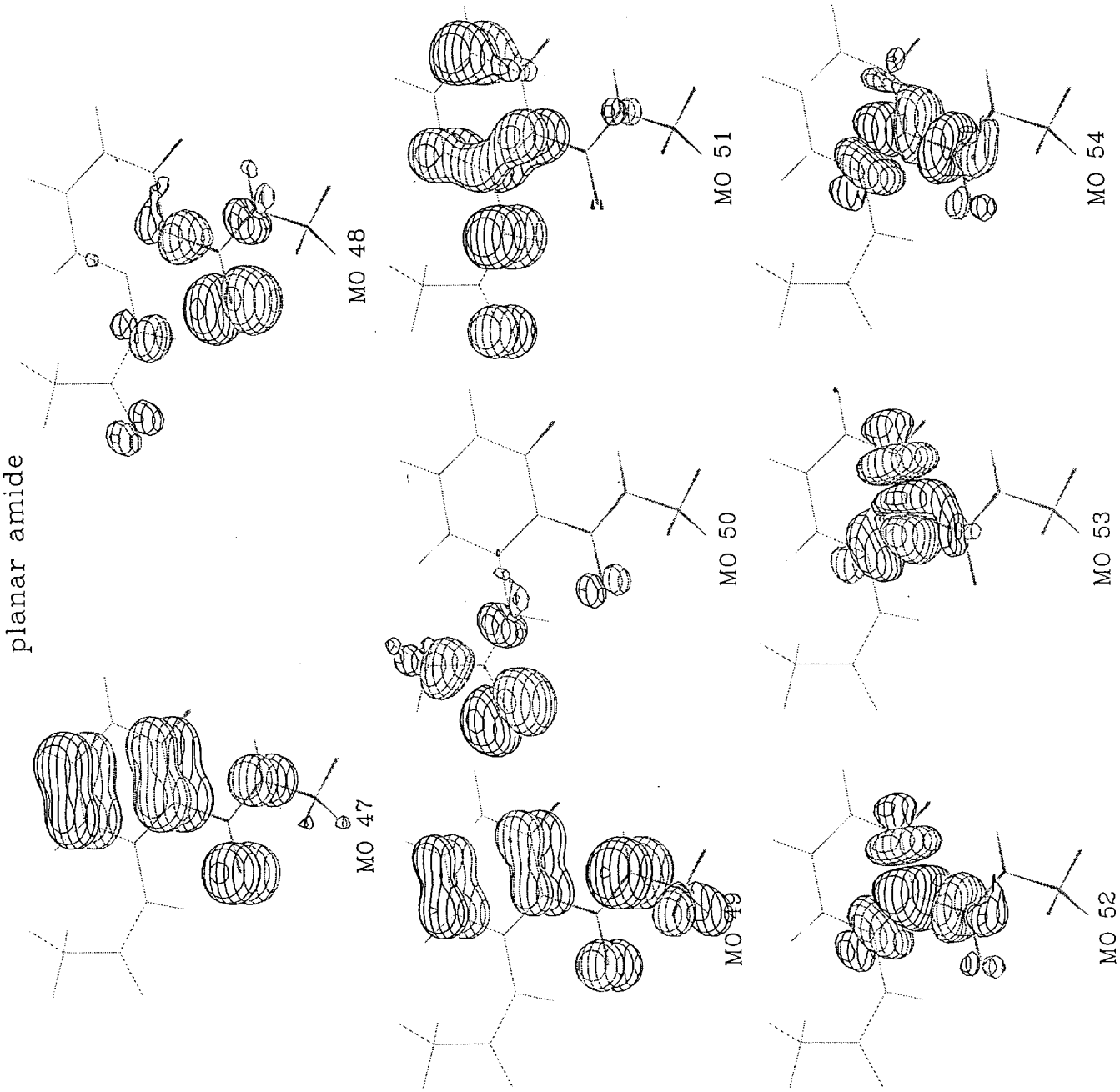

```
                26-Jan-2000
****************************************
%mem=26mw
----------------------------------------------
#t b3lyp rpa=(nstates=10) 6-31g* density=current
----------------------------------------------
------------------------------------------------------------------------
acetylated o-aminophenylcarboxamide td-b3lyp/6-31G*//b3lyp/6-31G* rest
ricted planar, C=O ... H-N contact
------------------------------------------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C                     0.9435   -0.28702   0.
C                     2.31407   0.02499   0.
C                     2.79006   1.32843   0.
C                     1.86661   2.37291   0.
C                     0.5037    2.11171   0.
C                     0.        0.79403   0.
C                     0.48681  -1.72006   0.
O                    -0.70948  -2.04997   0.
N                     1.42959  -2.70263   0.
C                     1.03143  -4.10187   0.
N                    -1.36005   0.49556   0.
C                    -2.54536   1.22476   0.
O                    -3.5988    0.60463   0.
C                    -2.54688   2.74206   0.
H                     3.05384  -0.76911   0.
H                     3.85771   1.52361   0.
H                     2.20554   3.40548   0.
H                    -0.17562   2.94896   0.
H                    -1.53921  -0.51556   0.
H                     2.41106  -2.48533   0.
H                     1.93264  -4.71918   0.
H                     0.43111  -4.33684   0.88478
H                     0.43111  -4.33684  -0.88478
H                    -3.59051   3.05918   0.
H                    -2.05098   3.14906   0.88795
H                    -2.05098   3.14906  -0.88795
------------------------------------------------------------------------
                      Z-MATRIX (ANGSTROMS AND DEGREES)
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z       J
------------------------------------------------------------------------
  1   1  C     0    0.943499         -0.287017          0.000000
  2   2  C     0    2.314067          0.024993          0.000000
  3   3  C     0    2.790063          1.328425          0.000000
  4   4  C     0    1.866613          2.372913          0.000000
  5   5  C     0    0.503700          2.111713          0.000000
  6   6  C     0    0.000000          0.794032          0.000000
  7   7  C     0    0.486813         -1.720059          0.000000
  8   8  O     0   -0.709478         -2.049967          0.000000
  9   9  N     0    1.429593         -2.702630          0.000000
 10  10  C     0    1.031429         -4.101874          0.000000
 11  11  N     0   -1.360048          0.495562          0.000000
 12  12  C     0   -2.545357          1.224764          0.000000
 13  13  O     0   -3.598801          0.604630          0.000000
 14  14  C     0   -2.546877          2.742056          0.000000
 15  15  H     0    3.053839         -0.769105          0.000000
```

16	16	H	0	3.857712	1.523607	0.000000
17	17	H	0	2.205535	3.405479	0.000000
18	18	H	0	-0.175624	2.948956	0.000000
19	19	H	0	-1.539211	-0.515562	0.000000
20	20	H	0	2.411065	-2.485334	0.000000
21	21	H	0	1.932644	-4.719179	0.000000
22	22	H	0	0.431109	-4.336841	0.884781
23	23	H	0	0.431109	-4.336841	-0.884781
24	24	H	0	-3.590506	3.059179	0.000000
25	25	H	0	-2.050978	3.149064	0.887954
26	26	H	0	-2.050978	3.149064	-0.887954

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.405634	0.000000			
3	C	2.453457	1.387626	0.000000		
4	C	2.815558	2.390176	1.394172	0.000000	
5	C	2.438715	2.762577	2.416815	1.387717	0.000000
6	C	1.434872	2.438509	2.840779	2.444813	1.410673
7	C	1.504052	2.526670	3.820761	4.319290	3.831809
8	O	2.416677	3.667054	4.864187	5.118409	4.334903
9	N	2.464036	2.867442	4.254443	5.094323	4.902568
10	C	3.815870	4.321596	5.707972	6.528430	6.235957
11	N	2.432850	3.704127	4.232857	3.733067	2.466881
12	C	3.802315	5.005342	5.336427	4.558917	3.175441
13	O	4.628987	5.941211	6.429733	5.744352	4.370562
14	C	4.621472	5.568771	5.520986	4.428901	3.115020
15	H	2.164704	1.085290	2.114051	3.358837	3.847378
16	H	3.430889	2.151438	1.085343	2.164670	3.405182
17	H	3.902212	3.382228	2.157736	1.086766	2.137773
18	H	3.424027	3.840328	3.379559	2.121923	1.078173
19	H	2.493207	3.891009	4.705624	4.465750	3.328071
20	H	2.643170	2.512200	3.832544	4.888660	4.977035
21	H	4.541197	4.759480	6.108083	7.092399	6.978751
22	H	4.176895	4.832594	6.200221	6.918404	6.509374
23	H	4.176895	4.832594	6.200221	6.918404	6.509374
24	H	5.635089	6.638544	6.611140	5.500101	4.202406
25	H	4.643491	5.440763	5.247749	4.091258	2.896712
26	H	4.643491	5.440763	5.247749	4.091258	2.896712

		6	7	8	9	10
6	C	0.000000				
7	C	2.560789	0.000000			
8	O	2.931158	1.240948	0.000000		
9	N	3.777616	1.361719	2.236424	0.000000	
10	C	5.003373	2.443287	2.690925	1.454792	0.000000
11	N	1.392413	2.884419	2.627348	4.243881	5.182237
12	C	2.581545	4.226824	3.754240	5.587902	6.416110
13	O	3.603782	4.700683	3.923656	6.018531	6.602288
14	C	3.206459	5.395715	5.132204	6.742175	7.722930
15	H	3.430646	2.737505	3.975319	2.525212	3.898396
16	H	3.926095	4.678069	5.799108	4.874099	6.295547
17	H	3.418193	5.406029	6.185402	6.157198	7.598610
18	H	2.162069	4.715774	5.027348	5.875129	7.153403
19	H	2.020942	2.357029	1.744378	3.687420	4.412462
20	H	4.070316	2.070843	3.150767	1.005239	2.125229
21	H	5.842141	3.329437	3.755729	2.078348	1.092362

22	H	5.224419	2.762877	2.704361	2.109610	1.094729
23	H	5.224419	2.762877	2.704361	2.109610	1.094729
24	H	4.245306	6.282169	5.865466	7.641979	8.523084
25	H	3.246714	5.562122	5.442243	6.866233	7.928795
26	H	3.246714	5.562122	5.442243	6.866233	7.928795
		11	12	13	14	15
11	N	0.000000				
12	C	1.391651	0.000000			
13	O	2.241408	1.222420	0.000000		
14	C	2.540728	1.517293	2.382254	0.000000	
15	H	4.591490	5.943611	6.792994	6.610316	0.000000
16	H	5.318073	6.410039	7.512929	6.519461	2.429556
17	H	4.602282	5.227475	6.444771	4.798495	4.259903
18	H	2.724335	2.930610	4.148976	2.380262	4.924775
19	H	1.026874	2.010240	2.344513	3.409907	4.600043
20	H	4.806978	6.191199	6.757689	7.204637	1.832648
21	H	6.167280	7.441972	7.677228	8.702651	4.106113
22	H	5.229073	6.369744	6.437480	7.730590	4.515561
23	H	5.229073	6.369744	6.437480	7.730590	4.515561
24	H	3.398099	2.111259	2.454563	1.090747	7.668317
25	H	2.882173	2.176190	3.107791	1.095460	6.496127
26	H	2.882173	2.176190	3.107791	1.095460	6.496127
		16	17	18	19	20
16	H	0.000000				
17	H	2.504223	0.000000			
18	H	4.277782	2.424527	0.000000		
19	H	5.769314	5.421963	3.723205	0.000000	
20	H	4.261971	5.894397	6.018510	4.414146	0.000000
21	H	6.532860	8.129240	7.952678	5.451988	2.284502
22	H	6.846115	7.992180	7.364360	4.389439	2.851516
23	H	6.846115	7.992180	7.364360	4.389439	2.851516
24	H	7.604862	5.806377	3.416660	4.121478	8.170709
25	H	6.192188	4.355699	2.084576	3.805240	7.241873
26	H	6.192188	4.355699	2.084576	3.805240	7.241873
		21	22	23	24	25
21	H	0.000000				
22	H	1.784272	0.000000			
23	H	1.784272	1.769562	0.000000		
24	H	9.539813	8.465066	8.465066	0.000000	
25	H	8.863800	7.886668	8.083447	1.779519	0.000000
26	H	8.863800	8.083447	7.886668	1.779519	1.775908
		26				
26	H	0.000000				

Interatomic angles:

C1-C2-C3=122.8863	C1-C2-C4= 92.0351	C1-C3-C4= 89.7002
C2-C3-C4=118.458	C2-C1-C5= 87.5648	C1-C5-C3= 60.6994
C2-C3-C5= 88.8495	C1-C5-C4= 90.4595	C2-C4-C5= 89.9406
C3-C4-C5=120.6314	C2-C1-C6=118.2884	C3-C1-C6= 89.9326
C3-C2-C6= 91.6782	C1-C6-C4= 89.1131	C4-C2-C6= 60.8269
C3-C4-C6= 91.2541	C1-C6-C5=117.9668	C2-C6-C5= 87.4633
C3-C5-C6= 92.009	C4-C5-C6=121.7691	C2-C1-C7=120.501
C3-C1-C7=148.8568	C3-C2-C7=153.7433	C4-C1-C7=178.5371
C4-C2-C7=122.8921	C5-C1-C7=151.9342	C5-C2-C7= 92.738
C6-C1-C7=121.2106	C6-C2-C7= 62.0651	C3-C6-C7= 89.884
C4-C6-C7=119.2675	C5-C6-C7=148.1212	C2-C1-O8=145.9809
C3-C1-O8=174.3367	C4-C1-O8=155.983	C5-C1-O8=126.4544
C6-C1-O8= 95.7307	C2-C6-O8= 85.6241	C3-C6-O8=114.8502

C4-C6-O8=144.2337	C5-C6-O8=173.0874	C1-C7-O8=123.0938
C2-C7-O8=151.7358	C6-C7-O8= 94.4588	C2-C1-N9= 91.4471
C3-C1-N9=119.8029	C3-C2-N9=177.9046	C4-C1-N9=149.4833
C4-C2-N9=151.2442	C5-C1-N9=179.0119	C5-C2-N9=121.0901
C6-C1-N9=150.2644	C6-C2-N9= 90.4172	C1-C7-N9=118.5078
C2-C7-N9= 89.8658	C6-C7-N9=147.1427	C1-O8-N9= 63.8117
C2-N9-O8= 90.9983	C6-O8-N9= 92.9604	O8-C7-N9=118.3985
C1-C7-C10=149.4442	C2-C7-C10=120.8022	C6-C7-C10=178.0792
C1-O8-C10= 96.5316	C6-O8-C10=125.6802	O8-C7-C10= 87.462
C1-N9-C10=152.7383	C2-N9-C10=177.918	C7-N9-C10=120.2999
O8-N9-C10= 91.0837	C2-C1-N11=148.4111	C3-C1-N11=120.0553
C4-C1-N11= 90.375	C5-C1-N11= 60.8464	C2-C5-N11= 90.0136
C3-C5-N11=120.1588	C4-C5-N11=149.9189	C1-C6-N11=118.7356
C2-C6-N11=149.239	C3-C6-N11=178.4651	C4-C6-N11=152.1513
C5-C6-N11=123.2976	C7-C1-N11= 91.0879	C2-C7-N11= 86.1316
C5-N11-C7= 91.1169	C7-C6-N11= 88.5811	O8-C1-N11= 65.608
C5-N11-O8=116.5938	C6-N11-O8= 88.0413	C7-O8-N11= 88.9188
N9-C1-N11=120.1417	N9-C7-N11=175.9973	N9-O8-N11=121.3041
C10-C7-N11=153.0662	C10-O8-N11=154.024	C1-C6-C12=140.718
C2-C6-C12=171.2214	C3-C6-C12=159.5525	C4-C6-C12=130.1689
C5-C6-C12=101.3152	C7-C6-C12=110.5635	O8-C6-C12= 85.5974
C1-N11-C12=167.1642	C5-N11-C12=107.4699	C6-N11-C12=136.0225
C7-N11-C12=161.4132	O8-N11-C12=135.9362	C1-N11-O13=164.0251
C5-N11-O13=136.2806	C6-N11-O13=164.8332	C7-N11-O13=132.6025
O8-N11-O13=107.1255	C6-C12-O13=139.9111	N11-C12-O13=117.916
C1-N11-C14=136.6117	C5-N11-C14= 76.9174	C6-N11-C14=105.47
C7-N11-C14=168.0343	O8-N11-C14=166.4888	C6-C12-C14= 99.6621
N11-C12-C14=121.6572	N11-O13-C14= 66.5853	O13-C12-C14=120.4268
C1-C2-H15=120.1467	C1-H15-C3= 69.9645	C3-C2-H15=116.9669
C4-C1-H15= 83.7288	C4-C2-H15=147.8182	C4-C3-H15=145.6872
C5-C1-H15=113.2575	C5-C2-H15=177.9722	C5-C3-H15=116.0786
C6-C1-H15=143.9811	C6-C2-H15=151.3549	C6-C3-H15= 86.3248
C7-C1-H15= 94.8083	C7-C2-H15= 89.2898	C3-H15-C7=103.1595
C6-C7-H15= 80.6316	O8-C1-H15=120.2882	O8-C7-H15=175.0904
N9-C1-H15= 65.7544	C2-H15-N9= 96.9967	C3-H15-N9=132.8006
C7-N9-H15= 83.8478	O8-N9-H15=113.064	C10-C7-H15= 97.4475
C10-N9-H15=155.8523	N11-C1-H15=174.1038	N11-C7-H15=109.4862
C1-C2-H16=148.6728	C1-C3-H16=149.1795	C2-C3-H16=120.4216
C1-C4-H16= 86.0383	C2-H16-C4= 67.2527	C4-C3-H16=121.1203
C5-C2-H16= 86.7918	C5-C3-H16=150.7289	C5-C4-H16=146.0502
C6-C2-H16=117.4647	C6-C3-H16=179.5173	C6-C4-H16=116.6729
C7-C2-H16=179.5298	N9-C2-H16=152.1181	C1-H15-H16= 96.4538
H15-C2-H16= 91.1804	H15-C3-H16= 93.1925	C4-H16-H15= 93.779
C7-H15-H16=129.6489	N9-H15-H16=159.29	C1-C3-H17=115.4629
C2-C3-H17=144.2207	C1-C4-H17=179.0325	C2-C4-H17=151.0387
C3-C4-H17=120.348	C1-C5-H17=116.8532	C2-C5-H17= 86.299
C3-H17-C5= 68.475	C5-C4-H17=119.0206	C6-C3-H17= 85.125
C6-C4-H17=148.3979	C6-C5-H17=148.1627	N11-C5-H17=176.3125
H15-C3-H17=171.4499	C2-H16-H17= 92.8707	H16-C3-H17= 95.3576
H16-C4-H17= 94.9292	C5-H17-H16= 94.0385	H15-H16-H17=119.397
C1-C4-H18= 86.6128	C2-C4-H18=116.5416	C3-C4-H18=147.2323
C1-C5-H18=151.3343	C2-C5-H18=178.1115	C3-C5-H18=147.9663
C4-C5-H18=118.2062	C1-C6-H18=143.546	C2-C6-H18=113.0426
C3-C6-H18= 83.8165	C4-H18-C6= 69.5889	C6-C5-H18=120.0248
C7-C6-H18=173.7005	O8-C6-H18=161.3334	C1-N11-H18= 82.9942
C4-H18-N11=100.018	N11-C5-H18= 91.875	N11-C6-H18= 97.7184
C7-N11-H18=114.4168	O8-N11-H18=139.8938	C4-H18-C12=128.2089

C5-H18-C12= 93.016	C12-C6-H18= 75.736	C12-N11-H18= 84.17
O13-N11-H18=112.9807	O13-C12-H18=174.4449	C4-H18-C14=159.2615
C5-H18-C14=124.0686	C6-H18-C14= 89.6726	N11-C14-H18= 67.139
C12-C14-H18= 94.9292	O13-C14-H18=121.1905	H16-C4-H18=172.6511
C3-H17-H18= 94.8645	H17-C4-H18= 92.4196	H17-C5-H18= 91.8125
C6-H18-H17= 96.194	N11-H18-H17=126.6231	C12-H18-H17=154.814
C14-H18-H17=174.1334	H16-H17-H18=120.4281	C2-C1-H19=172.4347
C3-C1-H19=144.0789	C4-C1-H19=114.3986	C5-C1-H19= 84.8699
C1-C6-H19= 90.7214	C2-C6-H19=121.2248	C3-C6-H19=150.4509
C4-C6-H19=179.8345	C5-C6-H19=151.3118	C1-C7-H19= 76.9442
C2-C7-H19=105.5862	C6-H19-C7= 71.1239	C1-O8-H19= 71.5585
C6-H19-O8=101.9894	C7-O8-H19=102.9848	N9-C1-H19= 96.1182
N9-C7-H19=164.5481	N9-O8-H19=135.3701	C10-C7-H19=133.6116
C10-O8-H19=168.09	C1-N11-H19= 81.284	C5-N11-H19=140.9783
C6-N11-H19=112.4257	C7-H19-N11=110.684	O8-H19-N11=141.5495
C1-H19-C12=114.7743	C6-H19-C12= 79.6419	C7-H19-C12=150.7658
O8-H19-C12=178.3686	C12-N11-H19=111.5518	C1-H19-O13=146.1991
C6-H19-O13=111.0668	C7-H19-O13=177.8093	O8-H19-O13=146.9438
O13-N11-H19= 82.7411	O13-C12-H19= 89.5496	C14-N11-H19=142.1043
C14-C12-H19=150.0236	C14-O13-H19= 92.3375	H15-C1-H19=161.8726
H15-C7-H19=128.9408	H18-C6-H19=125.7326	H18-N11-H19=164.2782
H18-C12-H19= 96.0055	C1-C2-H20= 79.388	C3-C1-H20= 97.4541
C3-C2-H20=157.7257	C4-C1-H20=127.1344	C4-C2-H20=171.423
C5-C1-H20=156.6631	C5-C2-H20=141.269	C6-C1-H20=172.6133
C6-C2-H20=110.5961	C1-C7-H20= 94.0115	C2-H20-C7= 66.0995
C6-C7-H20=122.6465	O8-C1-H20= 76.8826	O8-C7-H20=142.8947
C1-N9-H20= 88.8939	C2-H20-N9=100.271	C7-N9-H20=121.3322
O8-N9-H20=150.5485	C1-H20-C10=105.7944	C2-H20-C10=137.3081
C7-H20-C10= 71.2086	O8-C10-H20= 80.7915	C10-N9-H20=118.3678
N11-C1-H20=142.4906	N11-C7-H20=151.5011	C1-H15-H20= 82.3356
C2-H15-H20=116.4962	C3-H15-H20=152.3001	C7-H20-H15= 88.8446
N9-H20-H15=123.0161	C10-H20-H15=160.0532	H16-C2-H20=131.9392
H16-H15-H20=178.7895	H19-C1-H20=118.467	H19-C7-H20=170.9557
C1-N9-H21=177.3705	C2-N9-H21=148.0267	C7-N9-H21=150.1911
O8-N9-H21=120.9749	C7-C10-H21=137.2896	O8-C10-H21=164.7224
N9-C10-H21=108.5259	H15-N9-H21=125.9611	C1-H20-H21=134.1851
C2-H20-H21=165.6988	C7-H20-H21= 99.5993	H20-N9-H21= 88.4766
H20-C10-H21= 83.9309	H15-H20-H21=171.5561	C1-C7-H22=155.3027
C2-C7-H22=131.9678	C6-C7-H22=157.8224	C1-O8-H22=109.1717
C6-O8-H22=135.9221	C7-O8-H22= 79.5271	C1-N9-H22=131.7634
C2-N9-H22=151.9906	C7-N9-H22=103.372	O8-N9-H22= 76.9012
C7-C10-H22= 94.9911	O8-C10-H22= 78.9826	N9-C10-H22=110.8869
N11-C7-H22=135.6111	N11-O8-H22=157.4767	H15-C7-H22=110.36
H15-N9-H22=153.8411	H19-C7-H22=117.8184	H19-O8-H22=160.8128
C1-H20-H22= 98.8879	C2-H20-H22=128.4633	H20-C7-H22= 70.654
O8-H22-H20= 69.0388	H20-N9-H22=129.0179	H20-C10-H22=121.2818
H15-H20-H22=148.3853	C7-H22-H21= 91.5578	O8-H22-H21=111.9559
N9-H21-H22= 65.6946	H21-C10-H22=109.337	H20-H21-H22= 88.092
C1-C7-H23=155.3027	C2-C7-H23=131.9678	C6-C7-H23=157.8224
C1-O8-H23=109.1717	C6-O8-H23=135.9221	C7-O8-H23= 79.5271
C1-N9-H23=131.7634	C2-N9-H23=151.9906	C7-N9-H23=103.372
O8-N9-H23= 76.9012	C7-C10-H23= 94.9911	O8-C10-H23= 78.9826
N9-C10-H23=110.8869	N11-C7-H23=135.6111	N11-O8-H23=157.4767
H15-C7-H23=110.36	H15-N9-H23=153.8411	H19-C7-H23=117.8184
H19-O8-H23=160.8128	C1-H20-H23= 98.8879	C2-H20-H23=128.4633
H20-C7-H23= 70.654	O8-H23-H20= 69.0388	H20-N9-H23=129.0179
H20-C10-H23=121.2818	H15-H20-H23=148.3853	C7-H23-H21= 91.5578

O8-H23-H21=111.9559	N9-H21-H23= 65.6946	H21-C10-H23=109.337
H20-H21-H23= 88.092	C7-H22-H23= 71.3226	O8-H22-H23= 70.903
N9-H22-H23= 65.203	H22-C10-H23=107.8446	H20-H22-H23= 71.9236
H21-H22-H23= 60.2723	C6-C12-H24=129.2769	N11-C12-H24=151.2719
N11-O13-H24= 92.5955	O13-C12-H24= 90.8121	N11-C14-H24=134.7498
C12-C14-H24=106.9596	O13-C14-H24= 80.6983	H18-C12-H24= 83.6329
H18-C14-H24=158.1111	H19-C12-H24=179.6383	H19-O13-H24=118.3477
C1-C5-H25=120.7497	C2-C5-H25=148.0427	C3-C5-H25=161.8758
C4-C5-H25=143.0114	C6-C5-H25= 91.1233	C1-N11-H25=121.5428
C5-N11-H25= 65.0361	C6-N11-H25= 92.1093	C7-N11-H25=149.3935
O8-N11-H25=162.0543	C5-H25-C12= 76.0316	C6-C12-H25= 85.6152
N11-C12-H25=105.6548	O13-N11-H25= 73.4865	O13-C12-H25=130.1173
C5-H25-C14= 91.0146	N11-C14-H25= 96.7221	C12-C14-H25=111.7827
O13-C14-H25=122.2251	H17-C5-H25=119.0356	C4-H18-H25=153.1141
C5-H18-H25=129.8944	C6-H18-H25= 99.7154	N11-H18-H25= 72.2614
C12-H25-H18= 86.8865	C14-H25-H18= 91.5076	H17-H18-H25=149.936
H19-N11-H25=149.85	H19-C12-H25=130.6789	C5-H25-H24=126.2946
N11-H25-H24= 90.4104	C12-H24-H25= 67.3943	O13-H24-H25= 93.063
H24-C14-H25=108.9722	H18-H25-H24=124.1186	C1-C5-H26=120.7497
C2-C5-H26=148.0427	C3-C5-H26=161.8758	C4-C5-H26=143.0114
C6-C5-H26= 91.1233	C1-N11-H26=121.5428	C5-N11-H26= 65.0361
C6-N11-H26= 92.1093	C7-N11-H26=149.3935	O8-N11-H26=162.0543
C5-H26-C12= 76.0316	C6-C12-H26= 85.6152	N11-C12-H26=105.6548
O13-N11-H26= 73.4865	O13-C12-H26=130.1173	C5-H26-C14= 91.0146
N11-C14-H26= 96.7221	C12-C14-H26=111.7827	O13-C14-H26=122.2251
H17-C5-H26=119.0356	C4-H18-H26=153.1141	C5-H18-H26=129.8944
C6-H18-H26= 99.7154	N11-H18-H26= 72.2614	C12-H26-H18= 86.8865
C14-H26-H18= 91.5076	H17-H18-H26=149.936	H19-N11-H26=149.85
H19-C12-H26=130.6789	C5-H26-H24=126.2946	N11-H26-H24= 90.4104
C12-H24-H26= 67.3943	O13-H24-H26= 93.063	H24-C14-H26=108.9722
H18-H26-H24=124.1186	C5-H25-H26= 72.1492	N11-H25-H26= 72.0561
C12-H25-H26= 65.9188	H25-C14-H26=108.3045	H18-H25-H26= 64.7883
H24-H25-H26= 60.0671		

Framework group CS[SG(C10H8N2O2),X(H4)]
Deg. of freedom 47

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.943499	-0.287017	0.000000
2	6	0	2.314067	0.024993	0.000000
3	6	0	2.790063	1.328425	0.000000
4	6	0	1.866613	2.372913	0.000000
5	6	0	0.503700	2.111713	0.000000
6	6	0	0.000000	0.794032	0.000000
7	6	0	0.486813	-1.720059	0.000000
8	8	0	-0.709478	-2.049967	0.000000
9	7	0	1.429593	-2.702630	0.000000
10	6	0	1.031429	-4.101874	0.000000
11	7	0	-1.360048	0.495562	0.000000
12	6	0	-2.545357	1.224764	0.000000
13	8	0	-3.598801	0.604630	0.000000
14	6	0	-2.546877	2.742056	0.000000
15	1	0	3.053839	-0.769105	0.000000
16	1	0	3.857712	1.523607	0.000000
17	1	0	2.205535	3.405479	0.000000

```
  18          1             0       -0.175624    2.948956    0.000000
  19          1             0       -1.539211   -0.515562    0.000000
  20          1             0        2.411065   -2.485334    0.000000
  21          1             0        1.932644   -4.719179    0.000000
  22          1             0        0.431109   -4.336841    0.884781
  23          1             0        0.431109   -4.336841   -0.884781
  24          1             0       -3.590506    3.059179    0.000000
  25          1             0       -2.050978    3.149064    0.887954
  26          1             0       -2.050978    3.149064   -0.887954
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.8802545      0.5351898      0.3342249
 Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,C-12,O-16,N-14,C-12,N-14,C-12,O-16,C-
12,
 H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1,H-1
   234 basis functions      440 primitive gaussians
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       862.6031732995 Hartrees.
 Projected INDO Guess.
 Initial guess orbital symmetries:
       Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A') (A") (A') (A")
                 (A') (A') (A") (A') (A') (A') (A") (A') (A') (A")
                 (A') (A') (A') (A') (A") (A') (A") (A') (A") (A')
                 (A")
       Virtual   (A") (A") (A") (A') (A') (A") (A') (A') (A') (A')
                 (A') (A') (A') (A') (A") (A') (A') (A") (A') (A")
                 (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
                 (A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
                 (A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
                 (A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
                 (A") (A") (A") (A") (A") (A") (A") (A") (A") (A")
                 (A") (A") (A")
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
 SCF Done:  E(RB+HF-LYP) =  -648.271692170     A.U. after   16 cycles
            Convg  =    0.6915D-08             -V/T =  2.0095
            S**2   =   0.0000
 NROrb=    220 NOA=    37 NOB=    37 NVA=   183 NVB=   183
 Would need an additional  1113229624 words for in-memory AO integral storage.
 Orbital Symmetries:
       Occupied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A") (A') (A") (A') (A') (A") (A') (A')
                 (A') (A') (A") (A") (A') (A") (A") (A') (A") (A')
```

```
                (A")
     Virtual    (A") (A") (A") (A') (A") (A') (A') (A') (A') (A')
                (A") (A') (A") (A') (A') (A") (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A") (A') (A') (A') (A") (A") (A') (A') (A") (A')
                (A') (A") (A') (A') (A') (A') (A") (A") (A") (A')
                (A") (A') (A') (A') (A') (A") (A') (A') (A") (A')
                (A') (A') (A") (A") (A") (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A") (A") (A') (A')
                (A') (A') (A') (A') (A') (A') (A") (A') (A') (A")
                (A") (A') (A") (A') (A") (A') (A") (A") (A") (A")
                (A') (A") (A') (A') (A') (A') (A') (A') (A") (A')
                (A') (A') (A") (A') (A") (A') (A') (A') (A') (A")
                (A') (A") (A') (A') (A') (A') (A') (A') (A") (A")
                (A') (A") (A') (A') (A') (A") (A') (A") (A") (A')
                (A") (A") (A') (A') (A') (A") (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')
 Petite list used in FoFDir.
 MinBra= 0 MaxBra= 2 Meth= 1.
 IRaf=       0 NMat=   1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 1 JSym2E=1.
    40 initial guesses have been made.
 Iteration     1 Dimension    40
 New state      3 was old state      4
 New state      4 was old state      7
 New state      5 was old state      3
 New state      6 was old state      3
 New state      7 was old state     10
 New state     10 was old state      6
 Iteration     2 Dimension    60
 New state      4 was old state      5
 New state      5 was old state      4
 New state      8 was old state      9
 New state      9 was old state      8
 Iteration     3 Dimension    80
 New state      7 was old state      8
 New state      8 was old state      7
 Iteration     4 Dimension   100
 Iteration     5 Dimension   120
 Iteration     6 Dimension   134
 Iteration     7 Dimension   140
 Iteration     8 Dimension   144
 ********************************************************************
 Excited states from <AA,BB:AA,BB> singles matrix:
 ********************************************************************

 Ground to excited state Transition electric dipole moments (Au):
       state          X           Y           Z         Osc.
         1         0.6880     -0.8944      0.0000      0.1280
         2         0.0000      0.0000      0.0533      0.0003
         3         0.0000      0.0000      0.0075      0.0000
         4         1.2192     -0.5217      0.0000      0.2171
         5         0.0000      0.0000      0.0378      0.0002
         6        -0.5623     -0.6975      0.0000      0.1047
         7        -1.2985     -0.7882      0.0000      0.3312
```

8	0.0000	0.0000	-0.0106	0.0000
9	0.0316	-0.5309	0.0000	0.0413
10	0.8546	0.2742	0.0000	0.1217

Ground to excited state transition velocity dipole Moments (Au):

state	X	Y	Z	Osc.
1	-0.1050	0.1385	0.0000	0.1335
2	0.0000	0.0000	-0.0108	0.0005
3	0.0000	0.0000	-0.0069	0.0002
4	-0.2212	0.0854	0.0000	0.2024
5	0.0000	0.0000	-0.0097	0.0003
6	0.1183	0.1351	0.0000	0.1099
7	0.2737	0.1744	0.0000	0.3261
8	0.0000	0.0000	0.0051	0.0001
9	-0.0108	0.1033	0.0000	0.0328
10	-0.1898	-0.0502	0.0000	0.1134

Ground to excited state transition magnetic dipole Moments (Au):

state	X	Y	Z
1	0.0000	0.0000	1.0745
2	-0.6747	-0.2703	0.0000
3	0.0172	0.0093	0.0000
4	0.0000	0.0000	0.1723
5	-0.5771	-0.2538	0.0000
6	0.0000	0.0000	-0.1878
7	0.0000	0.0000	0.3279
8	0.1320	0.0368	0.0000
9	0.0000	0.0000	0.6724
10	0.0000	0.0000	0.2727

Ground to excited state transition densities written to RWF 633

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A' 4.1030 eV 302.17 nm f=0.1280

47 -> 53	-0.12293
49 -> 53	-0.11305
51 -> 52	0.64596
51 -> 53	-0.11657

This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A" 4.5538 eV 272.26 nm f=0.0003

48 -> 52	0.32012
50 -> 52	0.57308
50 -> 53	0.20335
50 -> 54	0.10059

Excited State 3: Singlet-A" 4.7107 eV 263.20 nm f=0.0000

48 -> 52	0.59766
50 -> 52	-0.25019
50 -> 53	-0.21464
50 -> 54	-0.10690

Excited State 4: Singlet-A' 5.0387 eV 246.06 nm f=0.2171

47 -> 52	0.18509
49 -> 52	0.31040
51 -> 52	0.11244
51 -> 53	0.54688

```
Excited State   5:    Singlet-A"      5.2063 eV  238.14 nm  f=0.0002
     48 -> 52          0.11549
     50 -> 52         -0.32111
     50 -> 53          0.58277
     50 -> 54          0.18376

Excited State   6:    Singlet-A'      5.3250 eV  232.83 nm  f=0.1047
     47 -> 52         -0.22207
     49 -> 52          0.57644
     51 -> 53         -0.23412

Excited State   7:    Singlet-A'      5.8592 eV  211.60 nm  f=0.3312
     46 -> 52         -0.13807
     47 -> 52          0.53671
     47 -> 53          0.20866
     49 -> 53         -0.10633
     49 -> 56          0.10347
     51 -> 53         -0.20543
     51 -> 54         -0.10226

Excited State   8:    Singlet-A"      5.8709 eV  211.18 nm  f=0.0000
     48 -> 53          0.69885

Excited State   9:    Singlet-A'      5.9615 eV  207.97 nm  f=0.0413
     46 -> 52         -0.25522
     49 -> 53          0.63329

Excited State  10:    Singlet-A'      6.1681 eV  201.01 nm  f=0.1217
     46 -> 52         -0.29190
     47 -> 52         -0.18794
     47 -> 53          0.53584
     51 -> 56          0.20103

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

           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') (A') (A') (A') (A') (A') (A')
                 (A') (A') (A") (A') (A") (A') (A') (A") (A') (A')
                 (A') (A') (A") (A") (A') (A") (A") (A') (A") (A')
                 (A")
       Virtual   (A") (A") (A") (A') (A") (A') (A') (A') (A') (A')
                 (A") (A') (A") (A') (A') (A") (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                 (A") (A') (A') (A') (A") (A") (A') (A') (A") (A')
                 (A') (A") (A') (A') (A') (A') (A") (A") (A") (A')
                 (A") (A') (A') (A') (A') (A") (A') (A') (A") (A')
                 (A') (A') (A") (A") (A") (A') (A') (A') (A') (A')
                 (A') (A') (A') (A') (A') (A') (A") (A") (A') (A')
                 (A') (A') (A') (A') (A') (A') (A") (A') (A') (A")
                 (A") (A') (A") (A') (A") (A') (A") (A") (A") (A")
```

```
                  (A')  (A")  (A')  (A')  (A')  (A')  (A')  (A')  (A")  (A')
                  (A')  (A')  (A")  (A')  (A")  (A')  (A')  (A')  (A')  (A")
                  (A')  (A")  (A')  (A')  (A')  (A')  (A')  (A')  (A")  (A")
                  (A')  (A")  (A')  (A')  (A')  (A")  (A')  (A")  (A")  (A')
                  (A")  (A")  (A')  (A')  (A')  (A")  (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 is 1-A'.
Alpha  occ. eigenvalues --  -19.12279 -19.10968 -14.36964 -14.35445 -10.29961
Alpha  occ. eigenvalues --  -10.28966 -10.25570 -10.22426 -10.21502 -10.21249
Alpha  occ. eigenvalues --  -10.20689 -10.19853 -10.19795 -10.19133  -1.04355
Alpha  occ. eigenvalues --   -1.02945  -0.93216  -0.92489  -0.85596  -0.77644
Alpha  occ. eigenvalues --   -0.75313  -0.73968  -0.71126  -0.64010  -0.63509
Alpha  occ. eigenvalues --   -0.60152  -0.57399  -0.54662  -0.51970  -0.48576
Alpha  occ. eigenvalues --   -0.47952  -0.46639  -0.45913  -0.44993  -0.44877
Alpha  occ. eigenvalues --   -0.43766  -0.41810  -0.40795  -0.40429  -0.39973
Alpha  occ. eigenvalues --   -0.39167  -0.38195  -0.37681  -0.35981  -0.35768
Alpha  occ. eigenvalues --   -0.30786  -0.26928  -0.26323  -0.25845  -0.24600
Alpha  occ. eigenvalues --   -0.21782
Alpha virt. eigenvalues --   -0.04601  -0.01607   0.04428   0.05460   0.05622
Alpha virt. eigenvalues --    0.09287   0.11332   0.12233   0.14215   0.14709
Alpha virt. eigenvalues --    0.15097   0.15490   0.17774   0.17898   0.18058
Alpha virt. eigenvalues --    0.19626   0.20470   0.21694   0.22321   0.23750
Alpha virt. eigenvalues --    0.25821   0.28099   0.29558   0.32095   0.33747
Alpha virt. eigenvalues --    0.35007   0.36952   0.40080   0.42934   0.48233
Alpha virt. eigenvalues --    0.49873   0.50828   0.51884   0.53003   0.53028
Alpha virt. eigenvalues --    0.53931   0.54673   0.55487   0.56687   0.57852
Alpha virt. eigenvalues --    0.58297   0.59368   0.59866   0.59926   0.61192
Alpha virt. eigenvalues --    0.63349   0.63356   0.64286   0.66500   0.67975
Alpha virt. eigenvalues --    0.70449   0.70769   0.72880   0.75293   0.76318
Alpha virt. eigenvalues --    0.78912   0.80083   0.80542   0.81077   0.81596
Alpha virt. eigenvalues --    0.83241   0.85176   0.85297   0.87436   0.88331
Alpha virt. eigenvalues --    0.88402   0.89090   0.90136   0.91377   0.92768
Alpha virt. eigenvalues --    0.93794   0.95631   0.96406   0.98517   0.99314
Alpha virt. eigenvalues --    1.02464   1.02605   1.04808   1.05153   1.05723
Alpha virt. eigenvalues --    1.09278   1.10777   1.14772   1.16624   1.19246
Alpha virt. eigenvalues --    1.22822   1.23170   1.26374   1.26447   1.26942
Alpha virt. eigenvalues --    1.31386   1.36226   1.37591   1.41114   1.42270
Alpha virt. eigenvalues --    1.42307   1.43305   1.45715   1.48535   1.48857
Alpha virt. eigenvalues --    1.49693   1.50225   1.52209   1.53661   1.59845
Alpha virt. eigenvalues --    1.63633   1.65934   1.70545   1.74112   1.74149
Alpha virt. eigenvalues --    1.75305   1.80259   1.80302   1.82696   1.83237
Alpha virt. eigenvalues --    1.85779   1.88678   1.90241   1.90678   1.93125
Alpha virt. eigenvalues --    1.93645   1.95044   1.96305   1.97568   1.99052
Alpha virt. eigenvalues --    2.02473   2.04154   2.04992   2.08414   2.09865
Alpha virt. eigenvalues --    2.10049   2.11186   2.12529   2.14498   2.16554
Alpha virt. eigenvalues --    2.21470   2.22552   2.24377   2.26734   2.29603
Alpha virt. eigenvalues --    2.30726   2.31774   2.33403   2.39433   2.40452
Alpha virt. eigenvalues --    2.46579   2.48463   2.49003   2.55249   2.57197
Alpha virt. eigenvalues --    2.57973   2.59931   2.62571   2.64197   2.65244
Alpha virt. eigenvalues --    2.67668   2.70733   2.72476   2.73841   2.76596
Alpha virt. eigenvalues --    2.87048   2.88401   2.97025   2.98767   3.04611
Alpha virt. eigenvalues --    3.12209   3.16327   3.27368   3.43322   3.96572
Alpha virt. eigenvalues --    3.99693   4.05596   4.07390   4.10140   4.12337
Alpha virt. eigenvalues --    4.16971   4.25991   4.27533   4.37167   4.39441
```

```
Alpha virt. eigenvalues --    4.52925   4.60591   4.75114
        Condensed to atoms (all electrons):
Total atomic charges:
              1
 1  C    0.044816
 2  C   -0.207797
 3  C   -0.131613
 4  C   -0.133246
 5  C   -0.163077
 6  C    0.329561
 7  C    0.605268
 8  O   -0.563018
 9  N   -0.612430
10  C   -0.288093
11  N   -0.746771
12  C    0.581163
13  O   -0.473299
14  C   -0.550668
15  H    0.115223
16  H    0.133378
17  H    0.138594
18  H    0.137707
19  H    0.397285
20  H    0.338004
21  H    0.147136
22  H    0.181379
23  H    0.181379
24  H    0.188784
25  H    0.175166
26  H    0.175166
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
              1
 1  C    0.044816
 2  C   -0.092573
 3  C    0.001765
 4  C    0.005349
 5  C   -0.025370
 6  C    0.329561
 7  C    0.605268
 8  O   -0.563018
 9  N   -0.274426
10  C    0.221802
11  N   -0.349486
12  C    0.581163
13  O   -0.473299
14  C   -0.011551
15  H    0.000000
16  H    0.000000
17  H    0.000000
18  H    0.000000
19  H    0.000000
20  H    0.000000
21  H    0.000000
22  H    0.000000
23  H    0.000000
24  H    0.000000
```

```
25  H    0.000000
26  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  3207.7366
Charge=     0.0000 electrons
Dipole moment (Debye):
   X=     6.1152    Y=     0.7570    Z=     0.0000  Tot=     6.1619
1\1\GINC-ORIGIN\SP\RTD-B3LYP-FC\6-31G(d)\C10H12N2O2\OSU2400\26-Jan-200
0\0\\#T B3LYP RPA=(NSTATES=10) 6-31G* DENSITY=CURRENT\\acetylated o-am
inophenylcarboxamide td-b3lyp/6-31G*//b3lyp/6-31G* restricted planar,
C=O ... H-N contact\\0,1\C,0,0.943499,-0.287017,0.\C,0,2.314067,0.0249
93,0.\C,0,2.790063,1.328425,0.\C,0,1.866613,2.372913,0.\C,0,0.5037,2.1
11713,0.\C,0,0.,0.794032,0.\C,0,0.486813,-1.720059,0.\O,0,-0.709478,-2
.049967,0.\N,0,1.429593,-2.70263,0.\C,0,1.031429,-4.101874,0.\N,0,-1.3
60048,0.495562,0.\C,0,-2.545357,1.224764,0.\O,0,-3.598801,0.60463,0.\C
,0,-2.546877,2.742056,0.\H,0,3.053839,-0.769105,0.\H,0,3.857712,1.5236
07,0.\H,0,2.205535,3.405479,0.\H,0,-0.175624,2.948956,0.\H,0,-1.539211
,-0.515562,0.\H,0,2.411065,-2.485334,0.\H,0,1.932644,-4.719179,0.\H,0,
0.431109,-4.336841,0.884781\H,0,0.431109,-4.336841,-0.884781\H,0,-3.59
0506,3.059179,0.\H,0,-2.050978,3.149064,0.887954\H,0,-2.050978,3.14906
4,-0.887954\\Version=SGI64-G98RevA.7\State=1-A'\HF=-648.2716922\RMSD=6
.915e-09\PG=CS [ SG(C10H8N2O2),X(H4)]\\@


WHAT, THEN, IS TIME?  IF NO ONE ASKS ME, I KNOW WHAT IT IS.
IF I WISH TO EXPLAIN WHAT IT IS TO HIM WHO ASKS ME, I DO NOT KNOW.
                                -- ST. AUGUSTINE (FIFTH CENTURY)
Job cpu time:  0 days  4 hours 26 minutes 25.5 seconds.
File lengths (MBytes):  RWF=  176 Int=    0 D2E=    0 Chk=   24 Scr=    1
Normal termination of Gaussian 98.
```