Development of a stereoselective Ugi reaction starting from an oxanorbornene β-amino acid derivative

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COMPUTATIONAL DATA

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INTERMEDIATE 15i_a

%mem=256MB

RB3LYP/6-31G SCRF=(PCM,Solvent=Methanol) Test

1/38=1/1;
2/17=6,18=5,40=1/2;
3/5=1,6=6,11=2,16=1,25=1,30=1,70=2201,72=3,74=-5/1,2,3;
4/7=1/1;
5/5=2,32=1,38=5,53=3/2;
6/7=2,8=2,9=2,10=2,28=1/1;
99/5=1,9=1/99;

[No Title]

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	0	-2.4604	2.7047	1.4908
C	0	-3.0522	1.6114	0.9846
C	0	-1.4863	3.1723	0.4463
C	0	-0.3807	2.1152	0.4054
C	0	-1.016	1.0392	-0.4975
C	0	-2.5116	1.4228	-0.4028
O	0	-2.301	2.8539	-0.724
C	0	0.9142	2.41	-0.2639
N	0	-0.3369	-0.2406	-0.329
O	0	1.3617	3.5287	-0.4808
O	0	1.5843	1.272	-0.6142
C	0	-0.9266	-1.1252	0.6861
C	0	-2.2309	-1.758	0.2491
C	0	-3.2557	-1.9625	1.1854
C	0	-4.4565	-2.5654	0.8059
C	0	-4.641	-2.9877	-0.5087
C	0	-3.6223	-2.8166	-1.4431
C	0	-2.4212	-2.2138	-1.0652
C	0	1.1091	-0.0112	-0.0843
H	0	1.3248	0.0053	0.9934
C	0	1.9424	-1.116	-0.7722
C	0	3.3727	-1.1381	-0.2782
C	0	3.7128	-1.862	0.8735
C	0	5.0265	-1.8623	1.3447
C	0	6.0102	-1.1396	0.6722
C	0	5.6821	-0.4161	-0.4728
C	0	4.3693	-0.4138	-0.9465
H	0	-2.5989	3.1279	2.4741
H	0	-3.7854	0.9859	1.4695
H	0	-1.2117	4.227	0.4722
H	0	-0.1423	1.7821	1.4258
H	0	-0.7776	1.2866	-1.5484
H	0	-3.1875	0.982	-1.1367
H	0	-0.2498	-1.9624	0.9002
H	0	-1.0565	-0.5842	1.6319
H	0	-3.1295	-1.6509	2.2209
H	0	-5.2472	-2.7106	1.5385
H	0	-5.5758	-3.4592	-0.8028
H	0	-3.7607	-3.158	-2.4664
H	0	-1.6326	-2.1009	-1.8071
H	0	1.5095	-2.1086	-0.5958
H	0	1.9408	-0.9686	-1.8603
H	0	2.9598	-2.4348	1.4117
H	0	5.284	-2.4282	2.2372
H	0	7.0336	-1.1412	1.04

H	0	6.4502	0.1476	-0.9974
H	0	4.1307	0.1598	-1.8404

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.460400	2.704700	1.490800
2	6	0	-3.052200	1.611400	0.984600
3	6	0	-1.486300	3.172300	0.446300
4	6	0	-0.380700	2.115200	0.405400
5	6	0	-1.016000	1.039200	-0.497500
6	6	0	-2.511600	1.422800	-0.402800
7	8	0	-2.301000	2.853900	-0.724000
8	6	0	0.914200	2.410000	-0.263900
9	7	0	-0.336900	-0.240600	-0.329000
10	8	0	1.361700	3.528700	-0.480800
11	8	0	1.584300	1.272000	-0.614200
12	6	0	-0.926600	-1.125200	0.686100
13	6	0	-2.230900	-1.758000	0.249100
14	6	0	-3.255700	-1.962500	1.185400
15	6	0	-4.456500	-2.565400	0.805900
16	6	0	-4.641000	-2.987700	-0.508700
17	6	0	-3.622300	-2.816600	-1.443100
18	6	0	-2.421200	-2.213800	-1.065200
19	6	0	1.109100	-0.011200	-0.084300
20	1	0	1.324800	0.005300	0.993400
21	6	0	1.942400	-1.116000	-0.772200
22	6	0	3.372700	-1.138100	-0.278200
23	6	0	3.712800	-1.862000	0.873500
24	6	0	5.026500	-1.862300	1.344700
25	6	0	6.010200	-1.139600	0.672200
26	6	0	5.682100	-0.416100	-0.472800
27	6	0	4.369300	-0.413800	-0.946500
28	1	0	-2.598900	3.127900	2.474100
29	1	0	-3.785400	0.985900	1.469500
30	1	0	-1.211700	4.227000	0.472200
31	1	0	-0.142300	1.782100	1.425800
32	1	0	-0.777600	1.286600	-1.548400
33	1	0	-3.187500	0.982000	-1.136700
34	1	0	-0.249800	-1.962400	0.900200
35	1	0	-1.056500	-0.584200	1.631900
36	1	0	-3.129500	-1.650900	2.220900
37	1	0	-5.247200	-2.710600	1.538500
38	1	0	-5.575800	-3.459200	-0.802800
39	1	0	-3.760700	-3.158000	-2.466400
40	1	0	-1.632600	-2.100900	-1.807100
41	1	0	1.509500	-2.108600	-0.595800
42	1	0	1.940800	-0.968600	-1.860300
43	1	0	2.959800	-2.434800	1.411700
44	1	0	5.284000	-2.428200	2.237200
45	1	0	7.033600	-1.141200	1.040000
46	1	0	6.450200	0.147600	-0.997400
47	1	0	4.130700	0.159800	-1.840400

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.342300	0.000000			
3	C	1.502831	2.275570	0.000000		
4	C	2.418833	2.779604	1.530191	0.000000	

5	C	2.968757	2.582662	2.379508	1.541626	0.000000
6	C	2.287271	1.500899	2.198400	2.381877	1.546912
7	O	2.225535	2.242191	1.461067	2.347078	2.235098
8	C	3.814937	4.234246	2.616846	1.487157	2.378935
9	N	4.061492	3.539534	3.683761	2.468006	1.458581
10	O	4.378885	5.030502	3.016229	2.412321	3.442578
11	O	4.779462	4.916145	3.763560	2.368923	2.613307
12	C	4.203358	3.477967	4.340423	3.298028	2.468507
13	C	4.637907	3.545187	4.990108	4.295270	3.139701
14	C	4.744315	3.585316	5.481169	5.049917	4.105924
15	C	5.676923	4.410176	6.470904	6.219370	5.150634
16	C	6.415328	5.089789	6.986398	6.710091	5.418180
17	C	6.359445	5.081921	6.633193	6.184462	4.749121
18	C	5.543132	4.385430	5.671750	5.006650	3.588716
19	C	4.753776	4.592581	4.141535	2.642137	2.406268
20	H	4.675672	4.662377	4.269835	2.775996	2.961600
21	C	6.253284	5.955761	5.624077	4.150203	3.670487
22	C	7.205659	7.101673	6.535620	5.013909	4.904020
23	C	7.703519	7.605398	7.249643	5.726603	5.714731
24	C	8.771118	8.801230	8.280754	6.777950	6.951562
25	C	9.338084	9.475900	8.651071	7.176943	7.448681
26	C	8.938424	9.084204	8.068911	6.628443	6.854418
27	C	7.893686	7.931535	7.006287	5.548511	5.595915
28	H	1.079425	2.173445	2.313401	3.197732	3.962152
29	H	2.170335	1.078870	3.333638	3.741605	3.397279
30	H	2.216798	3.239036	1.090169	2.270401	3.337767
31	H	2.495797	2.948103	2.167582	1.099548	2.239271
32	H	3.752274	3.419852	2.834951	2.159037	1.105637
33	H	3.224923	2.216837	3.193334	3.397108	2.264346
34	H	5.197825	4.542314	5.300953	4.109597	3.398563
35	H	3.578786	3.036853	3.962533	3.041014	2.677949
36	H	4.466765	3.489558	5.395607	5.003544	4.369579
37	H	6.090485	4.878987	7.067233	6.946588	6.009106
38	H	7.277361	5.939220	7.890567	7.715099	6.412534
39	H	7.191764	5.929465	7.330035	6.890448	5.387619
40	H	5.886866	4.856956	5.736362	4.923201	3.457669
41	H	6.578895	6.094684	6.160251	4.734527	4.036887
42	H	6.640299	6.299199	5.849143	4.475777	3.825069
43	H	7.469892	7.259359	7.220760	5.733592	5.614330
44	H	9.320918	9.347706	8.967156	7.489112	7.693598
45	H	10.253302	10.454819	9.568044	8.122728	8.480219
46	H	9.598369	9.816651	8.615168	7.245722	7.535847
47	H	7.811274	7.853777	6.771620	5.405547	5.391219

		6	7	8	9	10
6	C	0.000000				
7	O	1.481745	0.000000			
8	C	3.567907	3.278147	0.000000		
9	N	2.738917	3.686413	2.931752	0.000000	
10	O	4.409462	3.732274	1.224251	4.137138	0.000000
11	O	4.104123	4.196429	1.366305	2.461769	2.271572
12	C	3.192214	4.439661	4.097400	1.469929	5.315709
13	C	3.259027	4.713964	5.246622	2.494782	6.433407
14	C	3.812653	5.268299	6.213477	3.711838	7.365452
15	C	4.598840	6.029559	7.398885	4.864545	8.523210
16	C	4.898782	6.296526	7.749538	5.109220	8.859834
17	C	4.504264	5.866644	7.020519	4.320978	8.125830
18	C	3.697540	5.080595	5.757300	2.963075	6.901316
19	C	3.907335	4.499644	2.435662	1.484392	3.570982
20	H	4.321648	4.920408	2.744445	2.137862	3.819552
21	C	5.140046	5.811099	3.707862	2.481524	4.689922
22	C	6.418623	6.951667	4.316647	3.816965	5.085685
23	C	7.152762	7.807529	5.232191	4.524933	6.035018

24	C	8.406461	8.956245	6.144197	5.847841	6.769497
25	C	8.963403	9.325956	6.280538	6.488165	6.688123
26	C	8.397808	8.630521	5.546472	6.023275	5.850416
27	C	7.142513	7.431034	4.514145	4.749697	4.980546
28	H	3.345376	3.223610	4.511529	4.931613	4.957663
29	H	2.306286	3.241035	5.207588	4.078119	6.063179
30	H	3.212305	2.121997	2.891848	4.622407	2.831646
31	H	3.014375	3.229610	2.089387	2.684866	2.991279
32	H	2.082716	2.335982	2.402947	2.003370	3.277711
33	H	1.090759	2.111922	4.430001	3.205160	5.254627
34	H	4.274708	5.481076	4.672035	2.117337	5.886958
35	H	3.207081	4.349664	4.054991	2.116841	5.217963
36	H	4.088182	5.445372	6.246331	4.036032	7.368739
37	H	5.323265	6.690490	8.211701	5.805127	9.310424
38	H	5.777824	7.112366	8.766871	6.166842	9.852073
39	H	5.177106	6.427256	7.596599	4.980171	8.654106
40	H	3.893734	5.115653	5.405171	2.706351	6.512857
41	H	5.355117	6.258015	4.569714	2.640038	5.640410
42	H	5.259940	5.821989	3.875221	2.839504	4.739629
43	H	6.936116	7.759354	5.519439	4.325827	6.457462
44	H	9.086869	9.705746	6.982753	6.554807	7.632602
45	H	9.988324	10.305691	7.194319	7.550464	7.502749
46	H	9.071579	9.164186	6.025261	6.830972	6.131194
47	H	6.912453	7.061961	4.230204	4.733297	4.567862

		11	12	13	14	15
11	O	0.000000				
12	C	3.707016	0.000000			
13	C	4.947923	1.514135	0.000000		
14	C	6.093123	2.524892	1.403101	0.000000	
15	C	7.296135	3.814279	2.432122	1.396220	0.000000
16	C	7.543907	4.323566	2.809805	2.416623	1.393037
17	C	6.671762	3.828985	2.433140	2.787991	2.411844
18	C	5.328999	2.546749	1.404049	2.413450	2.786949
19	C	1.467382	2.445115	3.783922	4.946836	6.188077
20	H	2.063067	2.537965	4.038095	4.988996	6.329857
21	C	2.419864	3.218367	4.344151	5.618630	6.748117
22	C	3.019909	4.406135	5.662389	6.837942	8.031739
23	C	4.070101	4.701279	5.977312	6.976201	8.199805
24	C	5.050729	6.034606	7.340373	8.284338	9.524282
25	C	5.201849	6.936829	8.275093	9.316514	10.564213
26	C	4.434145	6.746909	8.058375	9.220914	10.442498
27	C	3.272395	5.587310	6.840977	8.067471	9.251758
28	H	5.520971	4.907381	5.381270	5.291909	6.216690
29	H	5.766917	3.639120	3.381543	3.009046	3.674571
30	H	4.210689	5.364054	6.075259	6.557172	7.535037
31	H	2.720836	3.100754	4.275416	4.875765	6.156083
32	H	2.539983	3.291196	3.822653	4.916431	5.823653
33	H	4.809073	3.588114	3.216073	3.750584	4.238880
34	H	4.014807	1.097634	2.095344	3.019400	4.250744
35	H	3.932463	1.097312	2.160823	2.633544	4.020874
36	H	6.229049	2.735825	2.169550	1.088706	2.144636
37	H	8.195402	4.680562	3.415855	2.156480	1.087654
38	H	8.584105	5.411048	3.897298	3.402340	2.153979
39	H	7.185024	4.701346	3.416757	3.875550	3.397537
40	H	4.811228	2.768840	2.168756	3.407149	3.875299
41	H	3.381477	2.923171	3.850632	5.089317	6.145452
42	H	2.588464	3.838054	4.740865	6.104731	7.112232
43	H	4.442594	4.164811	5.362188	6.237525	7.442147
44	H	5.959005	6.532631	7.802271	8.616823	9.846054
45	H	6.185045	7.968079	9.318633	10.323050	11.580395
46	H	5.008802	7.672768	8.974774	10.169643	11.382810
47	H	3.037220	5.797474	6.965194	8.259451	9.389868

		16	17	18	19	20
16	C	0.000000				
17	C	1.392885	0.000000			
18	C	2.415807	1.396001	0.000000		
19	C	6.488707	5.665929	4.275118	0.000000	
20	H	6.841427	6.194631	4.816093	1.099198	0.000000
21	C	6.849368	5.857306	4.509104	1.545373	2.180845
22	C	8.227608	7.287275	5.945231	2.536018	2.668000
23	C	8.541876	7.751231	6.442692	3.334981	3.033765
24	C	9.907683	9.136972	7.835777	4.562306	4.161000
25	C	10.874652	10.003593	8.675308	5.085898	4.833936
26	C	10.638647	9.657937	8.321426	4.607299	4.616642
27	C	9.380945	8.359769	7.026022	3.396230	3.634259
28	H	7.104071	7.192279	6.410303	5.490776	5.228626
29	H	4.520489	4.792582	4.303931	5.231122	5.225169
30	H	8.048240	7.687110	6.731300	4.863964	4.952599
31	H	6.836050	6.441198	5.231222	2.657504	2.344434
32	H	5.854612	4.993962	3.897140	2.717998	3.538723
33	H	4.273823	3.835661	3.287167	4.533736	5.084498
34	H	4.724286	4.194576	2.939554	2.573525	2.521883
35	H	4.817429	4.585037	3.433999	2.821966	2.534913
36	H	3.394464	3.876416	3.408372	5.095909	4.908212
37	H	2.152973	3.397275	3.874576	7.093856	7.131930
38	H	1.087501	2.153853	3.401673	7.555980	7.927634
39	H	2.153258	1.087590	2.156185	6.268309	6.916574
40	H	3.394514	2.145607	1.088601	3.853804	4.585313
41	H	6.213618	5.249243	3.960026	2.195686	2.651084
42	H	7.015959	5.876839	4.605405	2.182319	3.077587
43	H	7.859122	7.184685	5.927819	3.396608	2.966865
44	H	10.313032	9.644565	8.385817	5.353601	4.810845
45	H	11.920752	11.068918	9.745542	6.135198	5.822974
46	H	11.536189	10.509062	9.180553	5.420915	5.500296
47	H	9.413974	8.314193	7.011584	3.499028	3.990911

		21	22	23	24	25
21	C	0.000000				
22	C	1.513368	0.000000			
23	C	2.529656	1.402181	0.000000		
24	C	3.814433	2.427617	1.395649	0.000000	
25	C	4.316694	2.803510	2.416698	1.393635	0.000000
26	C	3.816393	2.427443	2.789497	2.413423	1.393602
27	C	2.532451	1.401587	2.416749	2.789204	2.416512
28	H	7.012315	7.837979	8.203571	9.182830	9.776247
29	H	6.500069	7.668391	8.042932	9.261609	10.055208
30	H	6.328075	7.096768	7.841407	8.761048	8.999791
31	H	4.192393	4.877131	5.333507	6.324929	6.852554
32	H	3.711250	4.971677	5.995246	7.209242	7.542661
33	H	5.554308	6.947523	7.729384	9.039756	9.610983
34	H	2.884277	3.897512	3.963962	5.295936	6.317957
35	H	3.880194	4.855214	4.995414	6.222452	7.153163
36	H	5.913454	6.984774	6.976899	8.205654	9.284073
37	H	7.718318	8.948510	9.024630	10.310484	11.399455
38	H	7.874951	9.259501	9.572832	10.934835	11.907626
39	H	6.290106	7.730046	8.287807	9.665309	10.459218
40	H	3.849892	5.321423	5.984646	7.371186	8.092183
41	H	1.097166	2.124677	2.659734	4.024362	4.775258
42	H	1.098040	2.140586	3.378137	4.537871	4.796125
43	H	2.746590	2.169719	1.088471	2.145575	3.395489
44	H	4.684511	3.412428	2.156138	1.087706	2.153388
45	H	5.404167	3.890996	3.402203	2.154362	1.087487
46	H	4.686967	3.411932	3.877128	3.398831	2.153613
47	H	2.749068	2.167851	3.409922	3.877655	3.396192

		26	27	28	29	30

26	C	0.000000				
27	C	1.395651	0.000000			
28	H	9.477295	8.532289	0.000000		
29	H	9.765843	8.619475	2.646728	0.000000	
30	H	8.365159	7.395762	2.672068	4.257143	0.000000
31	H	6.508487	5.550164	2.990818	3.729346	2.833815
32	H	6.766375	5.453826	4.784143	4.271417	3.594053
33	H	9.003624	7.686980	4.241369	2.673907	4.125817
34	H	6.282007	5.210043	5.822936	4.638647	6.278305
35	H	7.061639	6.009700	4.107065	3.152536	4.951428
36	H	9.296507	8.233762	4.814829	2.819135	6.425388
37	H	11.347231	10.194488	6.478960	3.975642	8.096453
38	H	11.666605	10.401929	7.936617	5.303564	8.930211
39	H	10.032892	8.714220	8.079038	5.715228	8.346915
40	H	7.623893	6.293627	6.826621	4.989889	6.739042
41	H	4.504473	3.342722	7.329677	6.471272	6.977491
42	H	4.028367	2.653384	7.495146	6.906302	6.509460
43	H	3.877810	3.410607	7.935457	7.563217	7.916038
44	H	3.398695	3.876910	9.647097	9.721083	9.465782
45	H	2.154272	3.402027	10.633293	11.034482	9.855199
46	H	1.087631	2.155900	10.140005	10.562000	8.803746
47	H	2.146819	1.088579	8.527136	8.619891	7.101512

		31	32	33	34	35
31	H	0.000000				
32	H	3.081394	0.000000			
33	H	4.059533	2.463716	0.000000		
34	H	3.782736	4.102465	4.631256	0.000000	
35	H	2.545116	3.700268	3.828745	1.756583	0.000000
36	H	4.619636	5.326158	4.267201	3.183387	2.404600
37	H	6.801254	6.744174	5.003434	5.093254	4.700241
38	H	7.871519	6.789791	5.053684	5.788514	5.883661
39	H	7.255800	5.431029	4.385916	5.008979	5.543754
40	H	5.267858	3.503299	3.517303	3.043155	3.802498
41	H	4.685388	4.203053	5.648556	2.313985	3.724352
42	H	4.764883	3.545830	5.534248	3.661520	4.618120
43	H	5.235023	6.048071	7.480519	3.284254	4.427626
44	H	6.915904	8.054409	9.735450	5.712047	6.630887
45	H	7.758097	8.579561	10.663812	7.330882	8.130825
46	H	7.211418	7.337712	9.674755	7.276193	7.987446
47	H	5.617691	5.044438	7.397787	5.586000	6.286290

		36	37	38	39	40
36	H	0.000000				
37	H	2.464404	0.000000			
38	H	4.289183	2.479933	0.000000		
39	H	4.963924	4.295238	2.480499	0.000000	
40	H	4.320647	4.962873	4.289805	2.465958	0.000000
41	H	5.446431	7.111303	7.215847	5.689938	3.367506
42	H	6.544438	8.139641	7.988784	6.137421	3.748883
43	H	6.192647	8.212612	8.877492	7.792804	5.618034
44	H	8.449346	10.558130	11.324302	10.220717	8.018905
45	H	10.244165	12.390705	12.952452	11.527326	9.172242
46	H	10.264634	12.305660	12.556733	10.832702	8.428702
47	H	8.513712	10.373098	10.411048	8.583348	6.190921

		41	42	43	44	45
41	H	0.000000				
42	H	1.756297	0.000000			
43	H	2.497966	3.727477	0.000000		
44	H	4.730210	5.486066	2.466455	0.000000	
45	H	5.841865	5.863288	4.290386	2.480072	0.000000
46	H	5.446305	4.724954	4.965425	4.296208	2.480395
47	H	3.683118	2.463604	4.321934	4.965347	4.291402

		46	47

46 H 0.000000
47 H 2.467970 0.000000
Stoichiometry C22H21NO3
Framework group C1[X(C22H21NO3)]
Deg. of freedom 135
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	-2.453932	2.747906	1.460526
2	6	0	-3.046515	1.652276	0.960314
3	6	0	-1.478715	3.208456	0.413938
4	6	0	-0.374152	2.150031	0.379871
5	6	0	-1.009971	1.069441	-0.517162
6	6	0	-2.505244	1.455080	-0.425629
7	8	0	-2.293008	2.884079	-0.755003
8	6	0	0.921458	2.439643	-0.290319
9	7	0	-0.332261	-0.210038	-0.340807
10	8	0	1.370216	3.556616	-0.513433
11	8	0	1.590633	1.298958	-0.633584
12	6	0	-0.923478	-1.088136	0.679045
13	6	0	-2.228142	-1.722159	0.244910
14	6	0	-3.253727	-1.920192	1.181740
15	6	0	-4.454896	-2.524085	0.804997
16	6	0	-4.639004	-2.953829	-0.507244
17	6	0	-3.619553	-2.789178	-1.441984
18	6	0	-2.418083	-2.185395	-1.066839
19	6	0	1.113816	0.019334	-0.096538
20	1	0	1.328864	0.041878	0.981183
21	6	0	1.946434	-1.090277	-0.777487
22	6	0	3.376404	-1.110937	-0.282471
23	6	0	3.715062	-1.828475	0.873626
24	6	0	5.028469	-1.827352	1.345643
25	6	0	6.013311	-1.109555	0.669573
26	6	0	5.686648	-0.392390	-0.479815
27	6	0	4.374145	-0.391529	-0.954343
28	1	0	-2.592617	3.176949	2.441264
29	1	0	-3.780643	1.030337	1.448379
30	1	0	-1.203073	4.263014	0.433884
31	1	0	-0.136720	1.822626	1.402337
32	1	0	-0.770671	1.310494	-1.569332
33	1	0	-3.181131	1.010701	-1.157379
34	1	0	-0.247652	-1.924755	0.898427
35	1	0	-1.053422	-0.541522	1.621605
36	1	0	-3.127857	-1.602708	2.215492
37	1	0	-5.246196	-2.664236	1.537932
38	1	0	-5.574094	-3.426094	-0.799186
39	1	0	-3.757661	-3.136378	-2.463370
40	1	0	-1.628910	-2.077595	-1.808888
41	1	0	1.512428	-2.081402	-0.595596
42	1	0	1.945657	-0.949198	-1.866426
43	1	0	2.961154	-2.397386	1.414672
44	1	0	5.284847	-2.388315	2.241576
45	1	0	7.036480	-1.110042	1.038017
46	1	0	6.455639	0.167485	-1.007199
47	1	0	4.136676	0.177108	-1.851708

Rotational constants (GHZ): 0.3018662 0.1392353 0.1052621

```
Standard basis: 6-31G (6D, 7F)
There are   276 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.
  276 basis functions,   656 primitive gaussians,   276 cartesian basis functions
   92 alpha electrons       92 beta electrons
      nuclear repulsion energy      2294.5957155213 Hartrees.
NAtoms=   47 NActive=   47 NUniq=   47 SFac= 1.00D+00 NAtFMM=   60 Big=F
--------------------------------------------------------------------------------
United Atom Topological Model (UA0  parameters set).
 Nord Group  Hybr  Charge Alpha Radius          Bonded to
  1   CH    *     0.00   1.00  2.125   C2   [d]  C3   [s]
  2   CH    *     0.00   1.00  2.125   C1   [d]  C6   [s]
  3   CH    *     0.00   1.00  2.125   C1   [s]  C4   [s]  O7   [s]
  4   CH    *     0.00   1.00  2.125   C3   [s]  C5   [s]  C8   [s]
  5   CH    *     0.00   1.00  2.125   C4   [s]  C6   [s]  N9   [s]
  6   CH    *     0.00   1.00  2.125   C2   [s]  C5   [s]  O7   [s]
  7   O     *     0.00   1.00  1.750   C3   [s]  C6   [s]
  8   C     *     0.00   1.00  1.925   C4   [s]  O10  [d]  O11  [s]
  9   N     *     0.00   1.00  1.830   C5   [s]  C12  [s]  C19  [s]
 10   O     *     0.00   1.00  1.750   C8   [d]
 11   O     *     0.00   1.00  1.750   C8   [s]  C19  [s]
 12   CH2   *     0.00   1.00  2.325   N9   [s]  C13  [s]
 13   C     *     0.00   1.00  1.925   C12  [s]  C14  [s]  C18  [s]
 14   CH    *     0.00   1.00  2.125   C13  [s]  C15  [s]
 15   CH    *     0.00   1.00  2.125   C14  [s]  C16  [s]
 16   CH    *     0.00   1.00  2.125   C15  [s]  C17  [s]
 17   CH    *     0.00   1.00  2.125   C16  [s]  C18  [s]
 18   CH    *     0.00   1.00  2.125   C13  [s]  C17  [s]
 19   CH    *     0.00   1.00  2.125   N9   [s]  O11  [s]  C21  [s]
 21   CH2   *     0.00   1.00  2.325   C19  [s]  C22  [s]
 22   C     *     0.00   1.00  1.925   C21  [s]  C23  [s]  C27  [s]
 23   CH    *     0.00   1.00  2.125   C22  [s]  C24  [s]
 24   CH    *     0.00   1.00  2.125   C23  [s]  C25  [s]
 25   CH    *     0.00   1.00  2.125   C24  [s]  C26  [s]
 26   CH    *     0.00   1.00  2.125   C25  [s]  C27  [s]
 27   CH    *     0.00   1.00  2.125   C22  [s]  C26  [s]
--------------------------------------------------------------------------------
Polarizable Continuum Model (PCM)
=================================
Model               : PCM.
Atomic radii        : UA0 (Simple United Atom Topological Model).
Polarization charges : Total charges.
Charge compensation  : None.
Solution method      : Matrix inversion.
Cavity              : GePol (RMin=0.200 OFac=0.890).
                    Default sphere list used, NSphG=   26.
                    Tesserae with average area of 0.200 Ang**2.
Solvent             : Methanol, Eps=  32.630000.
--------------------------------------------------------------------------------
One-electron integrals computed using PRISM.
NBasis=   276 RedAO= T  NBF=   276
NBsUse=   276 1.00D-06 NBFU=   276
Harris functional with IExCor=  402 diagonalized for initial guess.
ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 402 AccDes= 1.00D-06 IRadAn=         1 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)
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Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry


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          (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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          (A) (A) (A) (A)
The electronic state of the initial guess is 1-A.
Warning!  Cutoffs for single-point calculations used.
Requested convergence on RMS density matrix=1.00D-04 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-02.
Requested convergence on             energy=5.00D-05.
No special actions if energy rises.
EnCoef did     1 forward-backward iterations
Error on total polarization charges =  0.02518
SCF Done:  E(RB+HF-LYP) =  -1131.02734087     A.U. after   17 cycles
           Convg  =    0.1332D-07             -V/T =  2.0050
           S**2   =   0.0000
 --------------------------------------------------------------------
 Variational PCM results
 =======================
 <psi(f)|   H    |psi(f)>                 (a.u.) =   -1130.994508
 <psi(f)|H+V(f)/2|psi(f)>                 (a.u.) =   -1131.027341
 Total free energy in solution:
  with all non electrostatic terms        (a.u.) =   -1131.018649
 --------------------------------------------------------------------
 (Polarized solute)-Solvent              (kcal/mol) =     -20.60
 --------------------------------------------------------------------
 Cavitation energy                       (kcal/mol) =      30.73
 Dispersion energy                       (kcal/mol) =     -27.35
 Repulsion energy                        (kcal/mol) =       2.07
 Total non electrostatic                 (kcal/mol) =       5.45
 --------------------------------------------------------------------
 Partition over spheres:
 Sphere  on Atom  Surface  Charge   GEl    GCav    GDR
    1      C1      19.88  -0.041   -0.88   1.73   -1.77
    2      C2      11.02  -0.009   -0.33   1.35   -0.96
    3      C3       9.78  -0.058   -0.38   1.14   -0.99
    4      C4       4.42  -0.050   -0.96   0.60   -0.49
    5      C5       4.74  -0.040   -0.20   0.60   -0.53
    6      C6       7.00  -0.035   -0.28   0.96   -0.75
    7      O7       8.48   0.127   -2.66   0.97   -1.01
    8      C8       2.92  -0.017    0.00   0.51   -0.30
    9      N9       0.00   0.000    0.00   0.13    0.00
   10      O10     16.94   0.194   -4.48   1.94   -1.75
   11      O11      2.07   0.021   -0.31   0.71   -0.27
   12      C12     11.33  -0.041   -0.55   1.56   -1.16
   13      C13      0.05   0.000    0.00   0.04    0.00
```

14	C14	10.07	-0.024	-0.60	1.35	-1.00
15	C15	16.52	-0.018	-0.55	1.69	-1.51
16	C16	17.26	-0.014	-0.51	1.69	-1.55
17	C17	16.91	-0.017	-0.50	1.69	-1.57
18	C18	8.78	-0.002	-0.16	1.43	-0.92
19	C19	1.62	-0.024	-0.45	0.53	-0.24
20	C21	14.28	-0.042	-0.27	1.87	-1.43
21	C22	0.12	0.001	0.00	0.09	0.00
22	C23	12.77	-0.007	-0.54	1.58	-1.23
23	C24	17.55	-0.013	-0.55	1.69	-1.59
24	C25	17.56	-0.011	-0.51	1.69	-1.54
25	C26	17.55	-0.013	-0.48	1.69	-1.59
26	C27	11.11	-0.014	-0.30	1.52	-1.12
Added spheres:		94.29	0.124	-4.16	0.00	0.00

****

Population analysis using the SCF density.

****

Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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(A) (A) (A) (A)
The electronic state is 1-A.
Alpha occ. eigenvalues -- -19.20629 -19.15509 -19.15057 -14.34333 -10.33810
Alpha occ. eigenvalues -- -10.29097 -10.25077 -10.24641 -10.23312 -10.21825
Alpha occ. eigenvalues -- -10.20897 -10.19638 -10.19314 -10.19061 -10.18923
Alpha occ. eigenvalues -- -10.18804 -10.18397 -10.18326 -10.18293 -10.18270
Alpha occ. eigenvalues -- -10.18225 -10.18184 -10.18177 -10.18128 -10.18080
Alpha occ. eigenvalues -- -10.18065 -1.12778 -1.06701 -1.05215 -0.94696
Alpha occ. eigenvalues -- -0.86051 -0.85816 -0.82888 -0.79805 -0.78698
Alpha occ. eigenvalues -- -0.76823 -0.75801 -0.74505 -0.74453 -0.72175
Alpha occ. eigenvalues -- -0.68465 -0.65423 -0.65235 -0.60650 -0.60429
Alpha occ. eigenvalues -- -0.59844 -0.58539 -0.57644 -0.56313 -0.55602
Alpha occ. eigenvalues -- -0.54597 -0.53051 -0.51333 -0.50727 -0.50162
Alpha occ. eigenvalues -- -0.49560 -0.46919 -0.46125 -0.45793 -0.45142
Alpha occ. eigenvalues -- -0.44900 -0.44431 -0.43788 -0.42962 -0.41973
Alpha occ. eigenvalues -- -0.41865 -0.41597 -0.41199 -0.40588 -0.40033

Alpha occ. eigenvalues -- -0.39695 -0.39115 -0.38488 -0.37835 -0.36786
Alpha occ. eigenvalues -- -0.35910 -0.35747 -0.34697 -0.34494 -0.33951
Alpha occ. eigenvalues -- -0.33696 -0.33567 -0.33184 -0.31823 -0.28299
Alpha occ. eigenvalues -- -0.28028 -0.25125 -0.25021 -0.24854 -0.24438
Alpha occ. eigenvalues -- -0.24290 -0.21928
Alpha virt. eigenvalues -- -0.01311 -0.00622 -0.00030 0.00163 0.00315
Alpha virt. eigenvalues -- 0.00588 0.07880 0.09253 0.09513 0.09739
Alpha virt. eigenvalues -- 0.10256 0.10845 0.12101 0.12612 0.13428
Alpha virt. eigenvalues -- 0.13717 0.14261 0.15153 0.15551 0.15839
Alpha virt. eigenvalues -- 0.16286 0.16506 0.16918 0.17554 0.17628
Alpha virt. eigenvalues -- 0.18058 0.18491 0.18848 0.19287 0.20210
Alpha virt. eigenvalues -- 0.20590 0.20874 0.21280 0.22104 0.23146
Alpha virt. eigenvalues -- 0.23784 0.24681 0.24894 0.26443 0.26768
Alpha virt. eigenvalues -- 0.28347 0.28896 0.31489 0.31560 0.31599
Alpha virt. eigenvalues -- 0.32777 0.32921 0.34090 0.34874 0.34951
Alpha virt. eigenvalues -- 0.35486 0.35937 0.36618 0.37626 0.42270
Alpha virt. eigenvalues -- 0.48549 0.48795 0.49113 0.51071 0.52368
Alpha virt. eigenvalues -- 0.52793 0.53201 0.54223 0.54520 0.55011
Alpha virt. eigenvalues -- 0.55441 0.56443 0.56770 0.57490 0.57522
Alpha virt. eigenvalues -- 0.58275 0.58878 0.59039 0.59606 0.59993
Alpha virt. eigenvalues -- 0.60322 0.61531 0.62231 0.62660 0.62758
Alpha virt. eigenvalues -- 0.63211 0.63875 0.64356 0.64757 0.64804
Alpha virt. eigenvalues -- 0.64956 0.65323 0.65703 0.66143 0.66222
Alpha virt. eigenvalues -- 0.66977 0.67166 0.67362 0.67546 0.68661
Alpha virt. eigenvalues -- 0.70365 0.71047 0.71668 0.72849 0.74765
Alpha virt. eigenvalues -- 0.75764 0.75978 0.76458 0.78436 0.80246
Alpha virt. eigenvalues -- 0.82061 0.83679 0.83767 0.84925 0.85243
Alpha virt. eigenvalues -- 0.85469 0.85765 0.86154 0.86767 0.87208
Alpha virt. eigenvalues -- 0.87390 0.87616 0.88157 0.88967 0.89606
Alpha virt. eigenvalues -- 0.90777 0.91592 0.92198 0.93063 0.93568
Alpha virt. eigenvalues -- 0.94043 0.94620 0.95367 0.95790 0.97440
Alpha virt. eigenvalues -- 0.97832 0.99064 0.99603 1.00285 1.00688
Alpha virt. eigenvalues -- 1.01635 1.02857 1.03909 1.05096 1.05619
Alpha virt. eigenvalues -- 1.06252 1.07055 1.08008 1.09261 1.10450
Alpha virt. eigenvalues -- 1.12743 1.13211 1.15886 1.16123 1.16988
Alpha virt. eigenvalues -- 1.18538 1.19505 1.20008 1.20593 1.22773
Alpha virt. eigenvalues -- 1.23114 1.23767 1.25394 1.28398 1.29727
Alpha virt. eigenvalues -- 1.33251 1.35369 1.39732 1.41457 1.42372
Alpha virt. eigenvalues -- 1.46105 1.46689 1.48918 1.51726 1.52301
Alpha virt. eigenvalues -- 1.55149 1.56182 1.60828 1.68362 1.69449
Alpha virt. eigenvalues -- 1.79741 1.83535 1.90400 1.91627 1.92268
Alpha virt. eigenvalues -- 2.00010 2.05460 2.14171 2.53137

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	5.076060	0.634794	0.279079	-0.050980	-0.019000	-0.057823
2	C	0.634794	5.097455	-0.047691	-0.040374	-0.036488	0.265841
3	C	0.279079	-0.047691	5.362654	0.090672	-0.049214	-0.139129
4	C	-0.050980	-0.040374	0.090672	6.184215	0.154732	-0.013361
5	C	-0.019000	-0.036488	-0.049214	0.154732	5.439305	0.177480
6	C	-0.057823	0.265841	-0.139129	-0.013361	0.177480	5.363513
7	O	-0.090889	-0.108146	0.210187	-0.103860	-0.070790	0.198416
8	C	0.005753	0.001533	-0.002695	0.092563	-0.028592	0.001744
9	N	-0.000163	-0.001232	0.010119	-0.056562	0.124817	-0.012397
10	O	0.000134	-0.000017	0.005704	-0.121203	0.001651	-0.000253
11	O	-0.000148	-0.000032	0.004931	-0.145516	0.017682	0.000429
12	C	-0.000521	0.001900	-0.000042	-0.004964	-0.052294	-0.009996
13	C	0.000085	0.000476	0.000025	-0.001075	-0.003766	0.002726
14	C	0.000079	-0.001492	0.000005	0.000019	0.000434	0.000131
15	C	0.000003	-0.000292	0.000000	0.000000	0.000004	-0.000011
16	C	0.000000	-0.000010	0.000000	0.000000	0.000000	-0.000045
17	C	0.000000	-0.000011	0.000000	0.000003	-0.000042	-0.000321
18	C	-0.000004	-0.000142	-0.000006	0.000160	-0.000994	0.000249

19	C	-0.000171	-0.000003	0.000461	-0.005047	-0.044969	0.003623
20	H	-0.000044	-0.000062	-0.000307	0.001836	0.000559	0.000197
21	C	0.000000	0.000001	0.000020	-0.000758	0.001922	-0.000144
22	C	0.000000	0.000000	-0.000001	0.000035	-0.000124	0.000002
23	C	0.000000	0.000000	0.000000	0.000000	-0.000002	0.000000
24	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
25	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
26	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
27	C	0.000000	0.000000	0.000000	0.000010	0.000003	0.000000
28	H	0.354352	-0.028499	-0.032067	0.003271	-0.000128	0.005897
29	H	-0.025712	0.355451	0.005575	-0.000217	0.002259	-0.031186
30	H	-0.030133	0.002803	0.383243	-0.042162	0.000932	0.008490
31	H	-0.004432	0.002908	-0.025428	0.360920	-0.026267	-0.004638
32	H	0.000686	0.007224	-0.000588	-0.084057	0.422948	-0.056270
33	H	0.003355	-0.039410	0.006201	0.006956	-0.041785	0.388362
34	H	0.000012	0.000033	0.000014	-0.000209	0.005226	0.000263
35	H	0.000729	0.002424	-0.000957	0.007395	-0.004112	0.001059
36	H	0.000010	-0.000034	-0.000002	0.000006	-0.000014	-0.000001
37	H	0.000000	-0.000003	0.000000	0.000000	0.000000	-0.000001
38	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
39	H	0.000000	0.000000	0.000000	0.000000	0.000000	-0.000001
40	H	0.000000	-0.000011	-0.000002	0.000070	0.000482	-0.000149
41	H	0.000000	0.000000	0.000000	0.000031	0.000310	0.000002
42	H	0.000000	0.000000	-0.000001	0.000016	0.000044	0.000001
43	H	0.000000	0.000000	0.000000	0.000000	0.000002	0.000000
44	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
45	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
46	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
47	H	0.000000	0.000000	0.000000	0.000007	0.000000	0.000000

		7	8	9	10	11	12
1	C	-0.090889	0.005753	-0.000163	0.000134	-0.000148	-0.000521
2	C	-0.108146	0.001533	-0.001232	-0.000017	-0.000032	0.001900
3	C	0.210187	-0.002695	0.010119	0.005704	0.004931	-0.000042
4	C	-0.103860	0.092563	-0.056562	-0.121203	-0.145516	-0.004964
5	C	-0.070790	-0.028592	0.124817	0.001651	0.017682	-0.052294
6	C	0.198416	0.001744	-0.012397	-0.000253	0.000429	-0.009996
7	O	8.464022	0.003760	0.004384	-0.000093	-0.000032	0.000013
8	C	0.003760	4.741601	-0.015457	0.571313	0.106760	0.000755
9	N	0.004384	-0.015457	7.410319	-0.000069	-0.048951	0.224479
10	O	-0.000093	0.571313	-0.000069	8.087295	-0.091164	0.000002
11	O	-0.000032	0.106760	-0.048951	-0.091164	8.616992	0.001571
12	C	0.000013	0.000755	0.224479	0.000002	0.001571	5.181416
13	C	0.000028	-0.000084	-0.061791	0.000000	-0.000090	0.261950
14	C	0.000008	0.000000	0.001178	0.000000	0.000000	-0.037896
15	C	0.000000	0.000000	-0.000114	0.000000	0.000000	0.006313
16	C	0.000000	0.000000	-0.000009	0.000000	0.000000	0.000412
17	C	0.000000	0.000000	0.000573	0.000000	0.000000	0.006169
18	C	0.000016	-0.000002	0.001756	0.000000	-0.000002	-0.055632
19	C	-0.000166	-0.010817	0.157873	0.000970	0.143445	-0.026938
20	H	0.000003	-0.003241	-0.071663	0.000125	-0.047715	-0.000570
21	C	0.000001	0.001257	-0.051735	-0.000086	-0.045050	-0.003042
22	C	0.000000	0.000187	0.005507	0.000007	-0.002178	-0.000152
23	C	0.000000	-0.000003	0.000070	0.000000	-0.000239	-0.000033
24	C	0.000000	-0.000001	0.000002	0.000000	0.000007	0.000000
25	C	0.000000	0.000000	0.000000	0.000000	0.000001	0.000000
26	C	0.000000	-0.000003	0.000001	0.000000	-0.000007	0.000000
27	C	0.000000	0.000122	0.000025	-0.000003	0.003906	-0.000006
28	H	0.004159	-0.000108	-0.000008	0.000002	0.000000	0.000007
29	H	0.002912	0.000003	-0.000021	0.000000	0.000000	-0.000170
30	H	-0.023174	0.000459	-0.000100	0.005567	0.000163	-0.000004
31	H	0.003195	-0.031713	-0.006713	0.000761	0.000137	0.002551
32	H	0.005306	0.002532	-0.061219	0.000243	0.000968	0.006158

33	H	-0.021965	-0.000064	0.000594	0.000001	-0.000005	-0.000630
34	H	0.000001	-0.000013	-0.041827	0.000000	0.000117	0.374540
35	H	0.000008	0.000305	-0.062148	0.000002	-0.000162	0.365777
36	H	0.000000	0.000000	0.000053	0.000000	0.000000	-0.006654
37	H	0.000000	0.000000	0.000001	0.000000	0.000000	-0.000176
38	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000004
39	H	0.000000	0.000000	0.000002	0.000000	0.000000	-0.000175
40	H	0.000000	0.000000	0.011752	0.000000	0.000000	-0.008157
41	H	0.000000	-0.000058	-0.003017	0.000001	0.002759	0.000164
42	H	0.000000	0.000051	0.000650	-0.000010	-0.002310	0.000204
43	H	0.000000	0.000000	-0.000065	0.000000	0.000000	0.000013
44	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
45	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
46	H	0.000000	0.000000	0.000000	0.000000	-0.000001	0.000000
47	H	0.000000	0.000114	-0.000005	0.000003	0.001903	0.000000

		13	14	15	16	17	18
1	C	0.000085	0.000079	0.000003	0.000000	0.000000	-0.000004
2	C	0.000476	-0.001492	-0.000292	-0.000010	-0.000011	-0.000142
3	C	0.000025	0.000005	0.000000	0.000000	0.000000	-0.000006
4	C	-0.001075	0.000019	0.000000	0.000000	0.000003	0.000160
5	C	-0.003766	0.000434	0.000004	0.000000	-0.000042	-0.000994
6	C	0.002726	0.000131	-0.000011	-0.000045	-0.000321	0.000249
7	O	0.000028	0.000008	0.000000	0.000000	0.000000	0.000016
8	C	-0.000084	0.000000	0.000000	0.000000	0.000000	-0.000002
9	N	-0.061791	0.001178	-0.000114	-0.000009	0.000573	0.001756
10	O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
11	O	-0.000090	0.000000	0.000000	0.000000	0.000000	-0.000002
12	C	0.261950	-0.037896	0.006313	0.000412	0.006169	-0.055632
13	C	4.949791	0.516953	-0.043161	-0.030336	-0.041264	0.520959
14	C	0.516953	5.009270	0.511168	-0.059759	-0.039827	-0.058825
15	C	-0.043161	0.511168	4.936619	0.539532	-0.049519	-0.039676
16	C	-0.030336	-0.059759	0.539532	4.924453	0.532701	-0.057874
17	C	-0.041264	-0.039827	-0.049519	0.532701	4.952263	0.502537
18	C	0.520959	-0.058825	-0.039676	-0.057874	0.502537	5.002523
19	C	0.005487	-0.000109	0.000001	0.000000	-0.000002	0.000050
20	H	-0.000273	0.000023	0.000000	0.000000	0.000000	0.000044
21	C	-0.000399	-0.000004	0.000000	0.000000	0.000001	0.000062
22	C	-0.000021	0.000000	0.000000	0.000000	0.000000	0.000004
23	C	0.000002	0.000000	0.000000	0.000000	0.000000	0.000000
24	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
25	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
26	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
27	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
28	H	0.000000	-0.000001	0.000000	0.000000	0.000000	0.000000
29	H	0.000312	0.004428	0.000770	0.000011	-0.000034	-0.000051
30	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
31	H	-0.000067	-0.000007	0.000000	0.000000	0.000000	0.000005
32	H	0.000465	-0.000018	0.000000	0.000001	-0.000013	-0.000092
33	H	-0.000435	-0.000089	-0.000089	0.000074	0.000681	0.002149
34	H	-0.035650	-0.001500	-0.000209	0.000032	-0.000090	-0.004987
35	H	-0.059544	0.000589	0.000376	-0.000003	-0.000105	0.005815
36	H	-0.039170	0.355657	-0.033549	0.004464	0.000337	0.004976
37	H	0.003710	-0.030720	0.355673	-0.034310	0.004295	0.000736
38	H	0.000452	0.004793	-0.034537	0.357665	-0.034716	0.004643
39	H	0.003621	0.000749	0.004315	-0.034524	0.356894	-0.031528
40	H	-0.039457	0.005235	0.000307	0.004573	-0.035621	0.355051
41	H	-0.000319	-0.000001	0.000000	0.000000	0.000002	0.000193
42	H	0.000012	0.000000	0.000000	0.000000	0.000000	-0.000048
43	H	-0.000004	0.000000	0.000000	0.000000	0.000000	0.000000
44	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
45	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
46	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

47	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
		19	20	21	22	23	24
1	C	-0.000171	-0.000044	0.000000	0.000000	0.000000	0.000000
2	C	-0.000003	-0.000062	0.000001	0.000000	0.000000	0.000000
3	C	0.000461	-0.000307	0.000020	-0.000001	0.000000	0.000000
4	C	-0.005047	0.001836	-0.000758	0.000035	0.000000	0.000000
5	C	-0.044969	0.000559	0.001922	-0.000124	-0.000002	0.000000
6	C	0.003623	0.000197	-0.000144	0.000002	0.000000	0.000000
7	O	-0.000166	0.000003	0.000001	0.000000	0.000000	0.000000
8	C	-0.010817	-0.003241	0.001257	0.000187	-0.000003	-0.000001
9	N	0.157873	-0.071663	-0.051735	0.005507	0.000070	0.000002
10	O	0.000970	0.000125	-0.000086	0.000007	0.000000	0.000000
11	O	0.143445	-0.047715	-0.045050	-0.002178	-0.000239	0.000007
12	C	-0.026938	-0.000570	-0.003042	-0.000152	-0.000033	0.000000
13	C	0.005487	-0.000273	-0.000399	-0.000021	0.000002	0.000000
14	C	-0.000109	0.000023	-0.000004	0.000000	0.000000	0.000000
15	C	0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
16	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
17	C	-0.000002	0.000000	0.000001	0.000000	0.000000	0.000000
18	C	0.000050	0.000044	0.000062	0.000004	0.000000	0.000000
19	C	5.000939	0.384717	0.271489	-0.039955	-0.005240	-0.000016
20	H	0.384717	0.593622	-0.076416	0.006807	0.005356	-0.000248
21	C	0.271489	-0.076416	5.356494	0.236662	-0.049791	0.006073
22	C	-0.039955	0.006807	0.236662	4.921798	0.523695	-0.041420
23	C	-0.005240	0.005356	-0.049791	0.523695	5.008082	0.512012
24	C	-0.000016	-0.000248	0.006073	-0.041420	0.512012	4.936076
25	C	0.000026	0.000003	0.000409	-0.031571	-0.059374	0.538827
26	C	-0.000025	-0.000035	0.006015	-0.043966	-0.040589	-0.049327
27	C	-0.003965	0.000594	-0.040877	0.537831	-0.058894	-0.039366
28	H	0.000000	-0.000001	0.000000	0.000000	0.000000	0.000000
29	H	0.000002	-0.000001	0.000000	0.000000	0.000000	0.000000
30	H	-0.000013	0.000008	0.000000	0.000000	0.000000	0.000000
31	H	-0.000171	0.003133	0.000041	0.000007	-0.000003	0.000000
32	H	-0.002782	-0.000466	0.000612	-0.000066	0.000000	0.000000
33	H	-0.000088	0.000007	-0.000001	0.000000	0.000000	0.000000
34	H	0.000025	-0.002121	0.002386	-0.000734	0.000173	0.000003
35	H	-0.005586	0.009113	-0.000529	0.000122	-0.000011	0.000000
36	H	0.000000	0.000007	-0.000001	0.000000	0.000000	0.000000
37	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
38	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
39	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
40	H	-0.000427	0.000051	0.000149	0.000017	0.000000	0.000000
41	H	-0.031655	0.000224	0.366950	-0.041639	-0.003798	0.000321
42	H	-0.026952	0.005140	0.353878	-0.033433	0.004061	-0.000247
43	H	0.000178	0.001170	-0.005966	-0.040964	0.357256	-0.032372
44	H	-0.000001	0.000002	-0.000168	0.003906	-0.031121	0.355293
45	H	0.000000	0.000000	0.000002	0.000405	0.004895	-0.034888
46	H	-0.000001	0.000000	-0.000168	0.004028	0.000704	0.004345
47	H	0.000077	0.000115	-0.007274	-0.036620	0.004791	0.000300
		25	26	27	28	29	30
1	C	0.000000	0.000000	0.000000	0.354352	-0.025712	-0.030133
2	C	0.000000	0.000000	0.000000	-0.028499	0.355451	0.002803
3	C	0.000000	0.000000	0.000000	-0.032067	0.005575	0.383243
4	C	0.000000	0.000000	0.000010	0.003271	-0.000217	-0.042162
5	C	0.000000	0.000000	0.000003	-0.000128	0.002259	0.000932
6	C	0.000000	0.000000	0.000000	0.005897	-0.031186	0.008490
7	O	0.000000	0.000000	0.000000	0.004159	0.002912	-0.023174
8	C	0.000000	-0.000003	0.000122	-0.000108	0.000003	0.000459
9	N	0.000000	0.000001	0.000025	-0.000008	-0.000021	-0.000100
10	O	0.000000	0.000000	-0.000003	0.000002	0.000000	0.005567
11	O	0.000001	-0.000007	0.003906	0.000000	0.000000	0.000163
12	C	0.000000	0.000000	-0.000006	0.000007	-0.000170	-0.000004

13	C	0.000000	0.000000	0.000000	0.000000	0.000312	0.000000
14	C	0.000000	0.000000	0.000000	-0.000001	0.004428	0.000000
15	C	0.000000	0.000000	0.000000	0.000000	0.000770	0.000000
16	C	0.000000	0.000000	0.000000	0.000000	0.000011	0.000000
17	C	0.000000	0.000000	0.000000	0.000000	-0.000034	0.000000
18	C	0.000000	0.000000	0.000000	0.000000	-0.000051	0.000000
19	C	0.000026	-0.000025	-0.003965	0.000000	0.000002	-0.000013
20	H	0.000003	-0.000035	0.000594	-0.000001	-0.000001	0.000008
21	C	0.000409	0.006015	-0.040877	0.000000	0.000000	0.000000
22	C	-0.031571	-0.043966	0.537831	0.000000	0.000000	0.000000
23	C	-0.059374	-0.040589	-0.058894	0.000000	0.000000	0.000000
24	C	0.538827	-0.049327	-0.039366	0.000000	0.000000	0.000000
25	C	4.924672	0.536404	-0.059544	0.000000	0.000000	0.000000
26	C	0.536404	4.947787	0.511800	0.000000	0.000000	0.000000
27	C	-0.059544	0.511800	4.966752	0.000000	0.000000	0.000000
28	H	0.000000	0.000000	0.000000	0.511216	-0.001718	-0.001014
29	H	0.000000	0.000000	0.000000	-0.001718	0.509081	-0.000122
30	H	0.000000	0.000000	0.000000	-0.001014	-0.000122	0.506755
31	H	0.000000	0.000000	0.000000	0.001031	-0.000111	0.002204
32	H	0.000000	0.000000	0.000003	0.000009	-0.000073	-0.000253
33	H	0.000000	0.000000	0.000000	-0.000113	-0.001203	-0.000043
34	H	0.000000	0.000000	0.000000	0.000000	0.000011	0.000000
35	H	0.000000	0.000000	0.000000	-0.000002	-0.000001	0.000011
36	H	0.000000	0.000000	0.000000	0.000000	0.000896	0.000000
37	H	0.000000	0.000000	0.000000	0.000000	0.000011	0.000000
38	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
39	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
40	H	0.000000	0.000000	0.000000	0.000000	-0.000002	0.000000
41	H	0.000001	-0.000223	0.003448	0.000000	0.000000	0.000000
42	H	0.000014	0.000252	-0.003977	0.000000	0.000000	0.000000
43	H	0.004487	0.000365	0.004408	0.000000	0.000000	0.000000
44	H	-0.034371	0.004324	0.000720	0.000000	0.000000	0.000000
45	H	0.357822	-0.034925	0.004747	0.000000	0.000000	0.000000
46	H	-0.034926	0.355214	-0.030633	0.000000	0.000000	0.000000
47	H	0.004601	-0.034948	0.356966	0.000000	0.000000	0.000000

		31	32	33	34	35	36
1	C	-0.004432	0.000686	0.003355	0.000012	0.000729	0.000010
2	C	0.002908	0.007224	-0.039410	0.000033	0.002424	-0.000034
3	C	-0.025428	-0.000588	0.006201	0.000014	-0.000957	-0.000002
4	C	0.360920	-0.084057	0.006956	-0.000209	0.007395	0.000006
5	C	-0.026267	0.422948	-0.041785	0.005226	-0.004112	-0.000014
6	C	-0.004638	-0.056270	0.388362	0.000263	0.001059	-0.000001
7	O	0.003195	0.005306	-0.021965	0.000001	0.000008	0.000000
8	C	-0.031713	0.002532	-0.000064	-0.000013	0.000305	0.000000
9	N	-0.006713	-0.061219	0.000594	-0.041827	-0.062148	0.000053
10	O	0.000761	0.000243	0.000001	0.000000	0.000002	0.000000
11	O	0.000137	0.000968	-0.000005	0.000117	-0.000162	0.000000
12	C	0.002551	0.006158	-0.000630	0.374540	0.365777	-0.006654
13	C	-0.000067	0.000465	-0.000435	-0.035650	-0.059544	-0.039170
14	C	-0.000007	-0.000018	-0.000089	-0.001500	0.000589	0.355657
15	C	0.000000	0.000000	-0.000089	-0.000209	0.000376	-0.033549
16	C	0.000000	0.000001	0.000074	0.000032	-0.000003	0.004464
17	C	0.000000	-0.000013	0.000681	-0.000090	-0.000105	0.000337
18	C	0.000005	-0.000092	0.002149	-0.004987	0.005815	0.004976
19	C	-0.000171	-0.002782	-0.000088	0.000025	-0.005586	0.000000
20	H	0.003133	-0.000466	0.000007	-0.002121	0.009113	0.000007
21	C	0.000041	0.000612	-0.000001	0.002386	-0.000529	-0.000001
22	C	0.000007	-0.000066	0.000000	-0.000734	0.000122	0.000000
23	C	-0.000003	0.000000	0.000000	0.000173	-0.000011	0.000000
24	C	0.000000	0.000000	0.000000	0.000003	0.000000	0.000000
25	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
26	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

27	C	0.000000	0.000003	0.000000	0.000000	0.000000	0.000000
28	H	0.001031	0.000009	-0.000113	0.000000	-0.000002	0.000000
29	H	-0.000111	-0.000073	-0.001203	0.000011	-0.000001	0.000896
30	H	0.002204	-0.000253	-0.000043	0.000000	0.000011	0.000000
31	H	0.477561	0.003625	-0.000041	-0.000252	0.003620	0.000000
32	H	0.003625	0.547088	-0.006820	-0.000176	-0.000407	-0.000001
33	H	-0.000041	-0.006820	0.518406	0.000000	0.000266	0.000010
34	H	-0.000252	-0.000176	0.000000	0.557006	-0.039532	0.000181
35	H	0.003620	-0.000407	0.000266	-0.039532	0.620692	0.005757
36	H	0.000000	-0.000001	0.000010	0.000181	0.005757	0.555282
37	H	0.000000	0.000000	0.000000	0.000003	-0.000002	-0.003827
38	H	0.000000	0.000000	0.000000	0.000000	0.000000	-0.000159
39	H	0.000000	0.000000	0.000001	0.000002	0.000002	0.000011
40	H	0.000001	-0.000190	0.000244	-0.000002	0.000395	-0.000139
41	H	-0.000002	0.000004	0.000000	0.004406	0.000010	0.000000
42	H	0.000003	0.000042	0.000001	-0.000038	0.000009	0.000000
43	H	-0.000001	0.000000	0.000000	0.000656	0.000007	0.000000
44	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
45	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
46	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
47	H	0.000000	-0.000001	0.000000	0.000000	0.000000	0.000000

		37	38	39	40	41	42
1	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
2	C	-0.000003	0.000000	0.000000	-0.000011	0.000000	0.000000
3	C	0.000000	0.000000	0.000000	-0.000002	0.000000	-0.000001
4	C	0.000000	0.000000	0.000000	0.000070	0.000031	0.000016
5	C	0.000000	0.000000	0.000000	0.000482	0.000310	0.000044
6	C	-0.000001	0.000000	-0.000001	-0.000149	0.000002	0.000001
7	O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
8	C	0.000000	0.000000	0.000000	0.000000	-0.000058	0.000051
9	N	0.000001	0.000000	0.000002	0.011752	-0.003017	0.000650
10	O	0.000000	0.000000	0.000000	0.000000	0.000001	-0.000010
11	O	0.000000	0.000000	0.000000	0.000000	0.002759	-0.002310
12	C	-0.000176	0.000004	-0.000175	-0.008157	0.000164	0.000204
13	C	0.003710	0.000452	0.003621	-0.039457	-0.000319	0.000012
14	C	-0.030720	0.004793	0.000749	0.005235	-0.000001	0.000000
15	C	0.355673	-0.034537	0.004315	0.000307	0.000000	0.000000
16	C	-0.034310	0.357665	-0.034524	0.004573	0.000000	0.000000
17	C	0.004295	-0.034716	0.356894	-0.035621	0.000002	0.000000
18	C	0.000736	0.004643	-0.031528	0.355051	0.000193	-0.000048
19	C	0.000000	0.000000	0.000000	-0.000427	-0.031655	-0.026952
20	H	0.000000	0.000000	0.000000	0.000051	0.000224	0.005140
21	C	0.000000	0.000000	0.000000	0.000149	0.366950	0.353878
22	C	0.000000	0.000000	0.000000	0.000017	-0.041639	-0.033433
23	C	0.000000	0.000000	0.000000	0.000000	-0.003798	0.004061
24	C	0.000000	0.000000	0.000000	0.000000	0.000321	-0.000247
25	C	0.000000	0.000000	0.000000	0.000000	0.000001	0.000014
26	C	0.000000	0.000000	0.000000	0.000000	-0.000223	0.000252
27	C	0.000000	0.000000	0.000000	0.000000	0.003448	-0.003977
28	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
29	H	0.000011	0.000000	0.000000	-0.000002	0.000000	0.000000
30	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
31	H	0.000000	0.000000	0.000000	0.000001	-0.000002	0.000003
32	H	0.000000	0.000000	0.000000	-0.000190	0.000004	0.000042
33	H	0.000000	0.000000	0.000001	0.000244	0.000000	0.000001
34	H	0.000003	0.000000	0.000002	-0.000002	0.004406	-0.000038
35	H	-0.000002	0.000000	0.000002	0.000395	0.000010	0.000009
36	H	-0.003827	-0.000159	0.000011	-0.000139	0.000000	0.000000
37	H	0.554513	-0.004073	-0.000167	0.000011	0.000000	0.000000
38	H	-0.004073	0.557857	-0.004021	-0.000155	0.000000	0.000000
39	H	-0.000167	-0.004021	0.554103	-0.003849	0.000000	0.000000
40	H	0.000011	-0.000155	-0.003849	0.557611	0.000271	0.000219

41	H	0.000000	0.000000	0.000000	0.000271	0.554033	-0.028360
42	H	0.000000	0.000000	0.000000	0.000219	-0.028360	0.559673
43	H	0.000000	0.000000	0.000000	0.000000	0.002958	0.000126
44	H	0.000000	0.000000	0.000000	0.000000	-0.000002	0.000002
45	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
46	H	0.000000	0.000000	0.000000	0.000000	0.000003	-0.000004
47	H	0.000000	0.000000	0.000000	0.000000	0.000109	0.004342

		43	44	45	46	47
1	C	0.000000	0.000000	0.000000	0.000000	0.000000
2	C	0.000000	0.000000	0.000000	0.000000	0.000000
3	C	0.000000	0.000000	0.000000	0.000000	0.000000
4	C	0.000000	0.000000	0.000000	0.000000	0.000007
5	C	0.000002	0.000000	0.000000	0.000000	0.000000
6	C	0.000000	0.000000	0.000000	0.000000	0.000000
7	O	0.000000	0.000000	0.000000	0.000000	0.000000
8	C	0.000000	0.000000	0.000000	0.000000	0.000114
9	N	-0.000065	0.000000	0.000000	0.000000	-0.000005
10	O	0.000000	0.000000	0.000000	0.000000	0.000003
11	O	0.000000	0.000000	0.000000	-0.000001	0.001903
12	C	0.000013	0.000000	0.000000	0.000000	0.000000
13	C	-0.000004	0.000000	0.000000	0.000000	0.000000
14	C	0.000000	0.000000	0.000000	0.000000	0.000000
15	C	0.000000	0.000000	0.000000	0.000000	0.000000
16	C	0.000000	0.000000	0.000000	0.000000	0.000000
17	C	0.000000	0.000000	0.000000	0.000000	0.000000
18	C	0.000000	0.000000	0.000000	0.000000	0.000000
19	C	0.000178	-0.000001	0.000000	-0.000001	0.000077
20	H	0.001170	0.000002	0.000000	0.000000	0.000115
21	C	-0.005966	-0.000168	0.000002	-0.000168	-0.007274
22	C	-0.040964	0.003906	0.000405	0.004028	-0.036620
23	C	0.357256	-0.031121	0.004895	0.000704	0.004791
24	C	-0.032372	0.355293	-0.034888	0.004345	0.000300
25	C	0.004487	-0.034371	0.357822	-0.034926	0.004601
26	C	0.000365	0.004324	-0.034925	0.355214	-0.034948
27	C	0.004408	0.000720	0.004747	-0.030633	0.356966
28	H	0.000000	0.000000	0.000000	0.000000	0.000000
29	H	0.000000	0.000000	0.000000	0.000000	0.000000
30	H	0.000000	0.000000	0.000000	0.000000	0.000000
31	H	-0.000001	0.000000	0.000000	0.000000	0.000000
32	H	0.000000	0.000000	0.000000	0.000000	-0.000001
33	H	0.000000	0.000000	0.000000	0.000000	0.000000
34	H	0.000656	0.000000	0.000000	0.000000	0.000000
35	H	0.000007	0.000000	0.000000	0.000000	0.000000
36	H	0.000000	0.000000	0.000000	0.000000	0.000000
37	H	0.000000	0.000000	0.000000	0.000000	0.000000
38	H	0.000000	0.000000	0.000000	0.000000	0.000000
39	H	0.000000	0.000000	0.000000	0.000000	0.000000
40	H	0.000000	0.000000	0.000000	0.000000	0.000000
41	H	0.002958	-0.000002	0.000000	0.000003	0.000109
42	H	0.000126	0.000002	0.000000	-0.000004	0.004342
43	H	0.559495	-0.003887	-0.000162	0.000012	-0.000149
44	H	-0.003887	0.556382	-0.004103	-0.000167	0.000011
45	H	-0.000162	-0.004103	0.558945	-0.004113	-0.000158
46	H	0.000012	-0.000167	-0.004113	0.556481	-0.003991
47	H	-0.000149	0.000011	-0.000158	-0.003991	0.555977

Mulliken atomic charges:

		1
1	C	-0.075112
2	C	-0.068893
3	C	-0.060759
4	C	-0.232573
5	C	0.027787

6	C	-0.092699
7	O	-0.477304
8	C	0.562038
9	N	-0.458891
10	O	-0.460881
11	O	-0.518167
12	C	-0.226346
13	C	0.089853
14	C	-0.180473
15	C	-0.153921
16	C	-0.147046
17	C	-0.154890
18	C	-0.152066
19	C	0.235737
20	H	0.190306
21	C	-0.322016
22	C	0.071821
23	C	-0.171999
24	C	-0.155373
25	C	-0.147483
26	C	-0.158113
27	C	-0.154071
28	H	0.183717
29	H	0.178900
30	H	0.186382
31	H	0.238142
32	H	0.215576
33	H	0.185471
34	H	0.182251
35	H	0.148621
36	H	0.155902
37	H	0.154326
38	H	0.152249
39	H	0.154565
40	H	0.151724
41	H	0.172877
42	H	0.166640
43	H	0.152435
44	H	0.153179
45	H	0.151533
46	H	0.153216
47	H	0.153829

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

		1
1	C	0.108605
2	C	0.110007
3	C	0.125623
4	C	0.005568
5	C	0.243364
6	C	0.092772
7	O	-0.477304
8	C	0.562038
9	N	-0.458891
10	O	-0.460881
11	O	-0.518167
12	C	0.104526
13	C	0.089853
14	C	-0.024571
15	C	0.000405
16	C	0.005202
17	C	-0.000325

```
  18  C   -0.000342
  19  C    0.426043
  20  H    0.000000
  21  C    0.017502
  22  C    0.071821
  23  C   -0.019564
  24  C   -0.002194
  25  C    0.004050
  26  C   -0.004896
  27  C   -0.000242
  28  H    0.000000
  29  H    0.000000
  30  H    0.000000
  31  H    0.000000
  32  H    0.000000
  33  H    0.000000
  34  H    0.000000
  35  H    0.000000
  36  H    0.000000
  37  H    0.000000
  38  H    0.000000
  39  H    0.000000
  40  H    0.000000
  41  H    0.000000
  42  H    0.000000
  43  H    0.000000
  44  H    0.000000
  45  H    0.000000
  46  H    0.000000
  47  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>= 10099.9502
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=    -2.5632    Y=    -5.7256    Z=     4.9850  Tot=     8.0126
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=  -144.0866   YY=  -169.9834   ZZ=  -140.7681
  XY=    -1.3302   XZ=    -2.0459   YZ=    10.2315
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=     7.5261   YY=   -18.3707   ZZ=    10.8446
  XY=    -1.3302   XZ=    -2.0459   YZ=    10.2315
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=     7.2580  YYY=   -37.2529  ZZZ=     0.6482  XYY=   -29.4925
 XXY=   -50.7240  XXZ=    28.2844  XZZ=   -10.4443  YZZ=    -1.3863
 YYZ=    42.5976  XYZ=   -30.4090
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -8334.0345 YYYY= -4086.9590 ZZZZ=  -805.3031 XXXY=   260.3736
XXXZ=    22.4200 YYYX=   -66.9169 YYYZ=   146.9666 ZZZX=   -12.6718
ZZZY=    12.3257 XXYY= -2240.8021 XXZZ= -1546.3230 YYZZ=  -722.5379
XXYZ=   -32.2193 YYXZ=    25.2345 ZZXY=     5.0258
N-N= 2.294595715521D+03 E-N=-7.221647732981D+03  KE= 1.125392772119D+03

Test job not archived.
1|1|UNPC-UNK|SP|RB3LYP|6-31G|C22H21N1O3|PCUSER|18-Jul-2011|0||# RB3LYP
/6-31G SCRF=(PCM,SOLVENT=METHANOL) TEST||[No Title]||0,1|C,0,-2.4604,2
.7047,1.4908|C,0,-3.0522,1.6114,0.9846|C,0,-1.4863,3.1723,0.4463|C,0,-
0.3807,2.1152,0.4054|C,0,-1.016,1.0392,-0.4975|C,0,-2.5116,1.4228,-0.4
028|O,0,-2.301,2.8539,-0.724|C,0,0.9142,2.41,-0.2639|N,0,-0.3369,-0.24
06,-0.329|O,0,1.3617,3.5287,-0.4808|O,0,1.5843,1.272,-0.6142|C,0,-0.92
66,-1.1252,0.6861|C,0,-2.2309,-1.758,0.2491|C,0,-3.2557,-1.9625,1.1854
|C,0,-4.4565,-2.5654,0.8059|C,0,-4.641,-2.9877,-0.5087|C,0,-3.6223,-2.
8166,-1.4431|C,0,-2.4212,-2.2138,-1.0652|C,0,1.1091,-0.0112,-0.0843|H,
```

0,1.3248,0.0053,0.9934|C,0,1.9424,-1.116,-0.7722|C,0,3.3727,-1.1381,-0
.2782|C,0,3.7128,-1.862,0.8735|C,0,5.0265,-1.8623,1.3447|C,0,6.0102,-1
.1396,0.6722|C,0,5.6821,-0.4161,-0.4728|C,0,4.3693,-0.4138,-0.9465|H,0
,-2.5989,3.1279,2.4741|H,0,-3.7854,0.9859,1.4695|H,0,-1.2117,4.227,0.4
722|H,0,-0.1423,1.7821,1.4258|H,0,-0.7776,1.2866,-1.5484|H,0,-3.1875,0
.982,-1.1367|H,0,-0.2498,-1.9624,0.9002|H,0,-1.0565,-0.5842,1.6319|H,0
,-3.1295,-1.6509,2.2209|H,0,-5.2472,-2.7106,1.5385|H,0,-5.5758,-3.4592
,-0.8028|H,0,-3.7607,-3.158,-2.4664|H,0,-1.6326,-2.1009,-1.8071|H,0,1.
5095,-2.1086,-0.5958|H,0,1.9408,-0.9686,-1.8603|H,0,2.9598,-2.4348,1.4
117|H,0,5.284,-2.4282,2.2372|H,0,7.0336,-1.1412,1.04|H,0,6.4502,0.1476
,-0.9974|H,0,4.1307,0.1598,-1.8404||Version=x86-Win32-G03RevB.03|State
=1-A|HF=-1131.0273409|RMSD=1.332e-008|Dipole=-1.0049508,-2.2649857,1.9
48757|PG=C01 [X(C22H21N1O3)]||@

INTERMEDIATE 15i_b

%mem=256MB

RB3LYP/6-31G SCRF=(PCM,Solvent=Methanol) Test

1/38=1/1;
2/17=6,18=5,40=1/2;
3/5=1,6=6,11=2,16=1,25=1,30=1,70=2201,72=3,74=-5/1,2,3;
4/7=1/1;
5/5=2,32=1,38=5,53=3/2;
6/7=2,8=2,9=2,10=2,28=1/1;
99/5=1,9=1/99;

[No Title]

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	0	-0.2907	1.7476	2.432
C	0	-1.4188	1.2517	1.9003
C	0	0.3746	2.528	1.3329
C	0	0.8264	1.494	0.3017
C	0	-0.4637	1.2474	-0.4983
C	0	-1.5114	1.7877	0.5025
O	0	-0.8337	3.0821	0.7322
C	0	1.8357	1.8568	-0.7178
N	0	-0.3018	-0.0928	-1.0417
O	0	2.6461	2.7695	-0.6061
O	0	1.8108	1.05	-1.8123
C	0	-1.4955	-0.5742	-1.7609
C	0	-2.675	-0.8702	-0.8629
C	0	-2.5497	-1.7464	0.2253
C	0	-3.6456	-2.0261	1.0432
C	0	-4.8813	-1.4403	0.7775
C	0	-5.024	-0.5804	-0.3094
C	0	-3.9292	-0.3008	-1.1295
C	0	0.8822	-0.0875	-1.948
H	0	0.5269	0.0224	-2.9811
C	0	1.7021	-1.3991	-1.8896
C	0	2.4074	-1.6438	-0.5744
C	0	1.7711	-2.3504	0.4543
C	0	2.4083	-2.5432	1.6808
C	0	3.6892	-2.0364	1.8895
C	0	4.3363	-1.3401	0.8708
C	0	3.7004	-1.1458	-0.3562
H	0	0.1145	1.5435	3.411
H	0	-2.123	0.5807	2.3669
H	0	1.0683	3.3102	1.6419
H	0	1.2212	0.6109	0.8229

H	0	-0.5251	1.9435	-1.3546
H	0	-2.5161	1.973	0.1223
H	0	-1.7838	0.1448	-2.5395
H	0	-1.2642	-1.5145	-2.2788
H	0	-1.5921	-2.2111	0.4468
H	0	-3.5346	-2.7019	1.8878
H	0	-5.7351	-1.6587	1.4145
H	0	-5.9911	-0.1301	-0.5213
H	0	-4.0662	0.3676	-1.9776
H	0	1.0611	-2.2587	-2.1225
H	0	2.4638	-1.3734	-2.6805
H	0	0.7711	-2.7519	0.3093
H	0	1.9043	-3.0899	2.4744
H	0	4.1853	-2.1885	2.8452
H	0	5.3387	-0.9503	1.0318
H	0	4.2229	-0.6004	-1.1401

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.290700	1.747600	2.432000
2	6	0	-1.418800	1.251700	1.900300
3	6	0	0.374600	2.528000	1.332900
4	6	0	0.826400	1.494000	0.301700
5	6	0	-0.463700	1.247400	-0.498300
6	6	0	-1.511400	1.787700	0.502500
7	8	0	-0.833700	3.082100	0.732200
8	6	0	1.835700	1.856800	-0.717800
9	7	0	-0.301800	-0.092800	-1.041700
10	8	0	2.646100	2.769500	-0.606100
11	8	0	1.810800	1.050000	-1.812300
12	6	0	-1.495500	-0.574200	-1.760900
13	6	0	-2.675000	-0.870200	-0.862900
14	6	0	-2.549700	-1.746400	0.225300
15	6	0	-3.645600	-2.026100	1.043200
16	6	0	-4.881300	-1.440300	0.777500
17	6	0	-5.024000	-0.580400	-0.309400
18	6	0	-3.929200	-0.300800	-1.129500
19	6	0	0.882200	-0.087500	-1.948000
20	1	0	0.526900	0.022400	-2.981100
21	6	0	1.702100	-1.399100	-1.889600
22	6	0	2.407400	-1.643800	-0.574400
23	6	0	1.771100	-2.350400	0.454300
24	6	0	2.408300	-2.543200	1.680800
25	6	0	3.689200	-2.036400	1.889500
26	6	0	4.336300	-1.340100	0.870800
27	6	0	3.700400	-1.145800	-0.356200
28	1	0	0.114500	1.543500	3.411000
29	1	0	-2.123000	0.580700	2.366900
30	1	0	1.068300	3.310200	1.641900
31	1	0	1.221200	0.610900	0.822900
32	1	0	-0.525100	1.943500	-1.354600
33	1	0	-2.516100	1.973000	0.122300
34	1	0	-1.783800	0.144800	-2.539500
35	1	0	-1.264200	-1.514500	-2.278800
36	1	0	-1.592100	-2.211100	0.446800
37	1	0	-3.534600	-2.701900	1.887800
38	1	0	-5.735100	-1.658700	1.414500
39	1	0	-5.991100	-0.130100	-0.521300
40	1	0	-4.066200	0.367600	-1.977600

41	1	0	1.061100	-2.258700	-2.122500
42	1	0	2.463800	-1.373400	-2.680500
43	1	0	0.771100	-2.751900	0.309300
44	1	0	1.904300	-3.089900	2.474400
45	1	0	4.185300	-2.188500	2.845200
46	1	0	5.338700	-0.950300	1.031800
47	1	0	4.222900	-0.600400	-1.140100

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.342100	0.000000			
3	C	1.503220	2.273141	0.000000		
4	C	2.418761	2.766795	1.528611	0.000000	
5	C	2.977715	2.581766	2.386625	1.537911	0.000000
6	C	2.283569	1.499905	2.189658	2.364718	1.546351
7	O	2.228241	2.248814	1.458717	2.337375	2.239901
8	C	3.801939	4.220470	2.605896	1.479760	2.388889
9	N	3.931131	3.422095	3.600671	2.365479	1.455208
10	O	4.347312	5.010905	2.996290	2.400481	3.463996
11	O	4.787174	4.924875	3.760244	2.373852	2.634182
12	C	4.941934	4.091965	4.763666	3.731352	2.444790
13	C	4.836748	3.703481	5.066494	4.382412	3.083344
14	C	4.709633	3.615683	5.296112	4.680180	3.719924
15	C	5.236882	4.054286	6.081592	5.739313	4.818352
16	C	5.828695	4.527301	6.609112	6.435398	5.326029
17	C	5.944660	4.608344	6.442374	6.237288	4.916592
18	C	5.488070	4.229900	5.708609	5.280660	3.847730
19	C	4.891593	4.679473	4.226441	2.750528	2.386427
20	H	5.739899	5.396758	4.991174	3.609998	2.940444
21	C	5.705191	5.579435	5.250607	3.733453	3.691933
22	C	5.274446	5.398876	5.017368	3.621174	4.075297
23	C	4.995590	5.024092	5.149848	3.961711	4.341191
24	C	5.124438	5.394084	5.474855	4.550089	5.231205
25	C	5.518384	6.074815	5.668344	4.814609	5.807883
26	C	5.777574	6.395191	5.556150	4.547021	5.622241
27	C	5.663453	6.086543	5.235533	3.957430	4.804927
28	H	1.079020	2.172181	2.314172	3.190141	3.962905
29	H	2.173296	1.078821	3.331537	3.714583	3.377445
30	H	2.216497	3.238805	1.090201	2.270074	3.344043
31	H	2.483371	2.922502	2.156874	1.098809	2.233739
32	H	3.798902	3.445528	2.893744	2.184475	1.105249
33	H	3.215264	2.210345	3.182723	3.381410	2.263622
34	H	5.432691	4.590237	5.033271	4.087285	2.669249
35	H	5.812111	5.014044	5.663201	4.481145	3.382170
36	H	4.615839	3.759479	5.206933	4.426959	3.758686
37	H	5.533271	4.484163	6.552985	6.256166	5.542641
38	H	6.502282	5.228468	7.406993	7.364178	6.316002
39	H	6.688968	5.355319	7.143227	7.056439	5.696506
40	H	5.966856	4.777915	5.945372	5.513757	3.992541
41	H	6.214602	5.886912	5.943363	4.473767	4.154007
42	H	6.592842	6.553584	5.974367	4.449335	4.494535
43	H	5.087119	4.832779	5.392802	4.246267	4.262787
44	H	5.312366	5.497461	5.933279	5.186004	5.766848
45	H	5.974797	6.643324	6.249309	5.595749	6.678144
46	H	6.397606	7.160091	6.068898	5.183483	6.390535
47	H	6.216558	6.671063	5.541843	4.242819	5.078434

		6	7	8	9	10
6	C	0.000000				
7	O	1.479024	0.000000			
8	C	3.563283	3.275600	0.000000		
9	N	2.717345	3.675545	2.911144	0.000000	

10	O	4.413358	3.741360	1.225662	4.131903	0.000000
11	O	4.115764	4.194913	1.359955	2.522478	2.260382
12	C	3.271361	4.474601	4.253788	1.474420	5.446719
13	C	3.206667	4.642780	5.272950	2.503677	6.451935
14	C	3.693883	5.149370	5.753627	3.064757	6.934040
15	C	4.403662	5.839282	6.944255	4.389243	8.081056
16	C	4.674595	6.069367	7.630523	5.108529	8.734902
17	C	4.313402	5.661930	7.291243	4.803456	8.374980
18	C	3.587619	4.948945	6.169182	3.634419	7.275662
19	C	3.905208	4.491564	2.490554	1.491061	3.615866
20	H	4.405272	5.000159	3.193823	2.112176	4.204544
21	C	5.119025	5.777999	3.462925	2.537906	4.462705
22	C	5.319013	5.877590	3.549874	3.156538	4.419864
23	C	5.282140	6.031108	4.367897	3.410526	5.301269
24	C	5.958954	6.561586	5.043922	4.556436	5.788890
25	C	6.602556	6.927843	5.038897	5.319548	5.514776
26	C	6.641865	6.804702	4.358534	5.169660	4.682608
27	C	6.041990	6.294268	3.552952	4.194797	4.062459
28	H	3.341041	3.231461	4.484158	4.762071	4.903995
29	H	2.303669	3.254465	5.178331	3.922872	6.031077
30	H	3.204854	2.120657	2.875667	4.545249	2.799163
31	H	2.992427	3.215225	2.074520	2.508277	2.954985
32	H	2.108526	2.397160	2.446714	2.072266	3.361404
33	H	1.090096	2.105362	4.433670	3.244310	5.273830
34	H	3.468009	4.498271	4.398899	2.120420	5.500100
35	H	4.324496	5.511822	4.838571	2.116096	6.036640
36	H	4.000002	5.354866	5.445541	2.892698	6.623995
37	H	5.115555	6.487290	7.510727	5.083342	8.623039
38	H	5.527120	6.853061	8.615246	6.164877	9.692074
39	H	4.979341	6.203891	8.077449	5.713173	9.111317
40	H	3.833351	5.016033	6.215886	3.906224	7.259828
41	H	5.466419	6.345370	4.417072	2.777904	5.485844
42	H	5.993852	6.509340	3.831565	3.460368	4.636808
43	H	5.084791	6.065458	4.840292	3.169721	5.902494
44	H	6.272669	6.973198	5.887673	5.119809	6.661255
45	H	7.331494	7.578546	5.880480	6.295555	6.233969
46	H	7.395990	7.378925	4.817875	6.070416	4.875420
47	H	6.425212	6.529588	3.451796	4.554147	3.758681

		11	12	13	14	15
11	O	0.000000				
12	C	3.684059	0.000000			
13	C	4.971009	1.511701	0.000000		
14	C	5.566473	2.535820	1.402714	0.000000	
15	C	6.883936	3.820199	2.431334	1.395776	0.000000
16	C	7.595582	4.319403	2.807790	2.415570	1.393095
17	C	7.185500	3.815390	2.430668	2.787045	2.412377
18	C	5.936201	2.529093	1.402965	2.414179	2.788855
19	C	1.474659	2.434202	3.800491	4.387838	5.762501
20	H	2.017537	2.436169	3.941531	4.782794	6.148260
21	C	2.452729	3.304795	4.526903	4.761431	6.131259
22	C	3.024051	4.217162	5.149027	5.022239	6.277069
23	C	4.086780	4.328126	4.867629	4.368818	5.458261
24	C	5.046765	5.564343	5.925308	5.228301	6.109307
25	C	5.172772	6.507270	7.031271	6.463554	7.383469
26	C	4.392010	6.443783	7.237738	6.928113	8.013179
27	C	3.242276	5.412697	6.401439	6.305760	7.529739
28	H	5.513968	5.815952	5.645660	5.298121	5.699726
29	H	5.758536	4.332007	3.583493	3.191225	3.296346
30	H	4.194199	5.765473	6.145084	6.376981	7.145306
31	H	2.735821	3.932041	4.496215	4.487056	5.539679
32	H	2.542491	2.728657	3.575017	4.495604	5.589695
33	H	4.828734	3.328107	3.013247	3.720978	4.256363

34	H	3.777480	1.098315	2.153010	3.436184	4.584195
35	H	4.031117	1.098128	2.100060	2.824324	4.119282
36	H	5.226666	2.750039	2.164717	1.087201	2.146341
37	H	7.506051	4.690208	3.414731	2.155670	1.087371
38	H	8.642332	5.406803	3.895189	3.401273	2.153801
39	H	7.995559	4.684469	3.414814	3.874670	3.397624
40	H	5.918794	2.746351	2.170286	3.409037	3.877104
41	H	3.406724	3.082937	4.180068	4.337337	5.677040
42	H	2.655757	4.142516	5.473952	5.806719	7.184478
43	H	4.476227	3.763719	4.097616	3.470706	4.535707
44	H	5.960144	5.985412	6.085608	5.167355	5.829356
45	H	6.149670	7.489567	7.908959	7.240135	8.037199
46	H	4.953401	7.392355	8.235028	7.969383	9.048487
47	H	2.998983	5.752059	6.908738	7.003267	8.289313

		16	17	18	19	20
16	C	0.000000				
17	C	1.393249	0.000000			
18	C	2.416941	1.396183	0.000000		
19	C	6.517388	6.149078	4.885183	0.000000	
20	H	6.746495	6.189817	4.836291	1.098004	0.000000
21	C	7.103258	6.957566	5.787534	1.547883	2.143159
22	C	7.415807	7.511774	6.501099	2.575865	3.479182
23	C	6.722140	7.063251	6.261206	3.417880	4.356626
24	C	7.427692	7.940564	7.286292	4.639788	5.644048
25	C	8.662872	9.103568	8.376556	5.138469	6.161294
26	C	9.218617	9.464948	8.567370	4.630923	5.586150
27	C	8.661269	8.742827	7.715103	3.405301	4.280875
28	H	6.387206	6.690031	6.353668	5.654061	6.583522
29	H	3.770789	4.114187	4.032891	5.300574	5.994562
30	H	7.662387	7.487353	6.759807	4.946350	5.698673
31	H	6.438167	6.457850	5.582982	2.877598	3.911368
32	H	5.913749	5.263327	4.083558	2.541176	2.728155
33	H	4.204055	3.604966	2.955338	4.481099	4.764009
34	H	4.807238	3.999770	2.605648	2.740692	2.355701
35	H	4.736020	4.345938	3.145820	2.598613	2.462382
36	H	3.394456	3.874140	3.405291	4.045603	4.607514
37	H	2.153602	3.398053	3.876221	6.407540	6.900998
38	H	1.087401	2.154118	3.402514	7.587077	7.833265
39	H	2.152943	1.087637	2.156497	7.019939	6.968371
40	H	3.394623	2.144522	1.088486	4.969372	4.714100
41	H	6.662724	6.567531	5.451836	2.185535	2.495192
42	H	8.118666	7.894182	6.665322	2.165999	2.406283
43	H	5.821437	6.219436	5.492800	3.493819	4.310813
44	H	7.186447	7.877085	7.402493	5.442124	6.430095
45	H	9.329438	9.866544	9.230751	6.188654	7.226184
46	H	10.234900	10.455678	9.538713	5.429919	6.340578
47	H	9.341792	9.284160	8.157610	3.475060	4.175832

		21	22	23	24	25
21	C	0.000000				
22	C	1.512309	0.000000			
23	C	2.530534	1.400852	0.000000		
24	C	3.815159	2.427931	1.395528	0.000000	
25	C	4.316980	2.804986	2.416092	1.393236	0.000000
26	C	3.816058	2.429299	2.788266	2.412620	1.393313
27	C	2.531537	1.402663	2.414574	2.787762	2.415877
28	H	6.267035	5.594612	5.162253	4.995621	5.282909
29	H	6.055476	5.841590	5.235781	5.546365	6.392088
30	H	5.920363	5.589928	5.826381	6.004948	5.959577
31	H	3.410135	2.905717	3.034395	3.477578	3.773176
32	H	4.052113	4.698616	5.194442	6.160273	6.642598
33	H	5.762986	6.148779	6.097712	6.861100	7.596317
34	H	3.867492	4.962546	5.275052	6.527632	7.370713

35	H	2.993949	4.049981	4.169126	5.497628	6.494865
36	H	4.119449	4.166615	3.366092	4.199553	5.477594
37	H	6.587038	6.518387	5.507171	5.948621	7.254390
38	H	8.142261	8.381900	7.598913	8.195622	9.443819
39	H	7.916308	8.533986	8.132237	9.012337	10.156483
40	H	6.033428	6.922586	6.883003	7.985975	8.993326
41	H	1.097286	2.141784	2.674398	4.044871	4.801299
42	H	1.098349	2.124136	3.355791	4.515800	4.777664
43	H	2.744447	2.164784	1.087303	2.145924	3.394743
44	H	4.684462	3.411671	2.155321	1.087519	2.153564
45	H	5.404421	3.892466	3.401614	2.153919	1.087480
46	H	4.686241	3.413699	3.875765	3.397908	2.153163
47	H	2.748473	2.169041	3.408216	3.876174	3.394909

		26	27	28	29	30
26	C	0.000000				
27	C	1.395582	0.000000			
28	H	5.708884	5.855152	0.000000		
29	H	6.902923	6.656430	2.650195	0.000000	
30	H	5.735827	5.547638	2.675944	4.261478	0.000000
31	H	3.675941	3.259249	2.965264	3.683547	2.824953
32	H	6.274364	5.328736	4.824938	4.273180	3.658662
33	H	7.648024	6.971424	4.233211	2.670441	4.116456
34	H	7.161752	6.042259	6.400653	4.937391	5.969785
35	H	6.427752	5.336627	6.604998	5.168165	6.640043
36	H	6.007025	5.458043	5.078975	3.429692	6.244257
37	H	8.052320	7.733189	5.801680	3.605220	7.575784
38	H	10.091096	9.613902	6.961172	4.355370	8.427807
39	H	10.490817	9.745977	7.452669	4.879460	8.145565
40	H	9.035022	8.077091	6.920838	4.764044	6.937057
41	H	4.531071	3.365155	6.780295	6.193173	6.721860
42	H	4.014860	2.642603	7.150796	7.094610	6.524314
43	H	3.875450	3.406354	5.338738	4.869882	6.213953
44	H	3.398229	3.875280	5.054602	5.450138	6.507936
45	H	2.154261	3.401663	5.551519	6.905931	6.434230
46	H	1.087507	2.156106	6.258746	7.733267	6.063035
47	H	2.145631	1.088562	6.495211	7.346053	5.743154

		31	32	33	34	35
31	H	0.000000				
32	H	3.093039	0.000000			
33	H	4.039006	2.479150	0.000000		
34	H	4.533543	2.494722	3.311157	0.000000	
35	H	4.507225	3.654884	4.415336	1.758188	0.000000
36	H	4.002473	4.652336	4.297182	3.808543	2.832254
37	H	5.892902	6.414826	5.099904	5.547070	4.891338
38	H	7.341062	6.912876	5.022050	5.873627	5.800880
39	H	7.373820	5.905198	4.112527	4.674406	5.229623
40	H	5.988205	3.925682	3.064262	2.361085	3.388838
41	H	4.115291	4.556774	5.978526	3.747554	2.446484
42	H	4.213705	4.657613	6.622196	4.512972	3.752233
43	H	3.431443	5.147376	5.758935	4.799380	3.517366
44	H	4.109744	6.774831	7.120763	7.014596	5.925723
45	H	4.551069	7.543183	8.345120	8.370749	7.510440
46	H	4.408491	6.960829	8.430347	8.042601	7.407880
47	H	3.785607	5.390820	7.323262	6.212414	5.678070

		36	37	38	39	40
36	H	0.000000				
37	H	2.467929	0.000000			
38	H	4.290226	2.480822	0.000000		
39	H	4.961752	4.295615	2.479814	0.000000	
40	H	4.318400	4.964448	4.289226	2.464499	0.000000
41	H	3.693648	6.115504	7.684966	7.538455	5.762608
42	H	5.189612	7.656049	9.169099	8.814379	6.794560

43	H	2.428186	4.586198	6.689334	7.300074	6.193599
44	H	4.136214	5.484184	7.844243	8.948295	8.211058
45	H	6.255492	7.795964	10.037028	10.914644	9.893447
46	H	7.068793	9.084949	11.103033	11.465130	9.962203
47	H	6.239137	8.588556	10.334783	10.243529	8.387348

		41	42	43	44	45
41	H	0.000000				
42	H	1.750054	0.000000			
43	H	2.498199	3.701945	0.000000		
44	H	4.746933	5.461905	2.466991	0.000000	
45	H	5.868867	5.844768	4.290101	2.480519	0.000000
46	H	5.473516	4.714365	4.962936	4.295822	2.480300
47	H	3.702978	2.462680	4.317943	4.963681	4.290232

		46	47
46	H	0.000000	
47	H	2.466696	0.000000

Stoichiometry C22H21NO3
Framework group C1[X(C22H21NO3)]
Deg. of freedom 135
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	-0.274830	1.762241	2.439431
2	6	0	-1.401974	1.261559	1.910191
3	6	0	0.380228	2.552881	1.341498
4	6	0	0.834279	1.527393	0.302815
5	6	0	-0.457749	1.276323	-0.492669
6	6	0	-1.504505	1.804276	0.515680
7	8	0	-0.834475	3.101985	0.749182
8	6	0	1.836490	1.902347	-0.719278
9	7	0	-0.289322	-0.059876	-1.043882
10	8	0	2.641243	2.819884	-0.606392
11	8	0	1.812045	1.101171	-1.817912
12	6	0	-1.483011	-0.545513	-1.760245
13	6	0	-2.656415	-0.854176	-0.858530
14	6	0	-2.520305	-1.735230	0.224440
15	6	0	-3.610584	-2.026609	1.045768
16	6	0	-4.851380	-1.447755	0.788734
17	6	0	-5.004774	-0.583125	-0.292944
18	6	0	-3.915604	-0.291842	-1.116467
19	6	0	0.890496	-0.041828	-1.955457
20	1	0	0.529787	0.071114	-2.986352
21	6	0	1.719438	-1.348164	-1.907692
22	6	0	2.432319	-1.595029	-0.596991
23	6	0	1.805446	-2.311306	0.430803
24	6	0	2.449479	-2.506265	1.653387
25	6	0	3.727881	-1.991954	1.859005
26	6	0	4.365668	-1.285956	0.841107
27	6	0	3.722923	-1.089486	-0.381974
28	1	0	0.136165	1.555723	3.415504
29	1	0	-2.099532	0.583383	2.376394
30	1	0	1.070055	3.338099	1.651513
31	1	0	1.237357	0.644240	0.817550
32	1	0	-0.527702	1.976493	-1.344986
33	1	0	-2.512140	1.984803	0.140989
34	1	0	-1.779657	0.175619	-2.533722
35	1	0	-1.247754	-1.481493	-2.284153

```
  36        1          0      -1.558613   -2.194628    0.439167
  37        1          0      -3.491222   -2.706083    1.886269
  38        1          0      -5.700798   -1.675253    1.428402
  39        1          0      -5.975826   -0.138240   -0.498105
  40        1          0      -4.060931    0.380077   -1.960391
  41        1          0       1.083173   -2.210825   -2.142256
  42        1          0       2.477355   -1.313169   -2.701862
  43        1          0       0.807517   -2.718765    0.288178
  44        1          0       1.952763   -3.060519    2.446339
  45        1          0       4.229318   -2.145739    2.811645
  46        1          0       5.366149   -0.890265    0.999659
  47        1          0       4.238191   -0.536459   -1.165317
---------------------------------------------------------------------
Rotational constants (GHZ):      0.3130871      0.1709984      0.1481115
Standard basis: 6-31G (6D, 7F)
There are   276 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.
  276 basis functions,   656 primitive gaussians,   276 cartesian basis functions
   92 alpha electrons       92 beta electrons
      nuclear repulsion energy      2388.6614447516 Hartrees.
NAtoms=   47 NActive=   47 NUniq=   47 SFac= 1.00D+00 NAtFMM=   60 Big=F
---------------------------------------------------------------------------
United Atom Topological Model (UA0  parameters set).
 Nord Group  Hybr  Charge Alpha Radius          Bonded to
  1   CH    *     0.00   1.00  2.125   C2   [d]  C3   [s]
  2   CH    *     0.00   1.00  2.125   C1   [d]  C6   [s]
  3   CH    *     0.00   1.00  2.125   C1   [s]  C4   [s]  O7   [s]
  4   CH    *     0.00   1.00  2.125   C3   [s]  C5   [s]  C8   [s]
  5   CH    *     0.00   1.00  2.125   C4   [s]  C6   [s]  N9   [s]
  6   CH    *     0.00   1.00  2.125   C2   [s]  C5   [s]  O7   [s]
  7   O     *     0.00   1.00  1.750   C3   [s]  C6   [s]
  8   C     *     0.00   1.00  1.925   C4   [s]  O10  [d]  O11  [s]
  9   N     *     0.00   1.00  1.830   C5   [s]  C12  [s]  C19  [s]
 10   O     *     0.00   1.00  1.750   C8   [d]
 11   O     *     0.00   1.00  1.750   C8   [s]  C19  [s]
 12   CH2   *     0.00   1.00  2.325   N9   [s]  C13  [s]
 13   C     *     0.00   1.00  1.925   C12  [s]  C14  [s]  C18  [s]
 14   CH    *     0.00   1.00  2.125   C13  [s]  C15  [s]
 15   CH    *     0.00   1.00  2.125   C14  [s]  C16  [s]
 16   CH    *     0.00   1.00  2.125   C15  [s]  C17  [s]
 17   CH    *     0.00   1.00  2.125   C16  [s]  C18  [s]
 18   CH    *     0.00   1.00  2.125   C13  [s]  C17  [s]
 19   CH    *     0.00   1.00  2.125   N9   [s]  O11  [s]  C21  [s]
 21   CH2   *     0.00   1.00  2.325   C19  [s]  C22  [s]
 22   C     *     0.00   1.00  1.925   C21  [s]  C23  [s]  C27  [s]
 23   CH    *     0.00   1.00  2.125   C22  [s]  C24  [s]
 24   CH    *     0.00   1.00  2.125   C23  [s]  C25  [s]
 25   CH    *     0.00   1.00  2.125   C24  [s]  C26  [s]
 26   CH    *     0.00   1.00  2.125   C25  [s]  C27  [s]
 27   CH    *     0.00   1.00  2.125   C22  [s]  C26  [s]
---------------------------------------------------------------------------
Polarizable Continuum Model (PCM)
=================================
Model               : PCM.
Atomic radii        : UA0 (Simple United Atom Topological Model).
Polarization charges : Total charges.
Charge compensation  : None.
Solution method      : Matrix inversion.
Cavity              : GePol (RMin=0.200 OFac=0.890).
                      Default sphere list used, NSphG=   26.
```

```
                Tesserae with average area of 0.200 Ang**2.
Solvent           : Methanol, Eps=  32.630000.
-----------------------------------------------------------------------------
One-electron integrals computed using PRISM.
NBasis=   276 RedAO= T  NBF=   276
NBsUse=   276 1.00D-06 NBFU=   276
Harris functional with IExCor=  402 diagonalized for initial guess.
ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 402 AccDes= 1.00D-06 IRadAn=         1 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)
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              (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)
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              (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)
              (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.
Warning!  Cutoffs for single-point calculations used.
Requested convergence on RMS density matrix=1.00D-04 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-02.
Requested convergence on             energy=5.00D-05.
No special actions if energy rises.
Error on total polarization charges =  0.02431
SCF Done:  E(RB+HF-LYP) =  -1131.02725493     A.U. after    8 cycles
           Convg  =    0.5587D-05             -V/T =  2.0050
           S**2   =   0.0000
--------------------------------------------------------------------
Variational PCM results
=======================
<psi(f)|   H    |psi(f)>                (a.u.) =   -1130.996922
<psi(f)|H+V(f)/2|psi(f)>                (a.u.) =   -1131.027255
Total free energy in solution:
 with all non electrostatic terms       (a.u.) =   -1131.016922
--------------------------------------------------------------------
(Polarized solute)-Solvent          (kcal/mol) =     -19.03
--------------------------------------------------------------------
Cavitation energy                   (kcal/mol) =      30.35
Dispersion energy                   (kcal/mol) =     -25.77
Repulsion energy                    (kcal/mol) =       1.91
Total non electrostatic             (kcal/mol) =       6.48
--------------------------------------------------------------------
Partition over spheres:
Sphere  on Atom  Surface  Charge   GEl    GCav    GDR
```

1	C1	16.94	-0.040	-0.70	1.73	-1.48
2	C2	10.54	-0.013	-0.35	1.49	-0.89
3	C3	9.56	-0.056	-0.20	1.13	-0.98
4	C4	0.00	0.000	0.00	0.50	-0.01
5	C5	3.42	-0.034	-0.30	0.48	-0.42
6	C6	6.80	-0.034	-0.34	0.85	-0.63
7	O7	8.61	0.130	-2.79	0.97	-1.03
8	C8	1.71	-0.008	0.04	0.39	-0.12
9	N9	0.00	0.000	0.00	0.09	0.00
10	O10	15.97	0.194	-4.82	1.93	-1.61
11	O11	6.14	0.067	-1.06	0.75	-0.67
12	C12	17.18	-0.061	-0.79	1.76	-1.52
13	C13	0.00	0.000	0.00	0.05	0.00
14	C14	6.16	0.005	-0.07	1.30	-0.57
15	C15	15.20	-0.025	-0.56	1.66	-1.44
16	C16	16.51	-0.020	-0.53	1.69	-1.50
17	C17	17.33	-0.020	-0.54	1.69	-1.53
18	C18	12.38	-0.023	-0.56	1.43	-1.18
19	C19	6.06	-0.053	-0.82	0.57	-0.54
20	C21	21.52	-0.063	-0.62	1.96	-1.78
21	C22	0.06	0.000	0.00	0.06	0.00
22	C23	7.75	0.001	-0.19	1.44	-0.66
23	C24	14.99	-0.023	-0.52	1.69	-1.36
24	C25	16.18	-0.018	-0.47	1.69	-1.49
25	C26	16.45	-0.020	-0.42	1.69	-1.48
26	C27	10.14	-0.020	-0.26	1.37	-0.98
Added spheres:		77.97	0.109	-2.16	0.00	0.00

****

Population analysis using the SCF density.

****

```
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)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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The electronic state is 1-A.
Alpha  occ. eigenvalues --  -19.20681 -19.15178 -19.14981 -14.34637 -10.33732
```

Alpha occ. eigenvalues -- -10.29101 -10.24653 -10.24359 -10.23338 -10.21682
Alpha occ. eigenvalues -- -10.20550 -10.19702 -10.19368 -10.19112 -10.18612
Alpha occ. eigenvalues -- -10.18531 -10.18524 -10.18460 -10.18420 -10.18412
Alpha occ. eigenvalues -- -10.18306 -10.18230 -10.18221 -10.18185 -10.18173
Alpha occ. eigenvalues -- -10.18099 -1.12600 -1.06661 -1.04848 -0.94913
Alpha occ. eigenvalues -- -0.86072 -0.85931 -0.82906 -0.79663 -0.78647
Alpha occ. eigenvalues -- -0.76767 -0.75695 -0.74676 -0.74465 -0.72524
Alpha occ. eigenvalues -- -0.68328 -0.65941 -0.64667 -0.60722 -0.60391
Alpha occ. eigenvalues -- -0.59865 -0.58554 -0.57929 -0.56101 -0.55448
Alpha occ. eigenvalues -- -0.55137 -0.51718 -0.51218 -0.50436 -0.49738
Alpha occ. eigenvalues -- -0.48652 -0.48072 -0.46509 -0.45926 -0.45556
Alpha occ. eigenvalues -- -0.44852 -0.44702 -0.44155 -0.42447 -0.42200
Alpha occ. eigenvalues -- -0.41849 -0.41402 -0.40823 -0.40603 -0.39994
Alpha occ. eigenvalues -- -0.39698 -0.39051 -0.38636 -0.37037 -0.36850
Alpha occ. eigenvalues -- -0.35952 -0.35290 -0.35176 -0.34453 -0.34103
Alpha occ. eigenvalues -- -0.33670 -0.33570 -0.33305 -0.30992 -0.28327
Alpha occ. eigenvalues -- -0.27717 -0.25273 -0.25075 -0.24859 -0.24463
Alpha occ. eigenvalues -- -0.24354 -0.22324
Alpha virt. eigenvalues -- -0.01035 -0.00510 -0.00189 0.00121 0.00318
Alpha virt. eigenvalues -- 0.00522 0.07495 0.08961 0.09595 0.09825
Alpha virt. eigenvalues -- 0.10834 0.11393 0.12716 0.13145 0.13529
Alpha virt. eigenvalues -- 0.13930 0.14258 0.14554 0.15175 0.15677
Alpha virt. eigenvalues -- 0.16187 0.16485 0.16750 0.17311 0.17711
Alpha virt. eigenvalues -- 0.18014 0.18039 0.18809 0.18923 0.19855
Alpha virt. eigenvalues -- 0.20612 0.21072 0.21621 0.22618 0.23611
Alpha virt. eigenvalues -- 0.24001 0.25644 0.26162 0.26561 0.27122
Alpha virt. eigenvalues -- 0.27775 0.29121 0.31275 0.31658 0.32190
Alpha virt. eigenvalues -- 0.32881 0.33516 0.33910 0.34425 0.35269
Alpha virt. eigenvalues -- 0.35561 0.36396 0.36811 0.37068 0.42099
Alpha virt. eigenvalues -- 0.47184 0.49039 0.49194 0.50480 0.52802
Alpha virt. eigenvalues -- 0.53401 0.53544 0.54103 0.54260 0.54800
Alpha virt. eigenvalues -- 0.55335 0.56462 0.56623 0.57221 0.57787
Alpha virt. eigenvalues -- 0.58186 0.58978 0.59477 0.59680 0.60335
Alpha virt. eigenvalues -- 0.61364 0.62087 0.62249 0.62454 0.62750
Alpha virt. eigenvalues -- 0.63057 0.63537 0.64049 0.64443 0.64758
Alpha virt. eigenvalues -- 0.65005 0.65403 0.65767 0.66298 0.66455
Alpha virt. eigenvalues -- 0.66690 0.67252 0.67564 0.68175 0.68546
Alpha virt. eigenvalues -- 0.70690 0.71123 0.72502 0.74084 0.74543
Alpha virt. eigenvalues -- 0.75820 0.76903 0.78194 0.80690 0.82104
Alpha virt. eigenvalues -- 0.82572 0.83573 0.84426 0.85084 0.85483
Alpha virt. eigenvalues -- 0.85932 0.86590 0.86771 0.87149 0.87340
Alpha virt. eigenvalues -- 0.87410 0.88119 0.88203 0.89296 0.89864
Alpha virt. eigenvalues -- 0.91011 0.91597 0.93184 0.93936 0.94924
Alpha virt. eigenvalues -- 0.95079 0.95936 0.96972 0.97758 0.97997
Alpha virt. eigenvalues -- 0.98251 0.99534 0.99945 1.00396 1.01311
Alpha virt. eigenvalues -- 1.02023 1.02755 1.04229 1.05326 1.05633
Alpha virt. eigenvalues -- 1.06666 1.07234 1.08435 1.09064 1.10152
Alpha virt. eigenvalues -- 1.14523 1.15551 1.15918 1.17270 1.17944
Alpha virt. eigenvalues -- 1.19710 1.20334 1.21763 1.22370 1.22908
Alpha virt. eigenvalues -- 1.23729 1.24944 1.26514 1.28179 1.29946
Alpha virt. eigenvalues -- 1.33772 1.36360 1.37499 1.41759 1.44285
Alpha virt. eigenvalues -- 1.45179 1.48633 1.49248 1.52422 1.54064
Alpha virt. eigenvalues -- 1.54918 1.60632 1.63214 1.69693 1.75602
Alpha virt. eigenvalues -- 1.81771 1.84021 1.86687 1.92631 1.93120
Alpha virt. eigenvalues -- 1.98963 2.06100 2.11096 2.46885

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	5.076045	0.636843	0.277324	-0.050621	-0.018417	-0.055586
2	C	0.636843	5.080092	-0.040325	-0.043716	-0.031561	0.256239
3	C	0.277324	-0.040325	5.358540	0.112553	-0.061983	-0.148499
4	C	-0.050621	-0.043716	0.112553	6.094769	0.198631	-0.013172
5	C	-0.018417	-0.031561	-0.061983	0.198631	5.425540	0.166117

6	C	-0.055586	0.256239	-0.148499	-0.013172	0.166117	5.417833
7	O	-0.090523	-0.103723	0.204745	-0.100224	-0.072092	0.197880
8	C	0.005953	0.001654	0.002803	0.078672	-0.022848	0.001484
9	N	-0.000513	0.001740	0.008239	-0.049670	0.114578	-0.017588
10	O	0.000160	-0.000026	0.004499	-0.123312	0.002662	-0.000186
11	O	-0.000138	-0.000042	0.004712	-0.137410	0.014676	0.000477
12	C	-0.000023	-0.000127	-0.000291	0.007353	-0.054708	-0.004983
13	C	0.000028	-0.000172	-0.000044	0.000154	-0.003682	0.004991
14	C	-0.000027	0.000847	0.000016	-0.000131	-0.000972	-0.000417
15	C	0.000003	-0.000973	0.000002	-0.000005	-0.000009	-0.000173
16	C	0.000002	-0.000199	0.000000	0.000000	0.000006	-0.000041
17	C	0.000001	0.000046	0.000000	0.000000	0.000006	-0.000558
18	C	0.000013	0.000046	-0.000004	-0.000012	0.000777	-0.001371
19	C	-0.000137	-0.000027	0.000554	-0.008864	-0.048134	0.004032
20	H	-0.000001	0.000016	0.000064	-0.000839	-0.004478	-0.000514
21	C	0.000005	-0.000008	-0.000060	-0.000818	0.006787	0.000023
22	C	-0.000024	-0.000010	0.000079	-0.001733	-0.000732	0.000002
23	C	0.000002	0.000032	0.000034	-0.001635	-0.000218	-0.000023
24	C	0.000009	-0.000004	-0.000008	-0.000307	-0.000011	0.000001
25	C	0.000000	0.000000	-0.000003	-0.000015	0.000004	0.000000
26	C	-0.000001	0.000000	0.000001	0.000016	0.000011	0.000000
27	C	-0.000001	0.000001	0.000036	-0.000374	-0.000013	-0.000001
28	H	0.353836	-0.028973	-0.032643	0.003070	-0.000101	0.006096
29	H	-0.026117	0.354351	0.005576	-0.000133	0.002266	-0.030895
30	H	-0.030873	0.002973	0.381729	-0.043824	0.002225	0.008467
31	H	-0.004651	0.004033	-0.023580	0.348439	-0.021488	-0.006079
32	H	0.000342	0.008317	0.002310	-0.075469	0.404219	-0.071924
33	H	0.003334	-0.038238	0.006668	0.005548	-0.040894	0.385565
34	H	-0.000003	0.000151	0.000032	-0.000222	-0.005903	-0.001737
35	H	0.000000	-0.000009	0.000004	-0.000296	0.006029	0.000251
36	H	0.000009	0.000321	0.000001	-0.000038	0.000120	-0.000161
37	H	0.000000	-0.000020	0.000000	0.000000	0.000001	-0.000001
38	H	0.000000	-0.000001	0.000000	0.000000	0.000000	0.000000
39	H	0.000000	0.000001	0.000000	0.000000	0.000000	-0.000003
40	H	0.000000	0.000006	0.000000	0.000001	-0.000018	-0.000086
41	H	0.000000	0.000000	0.000000	0.000110	0.000024	0.000001
42	H	0.000000	0.000000	0.000001	-0.000021	-0.000163	0.000000
43	H	-0.000003	-0.000002	0.000002	-0.000022	0.000040	-0.000007
44	H	0.000001	0.000000	0.000000	-0.000002	0.000000	0.000000
45	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
46	H	0.000000	0.000000	0.000000	-0.000001	0.000000	0.000000
47	H	0.000000	0.000000	-0.000001	0.000117	0.000000	0.000000

		7	8	9	10	11	12
1	C	-0.090523	0.005953	-0.000513	0.000160	-0.000138	-0.000023
2	C	-0.103723	0.001654	0.001740	-0.000026	-0.000042	-0.000127
3	C	0.204745	0.002803	0.008239	0.004499	0.004712	-0.000291
4	C	-0.100224	0.078672	-0.049670	-0.123312	-0.137410	0.007353
5	C	-0.072092	-0.022848	0.114578	0.002662	0.014676	-0.054708
6	C	0.197880	0.001484	-0.017588	-0.000186	0.000477	-0.004983
7	O	8.468555	0.004684	0.004171	-0.000097	-0.000031	0.000014
8	C	0.004684	4.741111	-0.012517	0.571142	0.095769	0.000481
9	N	0.004171	-0.012517	7.388014	-0.000043	-0.042396	0.234073
10	O	-0.000097	0.571142	-0.000043	8.097637	-0.093770	0.000004
11	O	-0.000031	0.095769	-0.042396	-0.093770	8.639044	0.000999
12	C	0.000014	0.000481	0.234073	0.000004	0.000999	5.162184
13	C	0.000046	-0.000012	-0.067450	0.000000	-0.000108	0.270771
14	C	0.000014	-0.000001	0.006720	0.000000	0.000000	-0.052758
15	C	0.000000	0.000000	0.000454	0.000000	0.000000	0.005934
16	C	0.000000	0.000000	-0.000010	0.000000	0.000000	0.000382
17	C	0.000000	0.000000	-0.000092	0.000000	0.000000	0.006684
18	C	0.000022	0.000000	-0.000490	0.000000	0.000000	-0.037044
19	C	-0.000177	-0.003527	0.190428	0.001013	0.143030	-0.028322

20	H	0.000002	0.000631	-0.065139	-0.000083	-0.039818	-0.001346
21	C	0.000002	-0.000361	-0.061525	0.000044	-0.058907	-0.002160
22	C	-0.000001	0.001365	-0.008901	-0.000094	-0.003109	0.000419
23	C	0.000000	0.000030	0.008208	-0.000001	-0.000250	-0.000079
24	C	0.000000	-0.000011	0.000026	0.000000	0.000014	0.000000
25	C	0.000000	-0.000020	-0.000005	0.000000	0.000000	0.000000
26	C	0.000000	0.000058	0.000018	-0.000036	-0.000012	0.000000
27	C	0.000000	0.003075	-0.000187	-0.000376	0.003559	-0.000004
28	H	0.004115	-0.000108	-0.000015	0.000003	0.000000	0.000000
29	H	0.002912	0.000003	0.000054	0.000000	0.000000	-0.000054
30	H	-0.022316	-0.000010	-0.000083	0.006416	0.000170	0.000003
31	H	0.003394	-0.031329	0.001903	0.000584	-0.000011	0.000517
32	H	0.004115	0.003091	-0.080344	-0.000137	-0.000312	-0.001672
33	H	-0.022102	-0.000058	0.000268	0.000002	-0.000003	0.000678
34	H	-0.000002	-0.000073	-0.060886	0.000000	-0.000049	0.361137
35	H	0.000001	-0.000005	-0.042196	0.000000	0.000090	0.374015
36	H	0.000000	0.000001	0.003776	0.000000	0.000000	-0.007074
37	H	0.000000	0.000000	0.000002	0.000000	0.000000	-0.000172
38	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000003
39	H	0.000000	0.000000	0.000001	0.000000	0.000000	-0.000177
40	H	0.000000	0.000000	0.000037	0.000000	0.000000	-0.007192
41	H	0.000000	0.000004	-0.003266	0.000000	0.003061	0.000883
42	H	0.000000	-0.000126	0.004486	-0.000008	-0.000574	-0.000097
43	H	0.000000	0.000005	0.000798	0.000000	0.000010	0.000163
44	H	0.000000	0.000000	-0.000002	0.000000	0.000000	0.000000
45	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
46	H	0.000000	-0.000004	0.000000	0.000001	-0.000002	0.000000
47	H	0.000000	0.000784	0.000027	0.000023	0.001304	0.000000

		13	14	15	16	17	18
1	C	0.000028	-0.000027	0.000003	0.000002	0.000001	0.000013
2	C	-0.000172	0.000847	-0.000973	-0.000199	0.000046	0.000046
3	C	-0.000044	0.000016	0.000002	0.000000	0.000000	-0.000004
4	C	0.000154	-0.000131	-0.000005	0.000000	0.000000	-0.000012
5	C	-0.003682	-0.000972	-0.000009	0.000006	0.000006	0.000777
6	C	0.004991	-0.000417	-0.000173	-0.000041	-0.000558	-0.001371
7	O	0.000046	0.000014	0.000000	0.000000	0.000000	0.000022
8	C	-0.000012	-0.000001	0.000000	0.000000	0.000000	0.000000
9	N	-0.067450	0.006720	0.000454	-0.000010	-0.000092	-0.000490
10	O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
11	O	-0.000108	0.000000	0.000000	0.000000	0.000000	0.000000
12	C	0.270771	-0.052758	0.005934	0.000382	0.006684	-0.037044
13	C	4.932786	0.517012	-0.039218	-0.030422	-0.045458	0.530349
14	C	0.517012	4.996432	0.507339	-0.058144	-0.039275	-0.061671
15	C	-0.039218	0.507339	4.946126	0.531979	-0.049451	-0.040891
16	C	-0.030422	-0.058144	0.531979	4.921792	0.540061	-0.058731
17	C	-0.045458	-0.039275	-0.049451	0.540061	4.937694	0.508349
18	C	0.530349	-0.061671	-0.040891	-0.058731	0.508349	5.001811
19	C	0.005502	0.000159	0.000002	0.000000	0.000001	-0.000070
20	H	-0.000225	0.000071	0.000000	0.000000	0.000000	0.000001
21	C	-0.000236	0.000014	0.000000	0.000000	0.000000	-0.000003
22	C	0.000064	-0.000026	0.000000	0.000000	0.000000	0.000000
23	C	-0.000017	-0.000802	0.000011	0.000000	0.000000	0.000000
24	C	-0.000001	-0.000018	0.000000	0.000000	0.000000	0.000000
25	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
26	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
27	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
28	H	0.000000	0.000000	-0.000001	0.000000	0.000000	0.000000
29	H	-0.000337	0.002145	0.002993	0.000692	-0.000005	-0.000251
30	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
31	H	-0.000085	0.000032	0.000002	0.000000	0.000000	0.000000
32	H	-0.002143	0.000213	0.000004	-0.000001	0.000005	-0.000005
33	H	0.000226	-0.000534	-0.000181	0.000055	0.000893	0.005254

34	H	-0.057181	0.006328	-0.000112	-0.000020	0.000502	-0.001777
35	H	-0.034041	-0.006589	-0.000010	0.000028	-0.000266	0.000645
36	H	-0.038427	0.353751	-0.034611	0.004467	0.000391	0.004738
37	H	0.003535	-0.031394	0.356429	-0.033658	0.004262	0.000749
38	H	0.000423	0.004685	-0.034654	0.357911	-0.034372	0.004811
39	H	0.003906	0.000694	0.004348	-0.034452	0.355872	-0.030735
40	H	-0.035947	0.004887	0.000342	0.004402	-0.033516	0.354621
41	H	-0.000198	0.000036	0.000001	0.000000	0.000000	-0.000001
42	H	0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
43	H	-0.000171	0.000048	0.000004	0.000000	0.000000	-0.000001
44	H	0.000000	0.000003	0.000000	0.000000	0.000000	0.000000
45	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
46	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
47	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

		19	20	21	22	23	24
1	C	-0.000137	-0.000001	0.000005	-0.000024	0.000002	0.000009
2	C	-0.000027	0.000016	-0.000008	-0.000010	0.000032	-0.000004
3	C	0.000554	0.000064	-0.000060	0.000079	0.000034	-0.000008
4	C	-0.008864	-0.000839	-0.000818	-0.001733	-0.001635	-0.000307
5	C	-0.048134	-0.004478	0.006787	-0.000732	-0.000218	-0.000011
6	C	0.004032	-0.000514	0.000023	0.000002	-0.000023	0.000001
7	O	-0.000177	0.000002	0.000002	-0.000001	0.000000	0.000000
8	C	-0.003527	0.000631	-0.000361	0.001365	0.000030	-0.000011
9	N	0.190428	-0.065139	-0.061525	-0.008901	0.008208	0.000026
10	O	0.001013	-0.000083	0.000044	-0.000094	-0.000001	0.000000
11	O	0.143030	-0.039818	-0.058907	-0.003109	-0.000250	0.000014
12	C	-0.028322	-0.001346	-0.002160	0.000419	-0.000079	0.000000
13	C	0.005502	-0.000225	-0.000236	0.000064	-0.000017	-0.000001
14	C	0.000159	0.000071	0.000014	-0.000026	-0.000802	-0.000018
15	C	0.000002	0.000000	0.000000	0.000000	0.000011	0.000000
16	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
17	C	0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
18	C	-0.000070	0.000001	-0.000003	0.000000	0.000000	0.000000
19	C	4.972168	0.382115	0.279632	-0.041893	-0.003879	0.000014
20	H	0.382115	0.574670	-0.064244	0.005353	0.000142	0.000003
21	C	0.279632	-0.064244	5.300439	0.300605	-0.045001	0.005916
22	C	-0.041893	0.005353	0.300605	4.860439	0.535533	-0.044460
23	C	-0.003879	0.000142	-0.045001	0.535533	4.974567	0.509766
24	C	0.000014	0.000003	0.005916	-0.044460	0.509766	4.949150
25	C	0.000024	0.000000	0.000463	-0.031077	-0.058593	0.535946
26	C	0.000019	0.000002	0.005962	-0.045323	-0.039097	-0.050127
27	C	-0.005117	0.000076	-0.047413	0.531372	-0.062164	-0.039924
28	H	0.000000	0.000000	0.000000	-0.000001	0.000001	0.000008
29	H	0.000001	0.000000	0.000000	0.000000	0.000001	0.000000
30	H	-0.000020	0.000000	0.000000	0.000000	-0.000001	0.000000
31	H	-0.001402	0.000168	-0.000715	0.003559	0.004189	0.001202
32	H	-0.004907	0.006695	-0.000661	-0.000012	0.000020	0.000000
33	H	-0.000075	-0.000010	0.000001	0.000000	0.000000	0.000000
34	H	-0.004820	0.013348	-0.000880	-0.000015	0.000014	0.000000
35	H	-0.001627	-0.002994	0.002224	0.000046	-0.000067	-0.000001
36	H	-0.000162	0.000023	-0.000059	0.000013	0.000975	0.000078
37	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
38	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
39	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
40	H	0.000001	0.000007	0.000000	0.000000	0.000000	0.000000
41	H	-0.028220	-0.000771	0.356868	-0.032994	-0.004686	0.000299
42	H	-0.030607	-0.000562	0.356786	-0.039633	0.004170	-0.000224
43	H	0.000134	-0.000004	-0.006661	-0.036117	0.353495	-0.035449
44	H	0.000000	0.000000	-0.000178	0.003877	-0.030425	0.355037
45	H	0.000000	0.000000	0.000004	0.000448	0.004671	-0.034692
46	H	0.000000	0.000000	-0.000174	0.003915	0.000700	0.004346
47	H	-0.000064	-0.000024	-0.006364	-0.038041	0.004635	0.000326

		25	26	27	28	29	30
1	C	0.000000	-0.000001	-0.000001	0.353836	-0.026117	-0.030873
2	C	0.000000	0.000000	0.000001	-0.028973	0.354351	0.002973
3	C	-0.000003	0.000001	0.000036	-0.032643	0.005576	0.381729
4	C	-0.000015	0.000016	-0.000374	0.003070	-0.000133	-0.043824
5	C	0.000004	0.000011	-0.000013	-0.000101	0.002266	0.002225
6	C	0.000000	0.000000	-0.000001	0.006096	-0.030895	0.008467
7	O	0.000000	0.000000	0.000000	0.004115	0.002912	-0.022316
8	C	-0.000020	0.000058	0.003075	-0.000108	0.000003	-0.000010
9	N	-0.000005	0.000018	-0.000187	-0.000015	0.000054	-0.000083
10	O	0.000000	-0.000036	-0.000376	0.000003	0.000000	0.006416
11	O	0.000000	-0.000012	0.003559	0.000000	0.000000	0.000170
12	C	0.000000	0.000000	-0.000004	0.000000	-0.000054	0.000003
13	C	0.000000	0.000000	0.000000	0.000000	-0.000337	0.000000
14	C	0.000000	0.000000	0.000000	0.000000	0.002145	0.000000
15	C	0.000000	0.000000	0.000000	-0.000001	0.002993	0.000000
16	C	0.000000	0.000000	0.000000	0.000000	0.000692	0.000000
17	C	0.000000	0.000000	0.000000	0.000000	-0.000005	0.000000
18	C	0.000000	0.000000	0.000000	0.000000	-0.000251	0.000000
19	C	0.000024	0.000019	-0.005117	0.000000	0.000001	-0.000020
20	H	0.000000	0.000002	0.000076	0.000000	0.000000	0.000000
21	C	0.000463	0.005962	-0.047413	0.000000	0.000000	0.000000
22	C	-0.031077	-0.045323	0.531372	-0.000001	0.000000	0.000000
23	C	-0.058593	-0.039097	-0.062164	0.000001	0.000001	-0.000001
24	C	0.535946	-0.050127	-0.039924	0.000008	0.000000	0.000000
25	C	4.923993	0.537812	-0.058755	0.000002	0.000000	0.000000
26	C	0.537812	4.942936	0.508510	0.000000	0.000000	0.000001
27	C	-0.058755	0.508510	5.003098	0.000000	0.000000	0.000001
28	H	0.000002	0.000000	0.000000	0.516216	-0.001734	-0.000909
29	H	0.000000	0.000000	0.000000	-0.001734	0.514785	-0.000125
30	H	0.000000	0.000001	0.000001	-0.000909	-0.000125	0.511384
31	H	0.000224	0.000227	0.000109	0.001154	-0.000093	0.002224
32	H	0.000000	0.000000	-0.000002	0.000011	-0.000064	-0.000225
33	H	0.000000	0.000000	0.000000	-0.000116	-0.001083	-0.000059
34	H	0.000000	0.000000	0.000000	0.000000	0.000001	0.000000
35	H	0.000000	0.000000	-0.000001	0.000000	-0.000001	0.000000
36	H	0.000000	0.000000	0.000000	0.000001	0.000038	0.000000
37	H	0.000000	0.000000	0.000000	0.000000	0.000063	0.000000
38	H	0.000000	0.000000	0.000000	0.000000	0.000002	0.000000
39	H	0.000000	0.000000	0.000000	0.000000	-0.000001	0.000000
40	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
41	H	0.000004	-0.000219	0.003891	0.000000	0.000000	0.000000
42	H	0.000001	0.000352	-0.004524	0.000000	0.000000	0.000000
43	H	0.004545	0.000357	0.004694	0.000000	-0.000001	0.000000
44	H	-0.034511	0.004315	0.000719	0.000000	0.000000	0.000000
45	H	0.357728	-0.034629	0.004757	0.000000	0.000000	0.000000
46	H	-0.034589	0.355525	-0.030749	0.000000	0.000000	0.000000
47	H	0.004537	-0.034144	0.357311	0.000000	0.000000	0.000000

		31	32	33	34	35	36
1	C	-0.004651	0.000342	0.003334	-0.000003	0.000000	0.000009
2	C	0.004033	0.008317	-0.038238	0.000151	-0.000009	0.000321
3	C	-0.023580	0.002310	0.006668	0.000032	0.000004	0.000001
4	C	0.348439	-0.075469	0.005548	-0.000222	-0.000296	-0.000038
5	C	-0.021488	0.404219	-0.040894	-0.005903	0.006029	0.000120
6	C	-0.006079	-0.071924	0.385565	-0.001737	0.000251	-0.000161
7	O	0.003394	0.004115	-0.022102	-0.000002	0.000001	0.000000
8	C	-0.031329	0.003091	-0.000058	-0.000073	-0.000005	0.000001
9	N	0.001903	-0.080344	0.000268	-0.060886	-0.042196	0.003776
10	O	0.000584	-0.000137	0.000002	0.000000	0.000000	0.000000
11	O	-0.000011	-0.000312	-0.000003	-0.000049	0.000090	0.000000
12	C	0.000517	-0.001672	0.000678	0.361137	0.374015	-0.007074
13	C	-0.000085	-0.002143	0.000226	-0.057181	-0.034041	-0.038427

14	C	0.000032	0.000213	-0.000534	0.006328	-0.006589	0.353751
15	C	0.000002	0.000004	-0.000181	-0.000112	-0.000010	-0.034611
16	C	0.000000	-0.000001	0.000055	-0.000020	0.000028	0.004467
17	C	0.000000	0.000005	0.000893	0.000502	-0.000266	0.000391
18	C	0.000000	-0.000005	0.005254	-0.001777	0.000645	0.004738
19	C	-0.001402	-0.004907	-0.000075	-0.004820	-0.001627	-0.000162
20	H	0.000168	0.006695	-0.000010	0.013348	-0.002994	0.000023
21	C	-0.000715	-0.000661	0.000001	-0.000880	0.002224	-0.000059
22	C	0.003559	-0.000012	0.000000	-0.000015	0.000046	0.000013
23	C	0.004189	0.000020	0.000000	0.000014	-0.000067	0.000975
24	C	0.001202	0.000000	0.000000	0.000000	-0.000001	0.000078
25	C	0.000224	0.000000	0.000000	0.000000	0.000000	0.000000
26	C	0.000227	0.000000	0.000000	0.000000	0.000000	0.000000
27	C	0.000109	-0.000002	0.000000	0.000000	-0.000001	0.000000
28	H	0.001154	0.000011	-0.000116	0.000000	0.000000	0.000001
29	H	-0.000093	-0.000064	-0.001083	0.000001	-0.000001	0.000038
30	H	0.002224	-0.000225	-0.000059	0.000000	0.000000	0.000000
31	H	0.484667	0.004373	-0.000064	0.000034	-0.000026	0.000071
32	H	0.004373	0.616247	-0.006548	0.012943	-0.000429	0.000020
33	H	-0.000064	-0.006548	0.518486	-0.000277	0.000003	-0.000011
34	H	0.000034	0.012943	-0.000277	0.629614	-0.041590	0.000236
35	H	-0.000026	-0.000429	0.000003	-0.041590	0.561071	0.000481
36	H	0.000071	0.000020	-0.000011	0.000236	0.000481	0.554103
37	H	0.000000	0.000000	0.000000	0.000002	0.000001	-0.003534
38	H	0.000000	0.000000	-0.000001	0.000000	0.000000	-0.000158
39	H	0.000000	0.000000	0.000004	-0.000001	0.000003	0.000011
40	H	0.000000	0.000054	0.000385	0.005888	0.000094	-0.000149
41	H	0.000003	-0.000014	0.000000	-0.000023	0.003476	0.000078
42	H	0.000057	0.000042	0.000000	0.000049	-0.000201	0.000003
43	H	-0.000019	0.000002	0.000000	0.000004	0.000129	0.004288
44	H	0.000011	0.000000	0.000000	0.000000	0.000000	-0.000004
45	H	-0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
46	H	0.000004	0.000000	0.000000	0.000000	0.000000	0.000000
47	H	-0.000019	0.000000	0.000000	0.000000	0.000000	0.000000

		37	38	39	40	41	42
1	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
2	C	-0.000020	-0.000001	0.000001	0.000006	0.000000	0.000000
3	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000001
4	C	0.000000	0.000000	0.000000	0.000001	0.000110	-0.000021
5	C	0.000001	0.000000	0.000000	-0.000018	0.000024	-0.000163
6	C	-0.000001	0.000000	-0.000003	-0.000086	0.000001	0.000000
7	O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
8	C	0.000000	0.000000	0.000000	0.000000	0.000004	-0.000126
9	N	0.000002	0.000000	0.000001	0.000037	-0.003266	0.004486
10	O	0.000000	0.000000	0.000000	0.000000	0.000000	-0.000008
11	O	0.000000	0.000000	0.000000	0.000000	0.003061	-0.000574
12	C	-0.000172	0.000003	-0.000177	-0.007192	0.000883	-0.000097
13	C	0.003535	0.000423	0.003906	-0.035947	-0.000198	0.000001
14	C	-0.031394	0.004685	0.000694	0.004887	0.000036	0.000000
15	C	0.356429	-0.034654	0.004348	0.000342	0.000001	0.000000
16	C	-0.033658	0.357911	-0.034452	0.004402	0.000000	0.000000
17	C	0.004262	-0.034372	0.355872	-0.033516	0.000000	0.000000
18	C	0.000749	0.004811	-0.030735	0.354621	-0.000001	0.000000
19	C	0.000000	0.000000	0.000000	0.000001	-0.028220	-0.030607
20	H	0.000000	0.000000	0.000000	0.000007	-0.000771	-0.000562
21	C	0.000000	0.000000	0.000000	0.000000	0.356868	0.356786
22	C	0.000000	0.000000	0.000000	0.000000	-0.032994	-0.039633
23	C	0.000000	0.000000	0.000000	0.000000	-0.004686	0.004170
24	C	0.000000	0.000000	0.000000	0.000000	0.000299	-0.000224
25	C	0.000000	0.000000	0.000000	0.000000	0.000004	0.000001
26	C	0.000000	0.000000	0.000000	0.000000	-0.000219	0.000352
27	C	0.000000	0.000000	0.000000	0.000000	0.003891	-0.004524

28	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
29	H	0.000063	0.000002	-0.000001	0.000000	0.000000	0.000000
30	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
31	H	0.000000	0.000000	0.000000	0.000000	0.000003	0.000057
32	H	0.000000	0.000000	0.000000	0.000054	-0.000014	0.000042
33	H	0.000000	-0.000001	0.000004	0.000385	0.000000	0.000000
34	H	0.000002	0.000000	-0.000001	0.005888	-0.000023	0.000049
35	H	0.000001	0.000000	0.000003	0.000094	0.003476	-0.000201
36	H	-0.003534	-0.000158	0.000011	-0.000149	0.000078	0.000003
37	H	0.551162	-0.003987	-0.000165	0.000011	0.000000	0.000000
38	H	-0.003987	0.555196	-0.004092	-0.000158	0.000000	0.000000
39	H	-0.000165	-0.004092	0.552800	-0.003801	0.000000	0.000000
40	H	0.000011	-0.000158	-0.003801	0.550573	0.000000	0.000000
41	H	0.000000	0.000000	0.000000	0.000000	0.564137	-0.033710
42	H	0.000000	0.000000	0.000000	0.000000	-0.033710	0.576972
43	H	-0.000005	0.000000	0.000000	0.000000	0.003076	0.000081
44	H	0.000000	0.000000	0.000000	0.000000	-0.000002	0.000003
45	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
46	H	0.000000	0.000000	0.000000	0.000000	0.000002	-0.000002
47	H	0.000000	0.000000	0.000000	0.000000	0.000111	0.003816

		43	44	45	46	47
1	C	-0.000003	0.000001	0.000000	0.000000	0.000000
2	C	-0.000002	0.000000	0.000000	0.000000	0.000000
3	C	0.000002	0.000000	0.000000	0.000000	-0.000001
4	C	-0.000022	-0.000002	0.000000	-0.000001	0.000117
5	C	0.000040	0.000000	0.000000	0.000000	0.000000
6	C	-0.000007	0.000000	0.000000	0.000000	0.000000
7	O	0.000000	0.000000	0.000000	0.000000	0.000000
8	C	0.000005	0.000000	0.000000	-0.000004	0.000784
9	N	0.000798	-0.000002	0.000000	0.000000	0.000027
10	O	0.000000	0.000000	0.000000	0.000001	0.000023
11	O	0.000010	0.000000	0.000000	-0.000002	0.001304
12	C	0.000163	0.000000	0.000000	0.000000	0.000000
13	C	-0.000171	0.000000	0.000000	0.000000	0.000000
14	C	0.000048	0.000003	0.000000	0.000000	0.000000
15	C	0.000004	0.000000	0.000000	0.000000	0.000000
16	C	0.000000	0.000000	0.000000	0.000000	0.000000
17	C	0.000000	0.000000	0.000000	0.000000	0.000000
18	C	-0.000001	0.000000	0.000000	0.000000	0.000000
19	C	0.000134	0.000000	0.000000	0.000000	-0.000064
20	H	-0.000004	0.000000	0.000000	0.000000	-0.000024
21	C	-0.006661	-0.000178	0.000004	-0.000174	-0.006364
22	C	-0.036117	0.003877	0.000448	0.003915	-0.038041
23	C	0.353495	-0.030425	0.004671	0.000700	0.004635
24	C	-0.035449	0.355037	-0.034692	0.004346	0.000326
25	C	0.004545	-0.034511	0.357728	-0.034589	0.004537
26	C	0.000357	0.004315	-0.034629	0.355525	-0.034144
27	C	0.004694	0.000719	0.004757	-0.030749	0.357311
28	H	0.000000	0.000000	0.000000	0.000000	0.000000
29	H	-0.000001	0.000000	0.000000	0.000000	0.000000
30	H	0.000000	0.000000	0.000000	0.000000	0.000000
31	H	-0.000019	0.000011	-0.000001	0.000004	-0.000019
32	H	0.000002	0.000000	0.000000	0.000000	0.000000
33	H	0.000000	0.000000	0.000000	0.000000	0.000000
34	H	0.000004	0.000000	0.000000	0.000000	0.000000
35	H	0.000129	0.000000	0.000000	0.000000	0.000000
36	H	0.004288	-0.000004	0.000000	0.000000	0.000000
37	H	-0.000005	0.000000	0.000000	0.000000	0.000000
38	H	0.000000	0.000000	0.000000	0.000000	0.000000
39	H	0.000000	0.000000	0.000000	0.000000	0.000000
40	H	0.000000	0.000000	0.000000	0.000000	0.000000
41	H	0.003076	-0.000002	0.000000	0.000002	0.000111

42	H	0.000081	0.000003	0.000000	-0.000002	0.003816
43	H	0.556403	-0.003844	-0.000162	0.000011	-0.000153
44	H	-0.003844	0.556739	-0.004084	-0.000167	0.000011
45	H	-0.000162	-0.004084	0.558389	-0.004097	-0.000159
46	H	0.000011	-0.000167	-0.004097	0.555379	-0.003937
47	H	-0.000153	0.000011	-0.000159	-0.003937	0.553602

Mulliken atomic charges:

		1
1	C	-0.076253
2	C	-0.059554
3	C	-0.063082
4	C	-0.196548
5	C	0.043708
6	C	-0.095452
7	O	-0.483382
8	C	0.558209
9	N	-0.454704
10	O	-0.466023
11	O	-0.529974
12	C	-0.228412
13	C	0.085778
14	C	-0.148686
15	C	-0.155682
16	C	-0.146100
17	C	-0.151776
18	C	-0.179127
19	C	0.233222
20	H	0.197663
21	C	-0.319347
22	C	0.077105
23	C	-0.154260
24	C	-0.156904
25	C	-0.147715
26	C	-0.152533
27	C	-0.171605
28	H	0.180089
29	H	0.175011
30	H	0.182851
31	H	0.228380
32	H	0.181847
33	H	0.182881
34	H	0.145292
35	H	0.181758
36	H	0.156395
37	H	0.156720
38	H	0.154391
39	H	0.155788
40	H	0.159559
41	H	0.168040
42	H	0.163630
43	H	0.154333
44	H	0.152502
45	H	0.151829
46	H	0.153838
47	H	0.156301

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

		1
1	C	0.103837
2	C	0.115458
3	C	0.119769
4	C	0.031832

```
  5  C    0.225555
  6  C    0.087429
  7  O   -0.483382
  8  C    0.558209
  9  N   -0.454704
 10  O   -0.466023
 11  O   -0.529974
 12  C    0.098638
 13  C    0.085778
 14  C    0.007709
 15  C    0.001038
 16  C    0.008290
 17  C    0.004012
 18  C   -0.019569
 19  C    0.430885
 20  H    0.000000
 21  C    0.012323
 22  C    0.077105
 23  C    0.000073
 24  C   -0.004402
 25  C    0.004114
 26  C    0.001305
 27  C   -0.015304
 28  H    0.000000
 29  H    0.000000
 30  H    0.000000
 31  H    0.000000
 32  H    0.000000
 33  H    0.000000
 34  H    0.000000
 35  H    0.000000
 36  H    0.000000
 37  H    0.000000
 38  H    0.000000
 39  H    0.000000
 40  H    0.000000
 41  H    0.000000
 42  H    0.000000
 43  H    0.000000
 44  H    0.000000
 45  H    0.000000
 46  H    0.000000
 47  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  8075.1749
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=    -4.3859    Y=    -6.4686    Z=     0.3458  Tot=     7.8229
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=  -147.3652   YY=  -172.4263   ZZ=  -135.5372
  XY=    -8.0845   XZ=     7.9177   YZ=    -0.0420
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=     4.4110   YY=   -20.6501   ZZ=    16.2390
  XY=    -8.0845   XZ=     7.9177   YZ=    -0.0420
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=   -62.9144  YYY=   -56.5830  ZZZ=     1.2744  XYY=   -26.9668
 XXY=   -19.8586  XXZ=    28.1493  XZZ=     4.6130  YZZ=   -10.2582
 YYZ=    13.8278  XYZ=    32.4051
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -5928.7361 YYYY= -3083.8415 ZZZZ= -1597.0357 XXXY=   -84.2735
XXXZ=    19.6974 YYYX=    16.7010 YYYZ=   -28.4957 ZZZX=    27.0566
ZZZY=    -4.1803 XXYY= -1743.6489 XXZZ= -1290.7588 YYZZ=  -708.4541
```

XXYZ= -62.6329 YYXZ= 41.8371 ZZXY= -12.7059
N-N= 2.388661444752D+03 E-N=-7.410025255113D+03 KE= 1.125414848510D+03

Test job not archived.
1|1|UNPC-UNK|SP|RB3LYP|6-31G|C22H21N1O3|PCUSER|19-Jul-2011|0||# RB3LYP
/6-31G SCRF=(PCM,SOLVENT=METHANOL) TEST||[No Title]||0,1|C,0,-0.2907,1
.7476,2.432|C,0,-1.4188,1.2517,1.9003|C,0,0.3746,2.528,1.3329|C,0,0.82
64,1.494,0.3017|C,0,-0.4637,1.2474,-0.4983|C,0,-1.5114,1.7877,0.5025|O
,0,-0.8337,3.0821,0.7322|C,0,1.8357,1.8568,-0.7178|N,0,-0.3018,-0.0928
,-1.0417|O,0,2.6461,2.7695,-0.6061|O,0,1.8108,1.05,-1.8123|C,0,-1.4955
,-0.5742,-1.7609|C,0,-2.675,-0.8702,-0.8629|C,0,-2.5497,-1.7464,0.2253
|C,0,-3.6456,-2.0261,1.0432|C,0,-4.8813,-1.4403,0.7775|C,0,-5.024,-0.5
804,-0.3094|C,0,-3.9292,-0.3008,-1.1295|C,0,0.8822,-0.0875,-1.948|H,0,
0.5269,0.0224,-2.9811|C,0,1.7021,-1.3991,-1.8896|C,0,2.4074,-1.6438,-0
.5744|C,0,1.7711,-2.3504,0.4543|C,0,2.4083,-2.5432,1.6808|C,0,3.6892,-
2.0364,1.8895|C,0,4.3363,-1.3401,0.8708|C,0,3.7004,-1.1458,-0.3562|H,0
,0.1145,1.5435,3.411|H,0,-2.123,0.5807,2.3669|H,0,1.0683,3.3102,1.6419
|H,0,1.2212,0.6109,0.8229|H,0,-0.5251,1.9435,-1.3546|H,0,-2.5161,1.973
,0.1223|H,0,-1.7838,0.1448,-2.5395|H,0,-1.2642,-1.5145,-2.2788|H,0,-1.
5921,-2.2111,0.4468|H,0,-3.5346,-2.7019,1.8878|H,0,-5.7351,-1.6587,1.4
145|H,0,-5.9911,-0.1301,-0.5213|H,0,-4.0662,0.3676,-1.9776|H,0,1.0611,
-2.2587,-2.1225|H,0,2.4638,-1.3734,-2.6805|H,0,0.7711,-2.7519,0.3093|H
,0,1.9043,-3.0899,2.4744|H,0,4.1853,-2.1885,2.8452|H,0,5.3387,-0.9503,
1.0318|H,0,4.2229,-0.6004,-1.1401||Version=x86-Win32-G03RevB.03|State=
1-A|HF=-1131.0272549|RMSD=5.587e-006|Dipole=-1.7432509,-2.5325413,0.14
16225|PG=C01 [X(C22H21N1O3)]||@

INTERMEDIATE 10i_a
%mem=256Mb

RB3LYP/6-31G SCRF=(PCM,Solvent=Methanol) Test

1/38=1/1;
2/17=6,18=5,40=1/2;
3/5=1,6=6,11=2,16=1,25=1,30=1,70=2201,72=3,74=-5/1,2,3;
4/7=1/1;
5/5=2,32=1,38=5,53=3/2;
6/7=2,8=2,9=2,10=2,28=1/1;
99/5=1,9=1/99;

[No Title]

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	0	2.9018	2.0773	0.5506
C	0	3.4062	0.8367	0.5079
C	0	1.809	2.0407	1.5762
C	0	0.6695	1.1911	0.9949
C	0	1.1795	-0.2588	1.2118
C	0	2.6741	0.0354	1.5419
O	0	2.4304	1.115	2.5125
C	0	-0.6471	1.3636	1.6968
N	0	0.6931	-1.1678	0.1376
O	0	-0.7835	1.9878	2.7455
O	0	-1.7249	0.7776	1.0965
C	0	1.3952	-2.4696	0.1877
C	0	2.7904	-2.4361	-0.3983
C	0	3.8666	-3.0106	0.2941
C	0	5.1466	-3.0132	-0.2634
C	0	5.3616	-2.4592	-1.5241
C	0	4.2967	-1.9068	-2.2327
C	0	3.0169	-1.8999	-1.6762

C	0	-1.4818	0.0331	-0.0108
C	0	-0.806	-1.3265	0.2876
N	0	-1.787	0.426	-1.2014
C	0	-2.4966	1.7048	-1.3389
C	0	-1.5806	2.9019	-1.2686
C	0	-1.785	3.9041	-0.3095
C	0	-0.9078	4.9859	-0.2199
C	0	0.1739	5.0827	-1.0932
C	0	0.3758	4.103	-2.0631
C	0	-0.4992	3.02	-2.1542
H	0	-1.0207	-1.5807	1.3355
C	0	-1.4997	-2.4107	-0.5847
C	0	-2.9859	-2.5346	-0.306
C	0	-3.4412	-3.0576	0.9133
C	0	-4.8088	-3.1492	1.1765
C	0	-5.7335	-2.7248	0.2245
C	0	-5.2924	-2.2134	-0.9941
C	0	-3.9256	-2.1212	-1.2602
H	0	3.1637	2.9126	-0.0802
H	0	4.1742	0.4683	-0.154
H	0	1.5701	2.9932	2.0513
H	0	0.5514	1.4623	-0.0584
H	0	0.7659	-0.639	2.1612
H	0	3.2388	-0.76	2.0287
H	0	0.8908	-3.2212	-0.4247
H	0	1.4039	-2.8595	1.2137
H	0	3.719	-3.4628	1.273
H	0	5.9768	-3.4547	0.2833
H	0	6.3587	-2.465	-1.9579
H	0	4.4623	-1.4822	-3.22
H	0	2.1932	-1.469	-2.2427
H	0	-3.3068	1.7813	-0.6021
H	0	-2.9945	1.7135	-2.3162
H	0	-2.6262	3.8494	0.3795
H	0	-1.0717	5.759	0.5278
H	0	0.854	5.9289	-1.0255
H	0	1.215	4.1829	-2.7505
H	0	-0.3265	2.2569	-2.9115
H	0	-1.3264	-2.2158	-1.6506
H	0	-1.0857	-3.4047	-0.3842
H	0	-2.7381	-3.4066	1.6673
H	0	-5.1545	-3.5567	2.124
H	0	-6.7989	-2.7983	0.4301
H	0	-6.0144	-1.8874	-1.7393
H	0	-3.6004	-1.7173	-2.2175

Stoichiometry C30H28N2O3
Framework group C1[X(C30H28N2O3)]
Deg. of freedom 183
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	2.900173	2.079393	0.593873
2	6	0	3.401848	0.838093	0.540705
3	6	0	1.804788	2.035650	1.616430
4	6	0	0.664780	1.194188	1.024388
5	6	0	1.170943	-0.258861	1.228849

6	6	0	2.665398	0.028776	1.565329
7	8	0	2.421785	1.099744	2.545468
8	6	0	-0.653136	1.363098	1.724689
9	7	0	0.685102	-1.156581	0.144954
10	8	0	-0.790678	1.977705	2.778892
11	8	0	-1.730797	0.785261	1.116282
12	6	0	1.384109	-2.460407	0.184484
13	6	0	2.780811	-2.424600	-0.397790
14	6	0	3.854002	-3.008072	0.291771
15	6	0	5.135353	-3.008367	-0.262624
16	6	0	5.354697	-2.443013	-1.517522
17	6	0	4.292795	-1.881513	-2.223464
18	6	0	3.011656	-1.876910	-1.670027
19	6	0	-1.486687	0.050666	0.002607
20	6	0	-0.814719	-1.313236	0.289817
21	7	0	-1.788078	0.455465	-1.184974
22	6	0	-2.494424	1.737133	-1.312135
23	6	0	-1.575874	2.931406	-1.228335
24	6	0	-1.780335	3.924995	-0.260330
25	6	0	-0.900894	5.003882	-0.158412
26	6	0	0.183157	5.106414	-1.028137
27	6	0	0.385195	4.135431	-2.006735
28	6	0	-0.492045	3.055354	-2.110159
29	1	0	-1.032559	-1.576800	1.334751
30	6	0	-1.508752	-2.387572	-0.594342
31	6	0	-2.995907	-2.510671	-0.320425
32	6	0	-3.455378	-3.044083	0.892784
33	6	0	-4.823823	-3.135011	1.151793
34	6	0	-5.745223	-2.699535	0.201597
35	6	0	-5.299980	-2.177696	-1.011057
36	6	0	-3.932326	-2.086140	-1.272962
37	1	0	3.165518	2.919993	-0.028390
38	1	0	4.170623	0.474177	-0.122774
39	1	0	1.566897	2.984180	2.099906
40	1	0	0.549875	1.475568	-0.026592
41	1	0	0.754157	-0.647034	2.173618
42	1	0	3.227092	-0.772472	2.045979
43	1	0	0.879497	-3.205043	-0.436193
44	1	0	1.389411	-2.859973	1.206782
45	1	0	3.702979	-3.469132	1.266005
46	1	0	5.963205	-3.456906	0.281901
47	1	0	6.352839	-2.447021	-1.948939
48	1	0	4.461776	-1.448015	-3.206314
49	1	0	2.190328	-1.438798	-2.234436
50	1	0	-3.306247	1.808554	-0.576613
51	1	0	-2.989912	1.756184	-2.290513
52	1	0	-2.623340	3.865744	0.426082
53	1	0	-1.064860	5.770280	0.596141
54	1	0	0.865015	5.950371	-0.950816
55	1	0	1.226254	4.219870	-2.691315
56	1	0	-0.319232	2.299025	-2.874196
57	1	0	-1.332402	-2.183040	-1.657934
58	1	0	-1.097509	-3.384367	-0.402216
59	1	0	-2.754922	-3.401787	1.645163
60	1	0	-5.172767	-3.550621	2.094570
61	1	0	-6.811287	-2.772516	0.403911
62	1	0	-6.019410	-1.843031	-1.754899
63	1	0	-3.603867	-1.673990	-2.225622

Rotational constants (GHZ): 0.1367900 0.1076370 0.0749521
Standard basis: 6-31G (6D, 7F)
There are 371 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.
  371 basis functions,   882 primitive gaussians,   371 cartesian basis functions
  123 alpha electrons      123 beta electrons
       nuclear repulsion energy      3750.6237191624 Hartrees.
NAtoms=   63 NActive=   63 NUniq=   63 SFac= 1.00D+00 NAtFMM=   60 Big=T
-------------------------------------------------------------------------------
United Atom Topological Model (UA0  parameters set).
 Nord Group  Hybr  Charge Alpha Radius          Bonded to
  1   CH    *     0.00   1.00  2.125   C2   [d]  C3   [s]
  2   CH    *     0.00   1.00  2.125   C1   [d]  C6   [s]
  3   CH    *     0.00   1.00  2.125   C1   [s]  C4   [s]  O7   [s]
  4   CH    *     0.00   1.00  2.125   C3   [s]  C5   [s]  C8   [s]
  5   CH    *     0.00   1.00  2.125   C4   [s]  C6   [s]  N9   [s]
  6   CH    *     0.00   1.00  2.125   C2   [s]  C5   [s]  O7   [s]
  7   O     *     0.00   1.00  1.750   C3   [s]  C6   [s]
  8   C     *     0.00   1.00  1.925   C4   [s]  O10  [d]  O11  [s]
  9   N     *     0.00   1.00  1.830   C5   [s]  C12  [s]  C20  [s]
 10   O     *     0.00   1.00  1.750   C8   [d]
 11   O     *     0.00   1.00  1.750   C8   [s]  C19  [s]
 12   CH2   *     0.00   1.00  2.325   N9   [s]  C13  [s]
 13   C     *     0.00   1.00  1.925   C12  [s]  C14  [s]  C18  [s]
 14   CH    *     0.00   1.00  2.125   C13  [s]  C15  [s]
 15   CH    *     0.00   1.00  2.125   C14  [s]  C16  [s]
 16   CH    *     0.00   1.00  2.125   C15  [s]  C17  [s]
 17   CH    *     0.00   1.00  2.125   C16  [s]  C18  [s]
 18   CH    *     0.00   1.00  2.125   C13  [s]  C17  [s]
 19   C     *     0.00   1.00  1.925   O11  [s]  C20  [s]  N21  [d]
 20   CH    *     0.00   1.00  2.125   N9   [s]  C19  [s]  C30  [s]
 21   N     *     0.00   1.00  1.830   C19  [d]  C22  [s]
 22   CH2   *     0.00   1.00  2.325   N21  [s]  C23  [s]
 23   C     *     0.00   1.00  1.925   C22  [s]  C24  [s]  C28  [s]
 24   CH    *     0.00   1.00  2.125   C23  [s]  C25  [s]
 25   CH    *     0.00   1.00  2.125   C24  [s]  C26  [s]
 26   CH    *     0.00   1.00  2.125   C25  [s]  C27  [s]
 27   CH    *     0.00   1.00  2.125   C26  [s]  C28  [s]
 28   CH    *     0.00   1.00  2.125   C23  [s]  C27  [s]
 30   CH2   *     0.00   1.00  2.325   C20  [s]  C31  [s]
 31   C     *     0.00   1.00  1.925   C30  [s]  C32  [s]  C36  [s]
 32   CH    *     0.00   1.00  2.125   C31  [s]  C33  [s]
 33   CH    *     0.00   1.00  2.125   C32  [s]  C34  [s]
 34   CH    *     0.00   1.00  2.125   C33  [s]  C35  [s]
 35   CH    *     0.00   1.00  2.125   C34  [s]  C36  [s]
 36   CH    *     0.00   1.00  2.125   C31  [s]  C35  [s]
-------------------------------------------------------------------------------
Polarizable Continuum Model (PCM)
=================================
Model               : PCM.
Atomic radii        : UA0 (Simple United Atom Topological Model).
Polarization charges : Total charges.
Charge compensation  : None.
Solution method      : Matrix inversion.
Cavity              : GePol (RMin=0.200 OFac=0.890).
                      Default sphere list used, NSphG=   35.
                      Tesserae with average area of 0.200 Ang**2.
Solvent             : Methanol, Eps=  32.630000.
-------------------------------------------------------------------------------
One-electron integrals computed using PRISM.
NBasis=   371 RedAO= T  NBF=   371
NBsUse=   371 1.00D-06 NBFU=   371
Harris functional with IExCor=  402 diagonalized for initial guess.
```

```
ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 402 AccDes= 1.00D-06 IRadAn=         1 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)
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               (A) (A) (A) (A) (A) (A) (A) (A)
The electronic state of the initial guess is 1-A.
Warning!  Cutoffs for single-point calculations used.
Requested convergence on RMS density matrix=1.00D-04 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-02.
Requested convergence on             energy=5.00D-05.
No special actions if energy rises.
Error on total polarization charges =  0.02862
SCF Done:  E(RB+HF-LYP) =  -1494.73742770     A.U. after   10 cycles
           Convg  =    0.2134D-05             -V/T =  2.0051
           S**2   =   0.0000
--------------------------------------------------------------------
Variational PCM results
=======================
<psi(f)|   H    |psi(f)>                    (a.u.) =   -1494.703738
<psi(f)|H+V(f)/2|psi(f)>                    (a.u.) =   -1494.737428
Total free energy in solution:
 with all non electrostatic terms           (a.u.) =   -1494.722081
--------------------------------------------------------------------
(Polarized solute)-Solvent              (kcal/mol) =     -21.14
--------------------------------------------------------------------
Cavitation energy                       (kcal/mol) =      39.80
Dispersion energy                       (kcal/mol) =     -32.63
Repulsion energy                        (kcal/mol) =       2.45
Total non electrostatic                 (kcal/mol) =       9.63
--------------------------------------------------------------------
Partition over spheres:
```

```
Sphere  on Atom  Surface  Charge   GEl    GCav    GDR
   1      C1     12.23  -0.027   -0.55    1.69   -1.13
   2      C2      8.28  -0.001   -0.17    1.38   -0.75
   3      C3      6.20  -0.039   -0.16    1.05   -0.63
   4      C4      0.00   0.000    0.00    0.30    0.00
   5      C5      3.29  -0.035   -0.33    0.48   -0.40
   6      C6      6.73  -0.030   -0.28    0.81   -0.69
   7      O7      8.47   0.128   -2.94    0.97   -0.97
   8      C8      0.91  -0.004    0.02    0.25   -0.05
   9      N9      0.00   0.000    0.00    0.22    0.00
  10      O10    14.05   0.158   -3.66    1.86   -1.51
  11      O11     4.46   0.042   -0.67    0.76   -0.41
  12      C12    12.72  -0.043   -0.44    1.55   -1.26
  13      C13     0.20   0.001    0.00    0.04    0.00
  14      C14    12.60  -0.023   -0.56    1.39   -1.15
  15      C15    17.21  -0.018   -0.51    1.69   -1.53
  16      C16    16.57  -0.016   -0.49    1.69   -1.50
  17      C17    16.59  -0.020   -0.50    1.65   -1.47
  18      C18     9.54  -0.011   -0.25    1.31   -0.82
  19      C19     0.00   0.000    0.00    0.13    0.00
  20      C20     1.61  -0.024   -0.33    0.45   -0.17
  21      N21     1.63   0.032   -0.52    0.52   -0.16
  22      C22    19.20  -0.051   -0.28    2.16   -1.63
  23      C23     0.05   0.000    0.00    0.05    0.00
  24      C24    12.03  -0.028   -0.34    1.32   -1.00
  25      C25    16.43  -0.027   -0.45    1.69   -1.40
  26      C26    15.39  -0.027   -0.53    1.69   -1.36
  27      C27    13.89  -0.031   -0.56    1.64   -1.28
  28      C28    10.58  -0.030   -0.40    1.41   -1.00
  29      C30    14.41  -0.036   -0.23    1.63   -1.19
  30      C31     0.22   0.001    0.00    0.08    0.00
  31      C32    12.96  -0.021   -0.56    1.55   -1.21
  32      C33    17.13  -0.015   -0.51    1.69   -1.58
  33      C34    17.45  -0.011   -0.51    1.69   -1.56
  34      C35    16.34  -0.018   -0.48    1.69   -1.44
  35      C36    10.39  -0.013   -0.30    1.36   -0.88
Added spheres:   106.63   0.206   -3.63    0.00    0.00
-----------------------------------------------------------------

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

            Population analysis using the SCF density.

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

Orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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(A) (A) (A) (A) (A) (A) (A) (A)
The electronic state is 1-A.
Alpha occ. eigenvalues -- -19.22423 -19.16358 -19.15058 -14.34921 -14.34535
Alpha occ. eigenvalues -- -10.35099 -10.30340 -10.24860 -10.24549 -10.24030
Alpha occ. eigenvalues -- -10.23963 -10.21669 -10.21539 -10.21166 -10.20040
Alpha occ. eigenvalues -- -10.19444 -10.19412 -10.19006 -10.18701 -10.18686
Alpha occ. eigenvalues -- -10.18677 -10.18632 -10.18592 -10.18572 -10.18477
Alpha occ. eigenvalues -- -10.18313 -10.18267 -10.18257 -10.18212 -10.18168
Alpha occ. eigenvalues -- -10.18126 -10.18105 -10.18092 -10.18029 -10.18001
Alpha occ. eigenvalues -- -1.16258 -1.07300 -1.06650 -0.94721 -0.93547
Alpha occ. eigenvalues -- -0.86270 -0.85917 -0.85730 -0.82559 -0.80015
Alpha occ. eigenvalues -- -0.78975 -0.77495 -0.76762 -0.75627 -0.74894
Alpha occ. eigenvalues -- -0.74465 -0.74390 -0.73041 -0.70603 -0.68486
Alpha occ. eigenvalues -- -0.67620 -0.65186 -0.61545 -0.60875 -0.60412
Alpha occ. eigenvalues -- -0.60299 -0.59958 -0.59258 -0.58105 -0.57531
Alpha occ. eigenvalues -- -0.55963 -0.55336 -0.53574 -0.52091 -0.51280
Alpha occ. eigenvalues -- -0.50978 -0.50835 -0.50193 -0.49594 -0.48957
Alpha occ. eigenvalues -- -0.47566 -0.46633 -0.46038 -0.45951 -0.45400
Alpha occ. eigenvalues -- -0.45157 -0.44793 -0.44625 -0.43863 -0.43198
Alpha occ. eigenvalues -- -0.42410 -0.42242 -0.41901 -0.41790 -0.41520
Alpha occ. eigenvalues -- -0.41179 -0.40632 -0.40596 -0.40364 -0.40009
Alpha occ. eigenvalues -- -0.38967 -0.38241 -0.37341 -0.36677 -0.36309
Alpha occ. eigenvalues -- -0.35894 -0.35583 -0.35192 -0.34959 -0.34316
Alpha occ. eigenvalues -- -0.34253 -0.33940 -0.33742 -0.33575 -0.33200
Alpha occ. eigenvalues -- -0.32488 -0.31214 -0.28564 -0.27928 -0.26890
Alpha occ. eigenvalues -- -0.25457 -0.25164 -0.25012 -0.24861 -0.24788
Alpha occ. eigenvalues -- -0.24371 -0.24059 -0.22405
Alpha virt. eigenvalues -- -0.03938 -0.02035 -0.00508 -0.00283 -0.00131
Alpha virt. eigenvalues -- 0.00108 0.00231 0.00561 0.00699 0.08360
Alpha virt. eigenvalues -- 0.09182 0.10074 0.10350 0.10517 0.11289
Alpha virt. eigenvalues -- 0.12230 0.12782 0.13181 0.13302 0.13491
Alpha virt. eigenvalues -- 0.13724 0.14216 0.14499 0.15032 0.15660
Alpha virt. eigenvalues -- 0.15769 0.15954 0.16559 0.16712 0.16845
Alpha virt. eigenvalues -- 0.17345 0.17429 0.17698 0.17866 0.18174
Alpha virt. eigenvalues -- 0.18867 0.18929 0.19273 0.19941 0.20059
Alpha virt. eigenvalues -- 0.20433 0.20820 0.20961 0.21424 0.21763
Alpha virt. eigenvalues -- 0.22326 0.22634 0.23969 0.24464 0.25322
Alpha virt. eigenvalues -- 0.26032 0.26213 0.26578 0.27455 0.28256
Alpha virt. eigenvalues -- 0.29404 0.30923 0.31318 0.31562 0.31628
Alpha virt. eigenvalues -- 0.32425 0.32517 0.33526 0.33570 0.33804
Alpha virt. eigenvalues -- 0.34757 0.35170 0.35226 0.35870 0.36176
Alpha virt. eigenvalues -- 0.36344 0.37485 0.42174 0.43061 0.46395
Alpha virt. eigenvalues -- 0.48340 0.48791 0.49301 0.49732 0.50043
Alpha virt. eigenvalues -- 0.51647 0.52019 0.52764 0.53547 0.53767
Alpha virt. eigenvalues -- 0.54747 0.55139 0.55582 0.56020 0.56085
Alpha virt. eigenvalues -- 0.56482 0.56824 0.57031 0.57307 0.57999
Alpha virt. eigenvalues -- 0.58512 0.59184 0.59397 0.59674 0.60054

Alpha virt. eigenvalues --	0.60695	0.61182	0.61795	0.62143	0.62258
Alpha virt. eigenvalues --	0.62415	0.62671	0.63000	0.63385	0.63501
Alpha virt. eigenvalues --	0.63811	0.64142	0.64564	0.64724	0.65024
Alpha virt. eigenvalues --	0.65232	0.65415	0.65592	0.65756	0.65883
Alpha virt. eigenvalues --	0.66186	0.66522	0.66746	0.67103	0.67543
Alpha virt. eigenvalues --	0.67800	0.68938	0.69330	0.70058	0.70477
Alpha virt. eigenvalues --	0.70686	0.71617	0.71865	0.73128	0.73501
Alpha virt. eigenvalues --	0.75207	0.75772	0.76652	0.77490	0.79188
Alpha virt. eigenvalues --	0.80352	0.81650	0.82548	0.82881	0.83562
Alpha virt. eigenvalues --	0.83951	0.84139	0.84747	0.85203	0.85623
Alpha virt. eigenvalues --	0.85981	0.86425	0.86527	0.86932	0.87039
Alpha virt. eigenvalues --	0.87517	0.87994	0.88251	0.88453	0.88854
Alpha virt. eigenvalues --	0.89986	0.90225	0.90558	0.90730	0.91630
Alpha virt. eigenvalues --	0.92393	0.92552	0.93416	0.93852	0.94466
Alpha virt. eigenvalues --	0.94845	0.95428	0.96602	0.96919	0.97425
Alpha virt. eigenvalues --	0.97684	0.98311	0.98782	0.99272	0.99613
Alpha virt. eigenvalues --	1.00271	1.01170	1.01876	1.02684	1.02906
Alpha virt. eigenvalues --	1.04080	1.04832	1.05115	1.05868	1.06209
Alpha virt. eigenvalues --	1.07520	1.08619	1.09253	1.09989	1.11150
Alpha virt. eigenvalues --	1.11869	1.13224	1.14172	1.15194	1.15663
Alpha virt. eigenvalues --	1.16631	1.17743	1.18421	1.19280	1.19994
Alpha virt. eigenvalues --	1.20614	1.21907	1.22035	1.22427	1.23708
Alpha virt. eigenvalues --	1.23761	1.25422	1.27251	1.28717	1.29893
Alpha virt. eigenvalues --	1.31718	1.34036	1.35858	1.37972	1.39356
Alpha virt. eigenvalues --	1.40804	1.42158	1.45408	1.46517	1.46912
Alpha virt. eigenvalues --	1.47613	1.49103	1.49435	1.51171	1.51297
Alpha virt. eigenvalues --	1.55242	1.56429	1.57402	1.66790	1.70328
Alpha virt. eigenvalues --	1.73114	1.78968	1.82394	1.84081	1.90431
Alpha virt. eigenvalues --	1.91407	1.91825	1.94372	1.96879	2.02879
Alpha virt. eigenvalues --	2.10080	2.15631	2.56318		

Condensed to atoms (all electrons):

Mulliken atomic charges:

		1
1	C	-0.070931
2	C	-0.057668
3	C	-0.065787
4	C	-0.202573
5	C	0.064365
6	C	-0.097484
7	O	-0.484103
8	C	0.550594
9	N	-0.447443
10	O	-0.446084
11	O	-0.501164
12	C	-0.217597
13	C	0.087683
14	C	-0.182228
15	C	-0.152844
16	C	-0.147473
17	C	-0.156642
18	C	-0.145120
19	C	0.387048
20	C	0.014108
21	N	-0.336341
22	C	-0.264270
23	C	0.068661
24	C	-0.171087
25	C	-0.149984
26	C	-0.146307
27	C	-0.149898
28	C	-0.159707
29	H	0.166168

30	C	-0.343309
31	C	0.073014
32	C	-0.168676
33	C	-0.156473
34	C	-0.147522
35	C	-0.156065
36	C	-0.158737
37	H	0.180709
38	H	0.173659
39	H	0.184563
40	H	0.221858
41	H	0.179931
42	H	0.186703
43	H	0.184054
44	H	0.140697
45	H	0.156837
46	H	0.153683
47	H	0.151941
48	H	0.153897
49	H	0.152624
50	H	0.176535
51	H	0.175842
52	H	0.163575
53	H	0.158985
54	H	0.156682
55	H	0.159081
56	H	0.161979
57	H	0.165153
58	H	0.167011
59	H	0.156742
60	H	0.153069
61	H	0.150803
62	H	0.151740
63	H	0.153525

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

		1
1	C	0.109778
2	C	0.115990
3	C	0.118776
4	C	0.019285
5	C	0.244295
6	C	0.089219
7	O	-0.484103
8	C	0.550594
9	N	-0.447443
10	O	-0.446084
11	O	-0.501164
12	C	0.107154
13	C	0.087683
14	C	-0.025391
15	C	0.000840
16	C	0.004468
17	C	-0.002745
18	C	0.007504
19	C	0.387048
20	C	0.180275
21	N	-0.336341
22	C	0.088106
23	C	0.068661
24	C	-0.007512
25	C	0.009001

```
  26  C    0.010375
  27  C    0.009183
  28  C    0.002272
  29  H    0.000000
  30  C   -0.011145
  31  C    0.073014
  32  C   -0.011934
  33  C   -0.003404
  34  C    0.003282
  35  C   -0.004325
  36  C   -0.005212
  37  H    0.000000
  38  H    0.000000
  39  H    0.000000
  40  H    0.000000
  41  H    0.000000
  42  H    0.000000
  43  H    0.000000
  44  H    0.000000
  45  H    0.000000
  46  H    0.000000
  47  H    0.000000
  48  H    0.000000
  49  H    0.000000
  50  H    0.000000
  51  H    0.000000
  52  H    0.000000
  53  H    0.000000
  54  H    0.000000
  55  H    0.000000
  56  H    0.000000
  57  H    0.000000
  58  H    0.000000
  59  H    0.000000
  60  H    0.000000
  61  H    0.000000
  62  H    0.000000
  63  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>= 15089.8614
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     1.6326    Y=    -2.3102    Z=    -4.3040  Tot=     5.1504
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=  -186.6692   YY=  -187.7895   ZZ=  -215.4386
  XY=    -0.4666   XZ=    -5.2538   YZ=   -18.5528
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=     9.9632   YY=     8.8429   ZZ=   -18.8061
  XY=    -0.4666   XZ=    -5.2538   YZ=   -18.5528
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=    -3.3042  YYY=    83.7016  ZZZ=   -62.3982  XYY=    37.4154
 XXY=   -33.6371  XXZ=   -32.6238  XZZ=    -2.6736  YZZ=   -44.9174
 YYZ=    34.0860  XYZ=   -12.2820
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -9493.1145 YYYY= -7614.6004 ZZZZ= -2462.4132 XXXY=  -132.8071
XXXZ=  -126.8388 YYYX=    76.1499 YYYZ=   -22.8130 ZZZX=   -81.0566
ZZZY=  -125.4806 XXYY= -2992.2134 XXZZ= -2078.9747 YYZZ= -1745.9342
XXYZ=  -139.3156 YYXZ=   -66.1775 ZZXY=    31.8819
N-N= 3.750623719162D+03 E-N=-1.097854888543D+04  KE= 1.487127366362D+03

Test job not archived.
1|1|UNPC-UNK|SP|RB3LYP|6-31G|C30H28N2O3|PCUSER|18-Jul-2011|0||# RB3LYP
```

/6-31G SCRF=(PCM,SOLVENT=METHANOL) TEST||[No Title]||0,1|C,0,2.9018,2.
0773,0.5506|C,0,3.4062,0.8367,0.5079|C,0,1.809,2.0407,1.5762|C,0,0.669
5,1.1911,0.9949|C,0,1.1795,-0.2588,1.2118|C,0,2.6741,0.0354,1.5419|O,0
,2.4304,1.115,2.5125|C,0,-0.6471,1.3636,1.6968|N,0,0.6931,-1.1678,0.13
76|O,0,-0.7835,1.9878,2.7455|O,0,-1.7249,0.7776,1.0965|C,0,1.3952,-2.4
696,0.1877|C,0,2.7904,-2.4361,-0.3983|C,0,3.8666,-3.0106,0.2941|C,0,5.
1466,-3.0132,-0.2634|C,0,5.3616,-2.4592,-1.5241|C,0,4.2967,-1.9068,-2.
2327|C,0,3.0169,-1.8999,-1.6762|C,0,-1.4818,0.0331,-0.0108|C,0,-0.806,
-1.3265,0.2876|N,0,-1.787,0.426,-1.2014|C,0,-2.4966,1.7048,-1.3389|C,0
,-1.5806,2.9019,-1.2686|C,0,-1.785,3.9041,-0.3095|C,0,-0.9078,4.9859,-
0.2199|C,0,0.1739,5.0827,-1.0932|C,0,0.3758,4.103,-2.0631|C,0,-0.4992,
3.02,-2.1542|H,0,-1.0207,-1.5807,1.3355|C,0,-1.4997,-2.4107,-0.5847|C,
0,-2.9859,-2.5346,-0.306|C,0,-3.4412,-3.0576,0.9133|C,0,-4.8088,-3.149
2,1.1765|C,0,-5.7335,-2.7248,0.2245|C,0,-5.2924,-2.2134,-0.9941|C,0,-3
.9256,-2.1212,-1.2602|H,0,3.1637,2.9126,-0.0802|H,0,4.1742,0.4683,-0.1
54|H,0,1.5701,2.9932,2.0513|H,0,0.5514,1.4623,-0.0584|H,0,0.7659,-0.63
9,2.1612|H,0,3.2388,-0.76,2.0287|H,0,0.8908,-3.2212,-0.4247|H,0,1.4039
,-2.8595,1.2137|H,0,3.719,-3.4628,1.273|H,0,5.9768,-3.4547,0.2833|H,0,
6.3587,-2.465,-1.9579|H,0,4.4623,-1.4822,-3.22|H,0,2.1932,-1.469,-2.24
27|H,0,-3.3068,1.7813,-0.6021|H,0,-2.9945,1.7135,-2.3162|H,0,-2.6262,3
.8494,0.3795|H,0,-1.0717,5.759,0.5278|H,0,0.854,5.9289,-1.0255|H,0,1.2
15,4.1829,-2.7505|H,0,-0.3265,2.2569,-2.9115|H,0,-1.3264,-2.2158,-1.65
06|H,0,-1.0857,-3.4047,-0.3842|H,0,-2.7381,-3.4066,1.6673|H,0,-5.1545,
-3.5567,2.124|H,0,-6.7989,-2.7983,0.4301|H,0,-6.0144,-1.8874,-1.7393|H
,0,-3.6004,-1.7173,-2.2175||Version=x86-Win32-G03RevB.03|State=1-A|HF=
-1494.7374277|RMSD=2.134e-006|Dipole=0.640313,-0.9233664,-1.6862383|PG
=C01 [X(C30H28N2O3)]||@

INTERMEDIATE 10i_b

%mem=256MB

RB3LYP/6-31G SCRF=(PCM,Solvent=Methanol) Test

1/38=1/1;
2/17=6,18=5,40=1/2;
3/5=1,6=6,11=2,16=1,25=1,30=1,70=2201,72=3,74=-5/1,2,3;
4/7=1/1;
5/5=2,32=1,38=5,53=3/2;
6/7=2,8=2,9=2,10=2,28=1/1;
99/5=1,9=1/99;

[No Title]

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	0	-3.0597	-2.7254	-0.7675
C	0	-1.9585	-3.4276	-1.072
C	0	-2.9624	-1.4435	-1.5448
C	0	-1.8131	-0.636	-0.9257
C	0	-0.5614	-1.3266	-1.5179
C	0	-1.2093	-2.6203	-2.0885
O	0	-2.3481	-1.9783	-2.7521
C	0	-1.7625	0.809	-1.3063
N	0	0.5118	-1.3378	-0.5177
O	0	-2.4839	1.311	-2.1638
O	0	-0.8389	1.5678	-0.6484
C	0	1.558	-2.3239	-0.8529
C	0	2.5966	-2.5002	0.2322
C	0	3.9526	-2.2579	-0.0305
C	0	4.9069	-2.4163	0.976
C	0	4.5176	-2.8233	2.2509
C	0	3.1741	-3.0753	2.5219

C	0	2.218	-2.9173	1.5179
C	0	-0.0521	0.9722	0.2809
C	0	1.0591	0.0394	-0.2521
N	0	-0.1768	1.2001	1.5454
C	0	1.8344	0.719	-1.4106
H	0	1.7491	-0.0552	0.5968
C	0	2.4883	2.0203	-1.0011
C	0	3.5827	2.0196	-0.1248
C	0	4.1725	3.221	0.2699
C	0	3.6776	4.4323	-0.2087
C	0	2.5949	4.4438	-1.0856
C	0	2.0028	3.2441	-1.4827
C	0	-1.2221	2.1403	1.9705
C	0	-2.6051	1.5341	1.9461
C	0	-3.6404	2.1447	1.2245
C	0	-4.9044	1.5557	1.1667
C	0	-5.1494	0.3592	1.8379
C	0	-4.1342	-0.2458	2.5758
C	0	-2.8695	0.3408	2.6347
H	0	-3.8171	-2.9779	-0.0411
H	0	-1.6494	-4.3726	-0.6529
H	0	-3.9059	-0.9404	-1.7606
H	0	-1.8971	-0.7084	0.1644
H	0	-0.2121	-0.7757	-2.4033
H	0	-0.6196	-3.1871	-2.8108
H	0	2.0343	-2.0799	-1.8102
H	0	1.1056	-3.3142	-0.9899
H	0	4.2794	-1.9433	-1.0196
H	0	5.9565	-2.2244	0.7651
H	0	5.2626	-2.9468	3.0334
H	0	2.8708	-3.3949	3.5161
H	0	1.1712	-3.1134	1.743
H	0	1.1754	0.9062	-2.2664
H	0	2.6288	0.0638	-1.7851
H	0	3.9872	1.0842	0.2589
H	0	5.0206	3.2121	0.9508
H	0	4.1391	5.3679	0.0986
H	0	2.2134	5.39	-1.4632
H	0	1.1617	3.2789	-2.1724
H	0	-1.18	3.0606	1.3738
H	0	-1.0044	2.4496	2.9999
H	0	-3.4709	3.0809	0.6952
H	0	-5.7023	2.034	0.6026
H	0	-6.1365	-0.0958	1.7963
H	0	-4.3284	-1.1739	3.1088
H	0	-2.0833	-0.1446	3.211

Stoichiometry C30H28N2O3
Framework group C1[X(C30H28N2O3)]
Deg. of freedom 183
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	-3.081309	-2.705878	-0.805782
2	6	0	-1.980702	-3.409833	-1.108369
3	6	0	-2.976728	-1.420718	-1.576726
4	6	0	-1.828039	-0.619361	-0.948577

5	6	0	-0.575557	-1.310830	-1.538103
6	6	0	-1.224465	-2.600041	-2.117649
7	8	0	-2.358319	-1.951745	-2.783594
8	6	0	-1.771547	0.827215	-1.322298
9	7	0	0.492921	-1.329688	-0.532975
10	8	0	-2.487500	1.335203	-2.180836
11	8	0	-0.848874	1.580343	-0.656625
12	6	0	1.537864	-2.317240	-0.867821
13	6	0	2.570876	-2.501485	0.221286
14	6	0	3.928774	-2.261876	-0.033977
15	6	0	4.877905	-2.427619	0.976220
16	6	0	4.481495	-2.839333	2.247410
17	6	0	3.136031	-3.088716	2.510987
18	6	0	2.185087	-2.923379	1.503279
19	6	0	-0.068124	0.978240	0.273587
20	6	0	1.042894	0.044706	-0.258507
21	7	0	-0.198082	1.200705	1.538525
22	6	0	1.825530	0.727376	-1.410249
23	1	0	1.728647	-0.055759	0.593155
24	6	0	2.481212	2.024906	-0.991736
25	6	0	3.571499	2.017055	-0.110359
26	6	0	4.162867	3.214938	0.292597
27	6	0	3.673660	4.429831	-0.182737
28	6	0	2.595106	4.448452	-1.064610
29	6	0	2.001454	3.252286	-1.469969
30	6	0	-1.242676	2.141944	1.963062
31	6	0	-2.627267	1.539832	1.929435
32	6	0	-3.657441	2.156697	1.205830
33	6	0	-4.922829	1.571596	1.139438
34	6	0	-5.174369	0.372744	1.803988
35	6	0	-4.164355	-0.238538	2.543825
36	6	0	-2.898278	0.344155	2.611310
37	1	0	-3.842811	-2.959527	-0.084086
38	1	0	-1.676256	-4.357625	-0.692176
39	1	0	-3.917773	-0.913930	-1.794608
40	1	0	-1.917338	-0.696509	0.140776
41	1	0	-0.220557	-0.756887	-2.419327
42	1	0	-0.633013	-3.165217	-2.839789
43	1	0	2.019325	-2.070228	-1.821760
44	1	0	1.083291	-3.305601	-1.011473
45	1	0	4.261086	-1.943690	-1.020089
46	1	0	5.929021	-2.237767	0.771097
47	1	0	5.222476	-2.968551	3.032798
48	1	0	2.827180	-3.411993	3.502285
49	1	0	1.136692	-3.117504	1.722597
50	1	0	1.171072	0.920381	-2.268242
51	1	0	2.619803	0.071621	-1.784048
52	1	0	3.971537	1.078751	0.270923
53	1	0	5.007747	3.200488	0.977393
54	1	0	4.136381	5.362687	0.131002
55	1	0	2.218070	5.397461	-1.439635
56	1	0	1.163689	3.292656	-2.163414
57	1	0	-1.195168	3.064842	1.370797
58	1	0	-1.028908	2.445902	2.994875
59	1	0	-3.482805	3.094820	0.681630
60	1	0	-5.716720	2.054761	0.573828
61	1	0	-6.162555	-0.079228	1.755700
62	1	0	-4.363685	-1.168508	3.071647
63	1	0	-2.116165	-0.146131	3.189032

Rotational constants (GHZ): 0.1468826 0.1022815 0.0816284
Standard basis: 6-31G (6D, 7F)

There are 371 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.
371 basis functions, 882 primitive gaussians, 371 cartesian basis functions
123 alpha electrons 123 beta electrons
nuclear repulsion energy 3766.0356916259 Hartrees.
NAtoms= 63 NActive= 63 NUniq= 63 SFac= 1.00D+00 NAtFMM= 60 Big=T

United Atom Topological Model (UA0 parameters set).

Nord	Group	Hybr	Charge	Alpha	Radius	Bonded to
1	CH	*	0.00	1.00	2.125	C2 [d] C3 [s]
2	CH	*	0.00	1.00	2.125	C1 [d] C6 [s]
3	CH	*	0.00	1.00	2.125	C1 [s] C4 [s] O7 [s]
4	CH	*	0.00	1.00	2.125	C3 [s] C5 [s] C8 [s]
5	CH	*	0.00	1.00	2.125	C4 [s] C6 [s] N9 [s]
6	CH	*	0.00	1.00	2.125	C2 [s] C5 [s] O7 [s]
7	O	*	0.00	1.00	1.750	C3 [s] C6 [s]
8	C	*	0.00	1.00	1.925	C4 [s] O10 [d] O11 [s]
9	N	*	0.00	1.00	1.830	C5 [s] C12 [s] C20 [s]
10	O	*	0.00	1.00	1.750	C8 [d]
11	O	*	0.00	1.00	1.750	C8 [s] C19 [s]
12	CH2	*	0.00	1.00	2.325	N9 [s] C13 [s]
13	C	*	0.00	1.00	1.925	C12 [s] C14 [s] C18 [s]
14	CH	*	0.00	1.00	2.125	C13 [s] C15 [s]
15	CH	*	0.00	1.00	2.125	C14 [s] C16 [s]
16	CH	*	0.00	1.00	2.125	C15 [s] C17 [s]
17	CH	*	0.00	1.00	2.125	C16 [s] C18 [s]
18	CH	*	0.00	1.00	2.125	C13 [s] C17 [s]
19	C	*	0.00	1.00	1.925	O11 [s] C20 [s] N21 [d]
20	CH	*	0.00	1.00	2.125	N9 [s] C19 [s] C22 [s]
21	N	*	0.00	1.00	1.830	C19 [d] C30 [s]
22	CH2	*	0.00	1.00	2.325	C20 [s] C24 [s]
24	C	*	0.00	1.00	1.925	C22 [s] C25 [s] C29 [s]
25	CH	*	0.00	1.00	2.125	C24 [s] C26 [s]
26	CH	*	0.00	1.00	2.125	C25 [s] C27 [s]
27	CH	*	0.00	1.00	2.125	C26 [s] C28 [s]
28	CH	*	0.00	1.00	2.125	C27 [s] C29 [s]
29	CH	*	0.00	1.00	2.125	C24 [s] C28 [s]
30	CH2	*	0.00	1.00	2.325	N21 [s] C31 [s]
31	C	*	0.00	1.00	1.925	C30 [s] C32 [s] C36 [s]
32	CH	*	0.00	1.00	2.125	C31 [s] C33 [s]
33	CH	*	0.00	1.00	2.125	C32 [s] C34 [s]
34	CH	*	0.00	1.00	2.125	C33 [s] C35 [s]
35	CH	*	0.00	1.00	2.125	C34 [s] C36 [s]
36	CH	*	0.00	1.00	2.125	C31 [s] C35 [s]

Polarizable Continuum Model (PCM)
==========
Model : PCM.
Atomic radii : UA0 (Simple United Atom Topological Model).
Polarization charges : Total charges.
Charge compensation : None.
Solution method : Matrix inversion.
Cavity : GePol (RMin=0.200 OFac=0.890).
Default sphere list used, NSphG= 35.
Tesserae with average area of 0.200 Ang**2.
Solvent : Methanol, Eps= 32.630000.

One-electron integrals computed using PRISM.
NBasis= 371 RedAO= T NBF= 371
NBsUse= 371 1.00D-06 NBFU= 371

```
Harris functional with IExCor=  402 diagonalized for initial guess.
ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 402 AccDes= 1.00D-06 IRadAn=         1 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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               (A) (A) (A) (A) (A) (A) (A) (A)
The electronic state of the initial guess is 1-A.
Warning!  Cutoffs for single-point calculations used.
Requested convergence on RMS density matrix=1.00D-04 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-02.
Requested convergence on             energy=5.00D-05.
No special actions if energy rises.
Error on total polarization charges =  0.02738
SCF Done:  E(RB+HF-LYP) =  -1494.74570262     A.U. after   10 cycles
           Convg  =    0.3286D-05             -V/T =  2.0051
           S**2   =   0.0000
--------------------------------------------------------------------
Variational PCM results
=======================
<psi(f)|   H    |psi(f)>                  (a.u.) =   -1494.711902
<psi(f)|H+V(f)/2|psi(f)>                  (a.u.) =   -1494.745703
Total free energy in solution:
 with all non electrostatic terms         (a.u.) =   -1494.728213
--------------------------------------------------------------------
(Polarized solute)-Solvent             (kcal/mol) =     -21.21
--------------------------------------------------------------------
Cavitation energy                      (kcal/mol) =      40.57
Dispersion energy                      (kcal/mol) =     -31.98
Repulsion energy                       (kcal/mol) =       2.39
Total non electrostatic                (kcal/mol) =      10.98
--------------------------------------------------------------------
```

```
Partition over spheres:
Sphere  on Atom  Surface  Charge   GEl    GCav    GDR
   1      C1      14.51  -0.036   -0.73   1.74   -1.18
   2      C2      14.69  -0.037   -0.83   1.67   -1.43
   3      C3       6.47  -0.042   -0.21   1.07   -0.64
   4      C4       0.00   0.000    0.00   0.34    0.00
   5      C5       2.38  -0.022   -0.19   0.39   -0.19
   6      C6      10.68  -0.063   -0.95   0.97   -0.97
   7      O7       8.89   0.129   -2.72   0.97   -0.95
   8      C8       0.00   0.000    0.00   0.21    0.00
   9      N9       0.00   0.000    0.00   0.20    0.00
  10      O10     13.26   0.156   -3.47   1.85   -1.40
  11      O11      0.75   0.009   -0.14   0.51   -0.08
  12      C12     12.89  -0.044   -0.49   1.51   -1.11
  13      C13      0.17   0.001    0.00   0.06    0.00
  14      C14      9.12  -0.022   -0.50   1.47   -0.96
  15      C15     14.53  -0.025   -0.52   1.69   -1.39
  16      C16     17.26  -0.015   -0.52   1.69   -1.54
  17      C17     17.03  -0.018   -0.52   1.69   -1.58
  18      C18      9.01  -0.009   -0.25   1.53   -0.85
  19      C19      0.00   0.000    0.00   0.12    0.00
  20      C20      0.00   0.000    0.00   0.43    0.00
  21      N21      2.47   0.045   -0.91   0.79   -0.25
  22      C22     10.79  -0.027   -0.20   1.43   -1.10
  23      C24      0.10   0.000    0.00   0.08    0.00
  24      C25      6.11   0.014   -0.08   1.54   -0.57
  25      C26     17.11  -0.017   -0.50   1.69   -1.58
  26      C27     16.86  -0.015   -0.48   1.69   -1.53
  27      C28     16.97  -0.018   -0.44   1.69   -1.50
  28      C29      9.85  -0.009   -0.21   1.47   -0.98
  29      C30     21.99  -0.048   -0.27   2.27   -1.77
  30      C31      0.25   0.001   -0.01   0.05    0.00
  31      C32     11.48  -0.029   -0.34   1.32   -1.01
  32      C33     14.24  -0.031   -0.43   1.69   -1.39
  33      C34     13.93  -0.029   -0.53   1.69   -1.36
  34      C35     14.70  -0.030   -0.59   1.69   -1.28
  35      C36     11.23  -0.023   -0.37   1.40   -0.99
Added spheres:   119.78   0.225   -3.84    0.00    0.00
--------------------------------------------------------------------

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

         Population analysis using the SCF density.

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

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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The electronic state is 1-A.

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Alpha  occ. eigenvalues -- -19.22646 -19.16342 -19.15286 -14.34908 -14.34185
Alpha  occ. eigenvalues -- -10.35122 -10.30483 -10.24947 -10.24756 -10.23820
Alpha  occ. eigenvalues -- -10.23803 -10.21590 -10.21499 -10.21337 -10.20032
Alpha  occ. eigenvalues -- -10.19543 -10.19515 -10.18951 -10.18934 -10.18875
Alpha  occ. eigenvalues -- -10.18670 -10.18664 -10.18616 -10.18563 -10.18459
Alpha  occ. eigenvalues -- -10.18446 -10.18354 -10.18346 -10.18316 -10.18282
Alpha  occ. eigenvalues -- -10.18253 -10.18220 -10.18191 -10.18143 -10.18034
Alpha  occ. eigenvalues --  -1.16350  -1.07465  -1.06798  -0.94833  -0.93812
Alpha  occ. eigenvalues --  -0.86244  -0.86013  -0.85881  -0.82787  -0.80077
Alpha  occ. eigenvalues --  -0.79206  -0.77616  -0.77062  -0.75489  -0.74865
Alpha  occ. eigenvalues --  -0.74584  -0.74497  -0.73100  -0.70745  -0.68551
Alpha  occ. eigenvalues --  -0.67887  -0.65466  -0.61897  -0.60848  -0.60618
Alpha  occ. eigenvalues --  -0.60467  -0.59931  -0.59292  -0.58388  -0.57590
Alpha  occ. eigenvalues --  -0.56082  -0.55657  -0.53672  -0.52253  -0.51646
Alpha  occ. eigenvalues --  -0.51386  -0.51058  -0.49957  -0.49243  -0.48287
Alpha  occ. eigenvalues --  -0.47974  -0.46573  -0.46285  -0.45846  -0.45425
Alpha  occ. eigenvalues --  -0.45166  -0.45060  -0.44573  -0.44265  -0.42719
Alpha  occ. eigenvalues --  -0.42521  -0.42243  -0.41999  -0.41934  -0.41851
Alpha  occ. eigenvalues --  -0.41533  -0.40932  -0.40796  -0.40322  -0.39918
Alpha  occ. eigenvalues --  -0.39454  -0.38377  -0.37546  -0.36601  -0.36363
Alpha  occ. eigenvalues --  -0.35978  -0.35658  -0.35227  -0.35152  -0.34733
Alpha  occ. eigenvalues --  -0.34242  -0.34060  -0.33755  -0.33634  -0.33251
Alpha  occ. eigenvalues --  -0.32881  -0.31166  -0.28587  -0.28018  -0.26895
Alpha  occ. eigenvalues --  -0.25417  -0.25218  -0.25058  -0.25025  -0.24859
Alpha  occ. eigenvalues --  -0.24819  -0.24495  -0.21674
Alpha virt. eigenvalues --  -0.03759  -0.01907  -0.00548  -0.00429  -0.00096
Alpha virt. eigenvalues --   0.00114   0.00220   0.00244   0.00447   0.08474
Alpha virt. eigenvalues --   0.09082   0.09442   0.10087   0.10556   0.11635
Alpha virt. eigenvalues --   0.11774   0.12107   0.12483   0.12975   0.13697
Alpha virt. eigenvalues --   0.13856   0.14177   0.14585   0.14992   0.15652
Alpha virt. eigenvalues --   0.15863   0.15907   0.16372   0.16559   0.16728
Alpha virt. eigenvalues --   0.17031   0.17446   0.17637   0.17958   0.18246
Alpha virt. eigenvalues --   0.18887   0.19224   0.19579   0.19696   0.20365
Alpha virt. eigenvalues --   0.20527   0.20584   0.21048   0.21819   0.21966
Alpha virt. eigenvalues --   0.22757   0.23439   0.24226   0.25152   0.25237
Alpha virt. eigenvalues --   0.25593   0.25726   0.27382   0.28191   0.28335
Alpha virt. eigenvalues --   0.29257   0.30620   0.31353   0.31440   0.31539
Alpha virt. eigenvalues --   0.32467   0.32764   0.33182   0.33486   0.33818
Alpha virt. eigenvalues --   0.34540   0.35055   0.35348   0.35936   0.36304
Alpha virt. eigenvalues --   0.36400   0.37710   0.41939   0.43665   0.46678
Alpha virt. eigenvalues --   0.47130   0.48961   0.49275   0.50285   0.51738
Alpha virt. eigenvalues --   0.52118   0.52502   0.53153   0.53296   0.53954
Alpha virt. eigenvalues --   0.54602   0.54703   0.55246   0.55725   0.56308
Alpha virt. eigenvalues --   0.56447   0.56827   0.57104   0.57667   0.57775
```

Alpha virt. eigenvalues --	0.58385	0.58642	0.59072	0.59675	0.60060
Alpha virt. eigenvalues --	0.60175	0.60715	0.61227	0.61682	0.62096
Alpha virt. eigenvalues --	0.62166	0.62744	0.62984	0.63208	0.63499
Alpha virt. eigenvalues --	0.63667	0.63904	0.64107	0.64679	0.64771
Alpha virt. eigenvalues --	0.64853	0.65359	0.65486	0.65687	0.65973
Alpha virt. eigenvalues --	0.66265	0.66403	0.66645	0.67071	0.67202
Alpha virt. eigenvalues --	0.68049	0.68574	0.68939	0.69632	0.70015
Alpha virt. eigenvalues --	0.70313	0.70780	0.71803	0.72607	0.73368
Alpha virt. eigenvalues --	0.74364	0.74696	0.75725	0.76691	0.77237
Alpha virt. eigenvalues --	0.80542	0.81467	0.82322	0.83081	0.83423
Alpha virt. eigenvalues --	0.84002	0.84083	0.85129	0.85420	0.85563
Alpha virt. eigenvalues --	0.86040	0.86501	0.86615	0.86874	0.87112
Alpha virt. eigenvalues --	0.87407	0.87740	0.87969	0.88696	0.88771
Alpha virt. eigenvalues --	0.89265	0.89773	0.90548	0.91336	0.92228
Alpha virt. eigenvalues --	0.92531	0.92975	0.93173	0.93813	0.94227
Alpha virt. eigenvalues --	0.94929	0.95438	0.96299	0.96476	0.96554
Alpha virt. eigenvalues --	0.97107	0.97653	0.98712	0.99625	0.99936
Alpha virt. eigenvalues --	1.00105	1.00176	1.01243	1.02428	1.03153
Alpha virt. eigenvalues --	1.04292	1.04636	1.05629	1.06218	1.06856
Alpha virt. eigenvalues --	1.07893	1.08196	1.09319	1.10316	1.10844
Alpha virt. eigenvalues --	1.11539	1.12484	1.13441	1.14492	1.15149
Alpha virt. eigenvalues --	1.16447	1.16968	1.17775	1.18257	1.18990
Alpha virt. eigenvalues --	1.20420	1.20634	1.21333	1.22378	1.23139
Alpha virt. eigenvalues --	1.23455	1.23871	1.24781	1.27756	1.28320
Alpha virt. eigenvalues --	1.29443	1.33023	1.36117	1.37679	1.38328
Alpha virt. eigenvalues --	1.40310	1.43237	1.44560	1.46410	1.46641
Alpha virt. eigenvalues --	1.47056	1.48310	1.48884	1.50146	1.52443
Alpha virt. eigenvalues --	1.55393	1.57255	1.62182	1.65552	1.68592
Alpha virt. eigenvalues --	1.75629	1.76775	1.79279	1.84010	1.89945
Alpha virt. eigenvalues --	1.91751	1.92477	1.94099	1.96270	2.01259
Alpha virt. eigenvalues --	2.05885	2.17873	2.56915		

Condensed to atoms (all electrons):

Mulliken atomic charges:

		1
1	C	-0.068769
2	C	-0.068563
3	C	-0.066940
4	C	-0.190902
5	C	0.051033
6	C	-0.097345
7	O	-0.481921
8	C	0.549909
9	N	-0.452245
10	O	-0.444045
11	O	-0.504712
12	C	-0.208167
13	C	0.072096
14	C	-0.175660
15	C	-0.153787
16	C	-0.145418
17	C	-0.156059
18	C	-0.144469
19	C	0.401325
20	C	-0.008321
21	N	-0.341765
22	C	-0.358154
23	H	0.182965
24	C	0.087173
25	C	-0.163045
26	C	-0.155418
27	C	-0.146692
28	C	-0.154492

29	C	-0.165678
30	C	-0.260948
31	C	0.066815
32	C	-0.169387
33	C	-0.149889
34	C	-0.145777
35	C	-0.151384
36	C	-0.160530
37	H	0.183986
38	H	0.185477
39	H	0.185953
40	H	0.218377
41	H	0.182690
42	H	0.194603
43	H	0.142127
44	H	0.175942
45	H	0.158714
46	H	0.154749
47	H	0.153316
48	H	0.155247
49	H	0.153036
50	H	0.161602
51	H	0.171059
52	H	0.140573
53	H	0.154247
54	H	0.151350
55	H	0.153046
56	H	0.153051
57	H	0.176452
58	H	0.175633
59	H	0.162620
60	H	0.158460
61	H	0.156200
62	H	0.158930
63	H	0.161726

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

		1
1	C	0.115216
2	C	0.116914
3	C	0.119013
4	C	0.027475
5	C	0.233724
6	C	0.097259
7	O	-0.481921
8	C	0.549909
9	N	-0.452245
10	O	-0.444045
11	O	-0.504712
12	C	0.109902
13	C	0.072096
14	C	-0.016946
15	C	0.000962
16	C	0.007898
17	C	-0.000813
18	C	0.008567
19	C	0.401325
20	C	0.174644
21	N	-0.341765
22	C	-0.025493
23	H	0.000000
24	C	0.087173

```
  25  C   -0.022472
  26  C   -0.001171
  27  C    0.004658
  28  C   -0.001445
  29  C   -0.012628
  30  C    0.091136
  31  C    0.066815
  32  C   -0.006767
  33  C    0.008572
  34  C    0.010422
  35  C    0.007546
  36  C    0.001196
  37  H    0.000000
  38  H    0.000000
  39  H    0.000000
  40  H    0.000000
  41  H    0.000000
  42  H    0.000000
  43  H    0.000000
  44  H    0.000000
  45  H    0.000000
  46  H    0.000000
  47  H    0.000000
  48  H    0.000000
  49  H    0.000000
  50  H    0.000000
  51  H    0.000000
  52  H    0.000000
  53  H    0.000000
  54  H    0.000000
  55  H    0.000000
  56  H    0.000000
  57  H    0.000000
  58  H    0.000000
  59  H    0.000000
  60  H    0.000000
  61  H    0.000000
  62  H    0.000000
  63  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>= 14547.4125
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     2.1351    Y=    -3.3852    Z=     3.0808  Tot=     5.0507
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=  -185.5729   YY=  -189.1707   ZZ=  -212.9101
  XY=     3.1814   XZ=   -14.8818   YZ=    -0.4597
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    10.3117   YY=     6.7139   ZZ=   -17.0256
  XY=     3.1814   XZ=   -14.8818   YZ=    -0.4597
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=   -22.7385  YYY=    31.9304  ZZZ=    40.8235  XYY=    -1.6333
 XXY=   -18.8759  XXZ=    67.6110  XZZ=    59.4565  YZZ=   -27.0389
 YYZ=    10.2162  XYZ=    21.7373
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -9456.9226 YYYY= -6052.8730 ZZZZ= -3153.2481 XXXY=     0.5454
XXXZ=   114.1379 YYYX=   225.4225 YYYZ=     2.1403 ZZZX=   -37.7258
ZZZY=  -103.6359 XXYY= -2767.6084 XXZZ= -2370.0800 YYZZ= -1563.0149
XXYZ=   -65.4880 YYXZ=    -4.2683 ZZXY=   -63.9261
N-N= 3.766035691626D+03 E-N=-1.100958993090D+04  KE= 1.487194854033D+03

Test job not archived.
```

1|1|UNPC-UNK|SP|RB3LYP|6-31G|C30H28N2O3|PCUSER|15-Jul-2011|0||# RB3LYP
/6-31G SCRF=(PCM,SOLVENT=METHANOL) TEST||[No Title]||0,1|C,0,-3.0597,-
2.7254,-0.7675|C,0,-1.9585,-3.4276,-1.072|C,0,-2.9624,-1.4435,-1.5448|
C,0,-1.8131,-0.636,-0.9257|C,0,-0.5614,-1.3266,-1.5179|C,0,-1.2093,-2.
6203,-2.0885|O,0,-2.3481,-1.9783,-2.7521|C,0,-1.7625,0.809,-1.3063|N,0
,0.5118,-1.3378,-0.5177|O,0,-2.4839,1.311,-2.1638|O,0,-0.8389,1.5678,-
0.6484|C,0,1.558,-2.3239,-0.8529|C,0,2.5966,-2.5002,0.2322|C,0,3.9526,
-2.2579,-0.0305|C,0,4.9069,-2.4163,0.976|C,0,4.5176,-2.8233,2.2509|C,0
,3.1741,-3.0753,2.5219|C,0,2.218,-2.9173,1.5179|C,0,-0.0521,0.9722,0.2
809|C,0,1.0591,0.0394,-0.2521|N,0,-0.1768,1.2001,1.5454|C,0,1.8344,0.7
19,-1.4106|H,0,1.7491,-0.0552,0.5968|C,0,2.4883,2.0203,-1.0011|C,0,3.5
827,2.0196,-0.1248|C,0,4.1725,3.221,0.2699|C,0,3.6776,4.4323,-0.2087|C
,0,2.5949,4.4438,-1.0856|C,0,2.0028,3.2441,-1.4827|C,0,-1.2221,2.1403,
1.9705|C,0,-2.6051,1.5341,1.9461|C,0,-3.6404,2.1447,1.2245|C,0,-4.9044
,1.5557,1.1667|C,0,-5.1494,0.3592,1.8379|C,0,-4.1342,-0.2458,2.5758|C,
0,-2.8695,0.3408,2.6347|H,0,-3.8171,-2.9779,-0.0411|H,0,-1.6494,-4.372
6,-0.6529|H,0,-3.9059,-0.9404,-1.7606|H,0,-1.8971,-0.7084,0.1644|H,0,-
0.2121,-0.7757,-2.4033|H,0,-0.6196,-3.1871,-2.8108|H,0,2.0343,-2.0799,
-1.8102|H,0,1.1056,-3.3142,-0.9899|H,0,4.2794,-1.9433,-1.0196|H,0,5.95
65,-2.2244,0.7651|H,0,5.2626,-2.9468,3.0334|H,0,2.8708,-3.3949,3.5161|
H,0,1.1712,-3.1134,1.743|H,0,1.1754,0.9062,-2.2664|H,0,2.6288,0.0638,-
1.7851|H,0,3.9872,1.0842,0.2589|H,0,5.0206,3.2121,0.9508|H,0,4.1391,5.
3679,0.0986|H,0,2.2134,5.39,-1.4632|H,0,1.1617,3.2789,-2.1724|H,0,-1.1
8,3.0606,1.3738|H,0,-1.0044,2.4496,2.9999|H,0,-3.4709,3.0809,0.6952|H,
0,-5.7023,2.034,0.6026|H,0,-6.1365,-0.0958,1.7963|H,0,-4.3284,-1.1739,
3.1088|H,0,-2.0833,-0.1446,3.211||Version=x86-Win32-G03RevB.03|State=1
-A|HF=-1494.7457026|RMSD=3.286e-006|Dipole=0.8494829,-1.3238782,1.2142
168|PG=C01 [X(C30H28N2O3)]||@