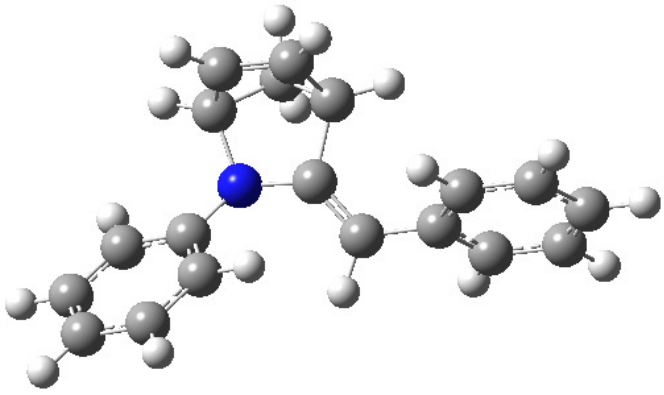
Calculations:

General Information:

All calculations were performed using the Gaussian 09[34a] and GaussView v5.08 programs at the Kohn Sham hybrid-DFT B3LYP[ii] level of theory and the GenECP method was employed using a 6-31G(d) basis set for all atoms (i.e. C, N, O).

Computations:

Enamine A



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%nproc=1
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Default route: MaxDisk=2000MB

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Title Card Required
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Symbolic Z-matrix:
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C                  14   B15      13   A14      12   D13      0
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H                  28   B36      27   A35      12   D34      0
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Input orientation:

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27	6	0	-1.192228	1.171057	-3.247285
28	6	0	-1.483348	2.518119	-5.716762
29	6	0	-0.785853	2.504450	-3.401639
30	6	0	-1.751613	0.532780	-4.366383
31	6	0	-1.896850	1.195809	-5.589004
32	6	0	-0.927589	3.173414	-4.622386
33	1	0	-0.323460	3.035032	-2.574025
34	1	0	-2.107451	-0.490719	-4.285325
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6	H	3.357823	4.285326	2.174974	2.649848	1.077420
7	C	2.242542	3.275587	2.316662	3.371938	1.521605
8	H	3.277389	4.256613	3.280877	4.296656	2.237821
9	C	1.538740	2.220229	2.311027	3.311673	2.310732
10	H	2.221129	2.628790	2.594484	3.434268	2.600720
11	H	2.213892	2.643292	3.326127	4.309982	3.325073
12	N	2.340158	3.330639	2.815420	3.780749	2.427327
13	C	1.543924	2.275652	2.479247	3.273590	2.813010
14	C	2.577621	2.878368	3.556437	4.117249	4.069304
15	H	3.549538	3.941482	4.435182	5.027021	4.732966
16	C	3.090948	2.865305	4.100291	4.382274	4.966346
17	C	5.222807	4.497252	6.086541	5.986524	7.241729
18	C	3.391769	3.037095	3.986425	3.909603	5.067474
19	C	4.070346	3.645636	5.287874	5.615454	6.138735
20	C	5.039724	4.389998	6.167921	6.310268	7.178346
21	C	4.509651	3.899868	5.096858	4.855860	6.286964
22	H	3.226148	3.101161	3.401700	3.164319	4.465997
23	H	4.404933	4.101707	5.750295	6.241773	6.428627
24	H	5.919035	5.235815	7.134298	7.321573	8.113029
25	H	5.101839	4.492926	5.424683	4.970317	6.667921
26	H	6.194256	5.394590	7.007981	6.819769	8.211846
27	C	3.652073	4.647856	3.809777	4.649274	3.169626
28	C	6.420484	7.407409	6.313627	6.967036	5.511796
29	C	4.296624	5.202146	4.280517	4.876902	3.856535
30	C	4.734692	5.755110	4.858840	5.759122	3.941603
31	C	6.022040	7.045113	6.016868	6.822560	5.064000
32	C	5.683083	6.599952	5.558685	6.093705	4.997406
33	H	3.992700	4.768566	3.957309	4.378335	3.866388
34	H	4.800642	5.794262	5.031464	6.020423	4.043796
35	H	6.881444	7.909979	6.881736	7.721713	5.833925
36	H	6.344842	7.191575	6.150984	6.538152	5.724696
37	H	7.495655	8.479228	7.338508	7.945889	6.515280

		6	7	8	9	10
6	H	0.000000				
7	C	2.316520	0.000000			
8	H	2.671075	1.091776	0.000000		
9	C	3.309412	1.539937	2.223211	0.000000	
10	H	3.440103	2.220902	2.627227	1.097730	0.000000
11	H	4.306908	2.214410	2.647270	1.097227	1.787347
12	N	3.210093	1.489455	2.221353	2.308967	3.322734
13	C	3.768597	2.335477	3.321576	2.332294	3.353945
14	C	4.966439	3.652603	4.586510	3.546255	4.551613
15	H	5.538242	4.169467	4.966798	4.307798	5.373004
16	C	5.887948	4.775689	5.779637	4.319491	5.163496
17	C	8.132495	7.285772	8.321246	6.516464	7.091800
18	C	5.878351	5.288526	6.364094	4.860700	5.542354
19	C	7.118589	5.739523	6.664885	5.074276	5.882610
20	C	8.146155	6.930606	7.892030	6.132445	6.809462
21	C	7.088264	6.561784	7.639393	5.956842	6.517856
22	H	5.148069	4.951086	6.033911	4.748277	5.385722
23	H	7.431509	5.775332	6.585089	5.126319	5.988937
24	H	9.108923	7.750389	8.659587	6.875953	7.529866
25	H	7.368217	7.156401	8.246696	6.595871	7.056205
26	H	9.086353	8.309111	9.346594	7.477441	7.979491
27	C	3.585145	2.467471	2.806262	3.647357	4.590243
28	C	5.471758	5.073828	5.053329	6.420485	7.285234
29	C	4.127573	3.601167	4.083354	4.703276	5.649692
30	C	4.161235	3.027640	2.829373	4.324858	5.152765
31	C	5.081089	4.351192	4.096097	5.705948	6.513145
32	C	5.052768	4.768952	5.046589	5.998716	6.914130
33	H	4.220137	3.874430	4.583423	4.746255	5.684814
34	H	4.316381	2.874999	2.355994	4.049885	4.770612

35	H	5.784136	5.041511	4.579623	6.384070	7.116358
36	H	5.731573	5.673223	6.037022	6.845004	7.759644
37	H	6.384776	6.127818	6.048081	7.496762	8.344199

		11	12	13	14	15
11	H	0.000000				
12	N	2.580708	0.000000			
13	C	2.591960	1.411761	0.000000		
14	C	3.576662	2.484617	1.342263	0.000000	
15	H	4.215559	2.773539	2.105662	1.086452	0.000000
16	C	4.346512	3.829599	2.484864	1.463176	2.165718
17	C	6.530945	6.554197	5.155091	4.263208	4.822707
18	C	5.147953	4.544071	3.192900	2.493289	3.243544
19	C	4.829229	4.789788	3.525796	2.472470	2.856954
20	C	5.929424	6.087213	4.754773	3.757583	4.176039
21	C	6.191458	5.895408	4.513211	3.770928	4.448789
22	H	5.244841	4.311301	3.108059	2.721575	3.476801
23	H	4.667249	4.761660	3.693438	2.689101	2.812305
24	H	6.538650	6.903260	5.626367	4.626556	4.932944
25	H	6.957873	6.600241	5.260266	4.645466	5.339920
26	H	7.488819	7.625547	6.221420	5.349200	5.889097
27	C	3.886660	1.406221	2.531631	3.193495	3.042967
28	C	6.627823	4.234013	5.233730	5.523595	4.962716
29	C	5.029196	2.462577	3.054013	3.287201	2.940977
30	C	4.426921	2.435609	3.758840	4.458517	4.195687
31	C	5.821878	3.724513	4.956332	5.476293	5.027046
32	C	6.293518	3.741960	4.444000	4.570754	4.036259
33	H	5.147275	2.717053	2.789629	2.781551	2.562326
34	H	4.020811	2.666765	4.039370	4.881593	4.731303
35	H	6.430433	4.590593	5.887014	6.450929	5.991437
36	H	7.180472	4.615993	5.106209	5.041648	4.464476
37	H	7.697479	5.320211	6.300763	6.523411	5.896841

		16	17	18	19	20
16	C	0.000000				
17	C	2.800168	0.000000			
18	C	1.400350	2.416900	0.000000		
19	C	1.398288	2.418220	2.416158	0.000000	
20	C	2.423781	1.394716	2.789480	1.396717	0.000000
21	C	2.424985	1.394460	1.395717	2.790510	2.414847
22	H	2.162852	3.398199	1.087294	3.405094	3.876687
23	H	2.161220	3.398895	3.405466	1.086945	2.150291
24	H	3.407296	2.154996	3.876416	2.155490	1.086940
25	H	3.408390	2.154234	2.154497	3.876942	3.399734
26	H	3.886174	1.086006	3.401177	3.402451	2.154168
27	C	4.629065	7.410204	5.312109	5.611154	6.942202
28	C	6.882804	9.567727	7.477047	7.811307	9.114313
29	C	4.586560	7.251128	5.081833	5.663968	6.915954
30	C	5.917166	8.714808	6.686599	6.776855	8.145618
31	C	6.922230	9.703122	7.647483	7.784859	9.147656
32	C	5.822666	8.409562	6.288521	6.835554	8.069283
33	H	3.873548	6.394659	4.179802	5.051059	6.200270
34	H	6.312912	9.083305	7.157552	7.069626	8.441304
35	H	7.907926	10.699605	8.682188	8.708025	10.087319
36	H	6.129794	8.528405	6.450062	7.151592	8.289358
37	H	7.847179	10.480678	8.413197	8.751871	10.034905

		21	22	23	24	25
21	C	0.000000				
22	H	2.149952	0.000000			
23	H	3.877403	4.310203	0.000000		
24	H	3.400238	4.963611	2.472589	0.000000	
25	H	1.086441	2.472434	4.963833	4.297999	0.000000
26	H	2.153976	4.293568	4.294145	2.482082	2.481453
27	C	6.702263	4.975654	5.532043	7.757407	7.371980
28	C	8.828824	7.044685	7.668868	9.891286	9.418569
29	C	6.447376	4.640089	5.721210	7.784500	7.031777
30	C	8.070009	6.374524	6.543933	8.887071	8.763187
31	C	9.030293	7.281127	7.539330	9.883581	9.689194
32	C	7.610868	5.818479	6.835825	8.902854	8.152086
33	H	5.513389	3.681198	5.285868	7.128181	6.040106

34	H	8.514381	6.914996	6.751960	9.124664	9.244610
35	H	10.064220	8.335413	8.386067	10.780373	10.741529
36	H	7.691792	5.939561	7.237732	9.135501	8.151504
37	H	9.740213	7.963936	8.595413	10.795006	10.302757

	26	27	28	29	30
26 H	0.000000				
27 C	8.492235	0.000000			
28 C	10.625288	2.828011	0.000000		
29 C	8.308792	1.402464	2.417950	0.000000	
30 C	9.800220	1.404525	2.416000	2.398105	0.000000
31 C	10.784431	2.445558	1.391334	2.780543	1.398393
32 C	9.445941	2.443435	1.391381	1.399223	2.778039
33 H	7.426728	2.163895	3.389592	1.086402	3.393145
34 H	10.162046	2.162558	3.389929	3.390952	1.086619
35 H	11.783462	3.424030	2.151886	3.866530	2.156211
36 H	9.518296	3.421665	2.152918	2.156026	3.864696
37 H	11.523495	3.914225	1.086215	3.403798	3.402271

	31	32	33	34	35
31 C	0.000000				
32 C	2.405149	0.000000			
33 H	3.866315	2.140071	0.000000		
34 H	2.142033	3.864137	4.306052	0.000000	
35 H	1.086045	3.391390	4.952360	2.459115	0.000000
36 H	3.392290	1.086704	2.454048	4.950837	4.292636
37 H	2.153209	2.153043	4.283830	4.285457	2.482363

	36	37	
36 H	0.000000		
37 H	2.483108	0.000000	

Stoichiometry C19H17N
Framework group C1[X(C19H17N)]
Deg. of freedom 105
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.679200	1.858421	-0.007864
2	1	0	1.741022	2.067247	-0.136162
3	6	0	0.058276	2.303804	1.305580
4	1	0	0.579037	2.429390	2.241251
5	6	0	-1.268717	2.401483	1.092719
6	1	0	-2.029857	2.626771	1.821242
7	6	0	-1.526520	2.049028	-0.364880
8	1	0	-2.445810	2.434444	-0.810228
9	6	0	-0.237727	2.645025	-0.960870
10	1	0	-0.162999	3.734330	-0.847553
11	1	0	-0.089768	2.384027	-2.016282
12	7	0	-1.222766	0.600750	-0.534292
13	6	0	0.163595	0.437743	-0.323343
14	6	0	0.910017	-0.670887	-0.447703
15	1	0	0.446094	-1.603274	-0.757229
16	6	0	2.354487	-0.730294	-0.222182
17	6	0	5.121200	-0.882087	0.181799
18	6	0	2.899126	-0.480522	1.043505
19	6	0	3.203805	-1.070144	-1.279713
20	6	0	4.584120	-1.142160	-1.078813
21	6	0	4.278574	-0.553320	1.243125
22	1	0	2.250281	-0.233222	1.880196
23	1	0	2.796432	-1.275281	-2.266331
24	1	0	5.239263	-1.403213	-1.905902
25	1	0	4.695157	-0.356540	2.227041
26	1	0	6.194375	-0.940183	0.337777
27	6	0	-2.254959	-0.304633	-0.230455
28	6	0	-4.368038	-2.094373	0.343458
29	6	0	-2.096787	-1.344303	0.697431

30	6	0	-3.502769	-0.189524	-0.864813
31	6	0	-4.549838	-1.072628	-0.583255
32	6	0	-3.140611	-2.230831	0.984351
33	1	0	-1.159618	-1.460765	1.234478
34	1	0	-3.661808	0.582816	-1.612434
35	1	0	-5.501623	-0.964647	-1.095054
36	1	0	-2.990882	-3.022630	1.713434
37	1	0	-5.178530	-2.783301	0.563329

```
Rotational constants (GHZ):      0.6416468      0.2097117      0.1799490
Standard basis: 6-311++G(d,p) (5D, 7F)
There are   559 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  559 basis functions,   873 primitive gaussians,   579 cartesian basis functions
   69 alpha electrons       69 beta electrons
      nuclear repulsion energy      1419.1213973029 Hartrees.
NAtoms=   37 NActive=   37 NUniq=   37 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=   559 RedAO= T  NBF=   559
NBsUse=   555 1.00D-06 NBFU=   555
Harris functional with IExCor=  402 diagonalized for initial guess.
ExpMin= 3.60D-02 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=3 IRadAn=         5 AccDes= 0.00D+00
HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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 The electronic state of the initial guess is 1-A.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -789.139215367     A.U. after   16 cycles
            Convg  =    0.4024D-08             -V/T =  2.0046
            S**2   =   0.0000
 Range of M.O.s used for correlation:     1   555
 NBasis=   559 NAE=    69 NBE=    69 NFC=     0 NFV=     0
 NROrb=    555 NOA=    69 NOB=    69 NVA=   486 NVB=   486

 **** Warning!!: The largest alpha MO coefficient is  0.12532621D+03

          Differentiating once with respect to magnetic field.
          Electric field/nuclear overlap derivatives assumed to be zero.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 2 Meth= 1.
 IRaf=       0 NMat=   6 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2 JSym2E=2.
          There are   6 degrees of freedom in the 1st order CPHF.
      6 vectors were produced by pass  0.
 AX will form   6 AO Fock derivatives at one time.
      6 vectors were produced by pass  1.
      6 vectors were produced by pass  2.
      6 vectors were produced by pass  3.
      6 vectors were produced by pass  4.
      6 vectors were produced by pass  5.
      3 vectors were produced by pass  6.
 Inv2:  IOpt= 1 Iter= 1 AM= 9.22D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension   39 with in-core refinement.
 Calculating magnetic properties, IRadAn=         0.
   Integrating Atom   1
   Integrating Atom   2
   Integrating Atom   3
   Integrating Atom   4
   Integrating Atom   5
   Integrating Atom   6
   Integrating Atom   7
   Integrating Atom   8
   Integrating Atom   9
   Integrating Atom  10
   Integrating Atom  11
   Integrating Atom  12
   Integrating Atom  13
   Integrating Atom  14
   Integrating Atom  15
   Integrating Atom  16
   Integrating Atom  17
   Integrating Atom  18
   Integrating Atom  19
   Integrating Atom  20
   Integrating Atom  21
   Integrating Atom  22
   Integrating Atom  23
   Integrating Atom  24
   Integrating Atom  25
   Integrating Atom  26
   Integrating Atom  27
   Integrating Atom  28
   Integrating Atom  29
   Integrating Atom  30
   Integrating Atom  31
```

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 Integrating Atom  32
 Integrating Atom  33
 Integrating Atom  34
 Integrating Atom  35
 Integrating Atom  36
 Integrating Atom  37
There are a total of      307076 grid points.
ElSum from orbitals=       77.5791956200

    Magnetic properties (single gauge origin)

Magnetic susceptibility (cgs-ppm):
 Isotropic =  -880.4149   Anisotropy=   719.8481
 XX=  -401.7580   YX=    21.8758   ZX=   -20.2295
 XY=    21.8748   YY= -1011.6221   ZY=    21.1121
 XZ=   -20.2285   YZ=    21.1093   ZZ= -1227.8645
 Eigenvalues: -1230.5043 -1010.2241  -400.5162
Magnetic shielding (ppm):
 1  C    Isotropic =   171.5563   Anisotropy =    37.3604
  XX=   149.1779   YX=    32.6778   ZX=    -6.8100
  XY=    -8.2343   YY=   182.8136   ZY=   -12.3319
  XZ=     2.9393   YZ=   -10.6504   ZZ=   182.6775
  Eigenvalues:   145.1209   173.0848   196.4633
 2  H    Isotropic =    45.8478   Anisotropy =    38.1181
  XX=    43.6208   YX=    37.6559   ZX=     1.6505
  XY=    13.2371   YY=    47.6288   ZY=    -0.5855
  XZ=    -0.5693   YZ=    -4.9131   ZZ=    46.2937
  Eigenvalues:    19.9051    46.3784    71.2598
 3  C    Isotropic =    60.7106   Anisotropy =   178.8044
  XX=    42.5591   YX=    29.2843   ZX=    10.1709
  XY=   -32.1221   YY=   165.7039   ZY=   -83.5094
  XZ=   -23.3117   YZ=   -24.7066   ZZ=   -26.1312
  Eigenvalues:   -40.8807    43.0989   179.9135
 4  H    Isotropic =    27.5296   Anisotropy =    46.4372
  XX=     9.0837   YX=    21.8496   ZX=    11.5003
  XY=     0.2969   YY=    29.9483   ZY=    -0.0183
  XZ=     1.8635   YZ=    35.2598   ZZ=    43.5568
  Eigenvalues:     4.2764    19.8247    58.4877
 5  C    Isotropic =    52.1307   Anisotropy =   167.7847
  XX=    45.3169   YX=   -14.8887   ZX=    -4.5223
  XY=    63.8139   YY=   149.4051   ZY=   -65.0876
  XZ=    28.1343   YZ=   -27.3872   ZZ=   -38.3300
  Eigenvalues:   -52.1476    44.5525   163.9871
 6  H    Isotropic =    16.0850   Anisotropy =    51.8723
  XX=    13.0325   YX=   -33.0234   ZX=   -15.0265
  XY=    -9.3686   YY=    17.2643   ZY=     1.0269
  XZ=   -16.2772   YZ=    28.7700   ZZ=    17.9583
  Eigenvalues:    -6.3448     3.9333    50.6666
 7  C    Isotropic =   135.1665   Anisotropy =    56.3794
  XX=   126.1097   YX=   -29.5931   ZX=     7.9248
  XY=    -8.9263   YY=   162.8828   ZY=    -7.2067
  XZ=     4.1362   YZ=    -8.4378   ZZ=   116.5069
  Eigenvalues:   113.5195   119.2271   172.7527
 8  H    Isotropic =    21.8542   Anisotropy =    64.0721
  XX=    28.7780   YX=   -36.8068   ZX=     5.9231
  XY=   -29.2104   YY=    22.3369   ZY=    -7.9510
  XZ=    19.3066   YZ=   -15.1913   ZZ=    14.4479
  Eigenvalues:    -7.6084     8.6022    64.5690
 9  C    Isotropic =   138.9723   Anisotropy =    45.0462
  XX=   123.0579   YX=     6.4941   ZX=    -4.9396
  XY=   -10.5650   YY=   131.4388   ZY=   -10.3441
  XZ=     2.9597   YZ=   -21.1053   ZZ=   162.4202
  Eigenvalues:   121.5247   126.3891   169.0031
10  H    Isotropic =    16.3349   Anisotropy =    61.0616
  XX=    -8.4407   YX=     6.4449   ZX=    -0.9264
  XY=    -6.8559   YY=    54.6305   ZY=   -15.5522
  XZ=     3.8703   YZ=    -7.3027   ZZ=     2.8149
  Eigenvalues:    -8.6601     0.6221    57.0427
```

11 H Isotropic = 42.2773 Anisotropy = 54.1317
XX= 25.5659 YX= 7.7428 ZX= -2.6521
XY= -3.3739 YY= 35.5822 ZY= -2.6110
XZ= 6.5935 YZ= -43.9525 ZZ= 65.6840
Eigenvalues: 21.0816 27.3853 78.3651
12 N Isotropic = 192.6390 Anisotropy = 52.3329
XX= 192.7892 YX= 0.7777 ZX= 2.9421
XY= -13.2100 YY= 165.2712 ZY= -6.6741
XZ= -33.4337 YZ= -14.2639 ZZ= 219.8566
Eigenvalues: 160.6114 189.7780 227.5276
13 C Isotropic = 97.4278 Anisotropy = 160.8877
XX= 10.6242 YX= -35.5109 ZX= -30.1692
XY= -26.8061 YY= 84.1722 ZY= -24.3681
XZ= -25.4204 YZ= -23.1188 ZZ= 197.4871
Eigenvalues: -6.6007 94.1979 204.6863
14 C Isotropic = 128.9458 Anisotropy = 149.1174
XX= 50.9291 YX= -30.1098 ZX= -32.5792
XY= -34.0649 YY= 116.3755 ZY= -16.5686
XZ= -44.1691 YZ= -12.2446 ZZ= 219.5327
Eigenvalues: 29.0102 129.4698 228.3574
15 H Isotropic = 59.2656 Anisotropy = 28.7481
XX= 32.6516 YX= 2.5780 ZX= 5.2421
XY= -11.6525 YY= 71.1721 ZY= 7.9194
XZ= -5.1464 YZ= 3.1090 ZZ= 73.9731
Eigenvalues: 32.1130 67.2528 78.4310
16 C Isotropic = 95.4462 Anisotropy = 213.3019
XX= -26.3647 YX= 29.1696 ZX= -11.9739
XY= 20.1697 YY= 224.3015 ZY= -39.0677
XZ= -19.0623 YZ= -38.9694 ZZ= 88.4017
Eigenvalues: -29.9828 78.6739 237.6474
17 C Isotropic = 27.0697 Anisotropy = 170.0584
XX= -29.6364 YX= 5.7188 ZX= -15.8470
XY= 11.1060 YY= 129.4428 ZY= -40.5401
XZ= -2.6085 YZ= -40.4696 ZZ= -18.5972
Eigenvalues: -36.4913 -22.7415 140.4420
18 C Isotropic = 95.9226 Anisotropy = 176.9898
XX= 35.9307 YX= 26.0560 ZX= 36.3637
XY= 38.7438 YY= 202.1634 ZY= -26.9843
XZ= 83.5683 YZ= -52.9257 ZZ= 49.6736
Eigenvalues: -28.7462 102.5981 213.9158
19 C Isotropic = 82.6075 Anisotropy = 180.2149
XX= 34.4305 YX= 11.2537 ZX= -21.1372
XY= -5.3152 YY= 194.8536 ZY= -36.5620
XZ= -93.6283 YZ= -33.2924 ZZ= 18.5385
Eigenvalues: -34.1053 79.1771 202.7508
20 C Isotropic = 38.8881 Anisotropy = 178.4713
XX= 9.2977 YX= 16.7851 ZX= 31.4276
XY= 7.3101 YY= 145.7798 ZY= -52.2771
XZ= -24.2553 YZ= -41.6893 ZZ= -38.4132
Eigenvalues: -50.3772 9.1725 157.8690
21 C Isotropic = 52.9946 Anisotropy = 182.3019
XX= 34.3106 YX= 4.1553 ZX= -28.9298
XY= 19.5964 YY= 160.9729 ZY= -43.4890
XZ= 36.4754 YZ= -60.0038 ZZ= -36.2997
Eigenvalues: -49.5568 34.0114 174.5292
22 H Isotropic = 61.5186 Anisotropy = 57.6535
XX= 29.4774 YX= 8.4738 ZX= -7.0524
XY= 12.7299 YY= 63.3516 ZY= 1.0987
XZ= 55.1601 YZ= -6.7492 ZZ= 91.7267
Eigenvalues: 18.5888 66.0127 99.9543
23 H Isotropic = 40.3527 Anisotropy = 64.8228
XX= 12.0829 YX= 7.5174 ZX= 7.2683
XY= -15.0877 YY= 43.1209 ZY= 5.2111
XZ= -68.6604 YZ= 18.5509 ZZ= 65.8542
Eigenvalues: -1.8863 39.3764 83.5679
24 H Isotropic = -15.2337 Anisotropy = 92.5627
XX= 13.4698 YX= -12.0013 ZX= -11.8257
XY= -23.7269 YY= -29.6508 ZY= 1.6430

XZ= -77.6628 YZ= 13.7700 ZZ= -29.5201
Eigenvalues: -58.0266 -34.1493 46.4748
25 H Isotropic = 2.3502 Anisotropy = 84.9055
XX= 17.3562 YX= -2.6816 ZX= 9.2419
XY= 17.6605 YY= -13.5667 ZY= 1.6549
XZ= 86.9035 YZ= -12.7184 ZZ= 3.2610
Eigenvalues: -41.2610 -10.6423 58.9538
26 H Isotropic = -34.1347 Anisotropy = 102.4823
XX= 32.1595 YX= -15.7240 ZX= 2.6867
XY= -4.8451 YY= -59.7788 ZY= -4.6018
XZ= 15.8290 YZ= -7.0563 ZZ= -74.7850
Eigenvalues: -77.0748 -59.5163 34.1868
27 C Isotropic = 86.2713 Anisotropy = 180.1723
XX= 24.4223 YX= -72.7915 ZX= -18.5684
XY= -72.3072 YY= 81.2445 ZY= 63.2831
XZ= -12.4746 YZ= 65.6916 ZZ= 153.1471
Eigenvalues: -28.5924 81.0201 206.3862
28 C Isotropic = 36.3694 Anisotropy = 167.0930
XX= 9.1706 YX= -48.3976 ZX= -26.1327
XY= -19.6288 YY= 33.1609 ZY= 80.1645
XZ= -39.0717 YZ= 80.3621 ZZ= 66.7767
Eigenvalues: -33.2078 -5.4487 147.7648
29 C Isotropic = 111.8512 Anisotropy = 201.8480
XX= 25.0755 YX= -35.1982 ZX= -52.5492
XY= -30.8915 YY= 131.1172 ZY= 72.7026
XZ= -104.6096 YZ= 35.3151 ZZ= 179.3610
Eigenvalues: -8.6495 97.7867 246.4165
30 C Isotropic = 78.8876 Anisotropy = 169.8334
XX= 75.8813 YX= -29.7785 ZX= -28.2189
XY= -59.5487 YY= 63.2932 ZY= 81.3200
XZ= 6.8320 YZ= 114.9608 ZZ= 97.4884
Eigenvalues: -26.9716 71.5245 192.1099
31 C Isotropic = 34.5013 Anisotropy = 175.0871
XX= 2.4319 YX= -6.9886 ZX= -68.8353
XY= -31.7908 YY= 45.6944 ZY= 71.8079
XZ= -41.1872 YZ= 90.2396 ZZ= 55.3777
Eigenvalues: -47.1705 -0.5516 151.2260
32 C Isotropic = 62.8394 Anisotropy = 186.1689
XX= 40.5264 YX= -27.5037 ZX= -38.9837
XY= 24.0140 YY= 68.1321 ZY= 103.5029
XZ= -88.7932 YZ= 88.9935 ZZ= 79.8599
Eigenvalues: -46.1564 47.7227 186.9521
33 H Isotropic = 70.8559 Anisotropy = 45.6735
XX= 34.6997 YX= -21.9079 ZX= 10.3126
XY= 10.5206 YY= 85.7956 ZY= -6.7376
XZ= -23.0462 YZ= -17.1153 ZZ= 92.0723
Eigenvalues: 33.0452 78.2176 101.3049
34 H Isotropic = 27.3308 Anisotropy = 70.6876
XX= 36.0326 YX= -5.5211 ZX= 5.0500
XY= -51.2968 YY= 10.5652 ZY= -9.2588
XZ= 56.2778 YZ= 4.5749 ZZ= 35.3947
Eigenvalues: -13.4992 21.0358 74.4559
35 H Isotropic = -19.8945 Anisotropy = 92.3020
XX= 33.5259 YX= 18.3319 ZX= 6.8831
XY= -11.5373 YY= -52.8720 ZY= 5.1421
XZ= 42.9976 YZ= 18.4816 ZZ= -40.3373
Eigenvalues: -61.2815 -40.0421 41.6402
36 H Isotropic = 15.6435 Anisotropy = 72.8971
XX= -9.1203 YX= -7.3157 ZX= 1.3757
XY= 53.2113 YY= 37.4970 ZY= -10.0815
XZ= -49.6682 YZ= -29.1611 ZZ= 18.5537
Eigenvalues: -25.1769 7.8657 64.2416
37 H Isotropic = -26.4570 Anisotropy = 95.3680
XX= 6.7093 YX= 29.3343 ZX= -7.4879
XY= 58.5740 YY= -31.6759 ZY= 3.7396
XZ= -23.1375 YZ= -1.5186 ZZ= -54.4044
Eigenvalues: -67.7408 -48.7519 37.1216
Current density tensor (au):

XX= -0.5698 YX= 1.7750 ZX= 1.6553
XY= 1.6669 YY= -4.8548 ZY= -3.2258
XZ= -2.6659 YZ= -4.1002 ZZ= 5.4112

Magnetic properties (IGAIM method)

Magnetic susceptibility (cgs-ppm):
Isotropic = -153.8548 Anisotropy= 75.2294
XX= -112.8371 YX= 4.2526 ZX= 20.3331
XY= 3.8613 YY= -200.7268 ZY= -4.4489
XZ= 19.8024 YZ= -4.3223 ZZ= -148.0003
Eigenvalues: -201.4873 -156.3751 -103.7019
Magnetic shielding (ppm):
1 C Isotropic = 128.8450 Anisotropy = 23.1887
XX= 118.2673 YX= 4.5097 ZX= -8.1928
XY= -15.0186 YY= 138.1141 ZY= -9.7614
XZ= 2.0370 YZ= -8.3000 ZZ= 130.1536
Eigenvalues: 114.8579 127.3729 144.3041
2 H Isotropic = 27.8280 Anisotropy = 5.8004
XX= 31.0239 YX= -0.9087 ZX= 0.8810
XY= -1.9831 YY= 28.1517 ZY= 0.1507
XZ= 0.2400 YZ= -1.1735 ZZ= 24.3083
Eigenvalues: 24.2197 27.5693 31.6949
3 C Isotropic = 36.5099 Anisotropy = 173.5289
XX= 40.1501 YX= 9.4241 ZX= -0.9881
XY= -32.7400 YY= 131.3976 ZY= -83.1567
XZ= -23.6352 YZ= -48.5399 ZZ= -62.0180
Eigenvalues: -84.1693 41.5032 152.1959
4 H Isotropic = 24.6258 Anisotropy = 3.6369
XX= 25.4448 YX= -0.4711 ZX= -0.0187
XY= -3.0932 YY= 25.0708 ZY= -1.9816
XZ= -0.6949 YZ= 1.0507 ZZ= 23.3617
Eigenvalues: 22.8265 24.0005 27.0504
5 C Isotropic = 37.3957 Anisotropy = 171.0583
XX= 39.2383 YX= 9.8434 ZX= 9.0678
XY= 75.0487 YY= 124.9751 ZY= -64.3309
XZ= 40.6323 YZ= -45.2244 ZZ= -52.0263
Eigenvalues: -78.7934 39.5459 151.4346
6 H Isotropic = 24.9474 Anisotropy = 3.5913
XX= 25.4727 YX= -0.6900 ZX= -0.0162
XY= 3.6127 YY= 25.4604 ZY= -0.9256
XZ= 2.4213 YZ= 1.8476 ZZ= 23.9092
Eigenvalues: 23.1994 24.3012 27.3416
7 C Isotropic = 110.1599 Anisotropy = 39.7611
XX= 104.9347 YX= -2.3475 ZX= 7.1715
XY= 13.5754 YY= 135.6065 ZY= -0.0498
XZ= -4.7538 YZ= 3.1756 ZZ= 89.9385
Eigenvalues: 89.8134 103.9989 136.6673
8 H Isotropic = 26.5432 Anisotropy = 6.6604
XX= 29.1660 YX= -0.9021 ZX= 2.3285
XY= -2.2361 YY= 27.3916 ZY= -1.4152
XZ= 3.2066 YZ= 0.4424 ZZ= 23.0720
Eigenvalues: 22.0003 26.6459 30.9834
9 C Isotropic = 121.2236 Anisotropy = 30.2816
XX= 125.3667 YX= 0.6370 ZX= -3.5882
XY= -3.9646 YY= 97.8309 ZY= -6.1983
XZ= -3.0098 YZ= -1.2025 ZZ= 140.4732
Eigenvalues: 97.3765 124.8830 141.4113
10 H Isotropic = 29.3924 Anisotropy = 8.5362
XX= 26.8021 YX= 1.1015 ZX= -0.2777
XY= 0.6922 YY= 33.9149 ZY= -3.7527
XZ= 0.5852 YZ= -1.9945 ZZ= 27.4603
Eigenvalues: 26.0521 27.0420 35.0832
11 H Isotropic = 29.1224 Anisotropy = 9.0611
XX= 26.5797 YX= 0.2856 ZX= -0.9737
XY= -0.5529 YY= 26.3296 ZY= -2.8567
XZ= -0.5321 YZ= -1.9181 ZZ= 34.4581
Eigenvalues: 25.5692 26.6349 35.1632

12 N Isotropic = 136.2422 Anisotropy = 56.5540
XX= 154.2591 YX= 12.0902 ZX= 0.5964
XY= -2.3648 YY= 117.3465 ZY= -5.2694
XZ= -52.5982 YZ= -5.3367 ZZ= 137.1209
Eigenvalues: 115.6845 119.0972 173.9448
13 C Isotropic = 31.6136 Anisotropy = 122.1637
XX= -34.3796 YX= -46.8056 ZX= -29.6495
XY= -33.3816 YY= 23.6079 ZY= -21.6664
XZ= -26.6827 YZ= -19.1094 ZZ= 105.6126
Eigenvalues: -61.9220 43.7067 113.0561
14 C Isotropic = 75.8229 Anisotropy = 115.3432
XX= 28.4036 YX= -40.3784 ZX= -35.5111
XY= -31.2216 YY= 58.2216 ZY= -18.7490
XZ= -40.3296 YZ= -13.2722 ZZ= 140.8435
Eigenvalues: -6.6054 81.3557 152.7183
15 H Isotropic = 25.0985 Anisotropy = 7.0901
XX= 28.8840 YX= -3.3505 ZX= -1.1475
XY= -0.5792 YY= 23.6838 ZY= 1.7483
XZ= -1.2938 YZ= -0.1358 ZZ= 22.7278
Eigenvalues: 22.2664 23.2039 29.8253
16 C Isotropic = 38.3101 Anisotropy = 191.5200
XX= -57.3178 YX= 19.6097 ZX= -12.7986
XY= 18.0607 YY= 155.1045 ZY= -35.4156
XZ= -14.8089 YZ= -36.4417 ZZ= 17.1437
Eigenvalues: -60.5493 9.4896 165.9901
17 C Isotropic = 53.1166 Anisotropy = 180.0118
XX= -52.9983 YX= 15.6102 ZX= -18.1472
XY= 12.9851 YY= 164.2865 ZY= -31.4817
XZ= -16.2372 YZ= -29.0137 ZZ= 48.0616
Eigenvalues: -56.2416 42.4669 173.1245
18 C Isotropic = 48.6736 Anisotropy = 160.0748
XX= 17.9214 YX= 17.9519 ZX= 45.7550
XY= 25.3519 YY= 147.1335 ZY= -26.0372
XZ= 43.0914 YZ= -43.6612 ZZ= -19.0341
Eigenvalues: -56.9108 47.5414 155.3902
19 C Isotropic = 49.9796 Anisotropy = 168.2305
XX= 31.8126 YX= 2.9329 ZX= -28.8451
XY= 5.7844 YY= 152.7542 ZY= -36.9728
XZ= -39.4895 YZ= -44.0257 ZZ= -34.6278
Eigenvalues: -55.2733 43.0789 162.1333
20 C Isotropic = 49.8604 Anisotropy = 182.0815
XX= 4.5068 YX= 24.2910 ZX= 43.7947
XY= 26.5891 YY= 157.0806 ZY= -48.9091
XZ= 43.6576 YZ= -48.5054 ZZ= -12.0062
Eigenvalues: -61.5350 39.8681 171.2481
21 C Isotropic = 49.8786 Anisotropy = 181.2438
XX= 26.9498 YX= 3.3132 ZX= -37.5402
XY= 2.7489 YY= 160.5309 ZY= -41.7512
XZ= -38.2565 YZ= -46.2730 ZZ= -37.8450
Eigenvalues: -62.1628 41.0907 170.7077
22 H Isotropic = 24.1727 Anisotropy = 8.6722
XX= 26.5240 YX= -0.4709 ZX= 3.5094
XY= -2.2097 YY= 21.6069 ZY= -2.1528
XZ= 4.3513 YZ= -0.5445 ZZ= 24.3871
Eigenvalues: 21.0115 21.5523 29.9541
23 H Isotropic = 24.2616 Anisotropy = 8.2588
XX= 28.3928 YX= -1.5864 ZX= -2.5175
XY= -1.2805 YY= 21.4823 ZY= 1.0400
XZ= -2.5936 YZ= 1.1945 ZZ= 22.9096
Eigenvalues: 20.8701 22.1473 29.7674
24 H Isotropic = 24.1568 Anisotropy = 5.2747
XX= 26.5024 YX= -0.1335 ZX= 2.0280
XY= -0.2568 YY= 21.5726 ZY= 0.7033
XZ= 1.8758 YZ= 0.7071 ZZ= 24.3953
Eigenvalues: 21.3078 23.4893 27.6732
25 H Isotropic = 24.1276 Anisotropy = 5.8524
XX= 27.5656 YX= -1.0650 ZX= -1.0160
XY= -1.1420 YY= 21.5955 ZY= 0.6769

XZ= -1.0799 YZ= 0.4289 ZZ= 23.2218
Eigenvalues: 21.3220 23.0316 28.0292
26 H Isotropic = 24.3316 Anisotropy = 4.8289
XX= 23.8711 YX= -0.4670 ZX= -0.5022
XY= -0.7323 YY= 21.9981 ZY= 1.2772
XZ= -0.4441 YZ= 1.3882 ZZ= 27.1257
Eigenvalues: 21.5735 23.8704 27.5509
27 C Isotropic = 30.9346 Anisotropy = 158.6510
XX= -18.8460 YX= -58.7490 ZX= -18.1074
XY= -62.9760 YY= 31.3493 ZY= 58.7686
XZ= -16.1647 YZ= 61.1625 ZZ= 80.3005
Eigenvalues: -62.7087 18.8105 136.7019
28 C Isotropic = 56.8660 Anisotropy = 173.6680
XX= 6.8913 YX= -69.8872 ZX= -14.4583
XY= -66.6991 YY= 57.8232 ZY= 66.8157
XZ= -13.3941 YZ= 72.5156 ZZ= 105.8835
Eigenvalues: -46.9386 44.8919 172.6447
29 C Isotropic = 58.3691 Anisotropy = 179.0181
XX= 0.0827 YX= -11.0749 ZX= -60.7043
XY= -37.6684 YY= 69.1631 ZY= 70.2866
XZ= -84.1562 YZ= 43.2890 ZZ= 105.8616
Eigenvalues: -36.9008 34.2936 177.7145
30 C Isotropic = 55.4233 Anisotropy = 161.6406
XX= 50.8722 YX= -20.7474 ZX= -28.2845
XY= -15.0112 YY= 54.5943 ZY= 83.8183
XZ= -33.9359 YZ= 105.4225 ZZ= 60.8032
Eigenvalues: -37.9092 40.9953 163.1836
31 C Isotropic = 49.2070 Anisotropy = 179.8864
XX= -24.1145 YX= -16.9057 ZX= -71.9126
XY= -17.3354 YY= 90.1660 ZY= 57.9472
XZ= -74.5642 YZ= 65.1907 ZZ= 81.5694
Eigenvalues: -62.8305 41.3201 169.1312
32 C Isotropic = 49.1061 Anisotropy = 179.9491
XX= 53.6875 YX= -15.4963 ZX= -36.7039
XY= -17.4692 YY= 34.3187 ZY= 106.0839
XZ= -43.3619 YZ= 107.8066 ZZ= 59.3121
Eigenvalues: -62.7384 40.9845 169.0722
33 H Isotropic = 24.1256 Anisotropy = 10.7431
XX= 24.6853 YX= 3.3404 ZX= -2.5899
XY= 3.2873 YY= 26.9145 ZY= -4.8912
XZ= -2.0915 YZ= -3.0029 ZZ= 20.7770
Eigenvalues: 18.7500 22.3391 31.2877
34 H Isotropic = 24.3355 Anisotropy = 9.0902
XX= 28.3891 YX= 2.3102 ZX= 2.4581
XY= 3.7814 YY= 23.0528 ZY= 0.7914
XZ= 2.1585 YZ= 0.3973 ZZ= 21.5647
Eigenvalues: 20.7654 21.8456 30.3957
35 H Isotropic = 24.1177 Anisotropy = 5.2514
XX= 24.1223 YX= 1.9380 ZX= -0.3405
XY= 1.7742 YY= 25.3067 ZY= -2.3585
XZ= -0.6308 YZ= -2.0811 ZZ= 22.9241
Eigenvalues: 21.4534 23.2810 27.6187
36 H Isotropic = 24.2393 Anisotropy = 5.9941
XX= 27.2378 YX= 2.1030 ZX= 0.8901
XY= 2.3106 YY= 23.3145 ZY= -0.5810
XZ= 0.2251 YZ= -0.9381 ZZ= 22.1655
Eigenvalues: 21.3168 23.1657 28.2354
37 H Isotropic = 24.6415 Anisotropy = 4.2706
XX= 25.3528 YX= -0.4585 ZX= 1.9791
XY= -0.1710 YY= 24.4302 ZY= -2.1841
XZ= 1.8130 YZ= -1.7342 ZZ= 24.1416
Eigenvalues: 21.8566 24.5794 27.4886
Current density tensor (au):
XX= -0.0120 YX= -0.0318 ZX= 0.0326
XY= 0.0040 YY= 0.0689 ZY= 0.0402
XZ= -0.0903 YZ= 0.0552 ZZ= -0.0790

Magnetic properties (CSGT method)

Magnetic susceptibility (cgs-ppm):
Isotropic = -153.9276 Anisotropy= 75.2225
XX= -112.8995 YX= 4.2628 ZX= 20.3117
XY= 3.8663 YY= -200.7904 ZY= -4.4470
XZ= 19.7964 YZ= -4.3222 ZZ= -148.0927
Eigenvalues: -201.5518 -156.4516 -103.7792
Magnetic shielding (ppm):
1 C Isotropic = 128.8329 Anisotropy = 23.1795
XX= 118.2644 YX= 4.5145 ZX= -8.1936
XY= -15.0163 YY= 138.0982 ZY= -9.7600
XZ= 2.0354 YZ= -8.2985 ZZ= 130.1361
Eigenvalues: 114.8532 127.3596 144.2859
2 H Isotropic = 27.8295 Anisotropy = 5.8017
XX= 31.0281 YX= -0.9064 ZX= 0.8818
XY= -1.9822 YY= 28.1520 ZY= 0.1508
XZ= 0.2396 YZ= -1.1735 ZZ= 24.3084
Eigenvalues: 24.2197 27.5714 31.6973
3 C Isotropic = 36.4903 Anisotropy = 173.5123
XX= 40.1343 YX= 9.4233 ZX= -0.9810
XY= -32.7406 YY= 131.3674 ZY= -83.1525
XZ= -23.6291 YZ= -48.5354 ZZ= -62.0309
Eigenvalues: -84.1799 41.4856 152.1651
4 H Isotropic = 24.6231 Anisotropy = 3.6329
XX= 25.4393 YX= -0.4701 ZX= -0.0153
XY= -3.0918 YY= 25.0684 ZY= -1.9810
XZ= -0.6925 YZ= 1.0512 ZZ= 23.3617
Eigenvalues: 22.8277 23.9966 27.0451
5 C Isotropic = 37.3761 Anisotropy = 171.0412
XX= 39.2267 YX= 9.8397 ZX= 9.0618
XY= 75.0449 YY= 124.9450 ZY= -64.3264
XZ= 40.6275 YZ= -45.2197 ZZ= -52.0435
Eigenvalues: -78.8051 39.5298 151.4036
6 H Isotropic = 24.9448 Anisotropy = 3.5871
XX= 25.4696 YX= -0.6912 ZX= -0.0210
XY= 3.6115 YY= 25.4579 ZY= -0.9250
XZ= 2.4180 YZ= 1.8482 ZZ= 23.9068
Eigenvalues: 23.2008 24.2973 27.3361
7 C Isotropic = 110.1473 Anisotropy = 39.7559
XX= 104.9272 YX= -2.3535 ZX= 7.1761
XY= 13.5699 YY= 135.5923 ZY= -0.0509
XZ= -4.7477 YZ= 3.1741 ZZ= 89.9225
Eigenvalues: 89.7968 103.9939 136.6513
8 H Isotropic = 26.5438 Anisotropy = 6.6656
XX= 29.1678 YX= -0.9043 ZX= 2.3285
XY= -2.2390 YY= 27.3918 ZY= -1.4167
XZ= 3.2088 YZ= 0.4414 ZZ= 23.0717
Eigenvalues: 21.9995 26.6443 30.9875
9 C Isotropic = 121.2048 Anisotropy = 30.2861
XX= 125.3395 YX= 0.6377 ZX= -3.5898
XY= -3.9645 YY= 97.8173 ZY= -6.1960
XZ= -3.0111 YZ= -1.1994 ZZ= 140.4577
Eigenvalues: 97.3633 124.8555 141.3955
10 H Isotropic = 29.3911 Anisotropy = 8.5393
XX= 26.8005 YX= 1.1018 ZX= -0.2773
XY= 0.6922 YY= 33.9162 ZY= -3.7532
XZ= 0.5857 YZ= -1.9945 ZZ= 27.4567
Eigenvalues: 26.0492 27.0402 35.0840
11 H Isotropic = 29.1211 Anisotropy = 9.0641
XX= 26.5783 YX= 0.2852 ZX= -0.9738
XY= -0.5534 YY= 26.3261 ZY= -2.8570
XZ= -0.5324 YZ= -1.9184 ZZ= 34.4588
Eigenvalues: 25.5658 26.6336 35.1638
12 N Isotropic = 136.2377 Anisotropy = 56.5569
XX= 154.2616 YX= 12.0913 ZX= 0.5966
XY= -2.3639 YY= 117.3408 ZY= -5.2695
XZ= -52.5967 YZ= -5.3371 ZZ= 137.1107
Eigenvalues: 115.6785 119.0923 173.9423

13 C Isotropic = 31.6077 Anisotropy = 122.1523
XX= -34.3794 YX= -46.8102 ZX= -29.6473
XY= -33.3856 YY= 23.6026 ZY= -21.6640
XZ= -26.6815 YZ= -19.1077 ZZ= 105.5999
Eigenvalues: -61.9258 43.7064 113.0426
14 C Isotropic = 75.8046 Anisotropy = 115.3238
XX= 28.3878 YX= -40.3790 ZX= -35.5059
XY= -31.2225 YY= 58.2122 ZY= -18.7438
XZ= -40.3268 YZ= -13.2663 ZZ= 140.8140
Eigenvalues: -6.6179 81.3446 152.6871
15 H Isotropic = 25.0984 Anisotropy = 7.0870
XX= 28.8820 YX= -3.3494 ZX= -1.1448
XY= -0.5790 YY= 23.6853 ZY= 1.7488
XZ= -1.2941 YZ= -0.1347 ZZ= 22.7278
Eigenvalues: 22.2661 23.2060 29.8230
16 C Isotropic = 38.2993 Anisotropy = 191.5056
XX= -57.3234 YX= 19.6075 ZX= -12.7964
XY= 18.0572 YY= 155.0851 ZY= -35.4131
XZ= -14.8086 YZ= -36.4387 ZZ= 17.1361
Eigenvalues: -60.5543 9.4824 165.9697
17 C Isotropic = 53.0922 Anisotropy = 179.9895
XX= -53.0086 YX= 15.6078 ZX= -18.1457
XY= 12.9818 YY= 164.2483 ZY= -31.4786
XZ= -16.2350 YZ= -29.0103 ZZ= 48.0368
Eigenvalues: -56.2515 42.4428 173.0852
18 C Isotropic = 48.6545 Anisotropy = 160.0551
XX= 17.9065 YX= 17.9490 ZX= 45.7521
XY= 25.3486 YY= 147.1028 ZY= -26.0325
XZ= 43.0909 YZ= -43.6561 ZZ= -19.0457
Eigenvalues: -56.9204 47.5260 155.3579
19 C Isotropic = 49.9588 Anisotropy = 168.2102
XX= 31.7947 YX= 2.9310 ZX= -28.8425
XY= 5.7809 YY= 152.7213 ZY= -36.9677
XZ= -39.4908 YZ= -44.0204 ZZ= -34.6397
Eigenvalues: -55.2848 43.0622 162.0989
20 C Isotropic = 49.8367 Anisotropy = 182.0596
XX= 4.4914 YX= 24.2877 ZX= 43.7912
XY= 26.5842 YY= 157.0439 ZY= -48.9043
XZ= 43.6512 YZ= -48.5003 ZZ= -12.0252
Eigenvalues: -61.5461 39.8464 171.2098
21 C Isotropic = 49.8556 Anisotropy = 181.2219
XX= 26.9338 YX= 3.3119 ZX= -37.5356
XY= 2.7472 YY= 160.4947 ZY= -41.7468
XZ= -38.2492 YZ= -46.2683 ZZ= -37.8616
Eigenvalues: -62.1745 41.0712 170.6702
22 H Isotropic = 24.1724 Anisotropy = 8.6702
XX= 26.5216 YX= -0.4722 ZX= 3.5067
XY= -2.2098 YY= 21.6067 ZY= -2.1524
XZ= 4.3519 YZ= -0.5441 ZZ= 24.3889
Eigenvalues: 21.0127 21.5520 29.9525
23 H Isotropic = 24.2588 Anisotropy = 8.2537
XX= 28.3856 YX= -1.5863 ZX= -2.5147
XY= -1.2811 YY= 21.4807 ZY= 1.0402
XZ= -2.5952 YZ= 1.1950 ZZ= 22.9101
Eigenvalues: 20.8686 22.1465 29.7612
24 H Isotropic = 24.1518 Anisotropy = 5.2668
XX= 26.4974 YX= -0.1349 ZX= 2.0234
XY= -0.2587 YY= 21.5684 ZY= 0.7033
XZ= 1.8693 YZ= 0.7073 ZZ= 24.3898
Eigenvalues: 21.3034 23.4891 27.6630
25 H Isotropic = 24.1228 Anisotropy = 5.8461
XX= 27.5591 YX= -1.0640 ZX= -1.0116
XY= -1.1407 YY= 21.5912 ZY= 0.6765
XZ= -1.0737 YZ= 0.4287 ZZ= 23.2182
Eigenvalues: 21.3178 23.0304 28.0202
26 H Isotropic = 24.3265 Anisotropy = 4.8189
XX= 23.8721 YX= -0.4674 ZX= -0.5009
XY= -0.7329 YY= 21.9929 ZY= 1.2753

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  XZ=   -0.4426   YZ=    1.3866   ZZ=   27.1145
  Eigenvalues:   21.5687   23.8716   27.5391
27  C   Isotropic =   30.9248   Anisotropy =  158.6384
  XX=  -18.8521   YX=  -58.7447   ZX=  -18.1056
  XY=  -62.9724   YY=   31.3387   ZY=   58.7629
  XZ=  -16.1620   YZ=   61.1583   ZZ=   80.2876
  Eigenvalues:  -62.7124   18.8031  136.6837
28  C   Isotropic =   56.8409   Anisotropy =  173.6459
  XX=    6.8737   YX=  -69.8774   ZX=  -14.4570
  XY=  -66.6892   YY=   57.7985   ZY=   66.8073
  XZ=  -13.3928   YZ=   72.5078   ZZ=  105.8505
  Eigenvalues:  -46.9487   44.8666  172.6048
29  C   Isotropic =   58.3506   Anisotropy =  178.9990
  XX=    0.0694   YX=  -11.0747   ZX=  -60.6950
  XY=  -37.6661   YY=   69.1419   ZY=   70.2789
  XZ=  -84.1499   YZ=   43.2810   ZZ=  105.8405
  Eigenvalues:  -36.9091   34.2776  177.6833
30  C   Isotropic =   55.4033   Anisotropy =  161.6211
  XX=   50.8556   YX=  -20.7458   ZX=  -28.2796
  XY=  -15.0116   YY=   54.5731   ZY=   83.8075
  XZ=  -33.9284   YZ=  105.4136   ZZ=   60.7814
  Eigenvalues:  -37.9201   40.9794  163.1507
31  C   Isotropic =   49.1833   Anisotropy =  179.8647
  XX=  -24.1274   YX=  -16.9004   ZX=  -71.9063
  XY=  -17.3320   YY=   90.1380   ZY=   57.9401
  XZ=  -74.5559   YZ=   65.1853   ZZ=   81.5392
  Eigenvalues:  -62.8415   41.2983  169.0931
32  C   Isotropic =   49.0826   Anisotropy =  179.9276
  XX=   53.6646   YX=  -15.4928   ZX=  -36.7003
  XY=  -17.4632   YY=   34.2980   ZY=  106.0721
  XZ=  -43.3607   YZ=  107.7941   ZZ=   59.2853
  Eigenvalues:  -62.7505   40.9640  169.0344
33  H   Isotropic =   24.1256   Anisotropy =   10.7382
  XX=   24.6853   YX=    3.3368   ZX=   -2.5856
  XY=    3.2867   YY=   26.9132   ZY=   -4.8905
  XZ=   -2.0906   YZ=   -3.0035   ZZ=   20.7783
  Eigenvalues:   18.7514   22.3410   31.2844
34  H   Isotropic =   24.3336   Anisotropy =    9.0860
  XX=   28.3855   YX=    2.3085   ZX=    2.4578
  XY=    3.7771   YY=   23.0508   ZY=    0.7900
  XZ=    2.1613   YZ=    0.3972   ZZ=   21.5645
  Eigenvalues:   20.7640   21.8459   30.3909
35  H   Isotropic =   24.1127   Anisotropy =    5.2440
  XX=   24.1221   YX=    1.9377   ZX=   -0.3388
  XY=    1.7727   YY=   25.2982   ZY=   -2.3557
  XZ=   -0.6278   YZ=   -2.0773   ZZ=   22.9176
  Eigenvalues:   21.4490   23.2803   27.6087
36  H   Isotropic =   24.2343   Anisotropy =    5.9880
  XX=   27.2277   YX=    2.1020   ZX=    0.8886
  XY=    2.3111   YY=   23.3130   ZY=   -0.5829
  XZ=    0.2221   YZ=   -0.9406   ZZ=   22.1622
  Eigenvalues:   21.3126   23.1640   28.2263
37  H   Isotropic =   24.6362   Anisotropy =    4.2605
  XX=   25.3491   YX=   -0.4538   ZX=    1.9756
  XY=   -0.1661   YY=   24.4258   ZY=   -2.1825
  XZ=    1.8094   YZ=   -1.7324   ZZ=   24.1337
  Eigenvalues:   21.8517   24.5803   27.4765
 Current density tensor (au):
  XX=   -0.0120   YX=   -0.0306   ZX=    0.0336
  XY=    0.0044   YY=    0.0679   ZY=    0.0399
  XZ=   -0.0910   YZ=    0.0545   ZZ=   -0.0782
 End of Minotr Frequency-dependent properties file   721 does not exist.

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        Population analysis using the SCF density.

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Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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Alpha virt. eigenvalues --	0.05909	0.06166	0.06681	0.07196	0.07721
Alpha virt. eigenvalues --	0.08102	0.08360	0.08731	0.08814	0.09774
Alpha virt. eigenvalues --	0.10077	0.10185	0.10515	0.10887	0.11196
Alpha virt. eigenvalues --	0.11308	0.11417	0.11694	0.11976	0.12105
Alpha virt. eigenvalues --	0.12119	0.12290	0.12508	0.12578	0.12650
Alpha virt. eigenvalues --	0.12843	0.13050	0.13317	0.13532	0.13657
Alpha virt. eigenvalues --	0.14097	0.14253	0.14358	0.14613	0.14859
Alpha virt. eigenvalues --	0.15382	0.15699	0.16065	0.16115	0.16384
Alpha virt. eigenvalues --	0.16770	0.17140	0.17232	0.17602	0.17795
Alpha virt. eigenvalues --	0.17977	0.18392	0.18668	0.19028	0.19843
Alpha virt. eigenvalues --	0.19974	0.20335	0.20635	0.20982	0.21218
Alpha virt. eigenvalues --	0.21581	0.21882	0.22263	0.22441	0.22766
Alpha virt. eigenvalues --	0.22860	0.23092	0.23699	0.23790	0.24393
Alpha virt. eigenvalues --	0.24681	0.25177	0.25519	0.25998	0.26113
Alpha virt. eigenvalues --	0.26549	0.26625	0.27064	0.27257	0.27356
Alpha virt. eigenvalues --	0.27847	0.28134	0.28481	0.28702	0.29120
Alpha virt. eigenvalues --	0.29306	0.29735	0.29815	0.30356	0.30414
Alpha virt. eigenvalues --	0.30762	0.31048	0.31277	0.31538	0.31787
Alpha virt. eigenvalues --	0.31988	0.32180	0.32590	0.32914	0.33426
Alpha virt. eigenvalues --	0.33963	0.34170	0.34463	0.35467	0.35682
Alpha virt. eigenvalues --	0.36569	0.36860	0.37158	0.37282	0.38103
Alpha virt. eigenvalues --	0.38595	0.39313	0.39596	0.40087	0.40696
Alpha virt. eigenvalues --	0.41150	0.41712	0.42774	0.43795	0.45358
Alpha virt. eigenvalues --	0.46509	0.49164	0.50377	0.51562	0.52258
Alpha virt. eigenvalues --	0.53218	0.54201	0.54341	0.54793	0.55133
Alpha virt. eigenvalues --	0.55603	0.56015	0.56151	0.56847	0.57368
Alpha virt. eigenvalues --	0.57862	0.58310	0.58470	0.59200	0.60187
Alpha virt. eigenvalues --	0.60731	0.61384	0.61470	0.62108	0.62650
Alpha virt. eigenvalues --	0.62963	0.63413	0.64205	0.64631	0.65408
Alpha virt. eigenvalues --	0.65709	0.66535	0.67307	0.67498	0.68396
Alpha virt. eigenvalues --	0.68776	0.68978	0.69904	0.70843	0.71250
Alpha virt. eigenvalues --	0.71545	0.72043	0.72274	0.72704	0.73019
Alpha virt. eigenvalues --	0.73231	0.73742	0.73978	0.75008	0.75341
Alpha virt. eigenvalues --	0.75879	0.76164	0.76701	0.76933	0.77844
Alpha virt. eigenvalues --	0.78443	0.79972	0.80039	0.80328	0.81050
Alpha virt. eigenvalues --	0.82266	0.82579	0.83176	0.83302	0.84444
Alpha virt. eigenvalues --	0.84740	0.85442	0.85859	0.86762	0.86864
Alpha virt. eigenvalues --	0.87172	0.87679	0.88699	0.89141	0.89734
Alpha virt. eigenvalues --	0.90188	0.90554	0.91469	0.92803	0.93434
Alpha virt. eigenvalues --	0.94425	0.94901	0.95830	0.96458	0.97913
Alpha virt. eigenvalues --	0.98749	0.99920	1.01035	1.02026	1.02701
Alpha virt. eigenvalues --	1.03333	1.04437	1.05047	1.05508	1.06085
Alpha virt. eigenvalues --	1.06868	1.07567	1.08073	1.08241	1.09487
Alpha virt. eigenvalues --	1.09726	1.10854	1.12408	1.14015	1.14286
Alpha virt. eigenvalues --	1.14866	1.16371	1.17446	1.18268	1.19565
Alpha virt. eigenvalues --	1.22310	1.25714	1.29446	1.31047	1.31499
Alpha virt. eigenvalues --	1.33618	1.34902	1.36498	1.39379	1.41030
Alpha virt. eigenvalues --	1.45173	1.46345	1.46824	1.48722	1.50591
Alpha virt. eigenvalues --	1.51168	1.52125	1.52975	1.53206	1.53589
Alpha virt. eigenvalues --	1.54466	1.54654	1.55426	1.55975	1.56828
Alpha virt. eigenvalues --	1.57521	1.57816	1.58095	1.58817	1.59841
Alpha virt. eigenvalues --	1.60047	1.60993	1.62558	1.63955	1.65418
Alpha virt. eigenvalues --	1.65887	1.66428	1.66861	1.67444	1.67627
Alpha virt. eigenvalues --	1.68757	1.69132	1.70190	1.70909	1.72066
Alpha virt. eigenvalues --	1.72847	1.74554	1.74868	1.75675	1.76121
Alpha virt. eigenvalues --	1.77492	1.78505	1.78754	1.79538	1.81650
Alpha virt. eigenvalues --	1.82556	1.83735	1.84246	1.85156	1.86469
Alpha virt. eigenvalues --	1.87415	1.88210	1.88973	1.89905	1.91188
Alpha virt. eigenvalues --	1.91472	1.92184	1.92404	1.93422	1.94094
Alpha virt. eigenvalues --	1.95395	1.95577	1.96014	1.96304	1.96377
Alpha virt. eigenvalues --	1.97665	1.97881	1.98629	1.99011	1.99961
Alpha virt. eigenvalues --	2.01199	2.01575	2.03145	2.03581	2.05471
Alpha virt. eigenvalues --	2.06186	2.06841	2.08202	2.09104	2.10632
Alpha virt. eigenvalues --	2.11088	2.12166	2.14365	2.16024	2.17350
Alpha virt. eigenvalues --	2.19748	2.21655	2.22960	2.24205	2.25455
Alpha virt. eigenvalues --	2.28380	2.30021	2.32708	2.32946	2.34810
Alpha virt. eigenvalues --	2.35745	2.37967	2.38308	2.41112	2.43486
Alpha virt. eigenvalues --	2.44071	2.45417	2.46656	2.46815	2.47769

Alpha virt. eigenvalues -- 2.48617 2.50131 2.51325 2.53447 2.54461
Alpha virt. eigenvalues -- 2.56032 2.58563 2.60818 2.62235 2.62959
Alpha virt. eigenvalues -- 2.64129 2.64916 2.66525 2.67218 2.67841
Alpha virt. eigenvalues -- 2.70002 2.70595 2.70952 2.71719 2.72477
Alpha virt. eigenvalues -- 2.73540 2.73663 2.74522 2.75086 2.75916
Alpha virt. eigenvalues -- 2.76622 2.77625 2.78064 2.79061 2.80193
Alpha virt. eigenvalues -- 2.81555 2.82151 2.82381 2.82676 2.83564
Alpha virt. eigenvalues -- 2.84551 2.84896 2.86217 2.86924 2.87924
Alpha virt. eigenvalues -- 2.88372 2.89179 2.91263 2.93858 2.94420
Alpha virt. eigenvalues -- 2.94870 2.95245 2.96039 2.96450 2.98322
Alpha virt. eigenvalues -- 2.99114 3.01389 3.02666 3.06734 3.07895
Alpha virt. eigenvalues -- 3.08921 3.11345 3.12044 3.12182 3.14597
Alpha virt. eigenvalues -- 3.18327 3.20161 3.20804 3.21971 3.29789
Alpha virt. eigenvalues -- 3.32927 3.35015 3.36585 3.37479 3.38572
Alpha virt. eigenvalues -- 3.39995 3.43163 3.48905 3.50568 3.51978
Alpha virt. eigenvalues -- 3.55331 3.55814 3.60435 3.62449 3.63020
Alpha virt. eigenvalues -- 3.64198 3.65221 3.74623 3.77970 3.89954
Alpha virt. eigenvalues -- 3.94245 3.99962 4.00303 4.03730 4.04288
Alpha virt. eigenvalues -- 4.08757 4.09438 4.13419 4.14353 4.15942
Alpha virt. eigenvalues -- 4.16480 4.17660 4.19207 4.22406 4.26137
Alpha virt. eigenvalues -- 4.35101 4.44658 4.84493 4.85295 4.90007
Alpha virt. eigenvalues -- 5.15512 23.62172 23.65137 23.78169 23.85054
Alpha virt. eigenvalues -- 23.87388 23.96007 23.97736 23.97895 23.98078
Alpha virt. eigenvalues -- 23.99702 24.02294 24.07344 24.07672 24.09144
Alpha virt. eigenvalues -- 24.09672 24.18603 24.19202 24.25777 24.27885
Alpha virt. eigenvalues -- 35.64386

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	13.519961	0.796895	-4.575653	-0.188148	3.358755	0.091521
2	H	0.796895	0.526642	-0.306086	-0.012321	0.138835	0.003751
3	C	-4.575653	-0.306086	10.613770	0.601196	-3.963666	-0.156493
4	H	-0.188148	-0.012321	0.601196	0.515171	-0.183892	-0.012632
5	C	3.358755	0.138835	-3.963666	-0.183892	10.939989	0.583342
6	H	0.091521	0.003751	-0.156493	-0.012632	0.583342	0.504490
7	C	-3.161815	-0.107068	3.193355	0.090323	-4.947262	-0.206828
8	H	-0.080981	-0.000251	0.112982	0.003839	-0.342424	-0.011673
9	C	-0.238385	0.011404	-0.082324	0.046810	0.406986	0.030824
10	H	-0.044011	-0.004342	-0.003405	0.000718	0.016591	0.000488
11	H	-0.166052	-0.018978	0.043876	-0.000018	0.071906	0.000378
12	N	-0.234283	0.035550	0.085470	0.006333	0.133016	0.009289
13	C	-1.355483	-0.183471	0.154746	-0.019157	0.505511	0.024426
14	C	-0.496441	-0.025510	-0.202615	-0.011378	0.300648	0.006012
15	H	0.124456	0.006445	-0.008366	0.000004	-0.001392	-0.000125
16	C	-1.881692	-0.154628	1.010506	0.024998	-0.659689	-0.015976
17	C	-0.007388	-0.004026	0.015689	0.001111	-0.004389	-0.000207
18	C	0.821237	0.083341	-0.331244	-0.024060	0.350090	0.008147
19	C	-0.864686	-0.106338	0.314004	0.013776	-0.206639	-0.003718
20	C	-0.017993	-0.020107	-0.012864	-0.002360	0.026389	0.000217
21	C	0.234835	0.056809	-0.070724	0.000384	0.007556	0.001383
22	H	0.004714	0.006294	-0.034886	-0.005222	0.040481	0.001460
23	H	-0.008694	0.000339	-0.005354	-0.000124	0.000733	0.000068
24	H	-0.002225	-0.000503	0.001303	0.000032	-0.000490	-0.000008
25	H	-0.003162	-0.000853	0.002353	0.000212	-0.002543	-0.000032
26	H	-0.000123	-0.000805	0.000647	0.000027	-0.000269	-0.000008
27	C	-0.103127	-0.008869	-0.280942	-0.015804	0.431993	0.006353
28	C	0.027988	0.001275	0.021399	0.001292	-0.008086	0.003503
29	C	-0.294893	0.000023	0.349466	0.012022	-0.521050	-0.021948
30	C	0.188709	0.011809	-0.156153	-0.003341	0.247327	0.014039
31	C	0.027390	0.001282	0.021091	-0.000038	-0.134315	-0.003277
32	C	0.204307	0.009944	-0.141261	-0.001800	0.137844	0.003986
33	H	-0.014417	-0.000402	0.060783	0.001685	-0.088745	-0.003651
34	H	0.029853	0.000954	-0.028694	-0.000547	0.056326	0.002843
35	H	-0.004304	-0.000149	0.002111	0.000013	-0.004480	-0.000561
36	H	-0.004576	-0.000202	-0.003431	-0.000147	0.003948	0.000159
37	H	0.000477	0.000028	0.000516	0.000030	-0.000791	-0.000092

		7	8	9	10	11	12
1	C	-3.161815	-0.080981	-0.238385	-0.044011	-0.166052	-0.234283
2	H	-0.107068	-0.000251	0.011404	-0.004342	-0.018978	0.035550

3	C	3.193355	0.112982	-0.082324	-0.003405	0.043876	0.085470
4	H	0.090323	0.003839	0.046810	0.000718	-0.000018	0.006333
5	C	-4.947262	-0.342424	0.406986	0.016591	0.071906	0.133016
6	H	-0.206828	-0.011673	0.030824	0.000488	0.000378	0.009289
7	C	12.888256	0.820781	-1.299005	-0.037953	-0.135687	-0.678150
8	H	0.820781	0.558753	-0.043282	-0.003621	-0.017496	-0.084455
9	C	-1.299005	-0.043282	7.947037	0.378541	0.393378	0.297358
10	H	-0.037953	-0.003621	0.378541	0.510285	-0.019061	0.010403
11	H	-0.135687	-0.017496	0.393378	-0.019061	0.554531	0.006890
12	N	-0.678150	-0.084455	0.297358	0.010403	0.006890	8.012116
13	C	-0.131624	-0.138710	-0.529622	0.028130	0.069546	-0.246227
14	C	-0.457299	-0.048408	-0.051439	0.001673	0.022878	-0.197515
15	H	-0.022375	-0.001373	-0.006657	0.000679	-0.000052	-0.047225
16	C	0.141639	-0.011808	-0.149694	-0.006537	0.055066	-0.262117
17	C	-0.006140	-0.000201	0.014756	0.000638	0.001207	0.001286
18	C	-0.466835	-0.021212	-0.366219	-0.003126	0.011197	-0.153953
19	C	0.278145	0.011495	0.118433	0.002953	-0.003310	0.060846
20	C	-0.042501	-0.001521	-0.022848	0.000395	0.004235	-0.028909
21	C	0.071558	0.002401	-0.001477	-0.000755	-0.004474	0.072736
22	H	-0.038451	-0.001886	-0.030048	0.000276	0.001053	-0.019145
23	H	0.005100	0.000257	-0.003816	-0.000251	0.000132	0.002325
24	H	0.000214	-0.000010	-0.001050	-0.000046	0.000009	-0.000714
25	H	0.002728	0.000058	-0.000702	-0.000068	-0.000022	0.000232
26	H	-0.000006	-0.000004	0.000335	0.000014	0.000041	-0.000019
27	C	-0.752052	-0.075999	-0.255566	-0.022766	0.004331	-0.278764
28	C	-0.002863	0.005114	0.035823	0.000518	-0.000384	0.082156
29	C	0.780072	0.066003	-0.028758	0.000974	-0.011577	-0.180067
30	C	-0.306452	0.011655	0.158416	0.005345	-0.001329	-0.015011
31	C	0.148134	0.012434	0.030871	0.003917	-0.004339	-0.014429
32	C	0.042246	0.021504	0.049240	0.000706	-0.000850	0.172453
33	H	0.113985	0.005262	-0.009406	-0.000115	-0.001283	-0.079077
34	H	-0.061220	-0.015157	0.000983	-0.000510	0.000643	-0.003236
35	H	0.008025	0.000911	-0.004199	-0.000053	0.000016	-0.009103
36	H	-0.001850	-0.000319	-0.001815	-0.000051	0.000082	-0.004238
37	H	-0.000878	0.000108	0.000727	-0.000007	0.000003	0.003434

		13	14	15	16	17	18
1	C	-1.355483	-0.496441	0.124456	-1.881692	-0.007388	0.821237
2	H	-0.183471	-0.025510	0.006445	-0.154628	-0.004026	0.083341
3	C	0.154746	-0.202615	-0.008366	1.010506	0.015689	-0.331244
4	H	-0.019157	-0.011378	0.000004	0.024998	0.001111	-0.024060
5	C	0.505511	0.300648	-0.001392	-0.659689	-0.004389	0.350090
6	H	0.024426	0.006012	-0.000125	-0.015976	-0.000207	0.008147
7	C	-0.131624	-0.457299	-0.022375	0.141639	-0.006140	-0.466835
8	H	-0.138710	-0.048408	-0.001373	-0.011808	-0.000201	-0.021212
9	C	-0.529622	-0.051439	-0.006657	-0.149694	0.014756	-0.366219
10	H	0.028130	0.001673	0.000679	-0.006537	0.000638	-0.003126
11	H	0.069546	0.022878	-0.000052	0.055066	0.001207	0.011197
12	N	-0.246227	-0.197515	-0.047225	-0.262117	0.001286	-0.153953
13	C	13.073365	2.848902	-0.250881	-4.790236	-0.301202	-2.415287
14	C	2.848902	10.262843	0.273669	-2.611662	-0.660005	-4.292426
15	H	-0.250881	0.273669	0.521427	0.260883	0.008606	0.177453
16	C	-4.790236	-2.611662	0.260883	16.141948	0.111347	1.707359
17	C	-0.301202	-0.660005	0.008606	0.111347	6.111057	1.096200
18	C	-2.415287	-4.292426	0.177453	1.707359	1.096200	18.833115
19	C	0.159925	1.696924	-0.108610	-1.223185	-1.000050	-6.377448
20	C	-0.172342	-0.484736	0.014128	0.151914	0.709934	1.239056
21	C	0.856096	1.301108	-0.042131	-1.460776	-0.115086	-3.909397
22	H	-0.081785	-0.089502	0.009493	-0.008906	0.031547	0.857824
23	H	0.019991	0.078778	-0.001982	-0.111246	-0.013639	-0.042985
24	H	-0.000383	0.004655	0.000283	0.026699	-0.056005	0.008062
25	H	0.015997	0.035824	-0.000608	0.057980	-0.097362	-0.215024
26	H	-0.009617	-0.019487	0.000522	0.023316	0.465686	0.066610
27	C	0.530302	-0.505431	-0.062048	-1.068031	-0.011978	-0.002276
28	C	0.010262	-0.065536	0.006811	-0.025433	-0.000422	-0.014347
29	C	-0.203655	-0.102746	-0.024408	-0.136254	-0.004024	-0.138380
30	C	-0.495204	0.112849	-0.002548	0.094019	0.000869	-0.025059
31	C	0.099235	0.003543	0.011628	0.020040	0.000327	0.008960
32	C	-0.547540	-0.077599	-0.033496	-0.102892	-0.000927	-0.044993

33	H	0.133238	-0.046667	0.000932	-0.062775	-0.003911	-0.083208
34	H	0.003919	-0.001751	-0.001258	-0.003639	-0.000020	0.002418
35	H	0.002801	0.001856	-0.000066	0.001017	0.000010	0.000281
36	H	-0.007089	0.010307	-0.002009	0.003762	0.000143	0.003396
37	H	-0.000145	-0.001962	0.000006	-0.001360	-0.000012	-0.000330

		19	20	21	22	23	24
1	C	-0.864686	-0.017993	0.234835	0.004714	-0.008694	-0.002225
2	H	-0.106338	-0.020107	0.056809	0.006294	0.000339	-0.000503
3	C	0.314004	-0.012864	-0.070724	-0.034886	-0.005354	0.001303
4	H	0.013776	-0.002360	0.000384	-0.005222	-0.000124	0.000032
5	C	-0.206639	0.026389	0.007556	0.040481	0.000733	-0.000490
6	H	-0.003718	0.000217	0.001383	0.001460	0.000068	-0.000008
7	C	0.278145	-0.042501	0.071558	-0.038451	0.005100	0.000214
8	H	0.011495	-0.001521	0.002401	-0.001886	0.000257	-0.000010
9	C	0.118433	-0.022848	-0.001477	-0.030048	-0.003816	-0.001050
10	H	0.002953	0.000395	-0.000755	0.000276	-0.000251	-0.000046
11	H	-0.003310	0.004235	-0.004474	0.001053	0.000132	0.000009
12	N	0.060846	-0.028909	0.072736	-0.019145	0.002325	-0.000714
13	C	0.159925	-0.172342	0.856096	-0.081785	0.019991	-0.000383
14	C	1.696924	-0.484736	1.301108	-0.089502	0.078778	0.004655
15	H	-0.108610	0.014128	-0.042131	0.009493	-0.001982	0.000283
16	C	-1.223185	0.151914	-1.460776	-0.008906	-0.111246	0.026699
17	C	-1.000050	0.709934	-0.115086	0.031547	-0.013639	-0.056005
18	C	-6.377448	1.239056	-3.909397	0.857824	-0.042985	0.008062
19	C	12.215714	-0.848740	1.537633	-0.144815	0.442733	-0.105746
20	C	-0.848740	6.324732	-0.691845	0.057298	-0.114133	0.442648
21	C	1.537633	-0.691845	8.200697	-0.231321	0.035760	0.002431
22	H	-0.144815	0.057298	-0.231321	0.558455	-0.002881	0.000519
23	H	0.442733	-0.114133	0.035760	-0.002881	0.543243	-0.017366
24	H	-0.105746	0.442648	0.002431	0.000519	-0.017366	0.549299
25	H	0.055410	-0.006742	0.465331	-0.021399	0.001250	-0.000151
26	H	-0.058863	-0.044928	-0.100024	0.002260	-0.000780	-0.017467
27	C	-0.141361	-0.001471	0.068008	-0.009446	-0.002598	-0.000050
28	C	0.003204	-0.000532	0.001462	-0.001985	-0.000024	-0.000002
29	C	0.065042	-0.029667	0.053272	-0.013368	0.002324	-0.000268
30	C	0.026665	-0.005913	0.002348	0.000853	0.001962	-0.000123
31	C	-0.001658	-0.000162	-0.000125	0.001189	-0.000095	-0.000007
32	C	0.026093	-0.008545	0.032968	-0.006506	0.002094	-0.000160
33	H	0.022509	-0.008080	0.013922	-0.009922	0.000410	0.000091
34	H	-0.002991	-0.000349	0.000364	0.000049	0.000043	-0.000005
35	H	0.000043	0.000025	-0.000016	0.000047	-0.000003	0.000000
36	H	-0.000715	0.000099	-0.000050	0.000545	0.000069	-0.000005
37	H	0.000014	-0.000022	0.000036	-0.000111	-0.000005	0.000000

		25	26	27	28	29	30
1	C	-0.003162	-0.000123	-0.103127	0.027988	-0.294893	0.188709
2	H	-0.000853	-0.000805	-0.008869	0.001275	0.000023	0.011809
3	C	0.002353	0.000647	-0.280942	0.021399	0.349466	-0.156153
4	H	0.000212	0.000027	-0.015804	0.001292	0.012022	-0.003341
5	C	-0.002543	-0.000269	0.431993	-0.008086	-0.521050	0.247327
6	H	-0.000032	-0.000008	0.006353	0.003503	-0.021948	0.014039
7	C	0.002728	-0.000006	-0.752052	-0.002863	0.780072	-0.306452
8	H	0.000058	-0.000004	-0.075999	0.005114	0.066003	0.011655
9	C	-0.000702	0.000335	-0.255566	0.035823	-0.028758	0.158416
10	H	-0.000068	0.000014	-0.022766	0.000518	0.000974	0.005345
11	H	-0.000022	0.000041	0.004331	-0.000384	-0.011577	-0.001329
12	N	0.000232	-0.000019	-0.278764	0.082156	-0.180067	-0.015011
13	C	0.015997	-0.009617	0.530302	0.010262	-0.203655	-0.495204
14	C	0.035824	-0.019487	-0.505431	-0.065536	-0.102746	0.112849
15	H	-0.000608	0.000522	-0.062048	0.006811	-0.024408	-0.002548
16	C	0.057980	0.023316	-1.068031	-0.025433	-0.136254	0.094019
17	C	-0.097362	0.465686	-0.011978	-0.000422	-0.004024	0.000869
18	C	-0.215024	0.066610	-0.002276	-0.014347	-0.138380	-0.025059
19	C	0.055410	-0.058863	-0.141361	0.003204	0.065042	0.026665
20	C	-0.006742	-0.044928	-0.001471	-0.000532	-0.029667	-0.005913
21	C	0.465331	-0.100024	0.068008	0.001462	0.053272	0.002348
22	H	-0.021399	0.002260	-0.009446	-0.001985	-0.013368	0.000853
23	H	0.001250	-0.000780	-0.002598	-0.000024	0.002324	0.001962
24	H	-0.000151	-0.017467	-0.000050	-0.000002	-0.000268	-0.000123

25	H	0.552130	-0.018939	0.000281	0.000047	0.000711	0.000005
26	H	-0.018939	0.555617	-0.000102	-0.000011	-0.000114	0.000002
27	C	0.000281	-0.000102	9.965877	0.222388	0.708461	-0.520171
28	C	0.000047	-0.000011	0.222388	6.060926	-0.713048	-0.600383
29	C	0.000711	-0.000114	0.708461	-0.713048	7.112575	-0.340400
30	C	0.000005	0.000002	-0.520171	-0.600383	-0.340400	6.571567
31	C	-0.000037	0.000005	-0.601904	0.416652	0.298977	-0.070584
32	C	0.000306	-0.000053	-1.279170	0.549666	-1.053876	0.878402
33	H	0.000859	-0.000201	0.051546	0.002724	0.490901	-0.041489
34	H	-0.000002	0.000000	-0.010853	0.011286	-0.022579	0.418929
35	H	-0.000001	0.000000	0.041505	-0.051120	0.047123	-0.123974
36	H	-0.000023	0.000006	0.013109	-0.076947	-0.071581	0.025386
37	H	0.000002	0.000000	0.025536	0.466974	-0.015872	-0.039857

		31	32	33	34	35	36
1	C	0.027390	0.204307	-0.014417	0.029853	-0.004304	-0.004576
2	H	0.001282	0.009944	-0.000402	0.000954	-0.000149	-0.000202
3	C	0.021091	-0.141261	0.060783	-0.028694	0.002111	-0.003431
4	H	-0.000038	-0.001800	0.001685	-0.000547	0.000013	-0.000147
5	C	-0.134315	0.137844	-0.088745	0.056326	-0.004480	0.003948
6	H	-0.003277	0.003986	-0.003651	0.002843	-0.000561	0.000159
7	C	0.148134	0.042246	0.113985	-0.061220	0.008025	-0.001850
8	H	0.012434	0.021504	0.005262	-0.015157	0.000911	-0.000319
9	C	0.030871	0.049240	-0.009406	0.000983	-0.004199	-0.001815
10	H	0.003917	0.000706	-0.000115	-0.000510	-0.000053	-0.000051
11	H	-0.004339	-0.000850	-0.001283	0.000643	0.000016	0.000082
12	N	-0.014429	0.172453	-0.079077	-0.003236	-0.009103	-0.004238
13	C	0.099235	-0.547540	0.133238	0.003919	0.002801	-0.007089
14	C	0.003543	-0.077599	-0.046667	-0.001751	0.001856	0.010307
15	H	0.011628	-0.033496	0.000932	-0.001258	-0.000066	-0.002009
16	C	0.020040	-0.102892	-0.062775	-0.003639	0.001017	0.003762
17	C	0.000327	-0.000927	-0.003911	-0.000020	0.000010	0.000143
18	C	0.008960	-0.044993	-0.083208	0.002418	0.000281	0.003396
19	C	-0.001658	0.026093	0.022509	-0.002991	0.000043	-0.000715
20	C	-0.000162	-0.008545	-0.008080	-0.000349	0.000025	0.000099
21	C	-0.000125	0.032968	0.013922	0.000364	-0.000016	-0.000050
22	H	0.001189	-0.006506	-0.009922	0.000049	0.000047	0.000545
23	H	-0.000095	0.002094	0.000410	0.000043	-0.000003	0.000069
24	H	-0.000007	-0.000160	0.000091	-0.000005	0.000000	-0.000005
25	H	-0.000037	0.000306	0.000859	-0.000002	-0.000001	-0.000023
26	H	0.000005	-0.000053	-0.000201	0.000000	0.000000	0.000006
27	C	-0.601904	-1.279170	0.051546	-0.010853	0.041505	0.013109
28	C	0.416652	0.549666	0.002724	0.011286	-0.051120	-0.076947
29	C	0.298977	-1.053876	0.490901	-0.022579	0.047123	-0.071581
30	C	-0.070584	0.878402	-0.041489	0.418929	-0.123974	0.025386
31	C	6.088853	-0.463250	0.016840	-0.088028	0.422390	0.002463
32	C	-0.463250	7.654431	-0.181264	0.021892	-0.016035	0.415989
33	H	0.016840	-0.181264	0.561562	-0.003049	0.000138	-0.015871
34	H	-0.088028	0.021892	-0.003049	0.577652	-0.020910	0.001202
35	H	0.422390	-0.016035	0.000138	-0.020910	0.548145	0.000274
36	H	0.002463	0.415989	-0.015871	0.001202	0.000274	0.546618
37	H	-0.061424	-0.044949	0.002196	-0.000639	-0.016978	-0.018172

		37
1	C	0.000477
2	H	0.000028
3	C	0.000516
4	H	0.000030
5	C	-0.000791
6	H	-0.000092
7	C	-0.000878
8	H	0.000108
9	C	0.000727
10	H	-0.000007
11	H	0.000003
12	N	0.003434
13	C	-0.000145
14	C	-0.001962
15	H	0.000006
16	C	-0.001360

17	C	-0.000012
18	C	-0.000330
19	C	0.000014
20	C	-0.000022
21	C	0.000036
22	H	-0.000111
23	H	-0.000005
24	H	0.000000
25	H	0.000002
26	H	0.000000
27	C	0.025536
28	C	0.466974
29	C	-0.015872
30	C	-0.039857
31	C	-0.061424
32	C	-0.044949
33	H	0.002196
34	H	-0.000639
35	H	-0.016978
36	H	-0.018172
37	H	0.557365

Mulliken atomic charges:

		1
1	C	0.317432
2	H	0.263288
3	C	-0.241105
4	H	0.161008
5	C	-0.688145
6	H	0.140551
7	C	0.279754
8	H	0.267236
9	C	-0.795609
10	H	0.183433
11	H	0.143517
12	N	0.544745
13	C	-0.656731
14	C	-0.512354
15	H	0.200184
16	C	0.916041
17	C	-0.283421
18	C	-0.346934
19	C	0.147312
20	C	-0.403760
21	C	-0.390899
22	H	0.177228
23	H	0.188365
24	H	0.166537
25	H	0.175954
26	H	0.156733
27	C	-0.058909
28	C	-0.370348
29	C	-0.059416
30	C	-0.023168
31	C	-0.192551
32	C	-0.218905
33	H	0.173950
34	H	0.136081
35	H	0.175220
36	H	0.181536
37	H	0.146151

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

		1
1	C	0.580720
2	H	0.000000
3	C	-0.080096
4	H	0.000000
5	C	-0.547594

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     6  H    0.000000
     7  C    0.546990
     8  H    0.000000
     9  C   -0.468659
    10  H    0.000000
    11  H    0.000000
    12  N    0.544745
    13  C   -0.656731
    14  C   -0.312169
    15  H    0.000000
    16  C    0.916041
    17  C   -0.126688
    18  C   -0.169705
    19  C    0.335676
    20  C   -0.237224
    21  C   -0.214946
    22  H    0.000000
    23  H    0.000000
    24  H    0.000000
    25  H    0.000000
    26  H    0.000000
    27  C   -0.058909
    28  C   -0.224197
    29  C    0.114534
    30  C    0.112913
    31  C   -0.017331
    32  C   -0.037370
    33  H    0.000000
    34  H    0.000000
    35  H    0.000000
    36  H    0.000000
    37  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  6158.9881
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=    -0.4107    Y=     1.3708    Z=     0.1623  Tot=     1.4401
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=  -111.6691   YY=  -117.0018   ZZ=  -114.9290
  XY=    -0.4927   XZ=     2.0406   YZ=    -1.4540
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=     2.8642   YY=    -2.4685   ZZ=    -0.3957
  XY=    -0.4927   XZ=     2.0406   YZ=    -1.4540
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=    -0.9521  YYY=    10.7989  ZZZ=     2.9695  XYY=   -21.0692
 XXY=    -6.0002  XXZ=   -12.0121  XZZ=    12.5846  YZZ=     2.6842
 YYZ=     1.4453  XYZ=    16.4466
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -5846.4059 YYYY= -1843.5306 ZZZZ=  -692.8227 XXXY=     3.6531
XXXZ=    81.2047 YYYX=    43.0160 YYYZ=   -45.0614 ZZZX=     8.0427
ZZZY=    11.0491 XXYY= -1347.6438 XXZZ= -1118.2771 YYZZ=  -406.4440
XXYZ=     3.1564 YYXZ=   -36.6692 ZZXY=   -18.1774
N-N= 1.419121397303D+03 E-N=-4.669204406748D+03  KE= 7.855302945904D+02
1|1|UNPC-UNK|SP|RB3LYP|6-311++G(d,p)|C19H17N1|PCUSER|19-Nov-2011|0||#
NMR=ALL B3LYP/6-311++G(D,P) GEOM=CONNECTIVITY||Title Card Required||0,
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93705588,2,-26.16711863,0|C,3,1.34750176,1,106.68498175,2,158.67680291
,0|H,5,1.07742007,3,127.15971149,1,175.44468837,0|C,5,1.52160507,3,107
.54056191,1,-1.10058382,0|H,7,1.09177562,5,116.84916426,3,-157.0035645
5,0|C,1,1.53874039,3,98.16393104,5,36.47165283,0|H,9,1.09772993,1,113.
75192534,3,63.13242498,0|H,9,1.0972265,1,113.19019619,3,-171.6851273,0
|N,7,1.4894546,5,107.43564778,3,67.80443,0|C,12,1.41176096,7,107.19012
424,5,-65.95782398,0|C,13,1.34226301,12,128.87395739,7,-175.60755616,0
|H,14,1.08645156,13,119.85181006,12,0.51967795,0|C,14,1.46317566,13,12
4.62736102,12,179.08649929,0|C,16,2.80016821,14,179.03594893,13,-156.5
1819107,0|C,16,1.4003496,14,121.0660487,13,64.08879684,0|C,16,1.398288
24,14,119.53341376,13,-117.3100443,0|C,17,1.39471646,16,59.94898537,14
,39.73777761,0|C,17,1.39446047,16,59.99844013,14,-139.91642182,0|H,18,
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1.08729435,16,120.26431855,14,-0.25992088,0|H,19,1.08694526,16,120.312
84834,14,0.86051786,0|H,20,1.08693974,17,120.02975175,16,179.94772825,
0|H,21,1.08644098,17,120.01862692,16,179.96611275,0|H,17,1.08600599,16
,179.94433968,14,101.45444488,0|C,12,1.40622118,7,116.85750332,5,85.36
052507,0|C,27,2.82801078,12,178.76242307,7,52.36762732,0|C,27,1.402463
55,12,122.51080709,7,-124.46656758,0|C,27,1.40452483,12,120.11679727,7
,55.58202096,0|C,28,1.39133353,27,59.84860777,12,3.24610673,0|C,28,1.3
9138061,27,59.76118658,12,-176.82731649,0|H,29,1.08640186,27,120.25279
998,12,1.6459509,0|H,30,1.08661907,27,119.93591823,12,1.75048798,0|H,3
1,1.08604512,28,120.09328154,27,179.49261136,0|H,32,1.08670419,28,120.
13505343,27,179.60963136,0|H,28,1.08621545,27,179.89659764,12,124.3863
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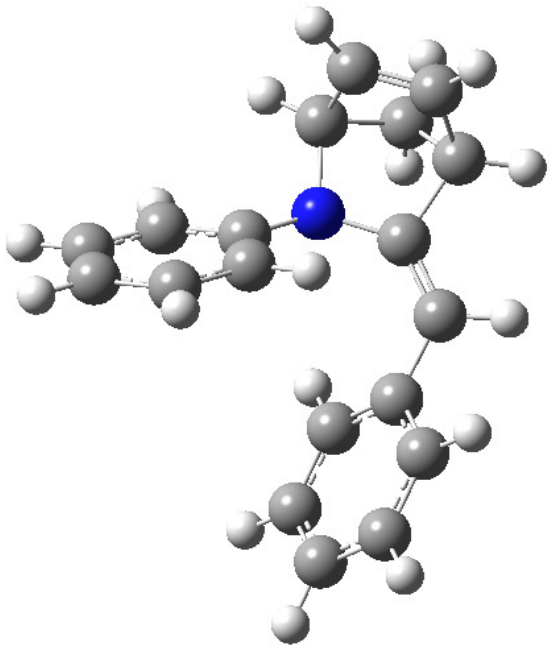
-009|Dipole=0.2811487,-0.4880498,-0.0616011|PG=C01 [X(C19H17N1)]||@

Job cpu time: 0 days 5 hours 46 minutes 1.0 seconds.
File lengths (MBytes): RWF=   181 Int=   0 D2E=   0 Chk=   20 Scr=   1
Normal termination of Gaussian 03 at Sat Nov 19 20:26:11 2011.

Enamine B



%chk=erb enamine 2.chk
%mem=65MW
%nproc=1
Will use up to   1 processors via shared memory.
Default route: MaxDisk=2000MB

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# nmr=all b3lyp/6-311++g(d,p) geom=connectivity
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1/38=1,57=2/1;
2/17=6,18=5,40=1/2;
3/5=4,6=6,7=1111,11=2,16=1,25=1,30=1,74=-5/1,2,8,3;
4//1;
5/5=2,38=5/2;
8/6=1,10=90,11=11,27=262144000/1;
10/13=100,45=7/2;
6/7=2,8=2,9=2,10=2,28=1/1;
99/9=1/99;
--------------------
Title Card Required
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Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C
H                  1    B1
C                  1    B2       2    A1
H                  3    B3       1    A2       2    D1       0
C                  3    B4       1    A3       2    D2       0
H                  5    B5       3    A4       1    D3       0
C                  5    B6       3    A5       1    D4       0
H                  7    B7       5    A6       3    D5       0
C                  1    B8       3    A7       5    D6       0
H                  9    B9       1    A8       3    D7       0
H                  9    B10      1    A9       3    D8       0
N                  7    B11      5    A10      3    D9       0
C                  12   B12      7    A11      5    D10      0
C                  13   B13      12   A12      7    D11      0
C                  12   B14      7    A13      5    D12      0
C                  15   B15      12   A14      7    D13      0
C                  15   B16      12   A15      7    D14      0
C                  15   B17      12   A16      7    D15      0
C                  16   B18      15   A17      12   D16      0
C                  16   B19      15   A18      12   D17      0
H                  17   B20      15   A19      12   D18      0
H                  18   B21      15   A20      12   D19      0
H                  19   B22      16   A21      15   D20      0
H                  20   B23      16   A22      15   D21      0
H                  16   B24      15   A23      12   D22      0
H                  14   B25      13   A24      12   D23      0
C                  14   B26      13   A25      12   D24      0
C                  27   B27      14   A26      13   D25      0
C                  27   B28      14   A27      13   D26      0
C                  27   B29      14   A28      13   D27      0
C                  28   B30      27   A29      14   D28      0
C                  28   B31      27   A30      14   D29      0
H                  29   B32      27   A31      14   D30      0
H                  30   B33      27   A32      14   D31      0
H                  31   B34      28   A33      27   D32      0
H                  32   B35      28   A34      27   D33      0
H                  28   B36      27   A35      14   D34      0
     Variables:
 B1                1.08939
 B2                1.51799
 B3                1.07857
 B4                1.34652
 B5                1.07742
 B6                1.52255
 B7                1.09181
 B8                1.53811
 B9                1.09744
 B10               1.09757
 B11               1.49378
 B12               1.41175
 B13               1.3436
 B14               1.41195
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B15	2.82356
B16	1.40211
B17	1.40492
B18	1.39139
B19	1.39159
B20	1.08633
B21	1.08646
B22	1.08623
B23	1.08634
B24	1.08678
B25	1.08811
B26	1.46925
B27	2.80785
B28	1.40149
B29	1.39961
B30	1.39312
B31	1.39347
B32	1.08742
B33	1.08779
B34	1.08672
B35	1.08653
B36	1.08626
A1	116.35322
A2	126.03082
A3	106.62769
A4	127.23746
A5	107.51824
A6	116.96717
A7	98.3599
A8	113.79606
A9	113.19365
A10	107.70215
A11	106.89937
A12	133.23543
A13	114.45138
A14	178.41962
A15	122.72009
A16	119.64373
A17	59.93473
A18	59.77098
A19	120.1073
A20	119.87242
A21	120.16681
A22	120.18028
A23	179.67233
A24	118.38907
A25	127.69838
A26	177.64826
A27	119.07392
A28	122.06546
A29	59.88027
A30	59.97042
A31	120.33512
A32	120.1806
A33	120.11848
A34	120.00203
A35	179.52915
D1	-25.50958
D2	159.3439
D3	175.3358
D4	-0.71372
D5	-157.46947
D6	36.26364
D7	63.09941
D8	-171.63943
D9	67.5394
D10	-66.09242
D11	-175.41009

D12	80.1892
D13	57.18049
D14	-117.75344
D15	62.03278
D16	4.92269
D17	-175.09469
D18	0.62169
D19	1.72753
D20	179.4282
D21	-179.81994
D22	120.08586
D23	-179.86916
D24	1.77697
D25	171.19265
D26	-139.82266
D27	43.61319
D28	-129.13163
D29	50.34683
D30	2.5003
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D32	-179.43263
D33	179.66078
D34	148.46613

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	1	0	0.000000	0.000000	1.089390
3	6	0	1.360234	0.000000	-0.673842
4	1	0	2.278184	0.375642	-0.250072
5	6	0	1.169587	-0.455133	-1.926687
6	1	0	1.902019	-0.523938	-2.713863
7	6	0	-0.311578	-0.773517	-2.078204
8	1	0	-0.587760	-1.484711	-2.859220
9	6	0	-0.569094	-1.275101	-0.645012
10	1	0	-0.013075	-2.186299	-0.390181
11	1	0	-1.633341	-1.431789	-0.427076
12	7	0	-1.061594	0.517126	-2.022660
13	6	0	-0.897741	1.031174	-0.718074
14	6	0	-1.401604	2.101115	-0.080416
15	6	0	-1.062513	1.245076	-3.232488
16	6	0	-1.095684	2.639156	-5.687675
17	6	0	-0.494852	2.521805	-3.349220
18	6	0	-1.647072	0.684362	-4.380396
19	6	0	-1.664633	1.372611	-5.597488
20	6	0	-0.511511	3.214375	-4.563229
21	1	0	-0.020131	2.987701	-2.490328
22	1	0	-2.119440	-0.292467	-4.324991
23	1	0	-2.131089	0.920501	-6.468068
24	1	0	-0.067906	4.204142	-4.624140
25	1	0	-1.112121	3.180062	-6.630135
26	1	0	-1.103908	2.276005	0.951458
27	6	0	-2.361208	3.085953	-0.598043
28	6	0	-4.203384	5.012224	-1.481152
29	6	0	-2.179256	4.441057	-0.290205
30	6	0	-3.491994	2.707492	-1.330848
31	6	0	-4.403530	3.665833	-1.777719
32	6	0	-3.092038	5.400389	-0.735505
33	1	0	-1.316722	4.761621	0.289246
34	1	0	-3.664030	1.660109	-1.568927
35	1	0	-5.268327	3.358315	-2.359552
36	1	0	-2.935071	6.449469	-0.500262
37	1	0	-4.912078	5.757527	-1.830786

Distance matrix (angstroms):

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1	C	0.000000				
2	H	1.089390	0.000000			
3	C	1.517992	2.226932	0.000000		
4	H	2.322448	2.669342	1.078574	0.000000	
5	C	2.299392	3.266772	1.346519	2.174906	0.000000
6	H	3.355181	4.284498	2.174794	2.649719	1.077422
7	C	2.239272	3.275525	2.316358	3.371869	1.522555
8	H	3.274899	4.259266	3.282517	4.299093	2.240070
9	C	1.538112	2.226634	2.312794	3.314803	2.310421
10	H	2.220882	2.639925	2.597373	3.439919	2.599322
11	H	2.213643	2.649055	3.327522	4.312559	3.325522
12	N	2.342126	3.328552	2.819925	3.783676	2.435706
13	C	1.544309	2.266316	2.482685	3.276469	2.818456
14	C	2.526984	2.783456	3.520595	4.067786	4.068679
15	C	3.623276	4.621448	3.737190	4.561905	3.094850
16	C	6.365164	7.354881	6.175370	6.787783	5.371322
17	C	4.221570	5.128902	4.118068	4.679793	3.695418
18	C	4.729594	5.753239	4.821906	5.706358	3.905471
19	C	5.998912	7.026337	5.939375	6.718230	4.984800
20	C	5.605079	6.522726	5.381725	5.868912	4.821072
21	H	3.889537	4.662740	3.759174	4.138098	3.685950
22	H	4.825258	5.821777	5.052183	6.032449	4.073821
23	H	6.872028	7.905949	6.827130	7.642122	5.780222
24	H	6.249968	7.093931	5.943000	6.268495	5.524173
25	H	7.436955	8.422629	7.190463	7.750106	6.367358
26	H	2.702607	2.533345	3.727438	4.061231	4.572922
27	C	3.931420	4.236253	4.835078	5.384313	5.174079
28	C	6.707059	7.028407	7.531798	8.063757	7.678496
29	C	4.955438	5.135701	5.691938	6.033074	6.153495
30	C	4.614726	5.038064	5.595202	6.316689	5.664588
31	C	5.999141	6.407006	6.919382	7.602918	6.932834
32	C	6.266248	6.484993	6.999337	7.370414	7.339448
33	H	4.948783	5.004700	5.546771	5.696580	6.189234
34	H	4.317709	4.821590	5.366597	6.220864	5.288297
35	H	6.678401	7.136439	7.619562	8.384276	7.495098
36	H	7.103559	7.262044	7.750834	8.008246	8.158213
37	H	7.786488	8.112031	8.592411	9.119387	8.694423

		6	7	8	9	10
6	H	0.000000				
7	C	2.316541	0.000000			
8	H	2.672679	1.091815	0.000000		
9	C	3.309197	1.540110	2.224185	0.000000	
10	H	3.439554	2.221369	2.630331	1.097442	0.000000
11	H	4.307245	2.215086	2.647898	1.097575	1.787711
12	N	3.216299	1.493777	2.220744	2.313557	3.327595
13	C	3.773620	2.334620	3.318173	2.330719	3.352951
14	C	4.973920	3.666446	4.608931	3.522879	4.517288
15	C	3.490965	2.443562	2.795793	3.645516	4.577595
16	C	5.275883	5.028861	5.026373	6.405244	7.247103
17	C	3.927495	3.536696	4.037437	4.662053	5.581600
18	C	4.102849	3.034641	2.853243	4.353691	5.180006
19	C	4.963185	4.338432	4.101470	5.721678	6.519934
20	C	4.818741	4.703042	4.999087	5.959122	6.843249
21	H	4.009519	3.794937	4.523356	4.677396	5.583991
22	H	4.338369	2.923667	2.432278	4.112346	4.848310
23	H	5.696176	5.044921	4.603335	6.416266	7.146951
24	H	5.466673	5.596272	5.978984	6.790195	7.665975
25	H	6.175908	6.082083	6.021201	7.480979	8.303178
26	H	5.505439	4.371067	5.378723	3.930025	4.785611
27	C	5.973534	4.613824	5.398982	4.715153	5.775256
28	C	8.333344	6.998387	7.561876	7.310106	8.400455
29	C	6.868923	5.820391	6.651874	5.949199	6.973105
30	C	6.438187	4.773994	5.324008	4.987460	6.077576
31	C	7.628270	6.045014	6.500604	6.356001	7.446396
32	C	7.997009	6.902964	7.627986	7.136918	8.194943
33	H	6.878670	6.103514	7.032843	6.154169	7.101740
34	H	6.087844	4.173827	4.584559	4.364368	5.432658

35	H	8.161575	6.459146	6.753687	6.818430	7.889160
36	H	8.770740	7.845008	8.603822	8.080085	9.117383
37	H	9.309595	7.992519	8.497494	8.350175	9.443513

		11	12	13	14	15
11	H	0.000000				
12	N	2.582838	0.000000			
13	C	2.586885	1.411750	0.000000		
14	C	3.557427	2.529218	1.343600	0.000000	
15	C	3.919412	1.411948	2.528870	3.283801	0.000000
16	C	6.673498	4.235151	5.227018	5.641314	2.823561
17	C	5.046383	2.469756	3.050775	3.418225	1.402106
18	C	4.484086	2.435091	3.754247	4.534013	1.404920
19	C	5.882075	3.724904	4.951099	5.571175	2.443776
20	C	6.320847	3.745962	4.438553	4.703959	2.439797
21	H	5.137251	2.721599	2.781921	2.915850	2.161967
22	H	4.089999	2.659927	4.031678	4.925540	2.162105
23	H	6.501893	4.590009	5.881822	6.536674	3.422891
24	H	7.199282	4.620520	5.100364	5.181400	3.417896
25	H	7.747179	5.321899	6.294135	6.644302	3.910324
26	H	3.991039	3.455550	2.092713	1.088105	4.309285
27	C	4.579193	3.212071	2.525522	1.469245	3.466372
28	C	7.017229	5.510897	5.230518	4.276282	5.208037
29	C	5.899752	4.432585	3.667786	2.474688	4.485359
30	C	4.626558	3.344122	3.148918	2.510180	3.414275
31	C	5.956839	4.598140	4.511633	3.786917	4.374793
32	C	6.992966	5.442952	4.889303	3.764560	5.255523
33	H	6.242731	4.840014	3.886705	2.687405	4.983304
34	H	3.871350	2.878360	2.961733	2.743852	3.115699
35	H	6.316066	5.087481	5.216518	4.661176	4.787136
36	H	7.988372	6.404710	5.792761	4.629900	6.169055
37	H	8.025383	6.505755	6.300114	5.362515	6.094763

		16	17	18	19	20
16	C	0.000000				
17	C	2.417259	0.000000			
18	C	2.415414	2.401485	0.000000		
19	C	1.391393	2.782759	1.398324	0.000000	
20	C	1.391586	1.397766	2.779189	2.406549	0.000000
21	H	3.391360	1.086331	3.394799	3.868766	2.142371
22	H	3.391076	3.392866	1.086461	2.144430	3.865247
23	H	2.152871	3.868935	2.156017	1.086229	3.393126
24	H	2.153280	2.153594	3.865492	3.393305	1.086341
25	H	1.086776	3.402753	3.402354	2.153720	2.152675
26	H	6.649062	4.350540	5.590798	6.634699	5.625233
27	C	5.263604	3.372020	4.536939	5.330592	4.377279
28	C	5.743178	4.842011	5.802649	6.052790	5.134334
29	C	5.792552	3.984761	5.579035	6.152029	4.748143
30	C	4.972817	3.618172	4.098357	4.829635	4.425889
31	C	5.223377	4.365338	4.822981	5.229824	4.807358
32	C	6.011141	4.675802	6.133030	6.472972	5.107763
33	H	6.346440	4.350940	6.207956	6.801476	5.156438
34	H	4.951668	3.735726	3.595074	4.506611	4.617354
35	H	5.385587	4.946237	4.934300	5.235825	5.244446
36	H	6.694108	5.431185	7.067590	7.305492	5.731245
37	H	6.258170	5.682203	6.549639	6.630342	5.770516

		21	22	23	24	25
21	H	0.000000				
22	H	4.304949	0.000000			
23	H	4.954985	2.462561	0.000000		
24	H	2.456657	4.951543	4.294077	0.000000	
25	H	4.285726	4.287988	2.483984	2.482567	0.000000
26	H	3.677903	5.955608	7.611955	5.989850	7.635309
27	C	3.011816	5.036101	6.260937	4.766450	6.160780
28	C	4.755705	6.369457	6.775392	5.256763	6.278913
29	C	3.408021	6.220075	7.110741	4.826689	6.551611
30	C	3.671069	4.455171	5.606820	4.980976	5.828341
31	C	4.492423	5.231997	5.890688	5.214358	5.883476
32	C	4.282181	6.799924	7.338603	5.069306	6.602771
33	H	3.543159	6.890526	7.815286	5.100166	7.100776

34	H	3.986161	3.714054	5.186377	5.360834	5.868417
35	H	5.262891	5.206405	5.715340	5.734821	5.961854
36	H	4.943791	7.794068	8.174997	5.501681	7.182444
37	H	5.660219	7.114936	7.255006	5.803606	6.642044

		26	27	28	29	30
26	H	0.000000				
27	C	2.153548	0.000000			
28	C	4.797002	2.807849	0.000000		
29	C	2.717637	1.401491	2.416956	0.000000	
30	C	3.331375	1.399612	2.416704	2.410699	0.000000
31	C	4.501948	2.428781	1.393119	2.785869	1.396069
32	C	4.069432	2.430971	1.393467	1.397061	2.786771
33	H	2.581104	2.164739	3.395574	1.087424	3.402347
34	H	3.644982	2.161711	3.396363	3.401964	1.087791
35	H	5.429233	3.410050	2.154323	3.872582	2.153407
36	H	4.783142	3.413520	2.153238	2.156177	3.873297
37	H	5.862084	3.894086	1.086263	3.402175	3.401366

		31	32	33	34	35
31	C	0.000000				
32	C	2.411412	0.000000			
33	H	3.873175	2.147065	0.000000		
34	H	2.147879	3.874463	4.310689	0.000000	
35	H	1.086725	3.397621	4.959898	2.466326	0.000000
36	H	3.396601	1.086530	2.468037	4.960988	4.296077
37	H	2.153281	2.154004	4.291031	4.291273	2.482483

		36	37
36	H	0.000000	
37	H	2.481458	0.000000

Stoichiometry C19H17N
Framework group C1[X(C19H17N)]
Deg. of freedom 105
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.258898	-2.101152	0.116812
2	1	0	2.237389	-3.189599	0.156692
3	6	0	3.072772	-1.403431	1.191565
4	1	0	3.301067	-1.796239	2.169780
5	6	0	3.353149	-0.172168	0.724133
6	1	0	3.855376	0.624918	1.246876
7	6	0	2.741721	-0.059359	-0.665688
8	1	0	3.169393	0.689342	-1.335466
9	6	0	2.967251	-1.514753	-1.116137
10	1	0	4.025912	-1.793538	-1.192902
11	1	0	2.463220	-1.757516	-2.060430
12	7	0	1.256080	-0.079939	-0.511365
13	6	0	0.911295	-1.361170	-0.029073
14	6	0	-0.262590	-1.967211	0.215811
15	6	0	0.691084	1.156127	-0.128589
16	6	0	-0.406683	3.660875	0.574007
17	6	0	-0.004387	1.330848	1.076273
18	6	0	0.822883	2.271500	-0.972611
19	6	0	0.280323	3.513035	-0.626884
20	6	0	-0.549970	2.569481	1.425382
21	1	0	-0.118493	0.498709	1.765214
22	1	0	1.333266	2.171014	-1.926450
23	1	0	0.388382	4.357517	-1.301470
24	1	0	-1.087630	2.675437	2.363376
25	1	0	-0.834919	4.622511	0.844105
26	1	0	-0.249103	-2.986280	0.596982
27	6	0	-1.613111	-1.430354	0.000032
28	6	0	-4.236739	-0.508895	-0.389204
29	6	0	-2.607320	-1.683832	0.954744

```
  30        6           0       -1.958291   -0.732712   -1.163180
  31        6           0       -3.260503   -0.266678   -1.353089
  32        6           0       -3.911097   -1.219353    0.764467
  33        1           0       -2.370199   -2.235248    1.861499
  34        1           0       -1.208329   -0.537213   -1.926479
  35        1           0       -3.509453    0.287566   -2.254093
  36        1           0       -4.671243   -1.412225    1.516481
  37        1           0       -5.249306   -0.144357   -0.536806
---------------------------------------------------------------------
Rotational constants (GHZ):      0.4831975      0.3179585      0.2278147
Standard basis: 6-311++G(d,p) (5D, 7F)
There are   559 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
  559 basis functions,   873 primitive gaussians,   579 cartesian basis functions
   69 alpha electrons       69 beta electrons
      nuclear repulsion energy      1462.6337746121 Hartrees.
NAtoms=   37 NActive=   37 NUniq=   37 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=   559 RedAO= T  NBF=   559
NBsUse=   555 1.00D-06 NBFU=   555
Harris functional with IExCor=  402 diagonalized for initial guess.
ExpMin= 3.60D-02 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=3 IRadAn=         5 AccDes= 0.00D+00
HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Initial guess orbital symmetries:
     Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A)
     Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               
```

```
              (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
              (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
              (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
              (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
              (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
              (A) (A) (A) (A) (A) (A)
 The electronic state of the initial guess is 1-A.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -789.139799188     A.U. after   15 cycles
            Convg  =    0.8605D-08             -V/T =  2.0046
            S**2   =   0.0000
 Range of M.O.s used for correlation:     1   555
 NBasis=   559 NAE=    69 NBE=    69 NFC=     0 NFV=     0
 NROrb=    555 NOA=    69 NOB=    69 NVA=   486 NVB=   486

 **** Warning!!: The largest alpha MO coefficient is  0.13599231D+03

          Differentiating once with respect to magnetic field.
          Electric field/nuclear overlap derivatives assumed to be zero.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 2 Meth= 1.
 IRaf=       0 NMat=   6 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 2 JSym2E=2.
          There are   6 degrees of freedom in the 1st order CPHF.
      6 vectors were produced by pass  0.
 AX will form   6 AO Fock derivatives at one time.
      6 vectors were produced by pass  1.
      6 vectors were produced by pass  2.
      6 vectors were produced by pass  3.
      6 vectors were produced by pass  4.
      6 vectors were produced by pass  5.
      4 vectors were produced by pass  6.
 Inv2:  IOpt= 1 Iter= 1 AM= 8.88D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension   40 with in-core refinement.
 Calculating magnetic properties, IRadAn=         0.
   Integrating Atom   1
   Integrating Atom   2
   Integrating Atom   3
   Integrating Atom   4
   Integrating Atom   5
   Integrating Atom   6
   Integrating Atom   7
   Integrating Atom   8
   Integrating Atom   9
   Integrating Atom  10
   Integrating Atom  11
   Integrating Atom  12
   Integrating Atom  13
   Integrating Atom  14
   Integrating Atom  15
   Integrating Atom  16
   Integrating Atom  17
   Integrating Atom  18
   Integrating Atom  19
   Integrating Atom  20
   Integrating Atom  21
   Integrating Atom  22
   Integrating Atom  23
   Integrating Atom  24
   Integrating Atom  25
   Integrating Atom  26
   Integrating Atom  27
   Integrating Atom  28
   Integrating Atom  29
   Integrating Atom  30
   Integrating Atom  31
```

```
 Integrating Atom  32
 Integrating Atom  33
 Integrating Atom  34
 Integrating Atom  35
 Integrating Atom  36
 Integrating Atom  37
There are a total of      305178 grid points.
ElSum from orbitals=       79.4761516011

    Magnetic properties (single gauge origin)

Magnetic susceptibility (cgs-ppm):
 Isotropic =  -714.6532   Anisotropy=   287.9715
 XX=  -523.5348   YX=   -11.7017   ZX=    -2.1915
 XY=   -11.7025   YY=  -685.3610   ZY=    10.3349
 XZ=    -2.1942   YZ=    10.3319   ZZ=  -935.0637
 Eigenvalues:  -935.4977  -685.7897  -522.6722
Magnetic shielding (ppm):
1  C    Isotropic =   144.6605   Anisotropy =    39.3440
 XX=   140.9274   YX=     2.6791   ZX=   -13.9180
 XY=   -45.2747   YY=   154.5264   ZY=     6.3945
 XZ=    -2.4482   YZ=    -5.8799   ZZ=   138.5277
 Eigenvalues:   122.6529   140.4388   170.8899
2  H    Isotropic =    19.8678   Anisotropy =    62.5677
 XX=    -1.1892   YX=    -5.1030   ZX=    -0.2985
 XY=   -46.0996   YY=    50.7268   ZY=    -5.3194
 XZ=     2.4374   YZ=    -3.0070   ZZ=    10.0657
 Eigenvalues:   -11.7062     9.7300    61.5796
3  C    Isotropic =    43.5043   Anisotropy =   171.1541
 XX=   111.2079   YX=    -8.1075   ZX=  -121.5966
 XY=   -60.6243   YY=    40.4756   ZY=     2.7806
 XZ=   -39.0873   YZ=    -1.1909   ZZ=   -21.1706
 Eigenvalues:   -61.0844    33.9902   157.6070
4  H    Isotropic =     9.6203   Anisotropy =    60.1399
 XX=     9.8547   YX=    -8.1950   ZX=    -0.1672
 XY=   -24.6622   YY=     1.7498   ZY=    -8.6476
 XZ=    50.1487   YZ=   -23.3465   ZZ=    17.2564
 Eigenvalues:   -12.6386    -8.2141    49.7135
5  C    Isotropic =    50.9924   Anisotropy =   168.6372
 XX=   112.2827   YX=  -112.8510   ZX=   -75.7136
 XY=    -0.8152   YY=    49.3080   ZY=     6.7198
 XZ=   -57.7130   YZ=   -23.4145   ZZ=    -8.6134
 Eigenvalues:   -49.1168    38.6769   163.4172
6  H    Isotropic =    16.8661   Anisotropy =    56.9401
 XX=    39.3878   YX=    -4.9988   ZX=     4.2824
 XY=    45.9795   YY=    -2.2326   ZY=    11.3753
 XZ=    29.0751   YZ=    -2.8196   ZZ=    13.4430
 Eigenvalues:   -10.9153     6.6874    54.8261
7  C    Isotropic =   135.0601   Anisotropy =    65.7829
 XX=   169.5887   YX=   -17.9765   ZX=   -17.5633
 XY=    22.2684   YY=   116.3407   ZY=   -11.1858
 XZ=   -29.2141   YZ=     6.0950   ZZ=   119.2509
 Eigenvalues:   109.6775   116.5875   178.9153
8  H    Isotropic =    28.8563   Anisotropy =    60.6115
 XX=    43.2415   YX=     6.7512   ZX=   -10.3375
 XY=    38.9562   YY=    12.5997   ZY=    -8.2789
 XZ=   -34.0803   YZ=    -6.2499   ZZ=    30.7277
 Eigenvalues:    -0.3515    17.6564    69.2640
9  C    Isotropic =   129.1402   Anisotropy =    41.3877
 XX=   114.8357   YX=     0.0191   ZX=    -0.0596
 XY=   -11.5823   YY=   125.8522   ZY=     9.0528
 XZ=   -21.7438   YZ=    17.2959   ZZ=   146.7327
 Eigenvalues:   111.1827   119.5059   156.7320
10  H    Isotropic =     1.9871   Anisotropy =    73.1918
 XX=    34.6447   YX=   -27.5699   ZX=   -17.9538
 XY=   -21.9920   YY=   -13.6985   ZY=     5.1544
 XZ=   -19.1052   YZ=     6.5108   ZZ=   -14.9849
 Eigenvalues:   -24.8753   -19.9450    50.7817
```

11 H Isotropic = 38.9164 Anisotropy = 57.1138
XX= 17.5259 YX= 5.0055 ZX= 4.4605
XY= -16.7942 YY= 38.5866 ZY= 7.1929
XZ= -46.5716 YZ= 25.3275 ZZ= 60.6368
Eigenvalues: 8.9303 30.8267 76.9923
12 N Isotropic = 198.3112 Anisotropy = 59.3900
XX= 164.2763 YX= 19.8522 ZX= -2.8495
XY= 4.3578 YY= 209.3030 ZY= -2.0641
XZ= -7.9894 YZ= 45.3097 ZZ= 221.3544
Eigenvalues: 159.2061 197.8230 237.9045
13 C Isotropic = 91.0883 Anisotropy = 150.6080
XX= 53.0450 YX= 38.8695 ZX= -11.1687
XY= 23.8627 YY= 40.1017 ZY= 42.9595
XZ= -2.4083 YZ= 39.9484 ZZ= 180.1182
Eigenvalues: 6.6212 75.1500 191.4937
14 C Isotropic = 111.9447 Anisotropy = 108.0336
XX= 99.4470 YX= 12.5886 ZX= -6.5060
XY= 25.0326 YY= 63.4627 ZY= 39.9237
XZ= -12.2907 YZ= 32.4623 ZZ= 172.9244
Eigenvalues: 44.7198 107.1472 183.9671
15 C Isotropic = 93.1910 Anisotropy = 170.6039
XX= 153.3936 YX= 58.4861 ZX= 57.4252
XY= 63.5116 YY= 7.1764 ZY= -2.7079
XZ= 57.4606 YZ= -11.1758 ZZ= 119.0031
Eigenvalues: -20.3462 92.9923 206.9270
16 C Isotropic = 52.9130 Anisotropy = 169.9274
XX= 112.9859 YX= 37.9840 ZX= 65.6567
XY= 58.3029 YY= 5.5175 ZY= 2.2788
XZ= 69.3515 YZ= 13.0244 ZZ= 40.2355
Eigenvalues: -21.5044 14.0455 166.1979
17 C Isotropic = 108.4584 Anisotropy = 187.9900
XX= 174.6971 YX= 45.7390 ZX= 67.2947
XY= 25.8637 YY= 39.8588 ZY= 44.4359
XZ= 58.0636 YZ= 76.8638 ZZ= 110.8193
Eigenvalues: 5.0734 86.5168 233.7851
18 C Isotropic = 85.5740 Anisotropy = 167.0173
XX= 149.8446 YX= 48.8676 ZX= 64.6215
XY= 42.6636 YY= 62.8901 ZY= -0.3415
XZ= 83.4559 YZ= -29.3124 ZZ= 43.9874
Eigenvalues: -11.1491 70.9523 196.9189
19 C Isotropic = 51.7630 Anisotropy = 175.7442
XX= 125.7177 YX= 33.4150 ZX= 60.3118
XY= 29.9963 YY= 13.5529 ZY= 54.7131
XZ= 67.3832 YZ= 27.5002 ZZ= 16.0186
Eigenvalues: -30.8942 17.2575 168.9259
20 C Isotropic = 70.1892 Anisotropy = 181.1478
XX= 130.3832 YX= 17.6725 ZX= 88.0684
XY= 35.8684 YY= 57.8883 ZY= 7.8370
XZ= 89.7438 YZ= 49.6138 ZZ= 22.2961
Eigenvalues: -29.4632 49.0765 190.9544
21 H Isotropic = 64.5906 Anisotropy = 39.3302
XX= 58.5415 YX= -5.0950 ZX= -5.3168
XY= 2.2220 YY= 45.0560 ZY= -12.4025
XZ= -3.2015 YZ= 15.7101 ZZ= 90.1742
Eigenvalues: 44.8720 58.0890 90.8107
22 H Isotropic = 33.3727 Anisotropy = 53.7738
XX= 29.0182 YX= 22.0145 ZX= -7.2369
XY= 7.3111 YY= 23.7031 ZY= -3.3601
XZ= -13.9070 YZ= -44.2481 ZZ= 47.3967
Eigenvalues: 6.2779 24.6182 69.2219
23 H Isotropic = -2.1118 Anisotropy = 69.6247
XX= -22.0560 YX= 9.4630 ZX= 1.9627
XY= 5.4424 YY= 31.7008 ZY= -9.0731
XZ= 2.2530 YZ= -44.6386 ZZ= -15.9802
Eigenvalues: -30.9816 -19.6585 44.3047
24 H Isotropic = 21.0496 Anisotropy = 57.0145
XX= 13.7501 YX= -27.0198 ZX= -10.8649
XY= -2.1760 YY= 15.2505 ZY= 3.4848

XZ= -10.7624 YZ= 48.6484 ZZ= 34.1483
Eigenvalues: -5.3843 9.4739 59.0593
25 H Isotropic = -7.7324 Anisotropy = 72.4653
XX= -26.3591 YX= -27.9895 ZX= 0.0815
XY= -6.8720 YY= 32.9960 ZY= 9.4421
XZ= 1.9893 YZ= 20.3683 ZZ= -29.8340
Eigenvalues: -36.7638 -27.0111 40.5779
26 H Isotropic = 28.8765 Anisotropy = 46.9847
XX= 1.7023 YX= 1.6047 ZX= 0.4425
XY= 3.5697 YY= 56.3212 ZY= -7.9597
XZ= -4.2618 YZ= -13.6597 ZZ= 28.6059
Eigenvalues: 1.5017 24.9280 60.1996
27 C Isotropic = 92.8991 Anisotropy = 210.5980
XX= -10.3467 YX= 51.3333 ZX= 8.0594
XY= 60.3776 YY= 180.9728 ZY= 68.4326
XZ= 5.5335 YZ= 69.0425 ZZ= 108.0710
Eigenvalues: -26.6000 71.9994 233.2977
28 C Isotropic = 45.2467 Anisotropy = 172.9577
XX= -2.5797 YX= 65.8222 ZX= 7.7017
XY= 39.0522 YY= 104.1192 ZY= 65.1632
XZ= 16.9710 YZ= 67.8130 ZZ= 34.2005
Eigenvalues: -29.3982 4.5864 160.5518
29 C Isotropic = 76.6193 Anisotropy = 173.2743
XX= 46.5435 YX= 37.8393 ZX= 1.8482
XY= 57.3663 YY= 145.2305 ZY= 76.0651
XZ= -45.3366 YZ= 75.6503 ZZ= 38.0838
Eigenvalues: -26.2359 63.9583 192.1355
30 C Isotropic = 98.8224 Anisotropy = 194.4466
XX= 29.5771 YX= 18.0733 ZX= 42.0787
XY= 14.9805 YY= 183.6214 ZY= 62.5623
XZ= 89.5618 YZ= 72.9608 ZZ= 83.2685
Eigenvalues: -18.0294 86.0430 228.4534
31 C Isotropic = 67.2076 Anisotropy = 186.0331
XX= 56.8884 YX= 42.6766 ZX= 2.0378
XY= 14.9612 YY= 124.2069 ZY= 89.7879
XZ= 47.6861 YZ= 100.5994 ZZ= 20.5276
Eigenvalues: -36.5357 46.9289 191.2297
32 C Isotropic = 45.6234 Anisotropy = 178.1917
XX= 13.2626 YX= 32.1170 ZX= 53.5799
XY= 32.9435 YY= 121.0825 ZY= 69.0159
XZ= 17.3985 YZ= 65.1014 ZZ= 2.5252
Eigenvalues: -36.7923 9.2447 164.4179
33 H Isotropic = 28.4919 Anisotropy = 60.4298
XX= 7.3829 YX= -1.2786 ZX= 1.1799
XY= 28.7646 YY= 37.3407 ZY= -10.5709
XZ= -48.9193 YZ= -24.8588 ZZ= 40.7521
Eigenvalues: -5.5184 22.2157 68.7784
34 H Isotropic = 61.6641 Anisotropy = 44.1543
XX= 35.0495 YX= -6.0682 ZX= -8.9276
XY= -9.1455 YY= 60.7397 ZY= -4.7842
XZ= 29.4600 YZ= 6.1623 ZZ= 89.2030
Eigenvalues: 31.2088 62.6831 91.1002
35 H Isotropic = 18.7938 Anisotropy = 64.6412
XX= 23.0400 YX= 0.6312 ZX= 6.2697
XY= -34.6554 YY= 5.5502 ZY= -9.8027
XZ= 59.3170 YZ= 3.1075 ZZ= 27.7911
Eigenvalues: -13.7251 8.2185 61.8879
36 H Isotropic = -8.5627 Anisotropy = 79.4101
XX= 21.8690 YX= 17.0781 ZX= -10.7852
XY= 17.3528 YY= -25.5712 ZY= 0.4049
XZ= -56.4096 YZ= -9.6951 ZZ= -21.9858
Eigenvalues: -41.5539 -28.5115 44.3774
37 H Isotropic = -13.6074 Anisotropy = 82.1695
XX= 39.1951 YX= 9.3806 ZX= 5.4229
XY= -26.9578 YY= -39.7038 ZY= 2.6441
XZ= 13.7432 YZ= 5.9970 ZZ= -40.3135
Eigenvalues: -46.3170 -35.6774 41.1723
Current density tensor (au):

XX= -2.0762 YX= 0.0082 ZX= 0.1279
XY= -1.8172 YY= -1.8613 ZY= -0.9078
XZ= 5.2124 YZ= 5.5685 ZZ= 3.9425

Magnetic properties (IGAIM method)

Magnetic susceptibility (cgs-ppm):
Isotropic = -155.1751 Anisotropy= 69.6490
XX= -167.0306 YX= -19.5971 ZX= -25.6760
XY= -19.8637 YY= -156.7139 ZY= -38.8273
XZ= -25.4480 YZ= -38.5229 ZZ= -141.7807
Eigenvalues: -211.2949 -145.4879 -108.7424
Magnetic shielding (ppm):
1 C Isotropic = 121.9986 Anisotropy = 24.8222
XX= 134.3740 YX= 7.1024 ZX= -12.6588
XY= -10.5309 YY= 116.9766 ZY= 8.3720
XZ= -6.5600 YZ= -4.1072 ZZ= 114.6452
Eigenvalues: 110.4582 116.9908 138.5467
2 H Isotropic = 27.9273 Anisotropy = 6.2450
XX= 26.4845 YX= -0.9937 ZX= -0.0169
XY= 0.3793 YY= 31.8378 ZY= -1.8258
XZ= -0.4011 YZ= -0.6977 ZZ= 25.4596
Eigenvalues: 25.1663 26.5250 32.0907
3 C Isotropic = 37.1883 Anisotropy = 175.3549
XX= 99.2866 YX= 3.6275 ZX= -119.9206
XY= -34.4356 YY= 43.9021 ZY= 11.9873
XZ= -72.9421 YZ= 16.2206 ZZ= -31.6236
Eigenvalues: -82.9367 40.4101 154.0916
4 H Isotropic = 24.5876 Anisotropy = 2.3986
XX= 25.0738 YX= 1.4463 ZX= -3.2267
XY= 0.2681 YY= 24.7537 ZY= 0.1833
XZ= 0.9617 YZ= -0.2817 ZZ= 23.9355
Eigenvalues: 23.1198 24.4564 26.1867
5 C Isotropic = 38.5050 Anisotropy = 171.1005
XX= 75.9096 YX= -108.3207 ZX= -77.1164
XY= -32.3598 YY= 55.3043 ZY= -4.9288
XZ= -73.5703 YZ= -22.2674 ZZ= -15.6989
Eigenvalues: -76.4984 39.4414 152.5720
6 H Isotropic = 25.0352 Anisotropy = 3.9980
XX= 25.5000 YX= -4.8890 ZX= -0.5724
XY= 1.0654 YY= 25.4464 ZY= -0.1693
XZ= 1.3944 YZ= -1.9840 ZZ= 24.1593
Eigenvalues: 23.2218 24.1833 27.7006
7 C Isotropic = 107.9379 Anisotropy = 45.0001
XX= 131.1506 YX= -20.7962 ZX= -11.5901
XY= -5.8185 YY= 105.8683 ZY= -10.0863
XZ= -6.5438 YZ= 5.0850 ZZ= 86.7947
Eigenvalues: 83.6847 102.1910 137.9379
8 H Isotropic = 26.5938 Anisotropy = 6.4980
XX= 27.7811 YX= 0.9417 ZX= -3.2676
XY= 0.6600 YY= 27.3783 ZY= -2.8637
XZ= -1.1136 YZ= -4.0144 ZZ= 24.6221
Eigenvalues: 21.9481 26.9075 30.9259
9 C Isotropic = 121.3505 Anisotropy = 30.3032
XX= 99.5031 YX= 9.5506 ZX= 2.6039
XY= 5.9987 YY= 125.7552 ZY= 5.2614
XZ= 6.6105 YZ= 4.4148 ZZ= 138.7932
Eigenvalues: 97.1262 125.3727 141.5526
10 H Isotropic = 29.2964 Anisotropy = 8.6643
XX= 31.7151 YX= -3.3134 ZX= -4.1302
XY= -2.6414 YY= 27.6978 ZY= 1.5798
XZ= -2.3883 YZ= 0.7021 ZZ= 28.4763
Eigenvalues: 25.8559 26.9607 35.0726
11 H Isotropic = 28.8376 Anisotropy = 8.5477
XX= 25.9070 YX= -0.5234 ZX= -0.6579
XY= -0.4048 YY= 26.8275 ZY= 2.5548
XZ= 0.2267 YZ= 2.2308 ZZ= 33.7783
Eigenvalues: 25.5978 26.3789 34.5361

12 N Isotropic = 137.4997 Anisotropy = 57.4152
XX= 116.5506 YX= 14.1348 ZX= -4.8329
XY= -4.5821 YY= 162.4711 ZY= -0.3599
XZ= 6.9304 YZ= 46.9357 ZZ= 133.4773
Eigenvalues: 115.7705 120.9520 175.7764
13 C Isotropic = 35.2454 Anisotropy = 121.9909
XX= 22.1193 YX= 40.1792 ZX= -13.1183
XY= 35.5778 YY= -20.8930 ZY= 41.1382
XZ= -4.8310 YZ= 40.1057 ZZ= 104.5101
Eigenvalues: -53.0163 42.1799 116.5727
14 C Isotropic = 76.5012 Anisotropy = 87.0345
XX= 100.4777 YX= 6.8424 ZX= -6.7850
XY= 24.3515 YY= 7.9892 ZY= 42.5404
XZ= -10.5381 YZ= 38.8036 ZZ= 121.0367
Eigenvalues: -7.9503 102.9296 134.5241
15 C Isotropic = 31.5826 Anisotropy = 159.5419
XX= 94.4362 YX= 51.0331 ZX= 53.1772
XY= 51.6394 YY= -43.0137 ZY= 0.1963
XZ= 53.5126 YZ= -7.4804 ZZ= 43.3253
Eigenvalues: -64.4508 21.2547 137.9439
16 C Isotropic = 56.1368 Anisotropy = 176.0561
XX= 125.3723 YX= 58.0874 ZX= 57.7267
XY= 61.9065 YY= -20.1866 ZY= -7.5180
XZ= 60.7131 YZ= -6.6861 ZZ= 63.2245
Eigenvalues: -49.0209 43.9237 173.5075
17 C Isotropic = 56.2866 Anisotropy = 179.0062
XX= 124.0298 YX= 45.9982 ZX= 65.3627
XY= 19.5686 YY= 5.4320 ZY= 56.5495
XZ= 55.3363 YZ= 64.7816 ZZ= 39.3980
Eigenvalues: -41.4128 34.6485 175.6241
18 C Isotropic = 54.5428 Anisotropy = 162.6140
XX= 119.4954 YX= 26.3869 ZX= 66.0172
XY= 32.0749 YY= 45.8556 ZY= -0.1346
XZ= 87.4064 YZ= 3.7230 ZZ= -1.7225
Eigenvalues: -40.3800 41.0564 162.9521
19 C Isotropic = 50.2618 Anisotropy = 179.1893
XX= 136.3559 YX= 20.4993 ZX= 50.7282
XY= 21.1800 YY= -11.0158 ZY= 62.9705
XZ= 57.2917 YZ= 64.8519 ZZ= 25.4453
Eigenvalues: -60.6986 41.7626 169.7213
20 C Isotropic = 49.8325 Anisotropy = 181.5808
XX= 110.4528 YX= 36.7916 ZX= 92.2715
XY= 33.8447 YY= 49.3318 ZY= 4.3207
XZ= 94.5801 YZ= 8.2672 ZZ= -10.2873
Eigenvalues: -62.3624 40.9734 170.8863
21 H Isotropic = 24.9564 Anisotropy = 7.9679
XX= 24.7843 YX= -1.8062 ZX= -3.5160
XY= -0.0460 YY= 25.1980 ZY= 4.4422
XZ= -1.6091 YZ= 3.7609 ZZ= 24.8868
Eigenvalues: 20.5309 24.0700 30.2683
22 H Isotropic = 24.3141 Anisotropy = 8.7024
XX= 22.5676 YX= -2.7551 ZX= 0.3556
XY= -1.0795 YY= 28.7055 ZY= -3.3440
XZ= 0.1012 YZ= -2.1223 ZZ= 21.6692
Eigenvalues: 20.6258 22.2008 30.1157
23 H Isotropic = 24.2427 Anisotropy = 4.8654
XX= 23.2144 YX= -1.4574 ZX= -2.1859
XY= -1.3714 YY= 25.6642 ZY= 1.0075
XZ= -1.7753 YZ= 1.5179 ZZ= 23.8495
Eigenvalues: 21.5059 23.7359 27.4863
24 H Isotropic = 24.6440 Anisotropy = 6.1822
XX= 22.1193 YX= -0.8229 ZX= -0.4051
XY= -0.5774 YY= 28.6646 ZY= 0.1951
XZ= -0.3739 YZ= 0.5007 ZZ= 23.1479
Eigenvalues: 21.9414 23.2250 28.7654
25 H Isotropic = 24.7830 Anisotropy = 3.9735
XX= 23.0424 YX= -0.0285 ZX= -2.1050
XY= 0.3883 YY= 25.4983 ZY= -1.4209

XZ= -1.6410 YZ= -0.9462 ZZ= 25.8082
Eigenvalues: 22.0533 24.8636 27.4320
26 H Isotropic = 25.2966 Anisotropy = 6.0929
XX= 28.9926 YX= 0.2237 ZX= -1.1866
XY= -0.4066 YY= 24.3644 ZY= -1.9256
XZ= -1.9192 YZ= -1.0190 ZZ= 22.5329
Eigenvalues: 21.4499 25.0814 29.3586
27 C Isotropic = 39.0308 Anisotropy = 192.3088
XX= -41.3464 YX= 51.7356 ZX= 9.0908
XY= 53.3729 YY= 115.8434 ZY= 65.8546
XZ= 8.4501 YZ= 67.4388 ZZ= 42.5954
Eigenvalues: -58.8328 8.6885 167.2366
28 C Isotropic = 54.0835 Anisotropy = 178.2352
XX= -31.8542 YX= 57.6311 ZX= 2.1206
XY= 58.4666 YY= 126.6285 ZY= 55.1135
XZ= 2.4067 YZ= 55.7352 ZZ= 67.4762
Eigenvalues: -52.9843 42.3278 172.9070
29 C Isotropic = 51.1375 Anisotropy = 164.8116
XX= 45.1192 YX= 35.0697 ZX= -2.0973
XY= 30.8981 YY= 109.3024 ZY= 80.2037
XZ= -9.6157 YZ= 88.5933 ZZ= -1.0092
Eigenvalues: -51.3432 43.7437 161.0119
30 C Isotropic = 50.5138 Anisotropy = 178.9285
XX= 5.2304 YX= 19.5601 ZX= 52.5755
XY= 20.6970 YY= 131.0316 ZY= 61.1217
XZ= 65.9804 YZ= 63.4431 ZZ= 15.2794
Eigenvalues: -54.0056 35.7474 169.7995
31 C Isotropic = 50.2056 Anisotropy = 182.9087
XX= 44.1876 YX= 39.9844 ZX= -4.3129
XY= 40.7393 YY= 110.1871 ZY= 93.3540
XZ= -3.7726 YZ= 95.2365 ZZ= -3.7578
Eigenvalues: -62.3215 40.7936 172.1448
32 C Isotropic = 50.2835 Anisotropy = 180.9977
XX= -0.3511 YX= 15.2107 ZX= 63.5014
XY= 13.4764 YY= 133.9233 ZY= 61.3119
XZ= 63.9700 YZ= 64.4783 ZZ= 17.2783
Eigenvalues: -61.3142 41.2161 170.9487
33 H Isotropic = 24.4275 Anisotropy = 7.7408
XX= 28.6305 YX= 0.2936 ZX= -3.0066
XY= -1.0003 YY= 22.4572 ZY= -0.3735
XZ= -2.3012 YZ= -0.5536 ZZ= 22.1950
Eigenvalues: 21.0255 22.6691 29.5881
34 H Isotropic = 24.1482 Anisotropy = 8.6216
XX= 26.4033 YX= -0.1395 ZX= 5.2822
XY= -1.1146 YY= 22.0851 ZY= -0.8824
XZ= 3.5823 YZ= -0.6412 ZZ= 23.9563
Eigenvalues: 20.5462 22.0025 29.8960
35 H Isotropic = 24.5694 Anisotropy = 6.0883
XX= 28.6101 YX= 0.1134 ZX= -0.2394
XY= -0.1977 YY= 21.8398 ZY= -0.2290
XZ= -0.3814 YZ= -0.0076 ZZ= 23.2582
Eigenvalues: 21.8293 23.2505 28.6282
36 H Isotropic = 24.3257 Anisotropy = 4.8350
XX= 26.1296 YX= -1.1454 ZX= 1.0764
XY= -1.3739 YY= 23.2607 ZY= -2.0585
XZ= 1.4663 YZ= -1.6689 ZZ= 23.5867
Eigenvalues: 21.5516 23.8764 27.5490
37 H Isotropic = 24.6640 Anisotropy = 4.2298
XX= 25.0475 YX= 0.6111 ZX= -1.0074
XY= 0.4436 YY= 22.8977 ZY= -2.1410
XZ= -0.7762 YZ= -1.9300 ZZ= 26.0470
Eigenvalues: 21.8967 24.6115 27.4839
Current density tensor (au):
XX= 0.0529 YX= 0.0048 ZX= -0.0519
XY= 0.0341 YY= 0.0158 ZY= -0.0354
XZ= -0.0904 YZ= -0.0148 ZZ= -0.0599

Magnetic properties (CSGT method)

Magnetic susceptibility (cgs-ppm):
Isotropic = -155.2367 Anisotropy= 69.6101
XX= -167.0835 YX= -19.6025 ZX= -25.6680
XY= -19.8630 YY= -156.7718 ZY= -38.8053
XZ= -25.4425 YZ= -38.5076 ZZ= -141.8549
Eigenvalues: -211.3411 -145.5391 -108.8300
Magnetic shielding (ppm):
1 C Isotropic = 121.9853 Anisotropy = 24.8142
XX= 134.3565 YX= 7.1020 ZX= -12.6574
XY= -10.5329 YY= 116.9733 ZY= 8.3706
XZ= -6.5580 YZ= -4.1082 ZZ= 114.6262
Eigenvalues: 110.4418 116.9860 138.5281
2 H Isotropic = 27.9271 Anisotropy = 6.2503
XX= 26.4818 YX= -0.9950 ZX= -0.0168
XY= 0.3779 YY= 31.8409 ZY= -1.8269
XZ= -0.4010 YZ= -0.6978 ZZ= 25.4586
Eigenvalues: 25.1650 26.5223 32.0940
3 C Isotropic = 37.1683 Anisotropy = 175.3378
XX= 99.2583 YX= 3.6296 ZX= -119.9150
XY= -34.4331 YY= 43.8835 ZY= 11.9788
XZ= -72.9360 YZ= 16.2138 ZZ= -31.6369
Eigenvalues: -82.9479 40.3927 154.0602
4 H Isotropic = 24.5845 Anisotropy = 2.3962
XX= 25.0704 YX= 1.4439 ZX= -3.2258
XY= 0.2659 YY= 24.7475 ZY= 0.1803
XZ= 0.9624 YZ= -0.2833 ZZ= 23.9355
Eigenvalues: 23.1206 24.4509 26.1819
5 C Isotropic = 38.4858 Anisotropy = 171.0841
XX= 75.8848 YX= -108.3129 ZX= -77.1104
XY= -32.3515 YY= 55.2917 ZY= -4.9267
XZ= -73.5640 YZ= -22.2659 ZZ= -15.7190
Eigenvalues: -76.5096 39.4252 152.5419
6 H Isotropic = 25.0329 Anisotropy = 3.9947
XX= 25.4988 YX= -4.8874 ZX= -0.5717
XY= 1.0672 YY= 25.4440 ZY= -0.1655
XZ= 1.3950 YZ= -1.9811 ZZ= 24.1557
Eigenvalues: 23.2234 24.1792 27.6960
7 C Isotropic = 107.9256 Anisotropy = 44.9959
XX= 131.1385 YX= -20.7920 ZX= -11.5936
XY= -5.8135 YY= 105.8560 ZY= -10.0925
XZ= -6.5474 YZ= 5.0778 ZZ= 86.7823
Eigenvalues: 83.6681 102.1859 137.9229
8 H Isotropic = 26.5941 Anisotropy = 6.5037
XX= 27.7817 YX= 0.9443 ZX= -3.2698
XY= 0.6621 YY= 27.3779 ZY= -2.8640
XZ= -1.1154 YZ= -4.0171 ZZ= 24.6227
Eigenvalues: 21.9470 26.9053 30.9299
9 C Isotropic = 121.3313 Anisotropy = 30.3079
XX= 99.4901 YX= 9.5482 ZX= 2.6066
XY= 5.9957 YY= 125.7282 ZY= 5.2649
XZ= 6.6137 YZ= 4.4179 ZZ= 138.7755
Eigenvalues: 97.1133 125.3439 141.5365
10 H Isotropic = 29.2948 Anisotropy = 8.6679
XX= 31.7157 YX= -3.3147 ZX= -4.1314
XY= -2.6427 YY= 27.6955 ZY= 1.5797
XZ= -2.3890 YZ= 0.7017 ZZ= 28.4731
Eigenvalues: 25.8528 26.9581 35.0733
11 H Isotropic = 28.8363 Anisotropy = 8.5506
XX= 25.9045 YX= -0.5221 ZX= -0.6574
XY= -0.4048 YY= 26.8256 ZY= 2.5554
XZ= 0.2272 YZ= 2.2313 ZZ= 33.7789
Eigenvalues: 25.5960 26.3764 34.5367
12 N Isotropic = 137.4966 Anisotropy = 57.4181
XX= 116.5459 YX= 14.1353 ZX= -4.8352
XY= -4.5825 YY= 162.4745 ZY= -0.3613
XZ= 6.9284 YZ= 46.9331 ZZ= 133.4693
Eigenvalues: 115.7653 120.9492 175.7753

13 C Isotropic = 35.2394 Anisotropy = 121.9781
XX= 22.1161 YX= 40.1844 ZX= -13.1194
XY= 35.5812 YY= -20.8953 ZY= 41.1326
XZ= -4.8323 YZ= 40.1012 ZZ= 104.4974
Eigenvalues: -53.0209 42.1810 116.5581
14 C Isotropic = 76.4825 Anisotropy = 87.0146
XX= 100.4623 YX= 6.8462 ZX= -6.7850
XY= 24.3554 YY= 7.9772 ZY= 42.5312
XZ= -10.5395 YZ= 38.7958 ZZ= 121.0080
Eigenvalues: -7.9602 102.9155 134.4922
15 C Isotropic = 31.5745 Anisotropy = 159.5290
XX= 94.4230 YX= 51.0307 ZX= 53.1713
XY= 51.6364 YY= -43.0176 ZY= 0.1958
XZ= 53.5086 YZ= -7.4820 ZZ= 43.3182
Eigenvalues: -64.4539 21.2502 137.9272
16 C Isotropic = 56.1110 Anisotropy = 176.0337
XX= 125.3378 YX= 58.0798 ZX= 57.7193
XY= 61.8984 YY= -20.2004 ZY= -7.5173
XZ= 60.7063 YZ= -6.6847 ZZ= 63.1957
Eigenvalues: -49.0316 43.8979 173.4668
17 C Isotropic = 56.2698 Anisotropy = 178.9870
XX= 124.0050 YX= 45.9962 ZX= 65.3549
XY= 19.5669 YY= 5.4190 ZY= 56.5421
XZ= 55.3286 YZ= 64.7775 ZZ= 39.3855
Eigenvalues: -41.4195 34.6345 175.5945
18 C Isotropic = 54.5235 Anisotropy = 162.5936
XX= 119.4671 YX= 26.3868 ZX= 66.0074
XY= 32.0727 YY= 45.8395 ZY= -0.1373
XZ= 87.3986 YZ= 3.7164 ZZ= -1.7360
Eigenvalues: -40.3906 41.0419 162.9193
19 C Isotropic = 50.2376 Anisotropy = 179.1671
XX= 136.3209 YX= 20.4971 ZX= 50.7214
XY= 21.1754 YY= -11.0287 ZY= 62.9656
XZ= 57.2868 YZ= 64.8432 ZZ= 25.4205
Eigenvalues: -60.7096 41.7400 169.6823
20 C Isotropic = 49.8097 Anisotropy = 181.5589
XX= 110.4232 YX= 36.7851 ZX= 92.2608
XY= 33.8392 YY= 49.3124 ZY= 4.3208
XZ= 94.5690 YZ= 8.2716 ZZ= -10.3066
Eigenvalues: -62.3739 40.9539 170.8489
21 H Isotropic = 24.9581 Anisotropy = 7.9643
XX= 24.7857 YX= -1.8057 ZX= -3.5156
XY= -0.0438 YY= 25.1978 ZY= 4.4375
XZ= -1.6104 YZ= 3.7605 ZZ= 24.8907
Eigenvalues: 20.5346 24.0720 30.2676
22 H Isotropic = 24.3124 Anisotropy = 8.6987
XX= 22.5656 YX= -2.7515 ZX= 0.3540
XY= -1.0777 YY= 28.7010 ZY= -3.3435
XZ= 0.1008 YZ= -2.1263 ZZ= 21.6704
Eigenvalues: 20.6250 22.2005 30.1115
23 H Isotropic = 24.2374 Anisotropy = 4.8584
XX= 23.2075 YX= -1.4548 ZX= -2.1837
XY= -1.3703 YY= 25.6628 ZY= 1.0043
XZ= -1.7721 YZ= 1.5123 ZZ= 23.8419
Eigenvalues: 21.5012 23.7347 27.4763
24 H Isotropic = 24.6394 Anisotropy = 6.1778
XX= 22.1169 YX= -0.8245 ZX= -0.4068
XY= -0.5779 YY= 28.6562 ZY= 0.1977
XZ= -0.3766 YZ= 0.5064 ZZ= 23.1451
Eigenvalues: 21.9377 23.2226 28.7579
25 H Isotropic = 24.7772 Anisotropy = 3.9634
XX= 23.0369 YX= -0.0314 ZX= -2.1032
XY= 0.3852 YY= 25.4974 ZY= -1.4176
XZ= -1.6391 YZ= -0.9426 ZZ= 25.7973
Eigenvalues: 22.0479 24.8642 27.4195
26 H Isotropic = 25.2954 Anisotropy = 6.0884
XX= 28.9881 YX= 0.2251 ZX= -1.1855
XY= -0.4050 YY= 24.3656 ZY= -1.9282

```
  XZ=   -1.9196   YZ=   -1.0197   ZZ=   22.5326
  Eigenvalues:   21.4489   25.0831   29.3544
27  C   Isotropic =   39.0205   Anisotropy =  192.2944
  XX=  -41.3523   YX=   51.7331   ZX=    9.0898
  XY=   53.3723   YY=  115.8269   ZY=   65.8476
  XZ=    8.4488   YZ=   67.4336   ZZ=   42.5870
  Eigenvalues:  -58.8387    8.6835  167.2168
28  C   Isotropic =   54.0594   Anisotropy =  178.2125
  XX=  -31.8658   YX=   57.6237   ZX=    2.1189
  XY=   58.4604   YY=  126.5945   ZY=   55.1068
  XZ=    2.4067   YZ=   55.7287   ZZ=   67.4494
  Eigenvalues:  -52.9941   42.3045  172.8677
29  C   Isotropic =   51.1169   Anisotropy =  164.7906
  XX=   45.1010   YX=   35.0666   ZX=   -2.0987
  XY=   30.8980   YY=  109.2734   ZY=   80.1925
  XZ=   -9.6196   YZ=   88.5842   ZZ=   -1.0236
  Eigenvalues:  -51.3536   43.7270  160.9773
30  C   Isotropic =   50.4959   Anisotropy =  178.9081
  XX=    5.2174   YX=   19.5589   ZX=   52.5681
  XY=   20.6955   YY=  131.0046   ZY=   61.1134
  XZ=   65.9769   YZ=   63.4349   ZZ=   15.2657
  Eigenvalues:  -54.0124   35.7321  169.7679
31  C   Isotropic =   50.1836   Anisotropy =  182.8862
  XX=   44.1703   YX=   39.9783   ZX=   -4.3126
  XY=   40.7336   YY=  110.1574   ZY=   93.3437
  XZ=   -3.7690   YZ=   95.2257   ZZ=   -3.7768
  Eigenvalues:  -62.3321   40.7752  172.1078
32  C   Isotropic =   50.2598   Anisotropy =  180.9752
  XX=   -0.3656   YX=   15.2075   ZX=   63.4945
  XY=   13.4757   YY=  133.8885   ZY=   61.3044
  XZ=   63.9619   YZ=   64.4720   ZZ=   17.2564
  Eigenvalues:  -61.3245   41.1939  170.9099
33  H   Isotropic =   24.4248   Anisotropy =    7.7358
  XX=   28.6237   YX=    0.2949   ZX=   -3.0049
  XY=   -0.9973   YY=   22.4548   ZY=   -0.3763
  XZ=   -2.3027   YZ=   -0.5541   ZZ=   22.1958
  Eigenvalues:   21.0246   22.6677   29.5820
34  H   Isotropic =   24.1495   Anisotropy =    8.6185
  XX=   26.4036   YX=   -0.1368   ZX=    5.2782
  XY=   -1.1139   YY=   22.0857   ZY=   -0.8830
  XZ=    3.5824   YZ=   -0.6424   ZZ=   23.9592
  Eigenvalues:   20.5494   22.0039   29.8952
35  H   Isotropic =   24.5656   Anisotropy =    6.0835
  XX=   28.6036   YX=    0.1121   ZX=   -0.2364
  XY=   -0.1994   YY=   21.8377   ZY=   -0.2304
  XZ=   -0.3761   YZ=   -0.0100   ZZ=   23.2554
  Eigenvalues:   21.8269   23.2485   28.6213
36  H   Isotropic =   24.3208   Anisotropy =    4.8273
  XX=   26.1266   YX=   -1.1436   ZX=    1.0719
  XY=   -1.3706   YY=   23.2543   ZY=   -2.0572
  XZ=    1.4607   YZ=   -1.6666   ZZ=   23.5815
  Eigenvalues:   21.5474   23.8760   27.5390
37  H   Isotropic =   24.6590   Anisotropy =    4.2207
  XX=   25.0478   YX=    0.6085   ZX=   -1.0062
  XY=    0.4417   YY=   22.8922   ZY=   -2.1387
  XZ=   -0.7739   YZ=   -1.9276   ZZ=   26.0369
  Eigenvalues:   21.8922   24.6119   27.4728
 Current density tensor (au):
  XX=    0.0520   YX=    0.0047   ZX=   -0.0532
  XY=    0.0325   YY=    0.0156   ZY=   -0.0364
  XZ=   -0.0876   YZ=   -0.0125   ZZ=   -0.0588
 End of Minotr Frequency-dependent properties file   721 does not exist.

 ******************************************************************

        Population analysis using the SCF density.

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Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(

Alpha virt. eigenvalues --	0.06079	0.06435	0.06658	0.07194	0.07586
Alpha virt. eigenvalues --	0.07773	0.08841	0.09058	0.09375	0.09522
Alpha virt. eigenvalues --	0.10030	0.10323	0.10622	0.10925	0.11084
Alpha virt. eigenvalues --	0.11254	0.11430	0.11663	0.11872	0.11985
Alpha virt. eigenvalues --	0.12232	0.12328	0.12598	0.12892	0.13017
Alpha virt. eigenvalues --	0.13088	0.13263	0.13635	0.13710	0.14147
Alpha virt. eigenvalues --	0.14285	0.14453	0.14609	0.14928	0.15108
Alpha virt. eigenvalues --	0.15342	0.15590	0.16105	0.16744	0.16900
Alpha virt. eigenvalues --	0.17325	0.17512	0.17739	0.18060	0.18399
Alpha virt. eigenvalues --	0.18569	0.18600	0.18809	0.18989	0.19682
Alpha virt. eigenvalues --	0.20044	0.20362	0.20998	0.21115	0.21517
Alpha virt. eigenvalues --	0.21624	0.21812	0.22059	0.22583	0.22728
Alpha virt. eigenvalues --	0.23147	0.23454	0.23986	0.24290	0.24838
Alpha virt. eigenvalues --	0.25066	0.25643	0.26039	0.26105	0.26300
Alpha virt. eigenvalues --	0.26785	0.27045	0.27154	0.27430	0.27931
Alpha virt. eigenvalues --	0.28105	0.28314	0.28722	0.29087	0.29424
Alpha virt. eigenvalues --	0.29601	0.30336	0.30445	0.30619	0.30879
Alpha virt. eigenvalues --	0.31286	0.31431	0.31673	0.31967	0.32069
Alpha virt. eigenvalues --	0.32625	0.32814	0.33106	0.33344	0.33748
Alpha virt. eigenvalues --	0.34196	0.34325	0.34665	0.35082	0.35615
Alpha virt. eigenvalues --	0.36100	0.36475	0.36993	0.37797	0.37931
Alpha virt. eigenvalues --	0.38294	0.38516	0.39360	0.39598	0.40435
Alpha virt. eigenvalues --	0.40484	0.41451	0.42587	0.43413	0.44700
Alpha virt. eigenvalues --	0.45906	0.49708	0.50668	0.51143	0.51923
Alpha virt. eigenvalues --	0.53125	0.54133	0.54472	0.55122	0.55653
Alpha virt. eigenvalues --	0.55792	0.56428	0.56711	0.57124	0.57499
Alpha virt. eigenvalues --	0.58282	0.58884	0.59170	0.59970	0.60204
Alpha virt. eigenvalues --	0.61240	0.62175	0.62314	0.62483	0.63187
Alpha virt. eigenvalues --	0.64046	0.64672	0.64724	0.65197	0.66101
Alpha virt. eigenvalues --	0.66696	0.67261	0.67608	0.67893	0.68467
Alpha virt. eigenvalues --	0.69369	0.69747	0.70803	0.71402	0.71474
Alpha virt. eigenvalues --	0.71934	0.72300	0.72766	0.73159	0.73383
Alpha virt. eigenvalues --	0.74228	0.75001	0.75159	0.75723	0.76224
Alpha virt. eigenvalues --	0.76724	0.77035	0.77728	0.78242	0.78690
Alpha virt. eigenvalues --	0.79303	0.80230	0.80823	0.81060	0.81268
Alpha virt. eigenvalues --	0.82409	0.82815	0.83370	0.84328	0.85104
Alpha virt. eigenvalues --	0.85465	0.86379	0.87003	0.87397	0.87581
Alpha virt. eigenvalues --	0.88091	0.88228	0.89125	0.89957	0.90491
Alpha virt. eigenvalues --	0.91861	0.92577	0.92996	0.93292	0.94399
Alpha virt. eigenvalues --	0.95381	0.96720	0.97085	0.98210	0.98798
Alpha virt. eigenvalues --	1.00168	1.00426	1.01285	1.01752	1.02866
Alpha virt. eigenvalues --	1.04639	1.05342	1.06019	1.06585	1.06851
Alpha virt. eigenvalues --	1.07523	1.08509	1.08913	1.10080	1.10432
Alpha virt. eigenvalues --	1.11630	1.12260	1.13705	1.14811	1.15314
Alpha virt. eigenvalues --	1.16228	1.17363	1.19212	1.20028	1.22493
Alpha virt. eigenvalues --	1.24929	1.27882	1.30600	1.32436	1.33208
Alpha virt. eigenvalues --	1.33440	1.35989	1.37209	1.39223	1.42106
Alpha virt. eigenvalues --	1.44235	1.46189	1.47826	1.49561	1.50202
Alpha virt. eigenvalues --	1.51380	1.51959	1.53215	1.53441	1.54062
Alpha virt. eigenvalues --	1.55208	1.55943	1.56594	1.56890	1.57268
Alpha virt. eigenvalues --	1.57642	1.58172	1.58571	1.58964	1.59903
Alpha virt. eigenvalues --	1.60829	1.61412	1.62513	1.64425	1.64851
Alpha virt. eigenvalues --	1.66547	1.67509	1.67632	1.67806	1.69027
Alpha virt. eigenvalues --	1.69108	1.70094	1.70732	1.70958	1.72659
Alpha virt. eigenvalues --	1.74699	1.75181	1.75424	1.76169	1.77778
Alpha virt. eigenvalues --	1.77919	1.78968	1.79974	1.81326	1.81922
Alpha virt. eigenvalues --	1.82382	1.83725	1.84399	1.85817	1.86698
Alpha virt. eigenvalues --	1.87574	1.87691	1.88564	1.90130	1.90399
Alpha virt. eigenvalues --	1.91390	1.92394	1.93437	1.94222	1.94332
Alpha virt. eigenvalues --	1.94663	1.95447	1.95869	1.96882	1.97159
Alpha virt. eigenvalues --	1.97730	1.98353	1.99522	2.00062	2.00337
Alpha virt. eigenvalues --	2.01290	2.01836	2.03669	2.04091	2.05285
Alpha virt. eigenvalues --	2.05959	2.07590	2.08459	2.10029	2.10689
Alpha virt. eigenvalues --	2.11803	2.13934	2.14733	2.16685	2.17991
Alpha virt. eigenvalues --	2.19843	2.21310	2.23105	2.24204	2.27062
Alpha virt. eigenvalues --	2.28704	2.30159	2.32479	2.33880	2.34435
Alpha virt. eigenvalues --	2.35449	2.36747	2.38343	2.40133	2.42921
Alpha virt. eigenvalues --	2.44413	2.46134	2.46852	2.47685	2.48018

Alpha virt. eigenvalues -- 2.48584 2.49352 2.50917 2.53746 2.55489
Alpha virt. eigenvalues -- 2.55771 2.59037 2.60582 2.61411 2.63931
Alpha virt. eigenvalues -- 2.64833 2.65666 2.66289 2.69053 2.69280
Alpha virt. eigenvalues -- 2.70947 2.71616 2.71901 2.73579 2.74214
Alpha virt. eigenvalues -- 2.74822 2.75621 2.76324 2.76908 2.77389
Alpha virt. eigenvalues -- 2.78127 2.78788 2.79312 2.79907 2.80685
Alpha virt. eigenvalues -- 2.81678 2.82550 2.84230 2.84483 2.85127
Alpha virt. eigenvalues -- 2.85848 2.86121 2.87598 2.88547 2.89204
Alpha virt. eigenvalues -- 2.90190 2.92147 2.92770 2.93589 2.95224
Alpha virt. eigenvalues -- 2.95533 2.95993 2.97032 2.97526 2.99628
Alpha virt. eigenvalues -- 2.99839 3.01850 3.03719 3.06803 3.07524
Alpha virt. eigenvalues -- 3.08943 3.11678 3.12713 3.13712 3.14076
Alpha virt. eigenvalues -- 3.18612 3.20165 3.21307 3.21575 3.30600
Alpha virt. eigenvalues -- 3.31329 3.35008 3.35904 3.38645 3.40522
Alpha virt. eigenvalues -- 3.41405 3.42961 3.49558 3.53036 3.53388
Alpha virt. eigenvalues -- 3.56824 3.58286 3.61428 3.62405 3.63574
Alpha virt. eigenvalues -- 3.64441 3.65583 3.74694 3.77734 3.88490
Alpha virt. eigenvalues -- 3.92781 4.00228 4.01069 4.04838 4.04883
Alpha virt. eigenvalues -- 4.08830 4.11113 4.14505 4.16221 4.16419
Alpha virt. eigenvalues -- 4.17596 4.19102 4.21959 4.22616 4.27901
Alpha virt. eigenvalues -- 4.34481 4.45475 4.84868 4.85654 4.89521
Alpha virt. eigenvalues -- 5.15170 23.64928 23.67058 23.78280 23.85123
Alpha virt. eigenvalues -- 23.87164 23.96441 23.98058 23.98524 23.99429
Alpha virt. eigenvalues -- 24.00085 24.02493 24.07841 24.08273 24.09653
Alpha virt. eigenvalues -- 24.10266 24.19494 24.19582 24.25757 24.26336
Alpha virt. eigenvalues -- 35.65546

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	17.019931	0.758335	-3.748012	-0.112955	2.960634	0.065740
2	H	0.758335	0.509262	-0.149372	-0.007490	0.048380	0.002453
3	C	-3.748012	-0.149372	8.583793	0.482152	-2.803327	-0.113655
4	H	-0.112955	-0.007490	0.482152	0.504224	-0.084681	-0.008875
5	C	2.960634	0.048380	-2.803327	-0.084681	10.715681	0.560548
6	H	0.065740	0.002453	-0.113655	-0.008875	0.560548	0.505519
7	C	-3.873929	-0.021405	3.310779	0.063380	-6.056622	-0.227145
8	H	-0.208795	-0.000697	0.152978	0.002898	-0.473924	-0.014479
9	C	0.658232	0.019786	-0.614706	0.024128	1.413344	0.060845
10	H	0.005031	-0.003365	0.007732	0.003832	0.021939	0.000459
11	H	-0.123268	-0.013775	0.012286	-0.001130	0.082556	0.000372
12	N	-0.784855	0.030028	0.121248	0.002392	0.067674	0.009414
13	C	-4.200281	-0.165822	0.857371	-0.011523	-0.117183	0.006914
14	C	-0.674708	-0.099323	0.208259	0.004562	-0.145546	-0.001932
15	C	1.316929	-0.000765	-0.733889	-0.024699	1.132674	0.013917
16	C	0.109297	0.003327	-0.050403	-0.000919	0.102409	0.014878
17	C	-0.614279	0.002933	0.455780	0.007547	-0.644502	-0.023593
18	C	0.370167	0.010304	-0.281735	-0.004101	0.547318	0.031110
19	C	-0.162944	-0.004049	0.147587	0.003075	-0.318576	-0.014037
20	C	-0.068967	0.004001	-0.012316	-0.001059	-0.018936	-0.005427
21	H	0.015108	-0.002016	-0.006454	-0.001787	-0.000007	-0.000232
22	H	0.066904	0.001250	-0.045899	-0.000876	0.115751	0.004935
23	H	-0.004696	-0.000152	0.004106	0.000070	-0.008550	-0.001082
24	H	-0.008203	-0.000204	0.002147	0.000108	-0.003780	-0.000688
25	H	0.002660	0.000061	-0.002160	-0.000063	0.003199	0.000332
26	H	-0.384608	-0.015707	0.070738	0.000649	-0.053093	-0.001193
27	C	-2.176255	-0.143557	0.360422	0.000292	-0.262781	-0.001678
28	C	0.001247	-0.000859	-0.007515	-0.000129	0.014854	0.000285
29	C	0.685140	0.017793	-0.215250	-0.002983	0.185749	0.004496
30	C	-1.223538	-0.040382	0.249259	0.004288	-0.246205	-0.007189
31	C	0.005822	0.000116	0.020654	-0.000009	-0.028970	-0.000786
32	C	0.053361	0.000420	-0.011643	0.000582	-0.002650	-0.000140
33	H	-0.004168	-0.000658	0.001152	-0.000015	0.002005	0.000040
34	H	-0.055500	-0.002760	0.022200	0.000604	-0.029988	-0.000739
35	H	-0.001310	-0.000013	0.000232	-0.000011	-0.000553	0.000003
36	H	-0.001098	-0.000010	0.000076	-0.000013	-0.000383	0.000004
37	H	-0.000737	-0.000034	-0.000001	0.000002	0.000128	0.000003

		7	8	9	10	11	12
1	C	-3.873929	-0.208795	0.658232	0.005031	-0.123268	-0.784855
2	H	-0.021405	-0.000697	0.019786	-0.003365	-0.013775	0.030028

3	C	3.310779	0.152978	-0.614706	0.007732	0.012286	0.121248
4	H	0.063380	0.002898	0.024128	0.003832	-0.001130	0.002392
5	C	-6.056622	-0.473924	1.413344	0.021939	0.082556	0.067674
6	H	-0.227145	-0.014479	0.060845	0.000459	0.000372	0.009414
7	C	15.419782	1.101633	-2.207847	-0.062436	-0.139431	-0.322493
8	H	1.101633	0.592427	-0.171689	-0.009025	-0.018303	-0.047322
9	C	-2.207847	-0.171689	7.664733	0.398849	0.404026	0.377661
10	H	-0.062436	-0.009025	0.398849	0.512588	-0.018535	0.023409
11	H	-0.139431	-0.018303	0.404026	-0.018535	0.556859	-0.021441
12	N	-0.322493	-0.047322	0.377661	0.023409	-0.021441	8.811079
13	C	0.303640	-0.002083	-0.168917	-0.038704	0.065391	-0.043889
14	C	0.087918	-0.006878	-0.328611	-0.009864	0.021952	-0.306940
15	C	-2.801544	-0.278925	-0.035366	-0.001932	0.039538	-1.837397
16	C	-0.077510	-0.011519	0.058927	0.000724	-0.000945	0.067854
17	C	1.081883	0.096873	-0.099801	0.003321	-0.017807	0.135890
18	C	-0.711292	-0.074755	0.138483	0.002645	0.003089	-0.016721
19	C	0.432325	0.080049	-0.017189	0.002804	-0.005750	0.206559
20	C	0.275470	0.049954	0.000472	0.001087	-0.002744	0.625411
21	H	0.010419	-0.001385	-0.024108	-0.000642	0.000952	-0.167077
22	H	-0.180669	-0.040292	0.026171	0.000369	0.001841	-0.026264
23	H	0.009132	0.001852	-0.004264	-0.000014	0.000075	-0.010039
24	H	0.003567	0.000476	-0.002196	-0.000045	0.000034	-0.001025
25	H	-0.003510	-0.000870	0.001089	-0.000005	0.000035	0.001091
26	H	0.095979	0.004434	-0.017336	-0.002051	0.001052	0.036626
27	C	0.143107	-0.027893	-0.739790	-0.025853	0.071856	-0.641105
28	C	-0.030666	-0.001505	0.002557	-0.000159	0.000291	-0.033291
29	C	-0.282566	-0.021898	-0.022932	-0.000217	0.017786	-0.381582
30	C	0.209790	0.039395	0.022135	0.002019	-0.036431	0.664728
31	C	0.036719	0.004639	0.041695	0.001975	-0.006950	0.058968
32	C	-0.007435	-0.000391	-0.009860	0.000128	-0.000911	-0.037020
33	H	-0.008567	-0.000386	0.002509	0.000014	0.000048	0.004057
34	H	0.043050	0.003445	-0.039050	-0.000503	-0.002673	-0.017406
35	H	0.001603	0.000081	0.000742	0.000017	0.000085	0.001672
36	H	0.000837	0.000031	-0.000313	-0.000003	0.000014	-0.000165
37	H	-0.000309	-0.000030	-0.000155	-0.000009	0.000023	0.000014

		13	14	15	16	17	18
1	C	-4.200281	-0.674708	1.316929	0.109297	-0.614279	0.370167
2	H	-0.165822	-0.099323	-0.000765	0.003327	0.002933	0.010304
3	C	0.857371	0.208259	-0.733889	-0.050403	0.455780	-0.281735
4	H	-0.011523	0.004562	-0.024699	-0.000919	0.007547	-0.004101
5	C	-0.117183	-0.145546	1.132674	0.102409	-0.644502	0.547318
6	H	0.006914	-0.001932	0.013917	0.014878	-0.023593	0.031110
7	C	0.303640	0.087918	-2.801544	-0.077510	1.081883	-0.711292
8	H	-0.002083	-0.006878	-0.278925	-0.011519	0.096873	-0.074755
9	C	-0.168917	-0.328611	-0.035366	0.058927	-0.099801	0.138483
10	H	-0.038704	-0.009864	-0.001932	0.000724	0.003321	0.002645
11	H	0.065391	0.021952	0.039538	-0.000945	-0.017807	0.003089
12	N	-0.043889	-0.306940	-1.837397	0.067854	0.135890	-0.016721
13	C	15.040772	1.931736	0.146745	0.105979	-0.049426	-0.277803
14	C	1.931736	8.616938	-0.345166	0.017223	-0.081158	0.010750
15	C	0.146745	-0.345166	13.096164	0.894034	-0.126917	-0.713526
16	C	0.105979	0.017223	0.894034	7.187706	-1.082914	-0.702904
17	C	-0.049426	-0.081158	-0.126917	-1.082914	7.732568	-0.254046
18	C	-0.277803	0.010750	-0.713526	-0.702904	-0.254046	7.452174
19	C	-0.125238	0.016780	-1.291488	-0.234714	0.363039	-0.521675
20	C	-0.632152	0.031489	-2.257990	-0.108858	-0.861482	0.484002
21	H	0.037803	0.015521	0.199544	-0.017534	0.456400	-0.014446
22	H	0.016962	-0.011329	0.084640	0.035858	-0.033108	0.508142
23	H	0.001182	0.000324	0.021565	-0.084744	0.058250	-0.130079
24	H	-0.002511	0.000464	-0.009842	-0.095055	-0.060298	0.023135
25	H	0.004674	0.000161	0.052330	0.500385	-0.028938	-0.038192
26	H	-0.054867	0.314210	-0.033052	-0.006553	0.025812	-0.010475
27	C	-4.298355	-1.400516	-0.164923	-0.010150	-0.604358	0.340479
28	C	0.107887	0.085427	0.140268	0.020805	-0.053143	-0.018570
29	C	-0.384003	0.180632	0.671582	0.032721	-0.428746	0.230457
30	C	-1.560875	-1.421160	-1.255077	-0.305331	0.508544	-0.351507
31	C	0.197271	0.159406	0.014658	0.020331	0.145317	-0.010091
32	C	-0.217185	-0.363389	0.027952	-0.055617	0.052986	-0.023850

33	H	0.040492	0.053272	-0.001749	0.003235	-0.005792	0.000737
34	H	0.025518	-0.002415	-0.014304	-0.007987	0.015286	-0.022861
35	H	-0.004105	0.006586	0.000253	0.003230	0.000316	0.001916
36	H	-0.008357	-0.006734	0.000826	-0.000482	0.002708	-0.000452
37	H	-0.002325	0.001712	0.002494	0.000545	-0.001809	-0.000188

		19	20	21	22	23	24
1	C	-0.162944	-0.068967	0.015108	0.066904	-0.004696	-0.008203
2	H	-0.004049	0.004001	-0.002016	0.001250	-0.000152	-0.000204
3	C	0.147587	-0.012316	-0.006454	-0.045899	0.004106	0.002147
4	H	0.003075	-0.001059	-0.001787	-0.000876	0.000070	0.000108
5	C	-0.318576	-0.018936	-0.000007	0.115751	-0.008550	-0.003780
6	H	-0.014037	-0.005427	-0.000232	0.004935	-0.001082	-0.000688
7	C	0.432325	0.275470	0.010419	-0.180669	0.009132	0.003567
8	H	0.080049	0.049954	-0.001385	-0.040292	0.001852	0.000476
9	C	-0.017189	0.000472	-0.024108	0.026171	-0.004264	-0.002196
10	H	0.002804	0.001087	-0.000642	0.000369	-0.000014	-0.000045
11	H	-0.005750	-0.002744	0.000952	0.001841	0.000075	0.000034
12	N	0.206559	0.625411	-0.167077	-0.026264	-0.010039	-0.001025
13	C	-0.125238	-0.632152	0.037803	0.016962	0.001182	-0.002511
14	C	0.016780	0.031489	0.015521	-0.011329	0.000324	0.000464
15	C	-1.291488	-2.257990	0.199544	0.084640	0.021565	-0.009842
16	C	-0.234714	-0.108858	-0.017534	0.035858	-0.084744	-0.095055
17	C	0.363039	-0.861482	0.456400	-0.033108	0.058250	-0.060298
18	C	-0.521675	0.484002	-0.014446	0.508142	-0.130079	0.023135
19	C	7.136974	0.224013	0.000434	-0.185754	0.452454	0.022869
20	C	0.224013	8.554700	-0.292991	-0.032911	0.003445	0.421419
21	H	0.000434	-0.292991	0.552238	-0.000371	0.001256	-0.012316
22	H	-0.185754	-0.032911	-0.000371	0.588812	-0.020625	0.000164
23	H	0.452454	0.003445	0.001256	-0.020625	0.549442	0.001081
24	H	0.022869	0.421419	-0.012316	0.000164	0.001081	0.542879
25	H	-0.088256	-0.074422	0.000369	0.000622	-0.017878	-0.018606
26	H	0.005818	0.002601	0.002666	-0.001419	0.000157	0.000501
27	C	-0.159054	-0.237491	0.095362	0.020165	-0.002021	0.000508
28	C	-0.027755	-0.084752	0.009925	0.003283	-0.000254	-0.001807
29	C	-0.121298	-0.313138	0.066874	0.016371	-0.001811	-0.002856
30	C	0.490417	0.642735	-0.077587	-0.060454	0.007144	0.009796
31	C	-0.027254	0.166749	-0.036452	0.003582	-0.001571	0.000333
32	C	0.050688	-0.089734	0.021322	-0.002774	0.001294	0.003813
33	H	-0.002090	0.009411	-0.003178	0.000236	-0.000067	-0.000449
34	H	0.025923	-0.001889	0.001226	-0.005380	0.000848	0.000905
35	H	-0.002615	0.002754	0.000322	0.000049	-0.000339	-0.000339
36	H	0.000489	-0.002957	0.000211	-0.000064	0.000007	-0.000163
37	H	-0.000626	-0.001190	-0.000147	0.000014	0.000021	-0.000036

		25	26	27	28	29	30
1	C	0.002660	-0.384608	-2.176255	0.001247	0.685140	-1.223538
2	H	0.000061	-0.015707	-0.143557	-0.000859	0.017793	-0.040382
3	C	-0.002160	0.070738	0.360422	-0.007515	-0.215250	0.249259
4	H	-0.000063	0.000649	0.000292	-0.000129	-0.002983	0.004288
5	C	0.003199	-0.053093	-0.262781	0.014854	0.185749	-0.246205
6	H	0.000332	-0.001193	-0.001678	0.000285	0.004496	-0.007189
7	C	-0.003510	0.095979	0.143107	-0.030666	-0.282566	0.209790
8	H	-0.000870	0.004434	-0.027893	-0.001505	-0.021898	0.039395
9	C	0.001089	-0.017336	-0.739790	0.002557	-0.022932	0.022135
10	H	-0.000005	-0.002051	-0.025853	-0.000159	-0.000217	0.002019
11	H	0.000035	0.001052	0.071856	0.000291	0.017786	-0.036431
12	N	0.001091	0.036626	-0.641105	-0.033291	-0.381582	0.664728
13	C	0.004674	-0.054867	-4.298355	0.107887	-0.384003	-1.560875
14	C	0.000161	0.314210	-1.400516	0.085427	0.180632	-1.421160
15	C	0.052330	-0.033052	-0.164923	0.140268	0.671582	-1.255077
16	C	0.500385	-0.006553	-0.010150	0.020805	0.032721	-0.305331
17	C	-0.028938	0.025812	-0.604358	-0.053143	-0.428746	0.508544
18	C	-0.038192	-0.010475	0.340479	-0.018570	0.230457	-0.351507
19	C	-0.088256	0.005818	-0.159054	-0.027755	-0.121298	0.490417
20	C	-0.074422	0.002601	-0.237491	-0.084752	-0.313138	0.642735
21	H	0.000369	0.002666	0.095362	0.009925	0.066874	-0.077587
22	H	0.000622	-0.001419	0.020165	0.003283	0.016371	-0.060454
23	H	-0.017878	0.000157	-0.002021	-0.000254	-0.001811	0.007144
24	H	-0.018606	0.000501	0.000508	-0.001807	-0.002856	0.009796

25	H	0.554183	-0.000145	0.002637	0.001064	0.002658	-0.009538
26	H	-0.000145	0.588284	0.188152	-0.013624	-0.112100	0.175953
27	C	0.002637	0.188152	18.101189	0.251196	-0.266423	-0.977164
28	C	0.001064	-0.013624	0.251196	6.272467	-0.310042	-0.560746
29	C	0.002658	-0.112100	-0.266423	-0.310042	12.454444	-6.094765
30	C	-0.009538	0.175953	-0.977164	-0.560746	-6.094765	16.063156
31	C	0.000345	-0.010290	-1.806603	0.068984	0.355101	-0.009115
32	C	-0.001544	0.024883	-0.734415	0.159751	-0.248914	1.108633
33	H	0.000065	-0.003021	-0.097632	0.002240	0.395367	-0.005858
34	H	-0.000498	0.004486	-0.046089	-0.017571	-0.115590	0.625610
35	H	0.000122	0.000415	0.045357	-0.067571	0.044537	-0.155480
36	H	0.000027	0.001040	-0.001670	-0.071057	-0.105500	0.026208
37	H	-0.000034	-0.000019	0.043566	0.472293	-0.020007	-0.002966

		31	32	33	34	35	36
1	C	0.005822	0.053361	-0.004168	-0.055500	-0.001310	-0.001098
2	H	0.000116	0.000420	-0.000658	-0.002760	-0.000013	-0.000010
3	C	0.020654	-0.011643	0.001152	0.022200	0.000232	0.000076
4	H	-0.000009	0.000582	-0.000015	0.000604	-0.000011	-0.000013
5	C	-0.028970	-0.002650	0.002005	-0.029988	-0.000553	-0.000383
6	H	-0.000786	-0.000140	0.000040	-0.000739	0.000003	0.000004
7	C	0.036719	-0.007435	-0.008567	0.043050	0.001603	0.000837
8	H	0.004639	-0.000391	-0.000386	0.003445	0.000081	0.000031
9	C	0.041695	-0.009860	0.002509	-0.039050	0.000742	-0.000313
10	H	0.001975	0.000128	0.000014	-0.000503	0.000017	-0.000003
11	H	-0.006950	-0.000911	0.000048	-0.002673	0.000085	0.000014
12	N	0.058968	-0.037020	0.004057	-0.017406	0.001672	-0.000165
13	C	0.197271	-0.217185	0.040492	0.025518	-0.004105	-0.008357
14	C	0.159406	-0.363389	0.053272	-0.002415	0.006586	-0.006734
15	C	0.014658	0.027952	-0.001749	-0.014304	0.000253	0.000826
16	C	0.020331	-0.055617	0.003235	-0.007987	0.003230	-0.000482
17	C	0.145317	0.052986	-0.005792	0.015286	0.000316	0.002708
18	C	-0.010091	-0.023850	0.000737	-0.022861	0.001916	-0.000452
19	C	-0.027254	0.050688	-0.002090	0.025923	-0.002615	0.000489
20	C	0.166749	-0.089734	0.009411	-0.001889	0.002754	-0.002957
21	H	-0.036452	0.021322	-0.003178	0.001226	0.000322	0.000211
22	H	0.003582	-0.002774	0.000236	-0.005380	0.000049	-0.000064
23	H	-0.001571	0.001294	-0.000067	0.000848	-0.000339	0.000007
24	H	0.000333	0.003813	-0.000449	0.000905	-0.000339	-0.000163
25	H	0.000345	-0.001544	0.000065	-0.000498	0.000122	0.000027
26	H	-0.010290	0.024883	-0.003021	0.004486	0.000415	0.001040
27	C	-1.806603	-0.734415	-0.097632	-0.046089	0.045357	-0.001670
28	C	0.068984	0.159751	0.002240	-0.017571	-0.067571	-0.071057
29	C	0.355101	-0.248914	0.395367	-0.115590	0.044537	-0.105500
30	C	-0.009115	1.108633	-0.005858	0.625610	-0.155480	0.026208
31	C	7.110113	-0.309694	0.036691	-0.140410	0.436431	0.007774
32	C	-0.309694	6.654095	-0.123659	0.055424	-0.006485	0.472006
33	H	0.036691	-0.123659	0.553279	-0.003851	0.001114	-0.018511
34	H	-0.140410	0.055424	-0.003851	0.558508	-0.018077	0.001780
35	H	0.436431	-0.006485	0.001114	-0.018077	0.550392	-0.000395
36	H	0.007774	0.472006	-0.018511	0.001780	-0.000395	0.557182
37	H	-0.085940	-0.084479	0.000071	-0.000139	-0.017936	-0.019482

		37
1	C	-0.000737
2	H	-0.000034
3	C	-0.000001
4	H	0.000002
5	C	0.000128
6	H	0.000003
7	C	-0.000309
8	H	-0.000030
9	C	-0.000155
10	H	-0.000009
11	H	0.000023
12	N	0.000014
13	C	-0.002325
14	C	0.001712
15	C	0.002494
16	C	0.000545

17	C	-0.001809
18	C	-0.000188
19	C	-0.000626
20	C	-0.001190
21	H	-0.000147
22	H	0.000014
23	H	0.000021
24	H	-0.000036
25	H	-0.000034
26	H	-0.000019
27	C	0.043566
28	C	0.472293
29	C	-0.020007
30	C	-0.002966
31	C	-0.085940
32	C	-0.084479
33	H	0.000071
34	H	-0.000139
35	H	-0.017936
36	H	-0.019482
37	H	0.560601

Mulliken atomic charges:

		1
1	C	0.338565
2	H	0.263966
3	C	-0.274612
4	H	0.158534
5	C	-0.674588
6	H	0.140602
7	C	0.384361
8	H	0.281881
9	C	-0.812256
10	H	0.184420
11	H	0.129935
12	N	0.450255
13	C	-0.524733
14	C	-0.559653
15	C	0.072437
16	C	-0.325329
17	C	-0.073339
18	C	0.024362
19	C	-0.351933
20	C	-0.398305
21	H	0.170780
22	H	0.152067
23	H	0.174479
24	H	0.186222
25	H	0.156550
26	H	0.175096
27	C	1.161487
28	C	-0.313809
29	C	0.090913
30	C	-0.448441
31	C	-0.419540
32	C	-0.355550
33	H	0.173615
34	H	0.160866
35	H	0.176997
36	H	0.166588
37	H	0.157110

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

		1
1	C	0.602532
2	H	0.000000
3	C	-0.116078
4	H	0.000000
5	C	-0.533985

```
     6  H    0.000000
     7  C    0.666241
     8  H    0.000000
     9  C   -0.497901
    10  H    0.000000
    11  H    0.000000
    12  N    0.450255
    13  C   -0.524733
    14  C   -0.384557
    15  C    0.072437
    16  C   -0.168779
    17  C    0.097442
    18  C    0.176428
    19  C   -0.177453
    20  C   -0.212083
    21  H    0.000000
    22  H    0.000000
    23  H    0.000000
    24  H    0.000000
    25  H    0.000000
    26  H    0.000000
    27  C    1.161487
    28  C   -0.156700
    29  C    0.264529
    30  C   -0.287575
    31  C   -0.242543
    32  C   -0.188962
    33  H    0.000000
    34  H    0.000000
    35  H    0.000000
    36  H    0.000000
    37  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  5063.7726
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     1.6244    Y=     0.0706    Z=     0.0680  Tot=     1.6274
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=  -113.8254   YY=  -114.6456   ZZ=  -113.4853
  XY=    -4.1173   XZ=    -4.1434   YZ=    -4.8163
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=     0.1600   YY=    -0.6602   ZZ=     0.5002
  XY=    -4.1173   XZ=    -4.1434   YZ=    -4.8163
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=    -5.3191  YYY=    12.5244  ZZZ=    -0.2174  XYY=    11.3498
 XXY=     4.6662  XXZ=     1.3634  XZZ=     1.2016  YZZ=     3.5818
 YYZ=     4.3996  XYZ=     0.9218
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -3868.4285 YYYY= -2362.6193 ZZZZ=  -732.8523 XXXY=   -21.4948
XXXZ=   -39.9035 YYYX=   -86.0844 YYYZ=   -43.9151 ZZZX=   -11.2403
ZZZY=   -20.8787 XXYY= -1114.5171 XXZZ=  -747.5266 YYZZ=  -521.2816
XXYZ=   -38.7879 YYXZ=   -39.7438 ZZXY=   -12.3244
N-N= 1.462633774612D+03 E-N=-4.756467768539D+03  KE= 7.854947475662D+02
1|1|UNPC-UNK|SP|RB3LYP|6-311++G(d,p)|C19H17N1|PCUSER|17-Nov-2011|0||#
NMR=ALL B3LYP/6-311++G(D,P) GEOM=CONNECTIVITY||Title Card Required||0,
1|C|H,1,1.0893902|C,1,1.51799177,2,116.3532174|H,3,1.0785736,1,126.030
8167,2,-25.5095755,0|C,3,1.34651885,1,106.62769277,2,159.34389535,0|H,
5,1.07742192,3,127.23746305,1,175.33580457,0|C,5,1.52255476,3,107.5182
3942,1,-0.71372017,0|H,7,1.09181454,5,116.96716519,3,-157.4694676,0|C,
1,1.53811248,3,98.35989637,5,36.2636352,0|H,9,1.09744203,1,113.7960627
5,3,63.09940722,0|H,9,1.0975746,1,113.19364727,3,-171.63943436,0|N,7,1
.49377676,5,107.70215006,3,67.53940134,0|C,12,1.41174962,7,106.8993736
6,5,-66.09242128,0|C,13,1.34360001,12,133.23542602,7,-175.41009221,0|C
,12,1.41194795,7,114.45137679,5,80.18920143,0|C,15,2.82356123,12,178.4
1962319,7,57.18048919,0|C,15,1.40210556,12,122.72009446,7,-117.7534378
1,0|C,15,1.40492028,12,119.64373255,7,62.03278172,0|C,16,1.39139283,15
,59.93473014,12,4.92269197,0|C,16,1.39158615,15,59.77098288,12,-175.09
468859,0|H,17,1.08633052,15,120.10730007,12,0.62169023,0|H,18,1.086460
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77,15,119.87241796,12,1.72752708,0|H,19,1.0862288,16,120.16681267,15,1
79.42820313,0|H,20,1.08634065,16,120.18028324,15,-179.81994153,0|H,16,
1.08677551,15,179.67233087,12,120.0858556,0|H,14,1.08810523,13,118.389
07498,12,-179.86915853,0|C,14,1.46924538,13,127.69838048,12,1.77697482
,0|C,27,2.80784864,14,177.64825527,13,171.19265458,0|C,27,1.40149135,1
4,119.07392058,13,-139.82266063,0|C,27,1.39961245,14,122.06546164,13,4
3.61318585,0|C,28,1.3931188,27,59.88027186,14,-129.13162614,0|C,28,1.3
934669,27,59.9704227,14,50.34682942,0|H,29,1.08742356,27,120.33512322,
14,2.5002951,0|H,30,1.08779088,27,120.18059687,14,-2.45796328,0|H,31,1
.0867249,28,120.11847919,27,-179.43263493,0|H,32,1.0865298,28,120.0020
2522,27,179.66077917,0|H,28,1.08626332,27,179.52915493,14,148.46613365
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Job cpu time: 0 days 6 hours 7 minutes 55.0 seconds.
File lengths (MBytes): RWF= 181 Int= 0 D2E= 0 Chk= 20 Scr= 1
Normal termination of Gaussian 03 at Thu Nov 17 20:01:23 2011.

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[i] McCarthy, D. G.; Hegarty, A. F *J. Chem. Soc., Perkin Trans. 2* **1980**, 579-591.

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