

NMR Spectrum of products

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Figure 1. ^1H NMR of **3a** 400 MHz DMSO- d_6

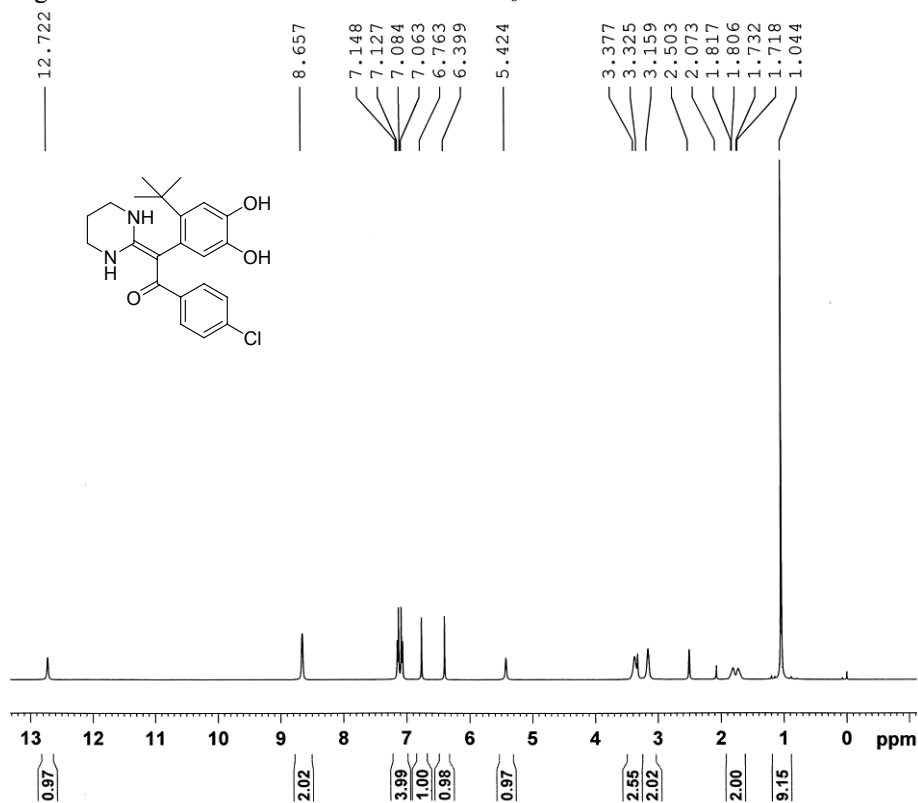


Figure 2. ^{13}C NMR of **3a** 100 MHz DMSO- d_6

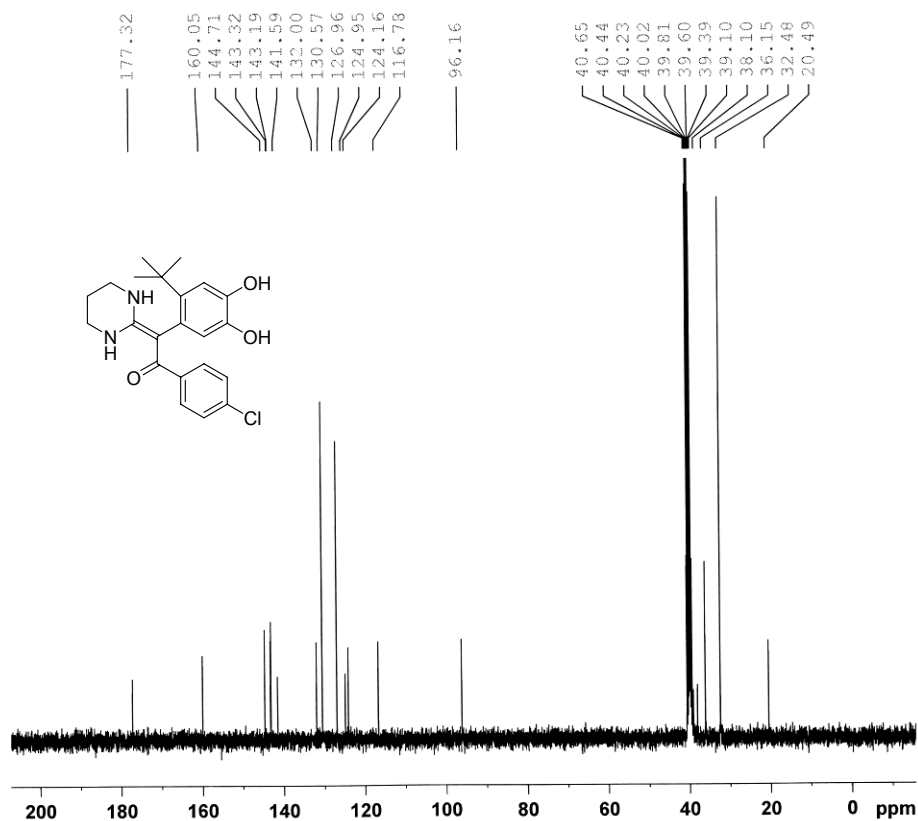


Figure 3. ^1H NMR of **3b** 400 MHz DMSO- d_6

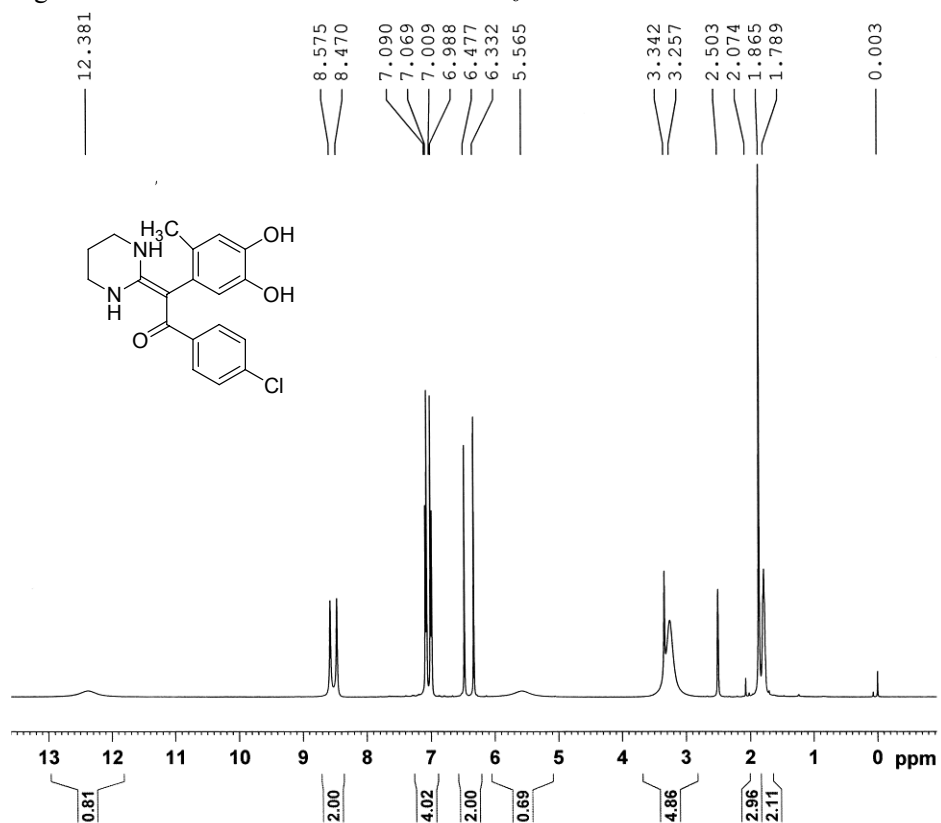


Figure 4. ^{13}C NMR of **3b** 100 MHz DMSO- d_6

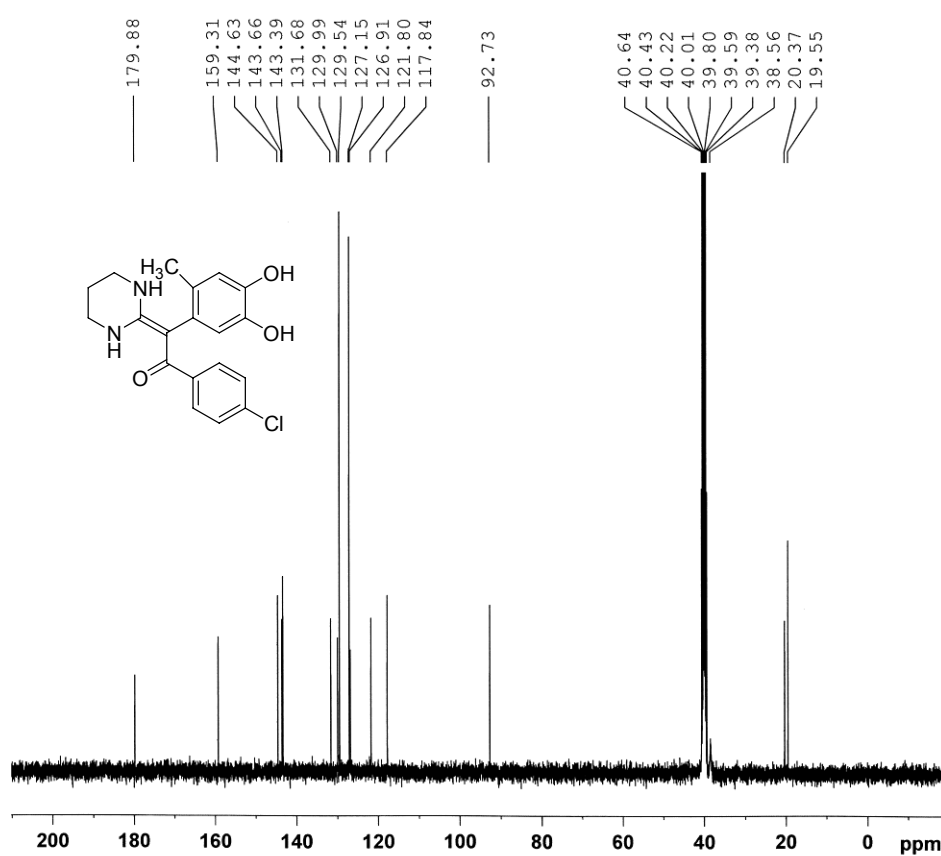


Figure 5. ^1H NMR of **3c** 400 MHz DMSO- d_6

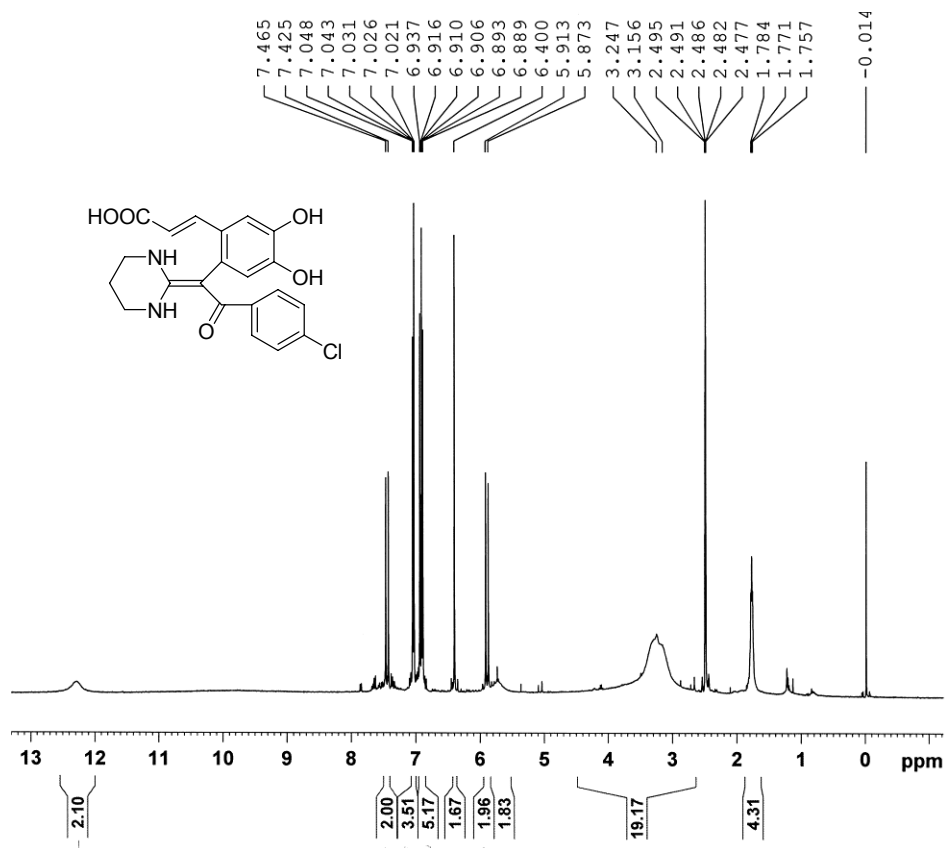


Figure 6. ^{13}C NMR of **3c** 100 MHz DMSO- d_6

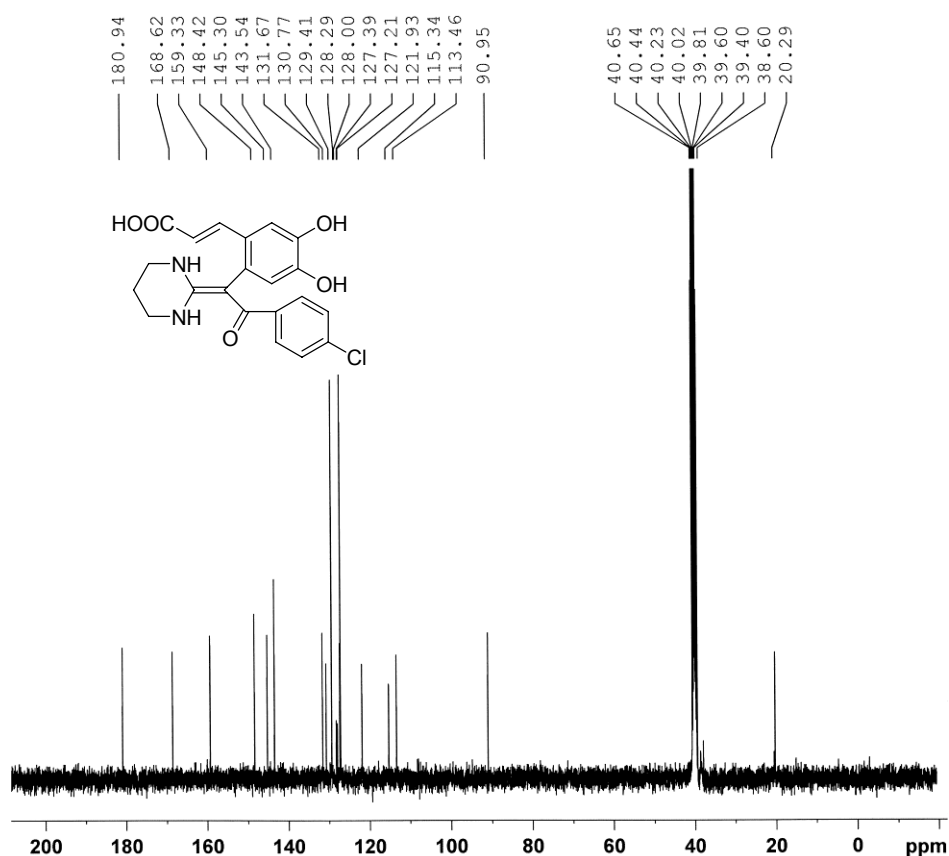


Figure 7. ¹H NMR of **3d** 400 MHz DMSO-d₆

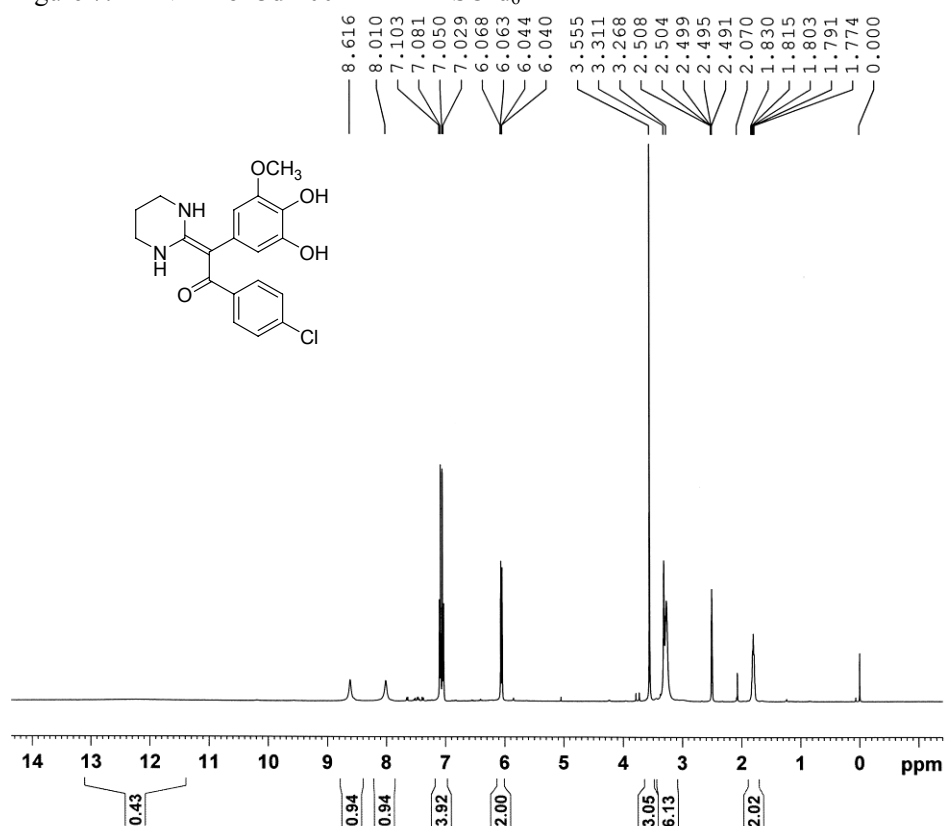


Figure 8. ¹³C NMR of **3d** 100 MHz DMSO-d₆

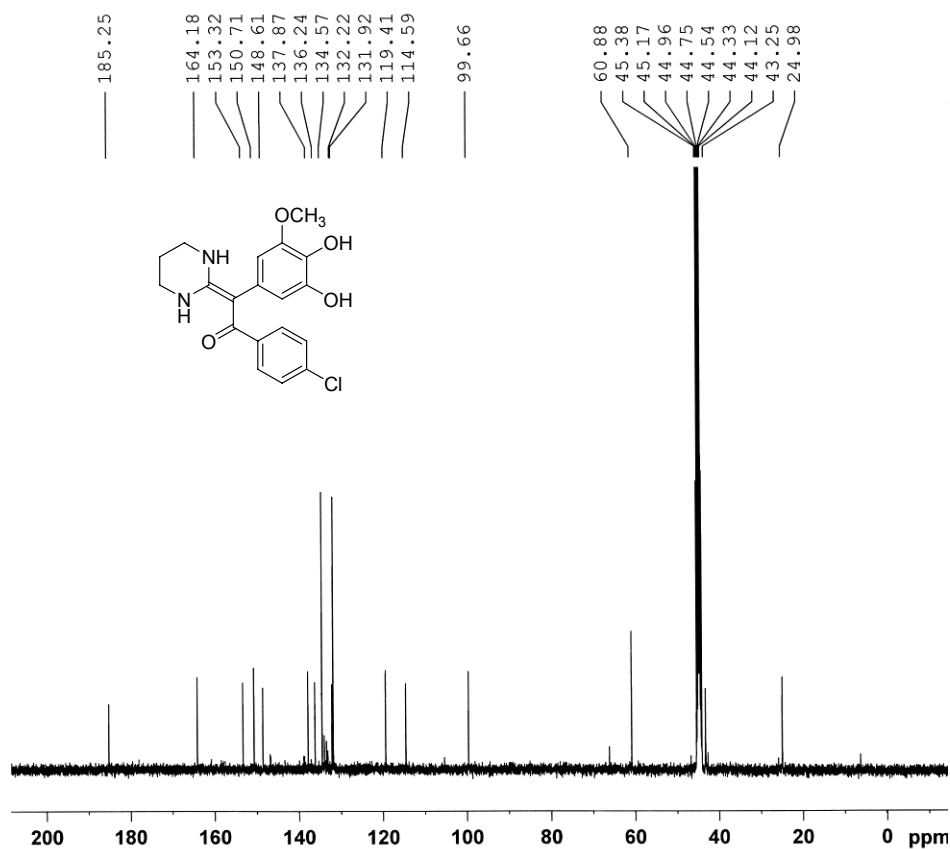


Figure 9. ¹H NMR of **3e** 400 MHz DMSO-d₆

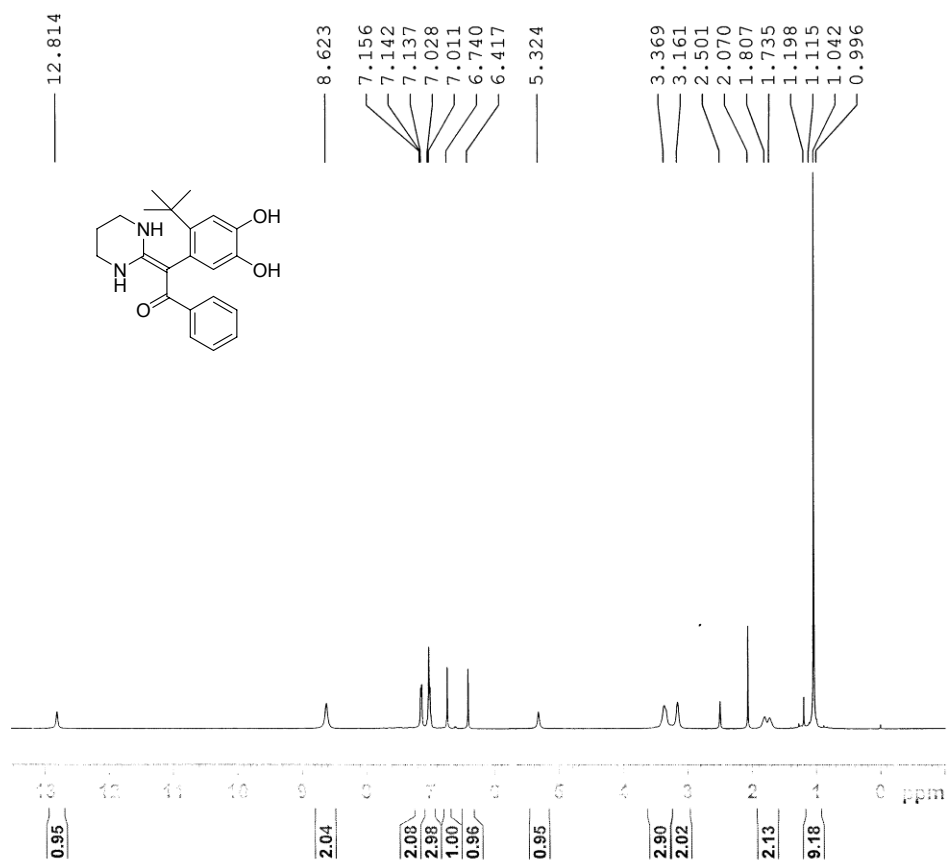


Figure 10. ^{13}C NMR of **3e** 100 MHz DMSO- d_6

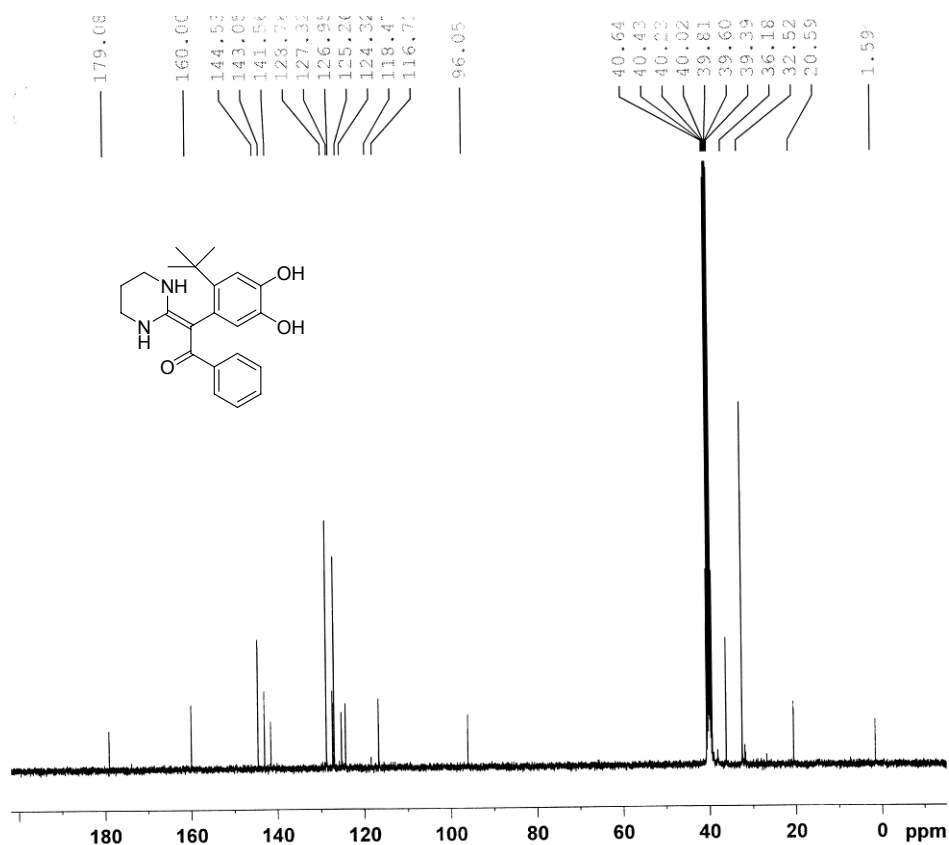


Figure 11. ^1H NMR of **3f** 400 MHz DMSO- d_6

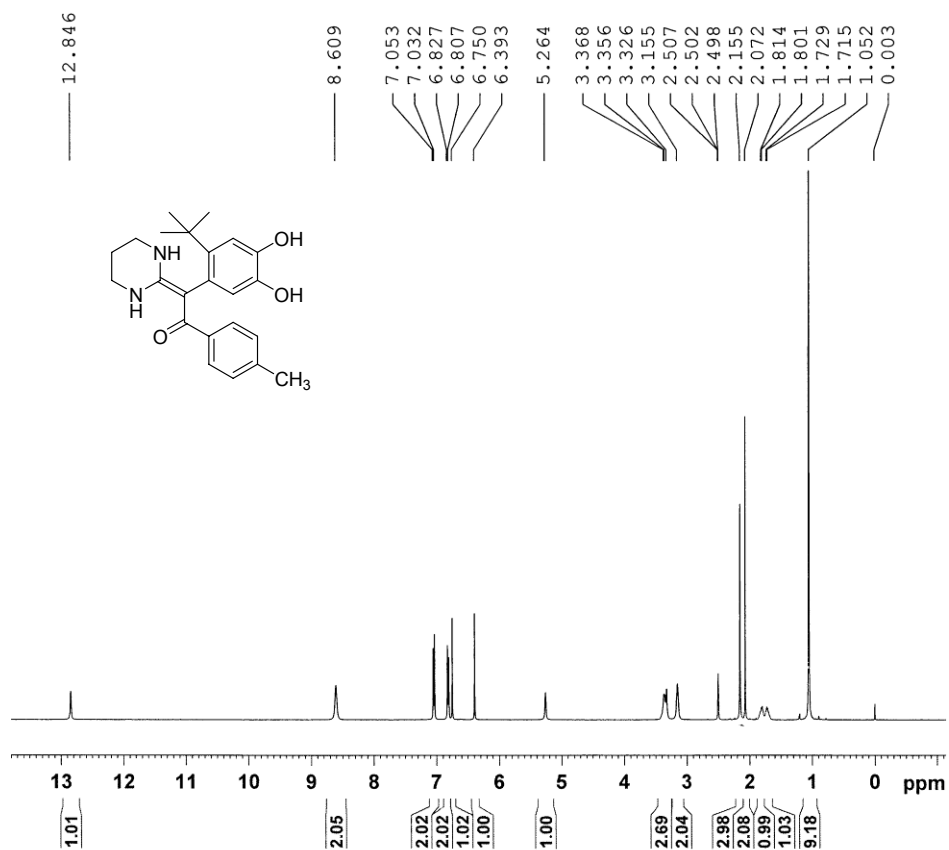


Figure 12. ^{13}C NMR of **3f** 100 MHz DMSO- d_6

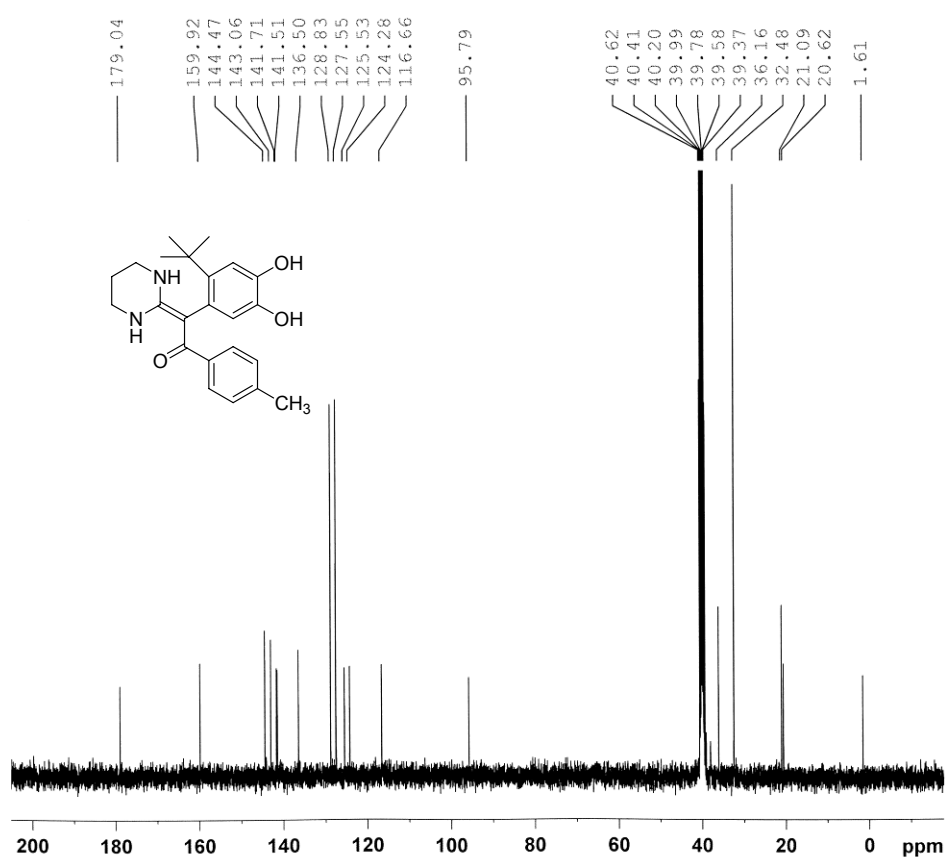


Figure 13. ^1H NMR of **3g** 400 MHz DMSO- d_6

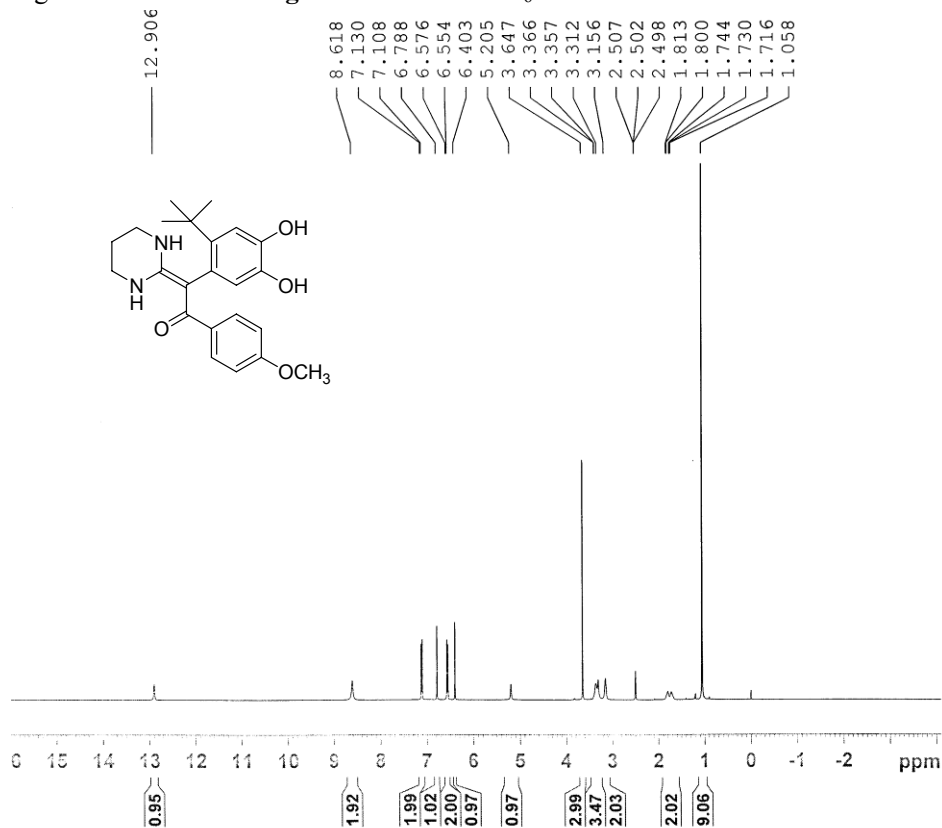


Figure 14. ^{13}C NMR of **3g** 100 MHz DMSO- d_6

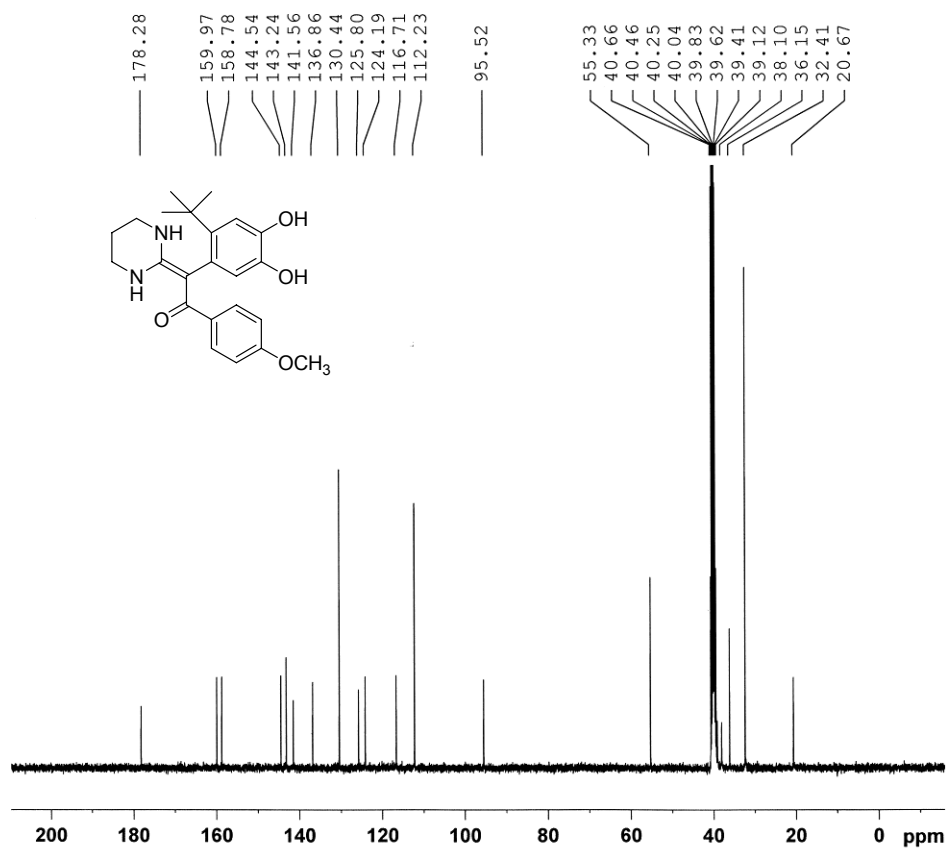


Figure 15. ¹H NMR of **3h** 400 MHz DMSO-d₆

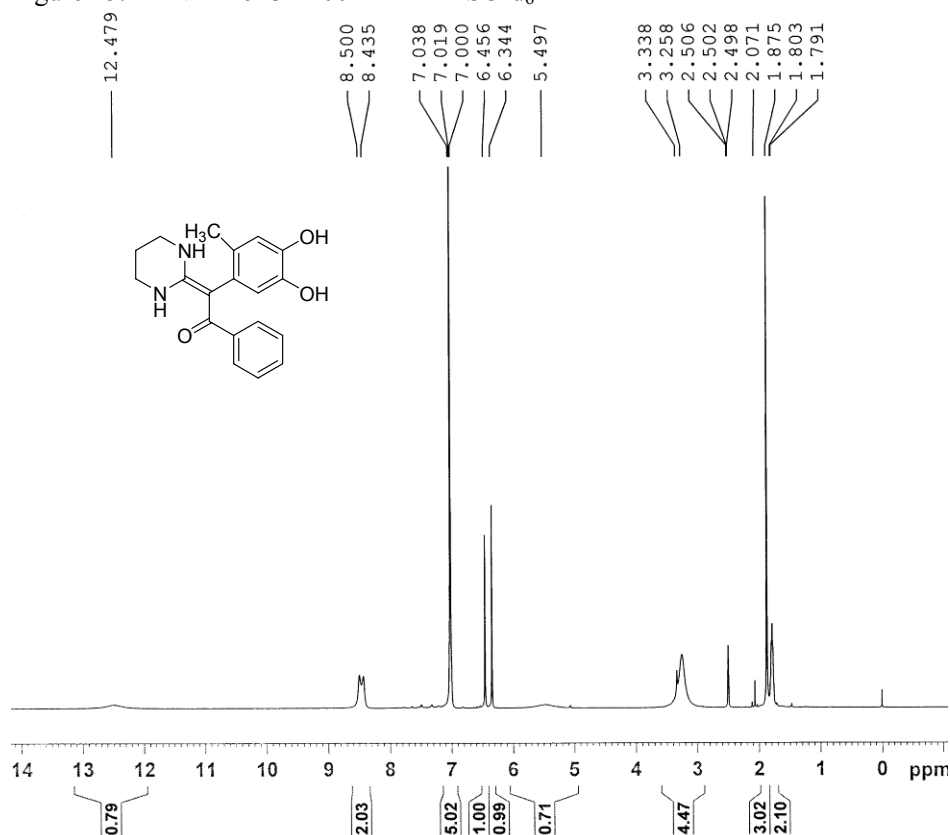


Figure 16. ¹³C NMR of **3h** 100 MHz DMSO-d₆

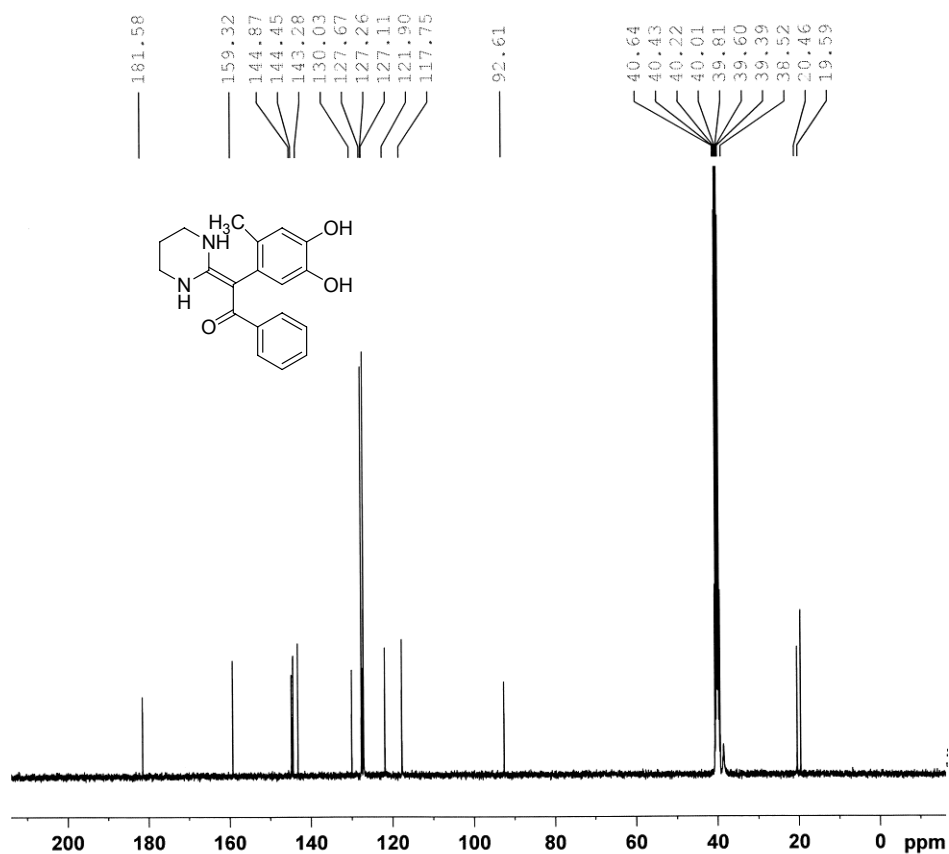


Figure 17. ¹H NMR of **3i** 400 MHz DMSO-d₆

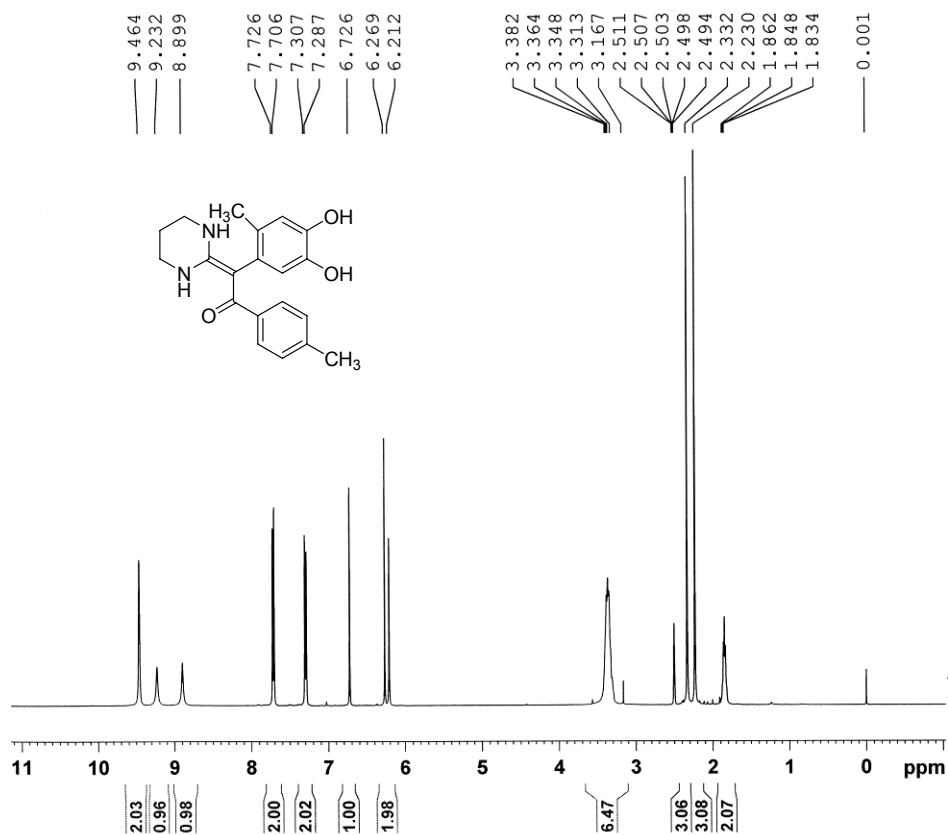


Figure 18. ¹³C NMR of **3i** 100 MHz DMSO-d₆

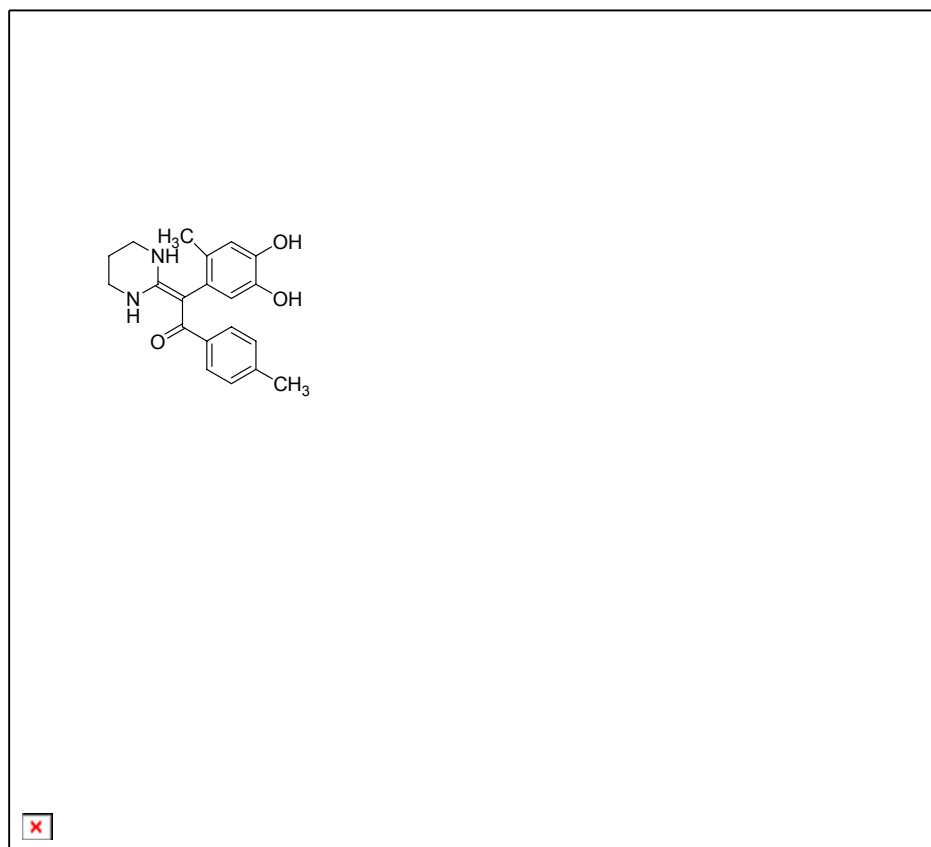


Figure 19. ^1H NMR of **3j** 400 MHz DMSO-d_6

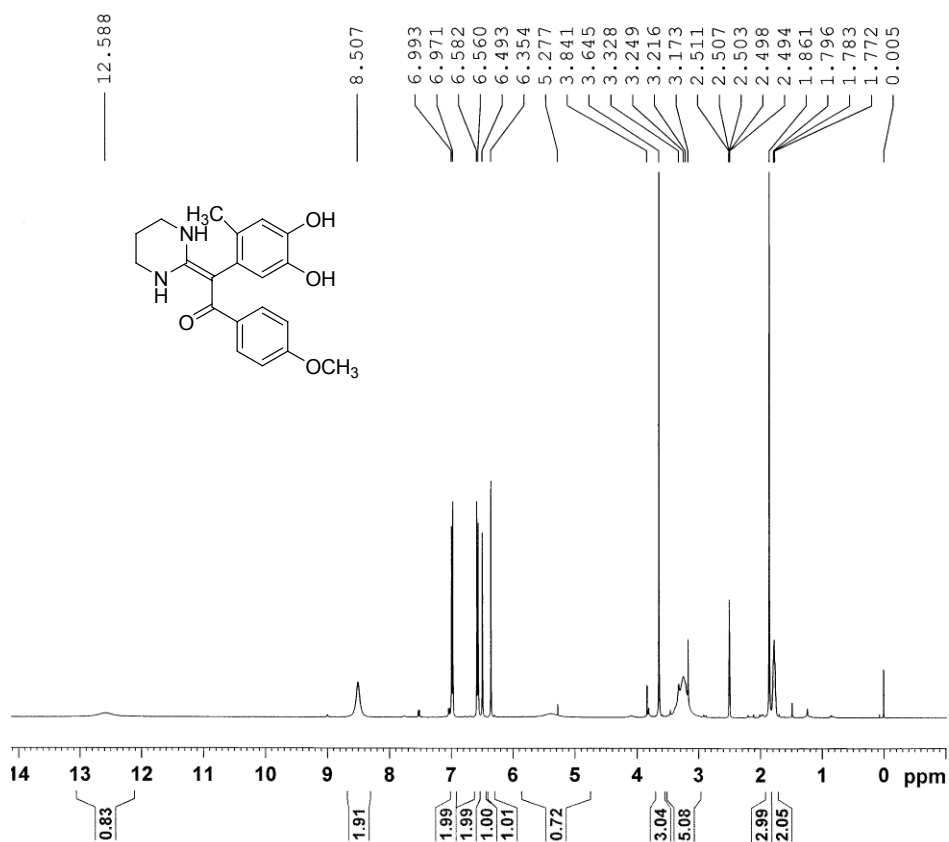


Figure 20. ^{13}C NMR of **3j** 100 MHz DMSO-d_6

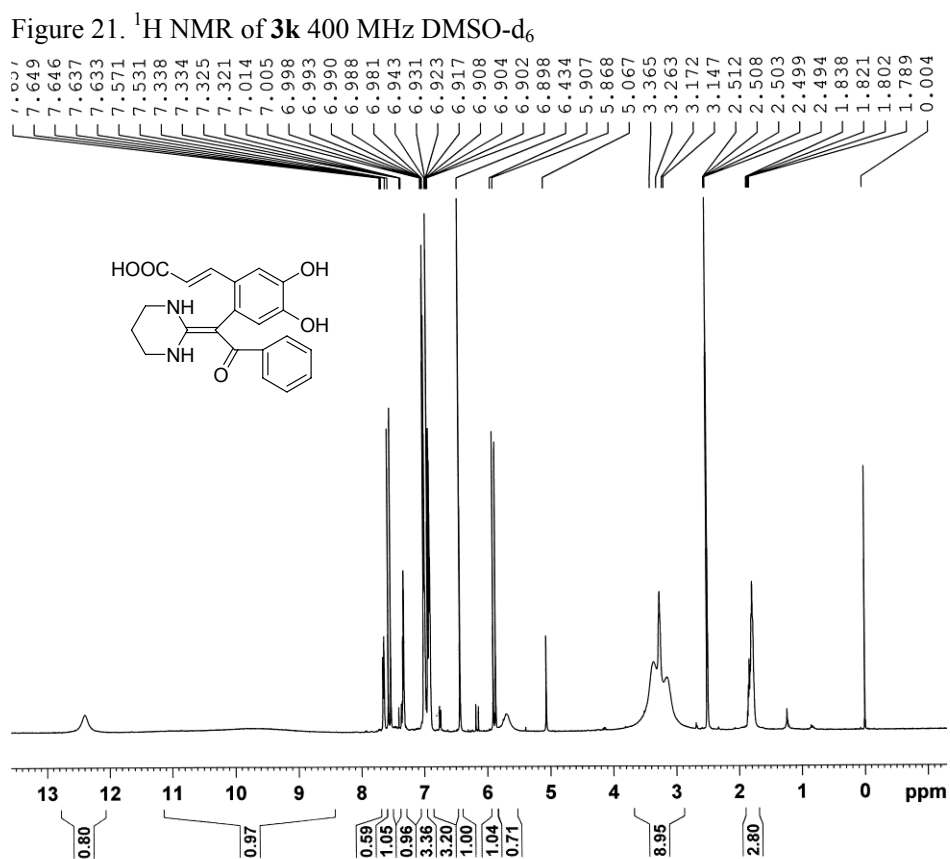
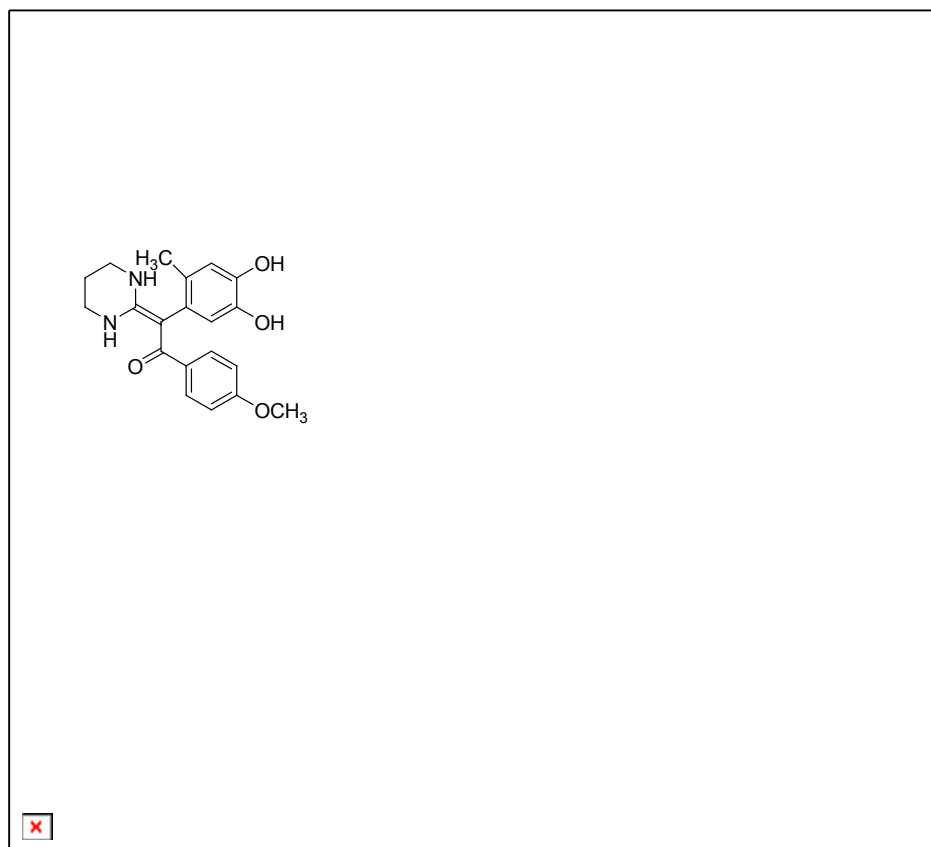


Figure 22. ¹³C NMR of **3k** 100 MHz DMSO-d₆

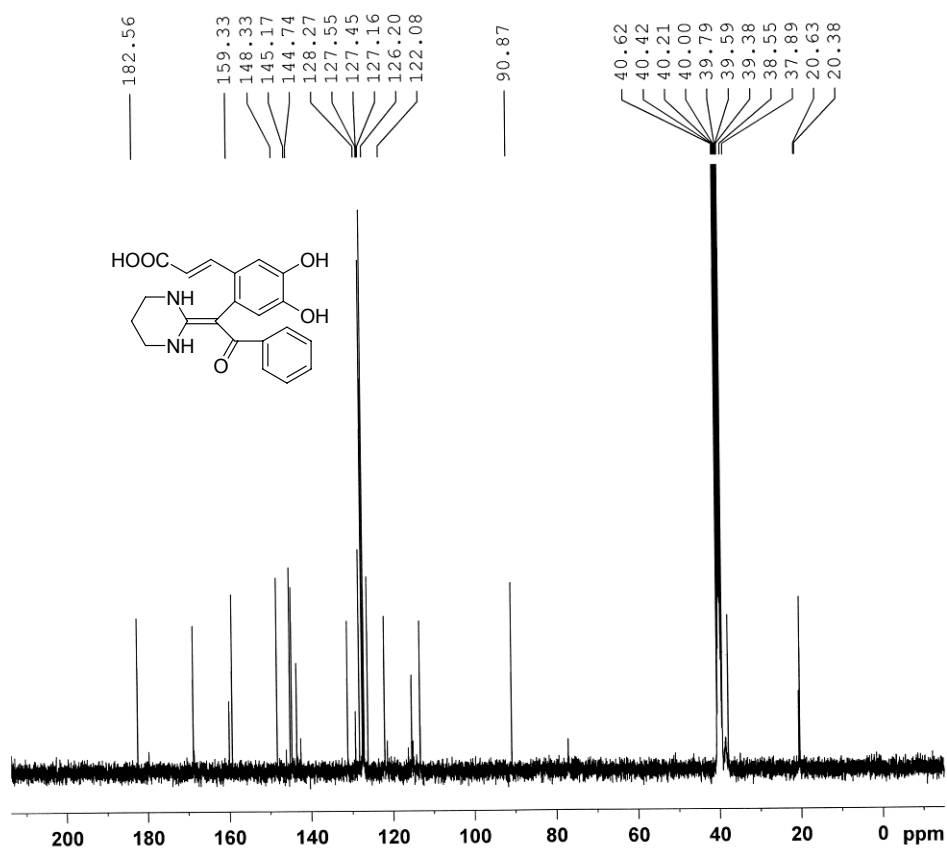


Figure 23. ¹H NMR of **3I** 400 MHz DMSO-d₆

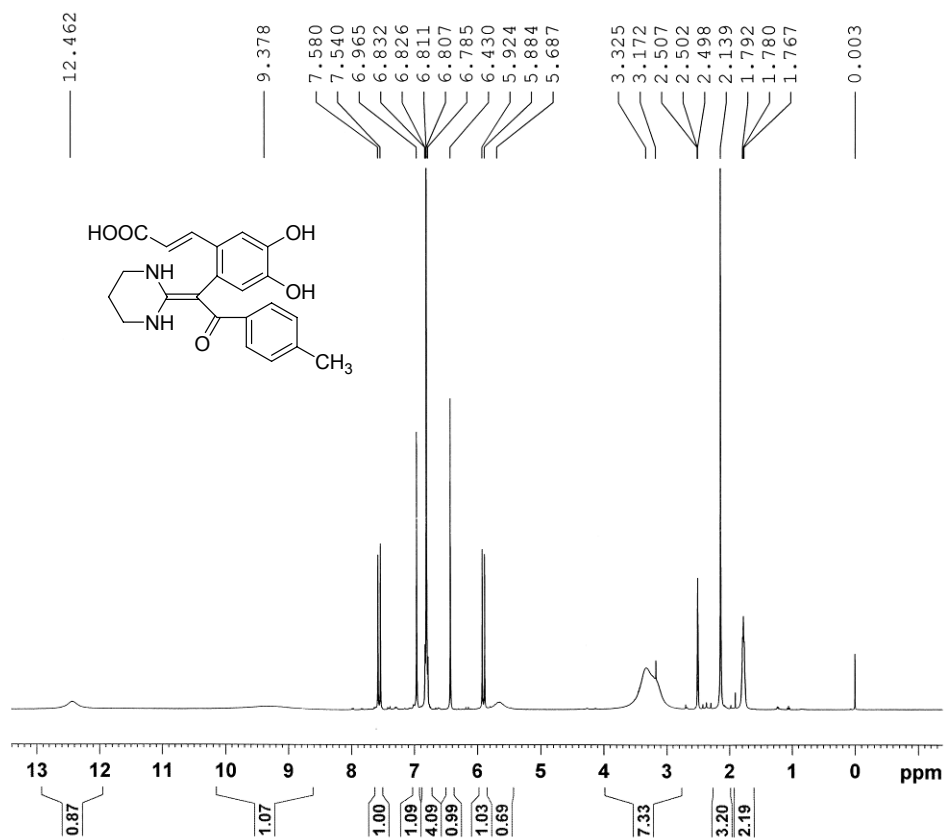


Figure 24. ^{13}C NMR of **3l** 100 MHz DMSO- d_6

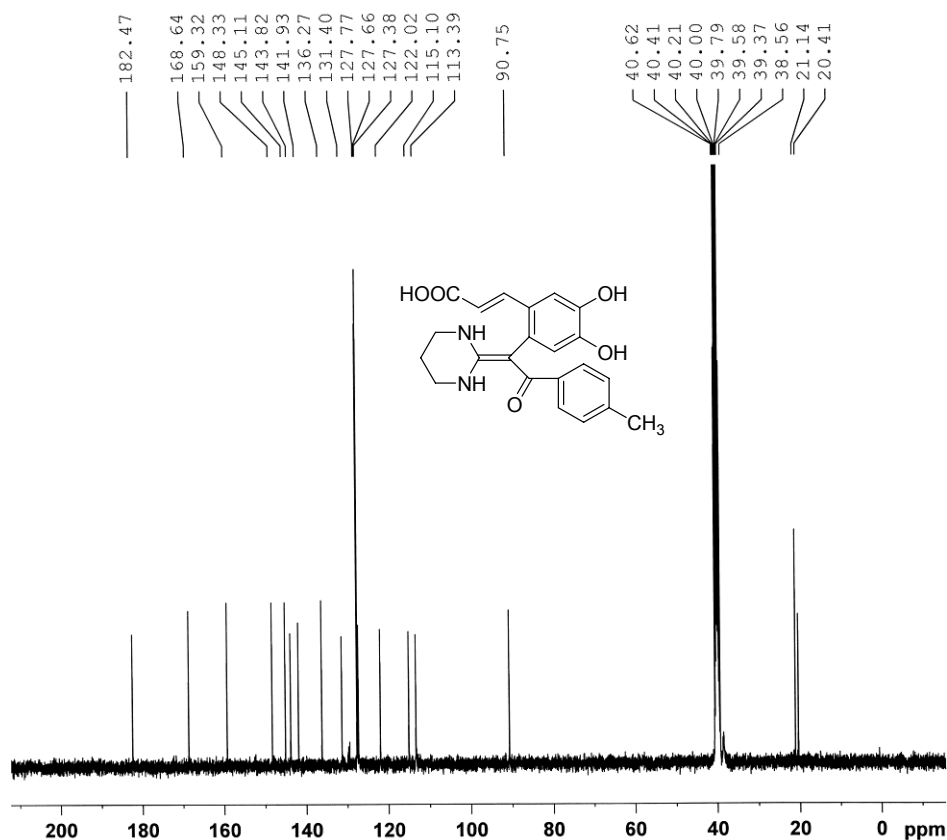


Figure 25. ^1H NMR of **3m** 400 MHz DMSO- d_6

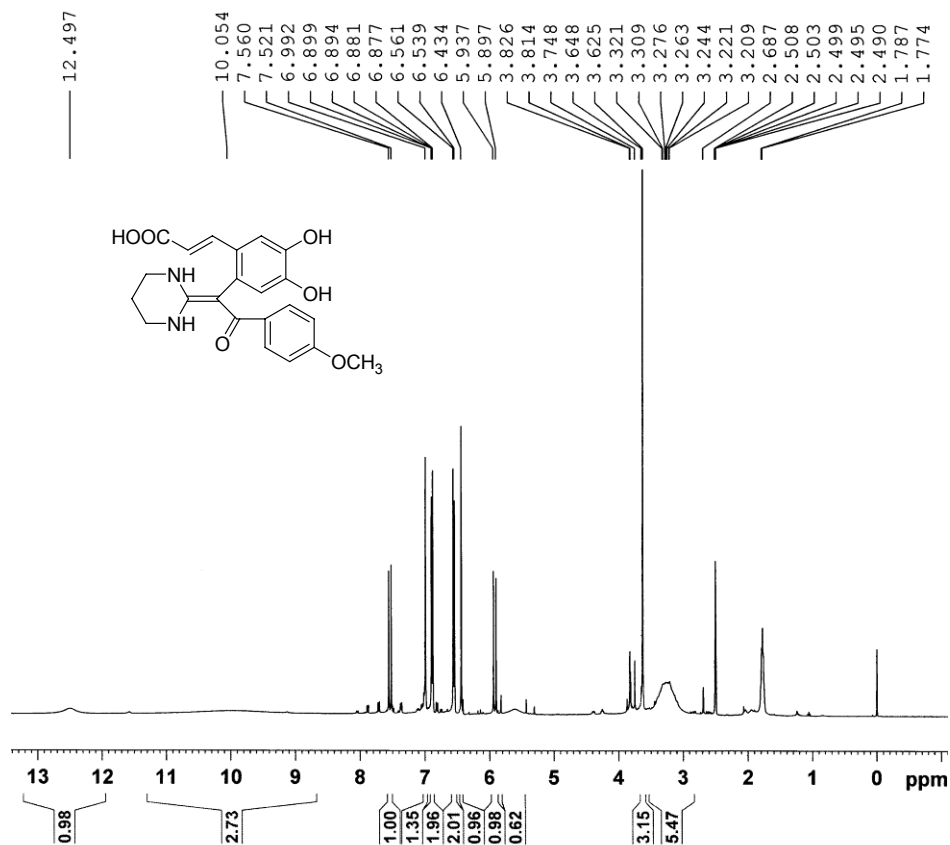


Figure 26. ^{13}C NMR of **3m** 100 MHz DMSO- d_6

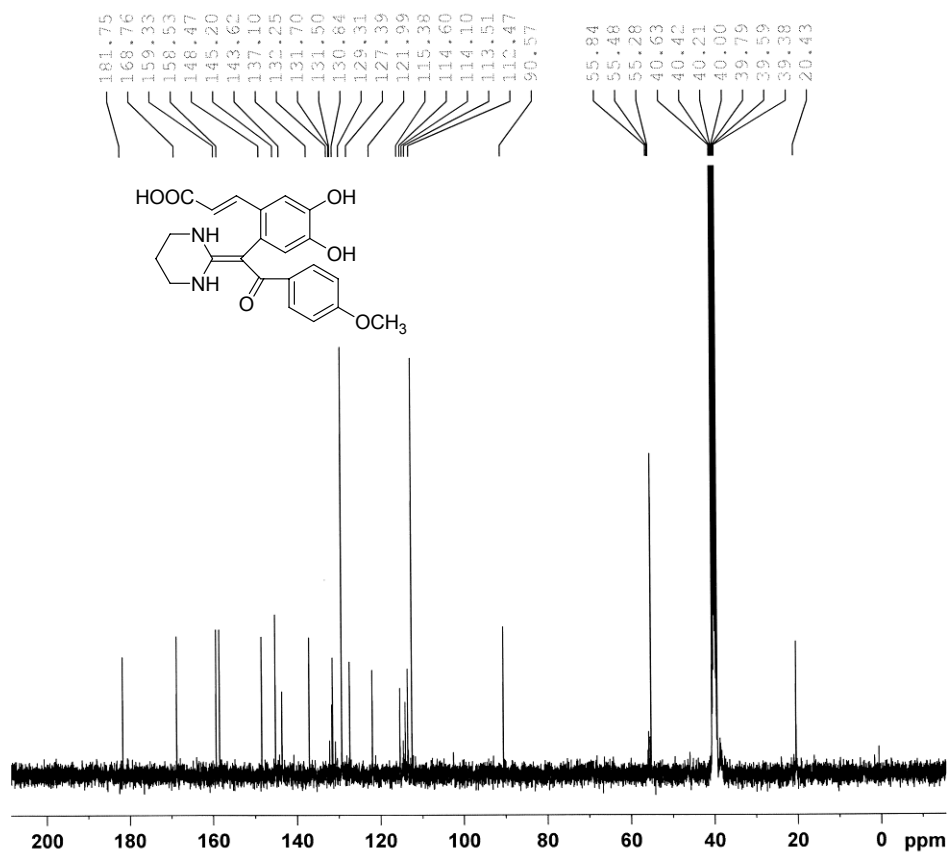


Figure 27. ^1H NMR of **3n** 400 MHz DMSO- d_6

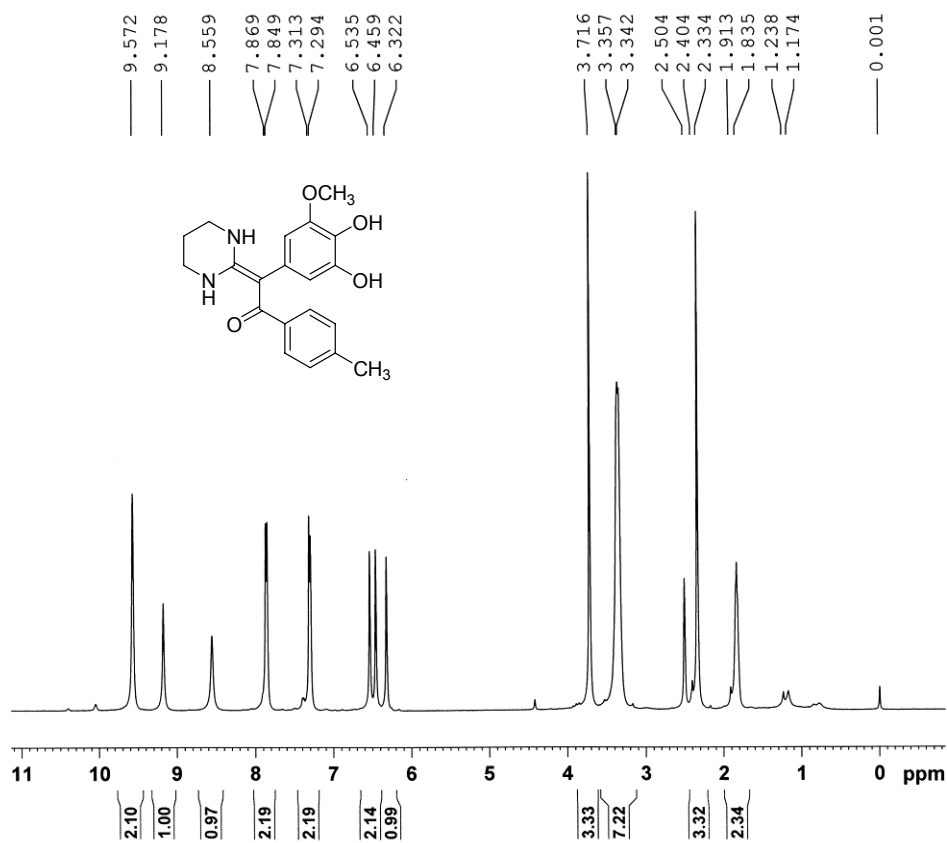
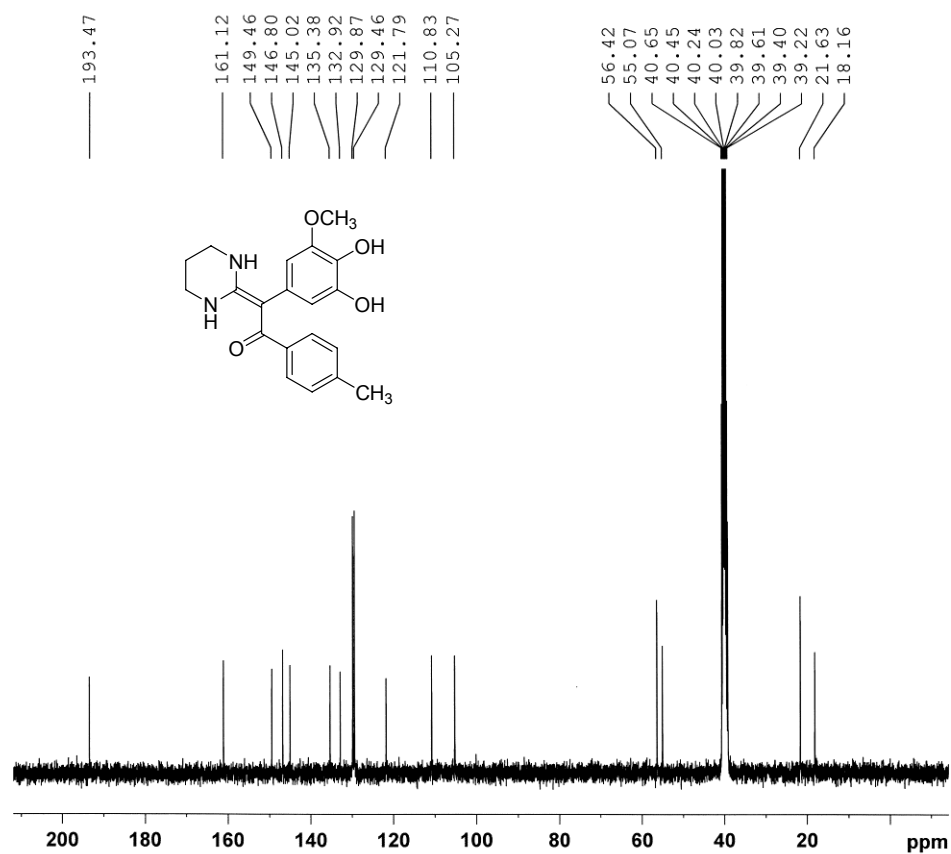
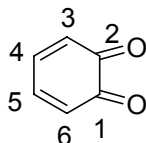


Figure 28. ^{13}C NMR of **3n** 100 MHz DMSO- d_6



Quantum calculation of benzoquinone



Entering Link 1 = C:\G03W\l1.exe PID= 2992.

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Cite this work as:

Gaussian 03, Revision B.05,

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Gaussian, Inc., Pittsburgh PA, 2003.

Gaussian 03: x86-Win32-G03RevB.05 8-Nov-2003

26-Feb-2010

%chk=zcc-1.chk

%mem=6MW

%nproc=1

Will use up to 1 processors via shared memory.

Default route: MaxDisk=2000MB

hf/3-21g pop=regular geom=connectivity

1/38=1,57=2/1;

2/17=6,18=5,40=1/2;

3/5=5,11=9,16=1,25=1,30=1/1,2,3;

4//1;

5/5=2,32=1,38=5/2;

6/28=1/1;

99/5=1,9=1/99;

Title Card Required

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C

C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
C	4	B4	3	A3	2	D2	0
C	1	B5	2	A4	3	D3	0
H	1	B6	6	A5	5	D4	0
H	4	B7	3	A6	2	D5	0
H	5	B8	4	A7	3	D6	0
H	6	B9	1	A8	2	D7	0
O	2	B10	1	A9	6	D8	0
O	3	B11	2	A10	1	D9	0

Variables:

B1 1.39516

B2	1.39471
B3	1.39543
B4	1.39483
B5	1.39483
B6	1.09961
B7	1.09968
B8	1.09976
B9	1.0996
B10	1.43
B11	1.43
A1	120.00863
A2	119.99416
A3	119.99399
A4	119.99846
A5	120.00432
A6	119.98114
A7	120.01134
A8	120.008
A9	119.98077
A10	120.01279
D1	-0.05684
D2	0.03411
D3	0.03235
D4	-179.97984
D5	-179.99644
D6	-180.
D7	179.98918
D8	179.95325
D9	179.96185

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.395160
3	6	0	1.207751	0.000000	2.092698
4	6	0	2.416260	-0.001199	1.395044
5	6	0	2.416182	-0.001678	0.000219
6	6	0	1.207976	-0.000682	-0.697382
7	1	0	-0.952317	0.000450	-0.549759
8	1	0	3.368403	-0.001258	1.945244
9	1	0	3.368463	-0.002623	-0.549903

10	1	0	1.208159	-0.000862	-1.796986
11	8	0	-1.238655	0.001710	2.109744
12	8	0	1.207855	0.000824	3.522698

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.395160	0.000000			
3	C	2.416205	1.394712	0.000000		
4	C	2.790065	2.416260	1.395427	0.000000	
5	C	2.416183	2.789946	2.416356	1.394825	0.000000
6	C	1.394829	2.416183	2.790080	2.416236	1.395138
7	H	1.099610	2.165553	3.412986	3.889675	3.413102
8	H	3.889745	3.413024	2.165678	1.099680	2.165606
9	H	3.413055	3.889707	3.413506	2.165528	1.099761
10	H	2.165365	3.413128	3.889684	3.412999	2.165471
11	O	2.446485	1.430000	2.446466	3.724139	4.219946
12	O	3.724019	2.446494	1.430000	2.446867	3.723965
		6	7	8	9	10
6	C	0.000000				
7	H	2.165331	0.000000			
8	H	3.413344	4.989355	0.000000		
9	H	2.165516	4.320781	2.495147	0.000000	
10	H	1.099604	2.494641	4.320988	2.494420	0.000000
11	O	3.723703	2.674874	4.609995	5.319707	4.609712
12	O	4.220080	4.609908	2.675132	4.610240	5.319684
		11	12			
11	O	0.000000				
12	O	2.825217	0.000000			

Stoichiometry C₆H₄O₂

Framework group C1[X(C₆H₄O₂)]

Deg. of freedom 30

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	-0.621924	-1.394959	-0.000015
2	6	0	0.586292	-0.697332	-0.000547
3	6	0	0.586447	0.697380	-0.000029
4	6	0	-0.622021	1.395105	-0.000177

5	6	0	-1.829909	0.697578	-0.000125
6	6	0	-1.829890	-0.697560	0.000353
7	1	0	-0.621828	-2.494570	0.000026
8	1	0	-0.621649	2.494785	0.000172
9	1	0	-2.782491	1.247179	-0.000241
10	1	0	-2.782245	-1.247241	0.000592
11	8	0	1.824497	-1.412698	0.000086
12	8	0	1.824784	1.412519	0.000251

Rotational constants (GHZ): 3.3788636 2.2933351 1.3661134

Standard basis: 3-21G (6D, 7F)

There are 80 symmetry adapted basis functions of A symmetry.

Integral buffers will be 262144 words long.

Raffenetti 1 integral format.

Two-electron integral symmetry is turned on.

80 basis functions, 132 primitive gaussians, 80 cartesian basis functions

28 alpha electrons 28 beta electrons

nuclear repulsion energy 321.4918512333 Hartrees.

NAtoms= 12 NActive= 12 NUniq= 12 SFac= 1.00D+00 NAtFMM= 60 Big=F

One-electron integrals computed using PRISM.

NBasis= 80 RedAO= T NBF= 80

NBsUse= 80 1.00D-06 NBFU= 80

Harris functional with IExCor= 205 diagonalized for initial guess.

ExpMin= 1.83D-01 ExpMax= 3.22D+02 ExpMxC= 3.22D+02 IAcc=1 IRadAn= 1

AccDes= 1.00D-06

HarFok: IExCor= 205 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)

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)

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.

Keep R1 integrals in memory in canonical form, NReq= 5951660.

SCF Done: E(RHF) = -376.969820563 A.U. after 7 cycles

Convg = 0.2533D-04 -V/T = 2.0046
S**2 = 0.0000

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)
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)

The electronic state is 1-A.

Alpha	occ. eigenvalues --	-20.50556	-20.50473	-11.30545	-11.30476	-11.24796
Alpha	occ. eigenvalues --	-11.24745	-11.23088	-11.23068	-1.33486	-1.29327
Alpha	occ. eigenvalues --	-1.19523	-1.05757	-1.03859	-0.88034	-0.84675
Alpha	occ. eigenvalues --	-0.73230	-0.70956	-0.65637	-0.62319	-0.60874
Alpha	occ. eigenvalues --	-0.58216	-0.55166	-0.54581	-0.47819	-0.46839
Alpha	occ. eigenvalues --	-0.45277	-0.44920	-0.33375		
Alpha	virt. eigenvalues --	-0.05309	0.13048	0.14309	0.21793	0.28841
Alpha	virt. eigenvalues --	0.30821	0.32676	0.34827	0.35998	0.40920
Alpha	virt. eigenvalues --	0.48832	0.49438	0.53098	0.54414	0.78300
Alpha	virt. eigenvalues --	0.80727	0.87779	0.88439	0.89411	0.97517
Alpha	virt. eigenvalues --	0.99812	0.99842	1.00211	1.02486	1.04048
Alpha	virt. eigenvalues --	1.05870	1.05949	1.09905	1.16210	1.21112
Alpha	virt. eigenvalues --	1.27790	1.31113	1.35839	1.42248	1.44650
Alpha	virt. eigenvalues --	1.49102	1.62959	1.66202	1.68698	1.71303
Alpha	virt. eigenvalues --	1.74405	1.84735	1.91461	1.94678	1.98670
Alpha	virt. eigenvalues --	1.98962	2.00596	2.13420	2.15257	2.61491
Alpha	virt. eigenvalues --	3.32283	3.79866			

Molecular Orbital Coefficients

		24	25	26	27	28
		(A)--O	(A)--O	(A)--O	(A)--O	(A)--O
EIGENVALUES --		-0.47819	-0.46839	-0.45277	-0.44920	-0.33375
1 1 C 1S		-0.01191	0.02438	0.00002	-0.00003	-0.00001
2 2S		0.00891	-0.01702	-0.00002	0.00001	0.00000
3 2PX		0.09836	-0.09994	-0.00019	0.00011	0.00014
4 2PY		-0.01001	-0.07276	-0.00004	0.00006	0.00000

5		2PZ	-0.00016	0.00016	-0.16963	0.10346	0.21478
6		3S	0.14426	-0.23907	-0.00006	0.00046	0.00025
7		3PX	0.08067	-0.07603	-0.00016	0.00010	0.00015
8		3PY	0.00299	-0.17296	0.00003	0.00035	0.00018
9		3PZ	-0.00020	0.00020	-0.16775	0.13351	0.29548
10	2	C 1S	-0.01885	-0.01443	-0.00003	-0.00002	0.00000
11		2S	0.01253	0.01145	0.00006	0.00005	0.00002
12		2PX	-0.05762	0.05918	0.00007	-0.00005	0.00000
13		2PY	0.01540	0.17476	0.00006	-0.00008	-0.00002
14		2PZ	-0.00006	-0.00001	-0.16737	-0.13373	-0.01283
15		3S	0.21832	0.15624	-0.00010	-0.00022	-0.00018
16		3PX	-0.00301	-0.08103	0.00011	0.00031	0.00020
17		3PY	0.23423	0.03983	-0.00018	-0.00011	-0.00007
18		3PZ	-0.00003	0.00003	-0.24661	-0.17028	-0.11331
19	3	C 1S	0.01886	-0.01440	-0.00003	0.00001	0.00000
20		2S	-0.01254	0.01145	0.00003	-0.00004	-0.00002
21		2PX	0.05756	0.05927	-0.00005	0.00000	0.00003
22		2PY	0.01552	-0.17476	-0.00011	0.00015	-0.00001
23		2PZ	0.00012	-0.00017	0.16746	-0.13366	0.01280
24		3S	-0.21851	0.15579	0.00035	0.00015	0.00013
25		3PX	0.00316	-0.08088	-0.00013	-0.00016	-0.00012
26		3PY	0.23421	-0.03951	-0.00028	0.00003	-0.00009
27		3PZ	0.00025	-0.00021	0.24675	-0.17017	0.11323
28	4	C 1S	0.01187	0.02439	0.00002	0.00001	-0.00001
29		2S	-0.00888	-0.01702	-0.00001	0.00000	0.00001
30		2PX	-0.09823	-0.10011	0.00000	0.00002	0.00002
31		2PY	-0.00999	0.07281	0.00000	-0.00007	0.00006
32		2PZ	0.00005	-0.00001	0.16959	0.10361	-0.21478
33		3S	-0.14392	-0.23912	-0.00009	-0.00021	-0.00004
34		3PX	-0.08061	-0.07623	0.00001	0.00000	0.00002
35		3PY	0.00290	0.17293	0.00006	0.00005	0.00011
36		3PZ	0.00001	0.00001	0.16770	0.13366	-0.29546
37	5	C 1S	-0.00948	-0.00789	0.00001	0.00000	0.00000
38		2S	0.00640	0.00435	-0.00001	-0.00001	0.00000
39		2PX	0.07405	0.03178	-0.00004	-0.00001	-0.00001
40		2PY	0.01338	-0.02678	0.00004	0.00012	-0.00007
41		2PZ	-0.00001	0.00009	0.08050	0.22488	-0.14754
42		3S	0.07106	0.07590	0.00002	0.00015	0.00008
43		3PX	0.11434	0.07902	-0.00002	0.00007	0.00004
44		3PY	-0.01821	-0.02892	0.00003	0.00005	-0.00009
45		3PZ	0.00001	0.00008	0.09878	0.24499	-0.20048
46	6	C 1S	0.00949	-0.00788	0.00000	0.00000	-0.00001
47		2S	-0.00640	0.00434	0.00000	0.00002	0.00002
48		2PX	-0.07411	0.03166	0.00004	0.00006	0.00002

49		2PY	0.01346	0.02680	-0.00005	0.00002	0.00008
50		2PZ	-0.00007	0.00011	-0.08056	0.22480	0.14758
51		3S	-0.07118	0.07592	-0.00004	-0.00023	-0.00006
52		3PX	-0.11443	0.07887	0.00003	-0.00008	-0.00005
53		3PY	-0.01815	0.02889	-0.00005	-0.00003	0.00006
54		3PZ	-0.00005	0.00010	-0.09884	0.24490	0.20053
55 7	H	1S	0.01825	0.03835	0.00000	-0.00002	0.00002
56		2S	-0.00337	0.03651	0.00005	0.00005	0.00007
57 8	H	1S	-0.01821	0.03837	0.00001	-0.00006	0.00002
58		2S	0.00339	0.03658	-0.00001	-0.00011	0.00003
59 9	H	1S	-0.03961	-0.02798	0.00003	0.00004	-0.00001
60		2S	-0.02609	-0.01848	0.00004	0.00007	-0.00001
61 10	H	1S	0.03961	-0.02791	-0.00003	0.00000	0.00000
62		2S	0.02607	-0.01841	-0.00003	-0.00002	-0.00003
63 11	O	1S	-0.00761	-0.00349	0.00001	0.00000	0.00001
64		2S	0.00777	0.00227	-0.00001	0.00001	0.00000
65		2PX	0.23040	-0.14417	-0.00004	0.00023	0.00015
66		2PY	0.28686	-0.30540	-0.00029	0.00015	-0.00004
67		2PZ	-0.00001	-0.00001	-0.22095	-0.16885	-0.22363
68		3S	0.04272	0.02707	-0.00003	-0.00009	-0.00008
69		3PX	0.24359	-0.16808	-0.00005	0.00028	0.00020
70		3PY	0.30120	-0.34892	-0.00032	0.00015	-0.00006
71		3PZ	-0.00003	-0.00002	-0.25373	-0.19981	-0.27632
72 12	O	1S	0.00761	-0.00348	0.00000	0.00000	0.00000
73		2S	-0.00777	0.00226	0.00000	-0.00001	-0.00001
74		2PX	-0.23012	-0.14438	0.00007	0.00001	-0.00002
75		2PY	0.28656	0.30567	-0.00009	-0.00002	-0.00007
76		2PZ	0.00021	-0.00005	0.22111	-0.16878	0.22356
77		3S	-0.04274	0.02697	0.00005	0.00005	0.00003
78		3PX	-0.24326	-0.16829	0.00006	0.00000	-0.00004
79		3PY	0.30087	0.34920	-0.00009	-0.00004	-0.00010
80		3PZ	0.00023	-0.00005	0.25392	-0.19974	0.27624
			29	30	31	32	33
			(A)--V	(A)--V	(A)--V	(A)--V	(A)--V
EIGENVALUES --			-0.05309	0.13048	0.14309	0.21793	0.28841
1 1	C	1S	0.00001	0.00001	-0.00006	0.04001	0.04036
2		2S	0.00001	0.00001	0.00007	-0.02622	-0.00981
3		2PX	-0.00012	0.00008	0.00008	0.00561	-0.02284
4		2PY	0.00000	0.00000	0.00008	0.07514	0.17949
5		2PZ	-0.12133	0.24587	0.06997	-0.00002	0.00002
6		3S	-0.00039	-0.00025	0.00048	-0.46927	-0.66873
7		3PX	-0.00012	0.00053	0.00010	-0.07728	-0.14521
8		3PY	-0.00041	-0.00033	0.00012	0.33601	0.69212
9		3PZ	-0.21783	0.54891	0.16506	-0.00003	0.00004

10	2	C	1S	-0.00003	-0.00006	0.00005	0.02827	-0.01076
11			2S	-0.00001	0.00002	-0.00001	-0.02820	0.01207
12			2PX	0.00001	0.00004	-0.00004	-0.03981	-0.03866
13			2PY	0.00000	0.00000	0.00002	0.02652	0.07072
14			2PZ	-0.15749	-0.18538	0.21888	0.00002	-0.00004
15			3S	0.00050	0.00075	-0.00051	-0.15994	0.04860
16			3PX	-0.00047	-0.00010	0.00012	-0.10157	-0.00736
17			3PY	0.00020	0.00050	0.00007	0.02896	0.01814
18			3PZ	-0.14880	-0.32859	0.36983	0.00005	-0.00010
19	3	C	1S	0.00002	0.00005	-0.00001	0.02830	0.01078
20			2S	0.00000	-0.00002	0.00002	-0.02822	-0.01208
21			2PX	0.00002	0.00002	0.00004	-0.03978	0.03844
22			2PY	0.00010	0.00016	0.00000	-0.02650	0.07069
23			2PZ	-0.15748	-0.18585	-0.21856	-0.00011	0.00006
24			3S	-0.00049	-0.00075	0.00003	-0.16018	-0.04869
25			3PX	0.00043	0.00028	-0.00008	-0.10152	0.00691
26			3PY	0.00018	0.00054	0.00007	-0.02892	0.01816
27			3PZ	-0.14881	-0.32925	-0.36926	-0.00019	0.00005
28	4	C	1S	-0.00001	0.00000	-0.00003	0.04000	-0.04031
29			2S	-0.00001	-0.00002	0.00004	-0.02621	0.00978
30			2PX	0.00005	0.00001	-0.00002	0.00563	0.02277
31			2PY	0.00001	-0.00005	-0.00001	-0.07519	0.17943
32			2PZ	-0.12134	0.24578	-0.07041	0.00003	0.00003
33			3S	0.00038	0.00027	0.00007	-0.46914	0.66798
34			3PX	0.00014	-0.00013	-0.00006	-0.07735	0.14497
35			3PY	-0.00025	-0.00042	0.00010	-0.33610	0.69156
36			3PZ	-0.21788	0.54864	-0.16614	-0.00003	0.00020
37	5	C	1S	0.00001	-0.00003	0.00000	0.05508	-0.04340
38			2S	0.00000	0.00005	0.00001	-0.02772	0.00902
39			2PX	-0.00001	0.00004	0.00000	0.10202	-0.09117
40			2PY	0.00004	-0.00005	0.00007	-0.06634	0.07343
41			2PZ	0.14518	-0.11699	0.24617	-0.00001	-0.00001
42			3S	-0.00019	0.00000	-0.00004	-0.75014	0.75222
43			3PX	-0.00014	-0.00031	-0.00004	0.36407	-0.37259
44			3PY	0.00018	-0.00018	0.00019	-0.26673	0.16531
45			3PZ	0.22457	-0.27387	0.58279	0.00005	-0.00010
46	6	C	1S	-0.00002	0.00001	0.00002	0.05508	0.04340
47			2S	0.00001	-0.00003	0.00000	-0.02772	-0.00903
48			2PX	0.00008	-0.00001	-0.00008	0.10194	0.09098
49			2PY	0.00003	-0.00007	-0.00002	0.06630	0.07342
50			2PZ	0.14521	-0.11738	-0.24596	0.00000	-0.00003
51			3S	0.00040	0.00020	-0.00023	-0.75023	-0.75210
52			3PX	0.00024	0.00030	-0.00024	0.36396	0.37209
53			3PY	0.00011	-0.00030	-0.00001	0.26658	0.16517

54		3PZ	0.22462	-0.27481	-0.58228	-0.00007	-0.00003
55	7	H 1S	-0.00002	-0.00004	-0.00001	0.05816	0.03676
56		2S	-0.00017	-0.00024	-0.00013	0.71465	1.15542
57	8	H 1S	-0.00002	0.00003	-0.00004	0.05818	-0.03672
58		2S	0.00005	0.00015	-0.00020	0.71471	-1.15444
59	9	H 1S	0.00001	-0.00001	-0.00002	0.05388	-0.01424
60		2S	-0.00004	-0.00016	-0.00012	0.96829	-0.82511
61	10	H 1S	-0.00003	0.00003	0.00002	0.05385	0.01419
62		2S	-0.00004	0.00012	0.00005	0.96815	0.82447
63	11	O 1S	-0.00002	0.00001	-0.00001	-0.01922	-0.00539
64		2S	-0.00001	-0.00003	0.00001	0.01020	0.00400
65		2PX	-0.00012	0.00004	0.00000	-0.07435	-0.03481
66		2PY	0.00004	-0.00001	0.00001	0.05179	0.00680
67		2PZ	0.25514	0.12866	-0.14109	-0.00006	0.00001
68		3S	0.00023	0.00005	0.00001	0.14546	0.02697
69		3PX	-0.00024	-0.00001	0.00000	-0.13943	-0.05191
70		3PY	0.00011	-0.00003	0.00000	0.09191	0.00982
71		3PZ	0.35594	0.20593	-0.21951	-0.00011	0.00002
72	12	O 1S	0.00001	0.00000	0.00000	-0.01922	0.00533
73		2S	0.00001	0.00001	0.00000	0.01020	-0.00397
74		2PX	-0.00002	-0.00001	-0.00003	-0.07437	0.03465
75		2PY	-0.00009	-0.00006	-0.00003	-0.05178	0.00666
76		2PZ	0.25510	0.12897	0.14087	0.00003	0.00000
77		3S	-0.00013	-0.00010	0.00006	0.14547	-0.02657
78		3PX	0.00001	0.00002	-0.00006	-0.13947	0.05159
79		3PY	-0.00010	-0.00009	-0.00007	-0.09190	0.00956
80		3PZ	0.35588	0.20638	0.21916	0.00005	0.00000

DENSITY MATRIX.

			1	2	3	4	5
1	1	C 1S	2.03846				
2		2S	0.10264	0.12064			
3		2PX	-0.00193	0.00289	0.32166		
4		2PY	0.00287	0.00604	-0.00358	0.30701	
5		2PZ	0.00000	0.00000	-0.00002	0.00000	0.21608
6		3S	-0.43089	0.22923	0.04119	-0.05334	0.00008
7		3PX	-0.00502	-0.00021	0.15000	-0.00299	0.00005
8		3PY	-0.05321	-0.00215	0.01829	0.28330	0.00005
9		3PZ	0.00001	0.00000	0.00006	0.00000	0.25147
10	2	C 1S	0.01723	-0.03578	-0.06709	-0.03850	0.00004
11		2S	-0.03283	0.02926	0.07283	0.04201	-0.00004
12		2PX	0.06433	-0.06328	-0.18098	-0.10934	0.00009
13		2PY	0.04296	-0.04323	-0.13042	-0.05324	0.00005
14		2PZ	-0.00001	0.00003	0.00006	0.00003	0.08575
15		3S	0.06045	0.04289	0.19867	0.07228	-0.00018

16		3PX	-0.03585	-0.02136	-0.12379	-0.04540	0.00013
17		3PY	-0.01078	0.00384	-0.02260	-0.03845	-0.00001
18		3PZ	0.00001	0.00002	0.00006	0.00002	0.05971
19 3	C	1S	-0.00523	0.00493	0.01152	0.01015	-0.00001
20		2S	0.00454	-0.00336	-0.01223	-0.01187	0.00000
21		2PX	-0.00145	0.00134	0.00228	0.00275	0.00001
22		2PY	-0.01563	0.01333	0.04000	0.03295	-0.00002
23		2PZ	-0.00001	0.00001	0.00001	0.00002	-0.01684
24		3S	0.01565	-0.04070	-0.10483	-0.06085	0.00010
25		3PX	0.00578	0.01315	0.04257	0.01722	-0.00008
26		3PY	-0.01842	0.02322	0.05692	0.03543	-0.00003
27		3PZ	0.00000	0.00001	0.00002	0.00001	-0.01035
28 4	C	1S	-0.00287	0.00050	-0.00338	0.00491	0.00000
29		2S	0.00050	-0.00354	0.00250	-0.00612	0.00000
30		2PX	-0.00338	0.00250	-0.00950	0.00356	0.00002
31		2PY	-0.00491	0.00612	-0.00357	0.01504	0.00002
32		2PZ	0.00000	0.00000	-0.00006	-0.00001	-0.08352
33		3S	0.01839	0.00685	0.02341	-0.00266	-0.00005
34		3PX	-0.00147	0.00172	-0.00592	0.00491	0.00000
35		3PY	-0.00917	-0.00778	-0.00998	-0.00156	0.00005
36		3PZ	0.00000	0.00000	-0.00008	-0.00001	-0.11617
37 5	C	1S	-0.00370	0.00406	-0.00741	0.00969	0.00001
38		2S	0.00398	-0.00244	0.00792	-0.01046	-0.00001
39		2PX	0.00480	-0.00506	0.00783	-0.00760	-0.00001
40		2PY	-0.01043	0.01160	-0.03039	0.02905	0.00001
41		2PZ	0.00000	-0.00001	0.00001	-0.00002	-0.00392
42		3S	-0.00459	-0.02646	0.06038	-0.05202	0.00001
43		3PX	-0.00005	-0.01850	0.04697	-0.02158	-0.00002
44		3PY	-0.01009	0.01980	-0.05463	0.04207	0.00000
45		3PZ	0.00000	-0.00001	-0.00001	-0.00001	-0.03063
46 6	C	1S	0.01742	-0.03090	0.06591	-0.03784	-0.00003
47		2S	-0.03135	0.02327	-0.06551	0.04030	0.00003
48		2PX	-0.06464	0.06717	-0.17922	0.10729	0.00011
49		2PY	0.03695	-0.03696	0.11684	-0.05088	0.00001
50		2PZ	0.00001	-0.00001	0.00014	-0.00001	0.17749
51		3S	0.05916	0.02896	-0.21142	0.07550	0.00007
52		3PX	0.02301	0.03281	-0.18148	0.04700	0.00010
53		3PY	0.00821	-0.00209	0.03480	-0.04339	0.00005
54		3PZ	-0.00002	-0.00001	0.00018	0.00001	0.20867
55 7	H	1S	-0.06454	0.06045	0.00396	-0.20030	0.00002
56		2S	-0.00878	0.01960	0.00222	-0.12977	0.00003
57 8	H	1S	-0.00082	0.00145	-0.00020	0.00312	0.00000
58		2S	0.00262	0.00239	-0.00242	0.00161	0.00000
59 9	H	1S	-0.00836	0.00770	-0.01934	0.01418	0.00001

60		2S	-0.00696	0.00445	-0.01580	0.01850	0.00001
61	10	H 1S	0.01092	-0.01199	0.03002	-0.00393	-0.00002
62		2S	0.02367	-0.01389	0.03234	-0.00701	-0.00002
63	11	O 1S	-0.00317	-0.00181	0.01035	-0.00440	0.00000
64		2S	0.00125	-0.00286	-0.01040	0.00123	0.00000
65		2PX	-0.02106	0.01203	0.05920	0.00773	-0.00002
66		2PY	-0.01078	0.00585	0.02272	0.00361	-0.00001
67		2PZ	-0.00001	0.00002	0.00002	0.00001	-0.01671
68		3S	0.01277	-0.00464	-0.02449	0.01232	-0.00006
69		3PX	-0.02502	0.01552	0.07840	0.00799	-0.00001
70		3PY	-0.01087	0.00964	0.03772	0.01225	-0.00003
71		3PZ	-0.00001	0.00002	0.00001	0.00000	-0.03165
72	12	O 1S	0.00122	0.00201	-0.00435	-0.00346	0.00000
73		2S	-0.00100	0.00027	0.00329	0.00219	0.00000
74		2PX	0.00405	-0.00558	-0.01441	-0.01182	0.00000
75		2PY	0.00921	-0.00459	-0.02398	-0.01472	0.00001
76		2PZ	0.00001	-0.00001	0.00001	-0.00002	0.02542
77		3S	-0.00226	-0.00441	0.00077	0.00588	0.00002
78		3PX	0.00376	-0.00503	-0.01390	-0.01360	0.00000
79		3PY	0.01112	-0.00675	-0.03337	-0.02150	0.00000
80		3PZ	0.00001	-0.00001	0.00001	-0.00002	0.03349
			6	7	8	9	10
6		3S	0.87259				
7		3PX	0.04358	0.08099			
8		3PY	0.06424	0.01918	0.33759		
9		3PZ	0.00009	0.00009	0.00009	0.30222	
10	2	C 1S	0.09989	-0.00009	0.06917	0.00002	2.03869
11		2S	0.00052	0.01928	-0.00510	-0.00001	0.09661
12		2PX	-0.21518	-0.09041	-0.16073	0.00007	0.00738
13		2PY	-0.14013	-0.07101	-0.08853	0.00002	-0.00443
14		2PZ	-0.00016	0.00003	-0.00013	0.06829	0.00000
15		3S	-0.19279	0.05238	-0.11622	-0.00016	-0.44451
16		3PX	0.06199	-0.04586	-0.00176	0.00014	0.12245
17		3PY	0.03024	-0.00008	-0.07585	-0.00006	-0.07745
18		3PZ	-0.00025	0.00002	-0.00021	0.02377	-0.00005
19	3	C 1S	-0.01400	0.02015	-0.00485	0.00001	0.01688
20		2S	-0.02083	-0.01311	-0.02244	-0.00001	-0.03701
21		2PX	0.02582	0.00447	0.00885	0.00001	-0.00534
22		2PY	0.15213	0.04077	0.11019	-0.00002	0.07873
23		2PZ	-0.00002	0.00000	-0.00001	-0.02890	0.00003
24		3S	-0.11237	-0.07653	-0.04278	0.00012	0.10357
25		3PX	0.02684	0.02512	0.01557	-0.00010	-0.04377
26		3PY	0.09279	0.04209	0.03348	-0.00005	-0.05244
27		3PZ	0.00001	0.00001	-0.00001	-0.00786	0.00000

28 4	C	1S	0.01839	-0.00147	0.00916	0.00000	-0.00523
29		2S	0.00686	0.00172	0.00779	0.00000	0.00493
30		2PX	0.02343	-0.00593	0.01001	0.00001	0.01152
31		2PY	0.00264	-0.00491	-0.00157	0.00003	-0.01015
32		2PZ	-0.00003	-0.00007	-0.00002	-0.11617	0.00000
33		3S	0.05687	0.01535	0.04501	-0.00007	-0.01398
34		3PX	0.01539	-0.00143	0.01094	0.00001	0.02014
35		3PY	-0.04498	-0.01090	-0.02930	0.00008	0.00483
36		3PZ	-0.00005	-0.00009	-0.00003	-0.15951	-0.00002
37 5	C	1S	-0.00753	-0.01135	0.00523	0.00000	-0.00355
38		2S	-0.02581	0.00898	-0.02710	0.00000	-0.00038
39		2PX	-0.01156	0.01064	-0.00238	-0.00001	0.00306
40		2PY	0.07161	-0.02892	0.07830	-0.00001	-0.00370
41		2PZ	0.00004	-0.00001	0.00003	-0.01826	0.00000
42		3S	-0.05248	0.03551	-0.06660	0.00005	0.03979
43		3PX	-0.03268	0.03238	-0.01486	0.00000	0.01955
44		3PY	0.05222	-0.03311	0.06270	-0.00002	-0.01042
45		3PZ	0.00004	-0.00003	0.00003	-0.05203	0.00000
46 6	C	1S	0.06078	-0.00257	0.02333	-0.00002	-0.00389
47		2S	0.03396	-0.01712	0.02871	0.00003	0.00546
48		2PX	0.13543	-0.09773	0.06759	0.00009	0.01243
49		2PY	-0.11396	0.06000	-0.09800	0.00005	-0.00273
50		2PZ	0.00015	0.00011	0.00014	0.21016	0.00000
51		3S	-0.12351	-0.06769	-0.00225	0.00002	-0.03414
52		3PX	-0.00815	-0.10264	-0.01952	0.00007	-0.00541
53		3PY	-0.02953	0.01559	-0.08254	0.00007	-0.01227
54		3PZ	0.00024	0.00015	0.00020	0.25123	0.00000
55 7	H	1S	0.20268	0.00281	-0.18518	0.00001	0.01140
56		2S	0.08892	0.00272	-0.10977	0.00005	0.03839
57 8	H	1S	-0.00412	-0.00195	-0.00514	0.00000	-0.00826
58		2S	-0.00870	-0.00206	-0.01241	0.00000	-0.00836
59 9	H	1S	0.02354	-0.01543	0.01773	0.00001	0.00049
60		2S	0.02026	-0.01308	0.02571	0.00001	0.00638
61 10	H	1S	-0.03190	0.03041	0.02337	-0.00002	-0.00879
62		2S	-0.03580	0.02236	0.01287	-0.00002	-0.00964
63 11	O	1S	0.07815	-0.01813	0.06539	-0.00002	0.00463
64		2S	-0.01691	0.00567	-0.00695	0.00001	0.00396
65		2PX	0.23622	0.06695	0.09453	-0.00003	0.05541
66		2PY	0.16083	0.03913	0.01871	-0.00007	-0.03465
67		2PZ	-0.00021	-0.00001	-0.00019	-0.06804	0.00004
68		3S	-0.08001	0.02972	-0.04098	-0.00006	-0.01403
69		3PX	0.27318	0.07846	0.11123	0.00000	0.07024
70		3PY	0.18056	0.04948	0.03042	-0.00010	-0.04219
71		3PZ	-0.00024	-0.00002	-0.00022	-0.09379	0.00009

72	12	O	1S	-0.06818	-0.00906	-0.03754	0.00002	-0.00315
73			2S	0.01553	0.00414	0.00998	-0.00001	-0.00084
74			2PX	-0.03579	-0.01340	-0.01079	0.00001	-0.00043
75			2PY	-0.09998	-0.01280	-0.09046	0.00000	-0.02198
76			2PZ	-0.00002	0.00001	-0.00001	0.04793	0.00000
77			3S	0.06105	0.00955	0.04475	0.00002	0.02345
78			3PX	-0.03813	-0.01337	-0.01520	0.00000	-0.00593
79			3PY	-0.12563	-0.01970	-0.11045	0.00000	-0.02642
80			3PZ	-0.00002	0.00002	-0.00001	0.06244	-0.00001
				11	12	13	14	15
11			2S	0.13181				
12			2PX	-0.01826	0.30929			
13			2PY	0.01121	0.03239	0.33884		
14			2PZ	-0.00001	-0.00001	0.00000	0.17823	
15			3S	0.25571	0.03512	0.00728	0.00016	0.95281
16			3PX	-0.06078	0.11081	0.00658	-0.00017	-0.20474
17			3PY	0.03161	0.02573	0.14802	0.00010	0.20722
18			3PZ	-0.00004	-0.00002	0.00002	0.21405	0.00026
19	3	C	1S	-0.03701	-0.00536	-0.07872	-0.00001	0.10360
20			2S	0.03359	0.00823	0.08397	0.00003	0.01221
21			2PX	0.00821	0.02159	0.01774	0.00000	0.00500
22			2PY	-0.08397	-0.01779	-0.26065	-0.00006	-0.25326
23			2PZ	-0.00004	-0.00001	-0.00010	0.06544	-0.00005
24			3S	0.01220	0.00502	0.25311	-0.00015	-0.30828
25			3PX	0.01191	0.01387	-0.07886	0.00010	0.06312
26			3PY	-0.00808	-0.00158	-0.15039	0.00006	0.13419
27			3PZ	-0.00001	0.00001	-0.00008	0.04304	0.00004
28	4	C	1S	0.00453	-0.00145	0.01563	0.00000	0.01567
29			2S	-0.00336	0.00133	-0.01333	-0.00001	-0.04070
30			2PX	-0.01223	0.00226	-0.04000	0.00000	-0.10488
31			2PY	0.01187	-0.00274	0.03295	0.00001	0.06088
32			2PZ	0.00000	0.00000	0.00000	-0.01685	0.00000
33			3S	-0.02083	0.02580	-0.15209	0.00010	-0.11247
34			3PX	-0.01311	0.00447	-0.04082	-0.00001	-0.07662
35			3PY	0.02244	-0.00884	0.11013	-0.00006	0.04285
36			3PZ	0.00001	0.00000	0.00002	-0.02890	0.00002
37	5	C	1S	0.00108	-0.00556	0.00113	0.00000	0.02185
38			2S	-0.00363	0.00826	-0.00357	0.00001	0.00610
39			2PX	-0.00427	0.00883	-0.01020	-0.00001	-0.00214
40			2PY	0.00479	-0.01487	-0.00683	-0.00001	0.00825
41			2PZ	0.00001	0.00000	0.00001	-0.02756	-0.00005
42			3S	-0.00551	-0.00865	0.02709	-0.00009	0.01146
43			3PX	0.00183	-0.01753	0.01659	-0.00007	0.02197
44			3PY	0.00162	0.00182	-0.01175	0.00002	-0.00191

45		3PZ	0.00002	0.00000	0.00001	-0.04037	-0.00004
46 6	C	1S	0.00470	-0.01215	-0.00480	0.00000	-0.00333
47		2S	-0.00374	0.01063	0.00431	-0.00001	-0.03281
48		2PX	-0.01472	0.03842	0.01733	0.00000	-0.08169
49		2PY	0.00251	-0.00990	-0.00388	0.00001	0.04042
50		2PZ	0.00001	-0.00002	-0.00001	0.01881	-0.00012
51		3S	-0.00874	0.12285	0.03397	0.00010	0.00015
52		3PX	-0.02001	0.10379	0.04230	0.00007	-0.04474
53		3PY	-0.00036	0.01162	0.00827	0.00004	0.01821
54		3PZ	0.00002	-0.00005	-0.00002	0.01552	-0.00014
55 7	H	1S	-0.01134	0.02239	0.02151	-0.00001	-0.03911
56		2S	-0.02469	0.00158	0.03585	-0.00005	-0.08062
57 8	H	1S	0.00771	0.00006	0.02029	0.00001	0.02438
58		2S	0.00464	-0.00039	0.01895	0.00003	0.04686
59 9	H	1S	0.00016	-0.00371	0.00049	0.00000	-0.00469
60		2S	-0.00035	-0.00955	0.00354	-0.00002	-0.00947
61 10	H	1S	0.00867	-0.01991	-0.01222	0.00001	0.02513
62		2S	0.00658	-0.01508	-0.00915	0.00003	0.02705
63 11	O	1S	0.00141	-0.01871	0.00975	-0.00001	-0.00790
64		2S	-0.00176	0.01578	-0.00872	0.00001	-0.02547
65		2PX	-0.06244	-0.19372	0.10570	-0.00013	-0.19758
66		2PY	0.03433	0.10759	-0.06991	0.00007	0.18489
67		2PZ	-0.00009	-0.00012	0.00007	0.17935	0.00008
68		3S	-0.00979	0.01699	-0.00341	0.00005	-0.06454
69		3PX	-0.06746	-0.22308	0.10371	-0.00015	-0.22682
70		3PY	0.03701	0.10752	-0.09996	0.00008	0.19562
71		3PZ	-0.00012	-0.00013	0.00007	0.20409	0.00004
72 12	O	1S	-0.00199	0.00775	0.00718	0.00000	0.07485
73		2S	-0.00196	-0.00397	-0.01005	0.00000	-0.01340
74		2PX	0.00088	0.00146	0.01210	0.00000	-0.03573
75		2PY	0.01128	0.01615	0.06353	0.00000	0.30079
76		2PZ	0.00001	0.00001	0.00002	0.01987	0.00006
77		3S	-0.01187	-0.03261	-0.00118	-0.00004	-0.09217
78		3PX	0.00146	0.00849	0.00176	0.00001	-0.02675
79		3PY	0.01702	0.02530	0.08660	0.00000	0.34055
80		3PZ	0.00001	0.00001	0.00003	0.01995	0.00006
			16	17	18	19	20
16		3PX	0.13857				
17		3PY	-0.00661	0.22507			
18		3PZ	-0.00026	0.00016	0.28541		
19 3	C	1S	-0.04376	0.05247	0.00001	2.03869	
20		2S	0.01191	0.00808	0.00003	0.09661	0.13179
21		2PX	0.01387	0.00155	-0.00002	0.00736	-0.01823
22		2PY	0.07888	-0.15047	-0.00006	0.00443	-0.01123

23		2PZ	-0.00003	-0.00003	0.04305	0.00000	0.00001
24		3S	0.06308	-0.13427	-0.00025	-0.44448	0.25571
25		3PX	-0.02239	-0.00439	0.00014	0.12246	-0.06079
26		3PY	0.00442	0.05089	0.00013	0.07746	-0.03160
27		3PZ	0.00000	0.00003	-0.00932	0.00005	-0.00001
28 4	C	1S	0.00577	0.01844	-0.00001	0.01722	-0.03280
29		2S	0.01315	-0.02323	-0.00001	-0.03575	0.02924
30		2PX	0.04258	-0.05696	-0.00001	-0.06707	0.07279
31		2PY	-0.01723	0.03545	0.00001	0.03848	-0.04199
32		2PZ	0.00000	-0.00002	-0.01034	-0.00001	0.00001
33		3S	0.02688	-0.09284	0.00013	0.09986	0.00049
34		3PX	0.02515	-0.04216	-0.00002	-0.00013	0.01928
35		3PY	-0.01560	0.03350	-0.00009	-0.06914	0.00510
36		3PZ	-0.00002	-0.00003	-0.00784	-0.00003	0.00002
37 5	C	1S	-0.01264	0.00198	0.00001	-0.00389	0.00470
38		2S	-0.00461	0.00405	0.00001	0.00546	-0.00374
39		2PX	-0.00215	-0.00001	0.00000	0.01243	-0.01472
40		2PY	-0.00446	-0.00545	-0.00001	0.00273	-0.00251
41		2PZ	0.00006	-0.00004	-0.02908	-0.00001	0.00000
42		3S	-0.01368	0.02085	-0.00011	-0.03416	-0.00872
43		3PX	-0.01607	0.01610	-0.00008	-0.00542	-0.02000
44		3PY	0.00495	-0.00986	0.00002	0.01226	0.00036
45		3PZ	0.00006	-0.00004	-0.03553	0.00000	-0.00001
46 6	C	1S	-0.00028	-0.00565	0.00000	-0.00355	0.00108
47		2S	0.02142	-0.00192	-0.00002	-0.00037	-0.00363
48		2PX	0.05431	0.00142	-0.00002	0.00306	-0.00427
49		2PY	-0.02755	0.01242	0.00001	0.00370	-0.00479
50		2PZ	0.00013	-0.00007	-0.01648	0.00000	-0.00001
51		3S	0.03840	-0.00161	0.00013	0.03980	-0.00552
52		3PX	0.04743	0.00597	0.00008	0.01956	0.00183
53		3PY	-0.00647	0.01493	0.00004	0.01042	-0.00162
54		3PZ	0.00016	-0.00007	-0.02889	-0.00001	-0.00002
55 7	H	1S	0.02097	0.03622	-0.00001	-0.00826	0.00771
56		2S	0.01336	0.01282	-0.00007	-0.00837	0.00465
57 8	H	1S	-0.00831	0.01463	0.00001	0.01140	-0.01134
58		2S	-0.01487	0.03267	0.00004	0.03838	-0.02469
59 9	H	1S	0.00299	-0.00296	0.00000	-0.00879	0.00867
60		2S	0.00299	-0.00343	-0.00003	-0.00964	0.00658
61 10	H	1S	-0.01607	-0.00831	0.00001	0.00049	0.00016
62		2S	-0.01794	-0.00544	0.00004	0.00638	-0.00035
63 11	O	1S	0.10882	-0.05949	0.00002	-0.00315	-0.00199
64		2S	-0.01812	0.01204	-0.00001	-0.00084	-0.00196
65		2PX	0.00770	0.13932	-0.00016	-0.00042	0.00088
66		2PY	0.10990	0.18092	0.00010	0.02198	-0.01129

67		2PZ	-0.00029	0.00016	0.26971	0.00000	0.00002
68		3S	-0.12093	0.08087	0.00003	0.02346	-0.01187
69		3PX	0.01193	0.13619	-0.00020	-0.00592	0.00146
70		3PY	0.11256	0.18253	0.00012	0.02642	-0.01703
71		3PZ	-0.00032	0.00017	0.31235	-0.00002	0.00003
72	12	O 1S	-0.06958	0.01857	0.00002	0.00463	0.00141
73		2S	0.01168	-0.00339	0.00000	0.00396	-0.00176
74		2PX	-0.01397	-0.01565	-0.00001	0.05543	-0.06246
75		2PY	-0.06065	0.17556	0.00008	0.03464	-0.03431
76		2PZ	0.00002	0.00004	-0.04969	0.00001	0.00000
77		3S	0.05742	-0.01131	-0.00007	-0.01405	-0.00978
78		3PX	-0.01528	-0.01428	0.00001	0.07027	-0.06750
79		3PY	-0.07147	0.19588	0.00009	0.04218	-0.03699
80		3PZ	0.00002	0.00004	-0.06328	0.00000	0.00001
			21	22	23	24	25
21		2PX	0.30925				
22		2PY	-0.03236	0.33883			
23		2PZ	0.00001	0.00004	0.17820		
24		3S	0.03504	-0.00715	-0.00004	0.95265	
25		3PX	0.11086	-0.00663	0.00004	-0.20476	0.13858
26		3PY	-0.02574	0.14795	-0.00001	-0.20711	0.00658
27		3PZ	-0.00002	-0.00002	0.21404	-0.00012	0.00002
28	4	C 1S	0.06430	-0.04295	0.00000	0.06039	-0.03582
29		2S	-0.06324	0.04321	-0.00001	0.04288	-0.02136
30		2PX	-0.18094	0.13041	-0.00001	0.19870	-0.12382
31		2PY	0.10931	-0.05326	-0.00001	-0.07234	0.04543
32		2PZ	-0.00004	-0.00001	0.08571	0.00006	-0.00003
33		3S	-0.21512	0.14011	0.00006	-0.19257	0.06186
34		3PX	-0.09039	0.07108	0.00000	0.05247	-0.04588
35		3PY	0.16071	-0.08851	-0.00006	0.11600	0.00186
36		3PZ	-0.00003	-0.00002	0.06826	0.00009	-0.00002
37	5	C 1S	-0.01215	0.00480	0.00000	-0.00332	-0.00028
38		2S	0.01063	-0.00431	0.00000	-0.03281	0.02143
39		2PX	0.03841	-0.01733	0.00001	-0.08168	0.05430
40		2PY	0.00990	-0.00388	0.00001	-0.04041	0.02754
41		2PZ	-0.00001	-0.00001	0.01880	0.00011	-0.00007
42		3S	0.12285	-0.03395	-0.00005	0.00010	0.03846
43		3PX	0.10380	-0.04229	-0.00003	-0.04478	0.04747
44		3PY	-0.01160	0.00828	0.00002	-0.01816	0.00646
45		3PZ	-0.00001	-0.00001	0.01552	0.00009	-0.00006
46	6	C 1S	-0.00556	-0.00114	0.00000	0.02184	-0.01265
47		2S	0.00826	0.00357	-0.00001	0.00609	-0.00460
48		2PX	0.00883	0.01021	-0.00001	-0.00215	-0.00215
49		2PY	0.01487	-0.00684	-0.00001	-0.00827	0.00447

50		2PZ	0.00000	0.00001	-0.02756	0.00011	-0.00010
51		3S	-0.00864	-0.02713	0.00002	0.01145	-0.01368
52		3PX	-0.01755	-0.01660	0.00001	0.02196	-0.01608
53		3PY	-0.00183	-0.01175	0.00000	0.00189	-0.00494
54		3PZ	0.00002	0.00003	-0.04037	0.00012	-0.00012
55 7	H	1S	0.00005	-0.02029	-0.00001	0.02437	-0.00831
56		2S	-0.00039	-0.01892	-0.00002	0.04684	-0.01487
57 8	H	1S	0.02239	-0.02152	0.00000	-0.03914	0.02099
58		2S	0.00160	-0.03587	0.00000	-0.08062	0.01337
59 9	H	1S	-0.01991	0.01222	0.00000	0.02514	-0.01608
60		2S	-0.01509	0.00916	-0.00001	0.02706	-0.01794
61 10	H	1S	-0.00371	-0.00049	0.00000	-0.00468	0.00298
62		2S	-0.00955	-0.00355	0.00001	-0.00944	0.00298
63 11	O	1S	0.00775	-0.00718	0.00000	0.07482	-0.06956
64		2S	-0.00397	0.01005	0.00000	-0.01340	0.01168
65		2PX	0.00146	-0.01208	-0.00002	-0.03580	-0.01396
66		2PY	-0.01614	0.06353	0.00002	-0.30067	0.06065
67		2PZ	-0.00001	-0.00004	0.01988	-0.00021	0.00015
68		3S	-0.03260	0.00118	0.00000	-0.09215	0.05740
69		3PX	0.00849	-0.00174	-0.00002	-0.02683	-0.01527
70		3PY	-0.02529	0.08660	0.00003	-0.34040	0.07146
71		3PZ	0.00000	-0.00003	0.01996	-0.00022	0.00017
72 12	O	1S	-0.01871	-0.00975	0.00000	-0.00789	0.10884
73		2S	0.01578	0.00871	0.00000	-0.02547	-0.01812
74		2PX	-0.19374	-0.10570	-0.00006	-0.19757	0.00762
75		2PY	-0.10757	-0.06987	-0.00009	-0.18495	-0.10982
76		2PZ	-0.00006	-0.00010	0.17936	-0.00002	-0.00007
77		3S	0.01697	0.00343	-0.00002	-0.06454	-0.12095
78		3PX	-0.22309	-0.10372	-0.00006	-0.22681	0.01185
79		3PY	-0.10749	-0.09991	-0.00010	-0.19570	-0.11246
80		3PZ	-0.00007	-0.00012	0.20410	0.00000	-0.00008
			26	27	28	29	30
26		3PY	0.22500				
27		3PZ	0.00000	0.28539			
28 4	C	1S	0.01079	0.00000	2.03846		
29		2S	-0.00385	-0.00002	0.10265	0.12063	
30		2PX	0.02259	-0.00002	-0.00191	0.00285	0.32161
31		2PY	-0.03845	-0.00001	-0.00287	-0.00603	0.00360
32		2PZ	-0.00004	0.05969	0.00000	0.00000	0.00000
33		3S	-0.03028	0.00005	-0.43084	0.22922	0.04121
34		3PX	0.00008	-0.00001	-0.00503	-0.00020	0.15003
35		3PY	-0.07582	-0.00008	0.05319	0.00217	-0.01830
36		3PZ	-0.00005	0.02378	-0.00001	0.00000	-0.00001
37 5	C	1S	0.00566	0.00000	0.01742	-0.03090	0.06591

38		2S	0.00191	0.00001	-0.03135	0.02328	-0.06551
39		2PX	-0.00143	0.00000	-0.06464	0.06718	-0.17918
40		2PY	0.01242	0.00000	-0.03696	0.03698	-0.11685
41		2PZ	-0.00004	-0.01646	0.00002	-0.00001	0.00000
42		3S	0.00159	-0.00004	0.05912	0.02901	-0.21140
43		3PX	-0.00599	-0.00003	0.02299	0.03284	-0.18144
44		3PY	0.01493	0.00001	-0.00820	0.00209	-0.03481
45		3PZ	-0.00003	-0.02885	0.00002	-0.00001	-0.00002
46	6	C 1S	-0.00198	0.00000	-0.00370	0.00406	-0.00741
47		2S	-0.00405	-0.00001	0.00397	-0.00244	0.00792
48		2PX	0.00002	-0.00001	0.00480	-0.00506	0.00783
49		2PY	-0.00546	-0.00001	0.01043	-0.01160	0.03039
50		2PZ	-0.00003	-0.02908	0.00000	0.00001	-0.00002
51		3S	-0.02085	0.00000	-0.00456	-0.02648	0.06035
52		3PX	-0.01609	0.00000	-0.00005	-0.01851	0.04695
53		3PY	-0.00984	0.00000	0.01009	-0.01981	0.05463
54		3PZ	-0.00002	-0.03553	0.00000	0.00001	-0.00002
55	7	H 1S	-0.01462	0.00000	-0.00082	0.00145	-0.00020
56		2S	-0.03265	-0.00001	0.00262	0.00239	-0.00241
57	8	H 1S	-0.03622	-0.00001	-0.06453	0.06045	0.00397
58		2S	-0.01282	0.00002	-0.00878	0.01961	0.00220
59	9	H 1S	0.00831	0.00000	0.01092	-0.01200	0.03001
60		2S	0.00544	-0.00001	0.02366	-0.01389	0.03235
61	10	H 1S	0.00295	0.00001	-0.00836	0.00770	-0.01934
62		2S	0.00342	0.00001	-0.00695	0.00444	-0.01578
63	11	O 1S	-0.01858	-0.00004	0.00122	0.00201	-0.00435
64		2S	0.00340	0.00001	-0.00101	0.00027	0.00329
65		2PX	0.01569	0.00005	0.00405	-0.00558	-0.01441
66		2PY	0.17548	0.00009	-0.00921	0.00459	0.02398
67		2PZ	0.00009	-0.04967	0.00000	-0.00001	-0.00002
68		3S	0.01134	0.00003	-0.00225	-0.00441	0.00077
69		3PX	0.01433	0.00005	0.00376	-0.00502	-0.01390
70		3PY	0.19579	0.00010	-0.01112	0.00675	0.03337
71		3PZ	0.00011	-0.06326	0.00000	-0.00001	-0.00001
72	12	O 1S	0.05946	0.00003	-0.00317	-0.00181	0.01035
73		2S	-0.01203	-0.00001	0.00125	-0.00286	-0.01040
74		2PX	-0.13925	-0.00004	-0.02106	0.01202	0.05920
75		2PY	0.18104	-0.00003	0.01079	-0.00584	-0.02273
76		2PZ	-0.00006	0.26972	0.00000	0.00000	-0.00001
77		3S	-0.08079	-0.00004	0.01275	-0.00462	-0.02444
78		3PX	-0.13612	-0.00004	-0.02501	0.01551	0.07839
79		3PY	0.18265	-0.00004	0.01087	-0.00964	-0.03774
80		3PZ	-0.00008	0.31236	0.00000	0.00000	-0.00001
			31	32	33	34	35

31		2PY	0.30698				
32		2PZ	0.00000	0.21607			
33		3S	0.05333	0.00000	0.87242		
34		3PX	0.00300	-0.00001	0.04366	0.08103	
35		3PY	0.28328	0.00002	-0.06414	-0.01918	0.33751
36		3PZ	0.00000	0.25147	-0.00001	-0.00001	0.00002
37 5	C	1S	0.03784	0.00001	0.06076	-0.00258	-0.02334
38		2S	-0.04030	-0.00001	0.03397	-0.01712	-0.02870
39		2PX	-0.10729	-0.00001	0.13540	-0.09771	-0.06757
40		2PY	-0.05088	0.00005	0.11398	-0.06002	-0.09798
41		2PZ	0.00000	0.17750	-0.00013	-0.00001	0.00007
42		3S	-0.07546	-0.00003	-0.12335	-0.06769	0.00226
43		3PX	-0.04699	-0.00001	-0.00810	-0.10264	0.01955
44		3PY	-0.04339	0.00004	0.02951	-0.01560	-0.08252
45		3PZ	-0.00003	0.20868	-0.00013	-0.00002	0.00004
46 6	C	1S	-0.00969	0.00000	-0.00752	-0.01135	-0.00523
47		2S	0.01045	0.00000	-0.02580	0.00898	0.02710
48		2PX	0.00760	0.00001	-0.01156	0.01064	0.00237
49		2PY	0.02905	0.00000	-0.07160	0.02892	0.07830
50		2PZ	-0.00002	-0.00391	-0.00008	-0.00002	0.00005
51		3S	0.05201	-0.00002	-0.05254	0.03549	0.06659
52		3PX	0.02158	0.00002	-0.03270	0.03236	0.01484
53		3PY	0.04206	-0.00001	-0.05224	0.03311	0.06268
54		3PZ	-0.00001	-0.03062	-0.00010	-0.00002	0.00007
55 7	H	1S	-0.00312	0.00000	-0.00411	-0.00196	0.00514
56		2S	-0.00161	-0.00001	-0.00868	-0.00206	0.01239
57 8	H	1S	0.20029	0.00003	0.20265	0.00283	0.18518
58		2S	0.12979	-0.00001	0.08889	0.00271	0.10980
59 9	H	1S	0.00394	0.00001	-0.03187	0.03041	-0.02337
60		2S	0.00702	0.00002	-0.03578	0.02237	-0.01288
61 10	H	1S	-0.01418	-0.00001	0.02354	-0.01543	-0.01772
62		2S	-0.01849	0.00000	0.02024	-0.01307	-0.02570
63 11	O	1S	0.00346	0.00000	-0.06814	-0.00905	0.03751
64		2S	-0.00219	0.00000	0.01553	0.00414	-0.00998
65		2PX	0.01181	-0.00002	-0.03577	-0.01342	0.01078
66		2PY	-0.01473	0.00000	0.09995	0.01284	-0.09040
67		2PZ	0.00000	0.02544	0.00012	-0.00002	-0.00009
68		3S	-0.00587	0.00000	0.06100	0.00952	-0.04473
69		3PX	0.01359	-0.00002	-0.03810	-0.01338	0.01519
70		3PY	-0.02151	0.00001	0.12560	0.01974	-0.11038
71		3PZ	0.00000	0.03352	0.00014	-0.00002	-0.00011
72 12	O	1S	0.00440	0.00000	0.07817	-0.01813	-0.06539
73		2S	-0.00123	0.00000	-0.01691	0.00566	0.00695
74		2PX	-0.00774	0.00001	0.23611	0.06693	-0.09450

75		2PY	0.00362	0.00000	-0.16078	-0.03924	0.01866
76		2PZ	0.00002	-0.01671	0.00000	0.00000	-0.00001
77		3S	-0.01232	0.00000	-0.07998	0.02969	0.04097
78		3PX	-0.00800	0.00002	0.27305	0.07844	-0.11120
79		3PY	0.01227	0.00001	-0.18051	-0.04960	0.03037
80		3PZ	0.00002	-0.03164	0.00001	0.00000	0.00000
			36	37	38	39	40
36		3PZ	0.30222				
37 5	C	1S	0.00001	2.03847			
38		2S	-0.00001	0.10103	0.12301		
39		2PX	-0.00001	0.00023	0.00556	0.31398	
40		2PY	0.00007	-0.00018	-0.00666	0.00882	0.32380
41		2PZ	0.21017	0.00000	0.00000	0.00001	-0.00002
42		3S	-0.00004	-0.41740	0.22776	-0.02395	0.02927
43		3PX	-0.00001	-0.04190	-0.00569	0.26502	-0.04372
44		3PY	0.00006	0.02757	-0.00093	-0.04158	0.19156
45		3PZ	0.25124	-0.00002	0.00000	0.00002	0.00004
46 6	C	1S	0.00001	0.01681	-0.03139	0.00040	0.07528
47		2S	-0.00001	-0.03139	0.02527	0.00061	-0.07936
48		2PX	0.00001	0.00041	0.00061	0.01321	0.00633
49		2PY	-0.00002	-0.07529	0.07936	-0.00631	-0.25003
50		2PZ	-0.01826	0.00002	-0.00003	0.00001	0.00009
51		3S	-0.00003	0.06270	0.02868	-0.02633	-0.19777
52		3PX	0.00003	0.01632	0.01532	-0.04403	-0.03680
53		3PY	-0.00003	0.01747	0.02887	-0.02471	-0.17256
54		3PZ	-0.05203	0.00000	-0.00002	0.00002	0.00008
55 7	H	1S	0.00000	-0.00828	0.00751	0.00234	-0.02283
56		2S	-0.00001	-0.00602	0.00329	0.00609	-0.01947
57 8	H	1S	0.00003	0.01067	-0.01141	-0.01934	-0.02462
58		2S	-0.00002	0.02222	-0.01238	-0.02500	-0.02587
59 9	H	1S	0.00001	-0.06342	0.06035	-0.17551	0.10158
60		2S	0.00002	-0.00857	0.01941	-0.11749	0.07246
61 10	H	1S	-0.00001	0.01082	-0.01143	0.01278	0.03121
62		2S	0.00000	0.02301	-0.01351	0.01242	0.03969
63 11	O	1S	0.00000	-0.00087	-0.00289	-0.00047	0.00003
64		2S	0.00000	-0.00055	0.00015	-0.00012	0.00028
65		2PX	-0.00005	0.00073	-0.00280	-0.00309	0.00062
66		2PY	-0.00002	-0.00086	0.00285	0.00222	-0.00092
67		2PZ	0.04796	0.00000	0.00001	0.00001	0.00000
68		3S	0.00000	0.00464	0.00316	-0.00033	0.00135
69		3PX	-0.00006	-0.00006	-0.00349	-0.00366	-0.00024
70		3PY	-0.00001	0.00014	0.00321	0.00166	-0.00128
71		3PZ	0.06249	0.00000	0.00001	0.00001	0.00000
72 12	O	1S	0.00000	0.00152	0.00184	-0.00559	-0.00233

73		2S	0.00000	-0.00107	0.00057	0.00375	0.00202
74		2PX	0.00003	0.01138	-0.00740	-0.03191	-0.01708
75		2PY	0.00000	-0.00173	-0.00181	-0.00087	0.00161
76		2PZ	-0.06802	0.00000	0.00000	-0.00001	-0.00003
77		3S	0.00000	-0.00407	-0.00248	0.01069	0.00180
78		3PX	0.00003	0.01261	-0.00909	-0.04224	-0.02115
79		3PY	0.00001	-0.00154	-0.00098	0.00136	0.00297
80		3PZ	-0.09375	0.00000	0.00000	-0.00001	-0.00004
			41	42	43	44	45
41		2PZ	0.19374				
42		3S	0.00004	0.70346			
43		3PX	0.00005	0.01009	0.27256		
44		3PY	-0.00001	0.00231	-0.07606	0.13523	
45		3PZ	0.21961	0.00005	0.00005	0.00002	0.25265
46 6	C	1S	-0.00002	0.06271	0.01632	-0.01747	0.00000
47		2S	0.00003	0.02868	0.01532	-0.02886	0.00001
48		2PX	0.00001	-0.02636	-0.04403	0.02472	0.00001
49		2PY	0.00009	0.19778	0.03681	-0.17255	0.00005
50		2PZ	0.08069	0.00003	0.00005	0.00003	0.06943
51		3S	-0.00001	-0.09292	-0.00175	-0.04816	-0.00005
52		3PX	0.00000	-0.00178	-0.08909	0.00388	0.00000
53		3PY	0.00004	0.04818	-0.00386	-0.10975	0.00001
54		3PZ	0.06943	0.00007	0.00007	0.00001	0.05279
55 7	H	1S	0.00001	0.02807	0.00637	-0.02423	0.00001
56		2S	0.00002	0.02329	0.01423	-0.02343	0.00002
57 8	H	1S	0.00001	-0.04601	-0.00631	-0.03696	-0.00001
58		2S	-0.00003	-0.04425	-0.01274	-0.02540	-0.00005
59 9	H	1S	-0.00002	0.18050	-0.17424	0.08997	0.00000
60		2S	0.00001	0.06969	-0.11514	0.06306	0.00002
61 10	H	1S	-0.00001	-0.04498	0.03619	0.02691	-0.00001
62		2S	-0.00001	-0.04009	0.02298	0.02504	-0.00001
63 11	O	1S	0.00000	0.03969	0.02935	-0.01468	0.00000
64		2S	0.00000	-0.00782	-0.00767	0.00366	0.00001
65		2PX	0.00001	0.02474	0.02349	-0.01683	0.00001
66		2PY	-0.00001	-0.03289	-0.02278	0.00158	0.00000
67		2PZ	-0.01025	-0.00010	-0.00006	0.00003	-0.00313
68		3S	-0.00003	-0.03651	-0.03235	0.01523	-0.00001
69		3PX	0.00003	0.03072	0.02887	-0.02070	0.00002
70		3PY	-0.00001	-0.04129	-0.02921	0.00281	-0.00001
71		3PZ	-0.01123	-0.00012	-0.00006	0.00003	-0.00111
72 12	O	1S	0.00000	-0.06713	-0.03768	0.00518	0.00000
73		2S	0.00000	0.01649	0.01082	0.00164	0.00000
74		2PX	0.00001	-0.11265	-0.08355	0.00159	0.00001
75		2PY	0.00002	0.02178	0.02078	0.00068	0.00004

76		2PZ	-0.07101	-0.00003	-0.00002	-0.00002	-0.09508
77		3S	0.00002	0.06334	0.04306	0.00014	0.00002
78		3PX	0.00001	-0.13296	-0.10233	0.00195	0.00001
79		3PY	0.00003	0.02644	0.02603	0.00048	0.00004
80		3PZ	-0.09251	-0.00003	-0.00002	-0.00003	-0.12233
			46	47	48	49	50
46 6	C	1S	2.03847				
47		2S	0.10103	0.12301			
48		2PX	0.00023	0.00555	0.31401		
49		2PY	0.00019	0.00665	-0.00881	0.32381	
50		2PZ	0.00000	0.00000	-0.00005	-0.00002	0.19372
51		3S	-0.41741	0.22777	-0.02395	-0.02929	-0.00009
52		3PX	-0.04191	-0.00568	0.26502	0.04371	-0.00009
53		3PY	-0.02757	0.00092	0.04158	0.19158	-0.00002
54		3PZ	0.00003	0.00001	-0.00003	0.00001	0.21960
55 7	H	1S	0.01067	-0.01141	-0.01934	0.02462	0.00000
56		2S	0.02222	-0.01238	-0.02501	0.02587	0.00004
57 8	H	1S	-0.00828	0.00751	0.00234	0.02284	-0.00002
58		2S	-0.00602	0.00329	0.00609	0.01947	-0.00004
59 9	H	1S	0.01082	-0.01143	0.01279	-0.03121	0.00000
60		2S	0.02301	-0.01351	0.01244	-0.03971	0.00002
61 10	H	1S	-0.06344	0.06037	-0.17552	-0.10161	0.00006
62		2S	-0.00856	0.01941	-0.11745	-0.07244	0.00004
63 11	O	1S	0.00152	0.00183	-0.00560	0.00233	0.00001
64		2S	-0.00107	0.00057	0.00375	-0.00202	0.00000
65		2PX	0.01138	-0.00740	-0.03192	0.01708	0.00006
66		2PY	0.00173	0.00182	0.00087	0.00161	-0.00001
67		2PZ	0.00001	-0.00002	-0.00005	-0.00001	-0.07104
68		3S	-0.00407	-0.00248	0.01071	-0.00181	-0.00007
69		3PX	0.01261	-0.00909	-0.04226	0.02116	0.00010
70		3PY	0.00154	0.00099	-0.00135	0.00296	-0.00003
71		3PZ	0.00001	-0.00002	-0.00005	-0.00002	-0.09255
72 12	O	1S	-0.00087	-0.00289	-0.00047	-0.00003	0.00000
73		2S	-0.00055	0.00015	-0.00012	-0.00028	0.00000
74		2PX	0.00073	-0.00280	-0.00309	-0.00063	0.00000
75		2PY	0.00086	-0.00285	-0.00222	-0.00091	0.00000
76		2PZ	0.00000	0.00000	-0.00001	0.00000	-0.01024
77		3S	0.00464	0.00316	-0.00033	-0.00135	0.00004
78		3PX	-0.00006	-0.00349	-0.00366	0.00024	-0.00001
79		3PY	-0.00014	-0.00321	-0.00166	-0.00128	0.00000
80		3PZ	0.00000	0.00000	-0.00002	0.00000	-0.01123
			51	52	53	54	55
51		3S	0.70351				
52		3PX	0.01015	0.27253			

53		3PY	-0.00232	0.07605	0.13525		
54		3PZ	-0.00012	-0.00011	0.00000	0.25265	
55 7	H	1S	-0.04606	-0.00634	0.03696	0.00000	0.17441
56		2S	-0.04428	-0.01277	0.02539	0.00005	0.10164
57 8	H	1S	0.02806	0.00636	0.02422	-0.00002	0.00110
58		2S	0.02329	0.01422	0.02342	-0.00004	0.00216
59 9	H	1S	-0.04498	0.03619	-0.02691	0.00000	-0.00639
60		2S	-0.04009	0.02300	-0.02505	0.00002	-0.01070
61 10	H	1S	0.18055	-0.17422	-0.08999	0.00005	-0.01561
62		2S	0.06968	-0.11507	-0.06305	0.00003	-0.01208
63 11	O	1S	-0.06710	-0.03767	-0.00518	0.00003	0.00776
64		2S	0.01649	0.01082	-0.00164	0.00000	-0.00274
65		2PX	-0.11270	-0.08357	-0.00160	0.00011	0.02229
66		2PY	-0.02186	-0.02082	0.00068	0.00001	0.00077
67		2PZ	0.00009	0.00004	0.00001	-0.09512	0.00000
68		3S	0.06337	0.04308	-0.00015	-0.00011	-0.01166
69		3PX	-0.13301	-0.10236	-0.00197	0.00016	0.02608
70		3PY	-0.02652	-0.02607	0.00049	-0.00001	-0.00369
71		3PZ	0.00011	0.00004	0.00001	-0.12240	0.00000
72 12	O	1S	0.03970	0.02936	0.01469	-0.00002	-0.00010
73		2S	-0.00781	-0.00767	-0.00366	0.00000	-0.00083
74		2PX	0.02472	0.02350	0.01681	-0.00002	0.00501
75		2PY	0.03293	0.02280	0.00159	-0.00001	0.00667
76		2PZ	0.00001	-0.00001	0.00001	-0.00313	0.00001
77		3S	-0.03651	-0.03234	-0.01524	0.00006	-0.00154
78		3PX	0.03070	0.02887	0.02068	-0.00004	0.00579
79		3PY	0.04133	0.02924	0.00282	-0.00002	0.00986
80		3PZ	0.00001	-0.00001	0.00002	-0.00110	0.00001
			56	57	58	59	60
56		2S	0.06907				
57 8	H	1S	0.00216	0.17440			
58		2S	0.00164	0.10164	0.06908		
59 9	H	1S	-0.00969	-0.01560	-0.00965	0.17747	
60		2S	-0.00924	-0.01208	-0.00586	0.10660	0.06873
61 10	H	1S	-0.00965	-0.00639	-0.00969	-0.01491	-0.00960
62		2S	-0.00586	-0.01070	-0.00924	-0.00959	-0.00423
63 11	O	1S	0.01793	-0.00010	-0.00589	0.00095	0.00720
64		2S	0.00094	-0.00083	0.00132	0.00020	-0.00131
65		2PX	0.03603	0.00501	0.01053	-0.00179	0.00361
66		2PY	-0.03669	-0.00667	0.00459	0.00056	-0.00355
67		2PZ	-0.00005	0.00001	0.00003	-0.00001	-0.00003
68		3S	0.00047	-0.00154	0.01300	0.00056	-0.00589
69		3PX	0.04100	0.00579	0.00909	-0.00256	0.00384
70		3PY	-0.04339	-0.00986	0.00290	0.00117	-0.00368

71		3PZ	-0.00006	0.00001	0.00003	-0.00001	-0.00003
72	12	O 1S	-0.00590	0.00776	0.01792	0.00009	-0.00539
73		2S	0.00132	-0.00274	0.00094	-0.00056	0.00100
74		2PX	0.01053	0.02227	0.03599	0.00789	0.00455
75		2PY	-0.00463	-0.00076	0.03670	-0.00007	0.00277
76		2PZ	0.00002	0.00001	0.00005	0.00000	-0.00001
77		3S	0.01301	-0.01165	0.00047	-0.00319	0.00581
78		3PX	0.00909	0.02605	0.04095	0.01149	0.00641
79		3PY	-0.00294	0.00370	0.04341	-0.00124	0.00172
80		3PZ	0.00003	0.00002	0.00006	-0.00001	-0.00001
			61	62	63	64	65
61	10	H 1S	0.17751				
62		2S	0.10658	0.06869			
63	11	O 1S	0.00009	-0.00539	2.06335		
64		2S	-0.00056	0.00100	0.07057	0.13931	
65		2PX	0.00789	0.00454	-0.04017	0.03580	0.39508
66		2PY	0.00007	-0.00279	0.02259	-0.01953	0.10721
67		2PZ	0.00002	0.00004	-0.00003	0.00002	-0.00003
68		3S	-0.00319	0.00581	-0.53736	0.40769	0.16564
69		3PX	0.01149	0.00640	0.00513	0.02791	0.42716
70		3PY	0.00124	-0.00173	-0.00242	-0.01602	0.11301
71		3PZ	0.00002	0.00005	0.00001	0.00002	-0.00003
72	12	O 1S	0.00095	0.00721	-0.00132	-0.00446	-0.00018
73		2S	0.00020	-0.00131	-0.00446	0.00048	-0.00249
74		2PX	-0.00179	0.00362	-0.00018	-0.00249	-0.01362
75		2PY	-0.00056	0.00356	-0.00402	0.00122	-0.00164
76		2PZ	0.00000	0.00000	0.00000	0.00000	0.00006
77		3S	0.00056	-0.00590	0.02402	-0.00071	0.01041
78		3PX	-0.00255	0.00385	-0.00767	-0.00161	-0.01855
79		3PY	-0.00117	0.00369	-0.00750	0.00060	-0.00949
80		3PZ	0.00000	0.00000	0.00001	-0.00001	0.00007
			66	67	68	69	70
66		2PY	0.51148				
67		2PZ	0.00003	0.28916			
68		3S	-0.09153	0.00016	1.47960		
69		3PX	0.11264	-0.00005	0.12648	0.46581	
70		3PY	0.55188	0.00005	-0.07403	0.11857	0.59834
71		3PZ	0.00003	0.34028	0.00015	-0.00007	0.00005
72	12	O 1S	0.00402	0.00000	0.02402	-0.00767	0.00750
73		2S	-0.00122	0.00000	-0.00071	-0.00161	-0.00060
74		2PX	0.00164	0.00000	0.01042	-0.01855	0.00950
75		2PY	0.01963	0.00004	0.03396	-0.01933	0.00938
76		2PZ	-0.00003	-0.10623	-0.00001	0.00006	-0.00004
77		3S	-0.03394	-0.00005	-0.02796	0.01719	-0.03734

78	3PX	0.01933	0.00002	0.01719	-0.02504	0.03021
79	3PY	0.00938	0.00006	0.03736	-0.03021	-0.00402
80	3PZ	-0.00004	-0.13122	-0.00002	0.00008	-0.00006
		71	72	73	74	75
71	3PZ	0.40122				
72 12	O 1S	-0.00002	2.06335			
73	2S	0.00001	0.07057	0.13931		
74	2PX	0.00000	-0.04017	0.03581	0.39501	
75	2PY	0.00003	-0.02258	0.01953	-0.10719	0.51153
76	2PZ	-0.13122	-0.00001	0.00001	-0.00001	0.00007
77	3S	-0.00004	-0.53736	0.40769	0.16567	0.09148
78	3PX	0.00002	0.00513	0.02792	0.42709	-0.11261
79	3PY	0.00004	0.00242	0.01601	-0.11299	0.55192
80	3PZ	-0.16179	0.00000	0.00000	-0.00001	0.00007
		76	77	78	79	80
76	2PZ	0.28918				
77	3S	0.00004	1.47959			
78	3PX	-0.00002	0.12651	0.46573		
79	3PY	0.00007	0.07397	-0.11854	0.59839	
80	3PZ	0.34031	0.00004	-0.00002	0.00007	0.40125

Full Mulliken population analysis:

		1	2	3	4	5
1 1	C 1S	2.03846				
2	2S	0.01965	0.12064			
3	2PX	0.00000	0.00000	0.32166		
4	2PY	0.00000	0.00000	0.00000	0.30701	
5	2PZ	0.00000	0.00000	0.00000	0.00000	0.21608
6	3S	-0.07770	0.17452	0.00000	0.00000	0.00000
7	3PX	0.00000	0.00000	0.07934	0.00000	0.00000
8	3PY	0.00000	0.00000	0.00000	0.14985	0.00000
9	3PZ	0.00000	0.00000	0.00000	0.00000	0.13302
10 2	C 1S	0.00000	-0.00016	-0.00078	-0.00026	0.00000
11	2S	-0.00015	0.00275	0.01009	0.00336	0.00000
12	2PX	-0.00074	0.00877	0.03027	0.01392	0.00000
13	2PY	-0.00029	0.00346	0.01661	0.00108	0.00000
14	2PZ	0.00000	0.00000	0.00000	0.00000	0.00457
15	3S	0.00291	0.01134	0.03548	0.00745	0.00000
16	3PX	0.00338	0.00889	0.01406	0.00761	0.00000
17	3PY	0.00059	-0.00092	0.00379	-0.00307	0.00000
18	3PZ	0.00000	0.00000	0.00000	0.00000	0.01055
19 3	C 1S	0.00000	0.00000	0.00000	0.00000	0.00000
20	2S	0.00000	0.00000	-0.00001	-0.00001	0.00000
21	2PX	0.00000	0.00000	0.00000	0.00000	0.00000
22	2PY	0.00000	-0.00002	-0.00007	-0.00009	0.00000

23		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
24		3S	0.00005	-0.00128	-0.00210	-0.00211	0.00000
25		3PX	-0.00004	-0.00066	-0.00054	-0.00097	0.00000
26		3PY	0.00021	-0.00201	-0.00321	-0.00275	0.00000
27		3PZ	0.00000	0.00000	0.00000	0.00000	-0.00021
28 4	C	1S	0.00000	0.00000	0.00000	0.00000	0.00000
29		2S	0.00000	0.00000	0.00000	0.00000	0.00000
30		2PX	0.00000	0.00000	0.00000	0.00000	0.00000
31		2PY	0.00000	0.00000	0.00000	-0.00001	0.00000
32		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
33		3S	0.00002	0.00007	0.00000	-0.00004	0.00000
34		3PX	0.00000	0.00000	-0.00004	0.00000	0.00000
35		3PY	0.00004	0.00031	0.00000	0.00008	0.00000
36		3PZ	0.00000	0.00000	0.00000	0.00000	-0.00077
37 5	C	1S	0.00000	0.00000	0.00000	0.00000	0.00000
38		2S	0.00000	0.00000	-0.00001	-0.00001	0.00000
39		2PX	0.00000	0.00000	-0.00001	-0.00001	0.00000
40		2PY	0.00000	-0.00001	-0.00005	-0.00008	0.00000
41		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
42		3S	-0.00002	-0.00083	-0.00121	-0.00181	0.00000
43		3PX	0.00000	-0.00092	-0.00059	-0.00122	0.00000
44		3PY	0.00012	-0.00171	-0.00308	-0.00327	0.00000
45		3PZ	0.00000	0.00000	0.00000	0.00000	-0.00061
46 6	C	1S	0.00000	-0.00014	-0.00076	-0.00025	0.00000
47		2S	-0.00014	0.00219	0.00909	0.00323	0.00000
48		2PX	-0.00075	0.00932	0.03000	0.01367	0.00000
49		2PY	-0.00025	0.00296	0.01489	0.00103	0.00000
50		2PZ	0.00000	0.00000	0.00000	0.00000	0.00948
51		3S	0.00285	0.00766	0.03777	0.00779	0.00000
52		3PX	0.00217	0.01367	0.02060	0.00788	0.00000
53		3PY	-0.00045	0.00050	0.00583	-0.00347	0.00000
54		3PZ	0.00000	0.00000	0.00000	0.00000	0.03690
55 7	H	1S	-0.00116	0.01142	0.00000	0.05746	0.00000
56		2S	-0.00070	0.00778	0.00000	0.03041	0.00000
57 8	H	1S	0.00000	0.00000	0.00000	0.00000	0.00000
58		2S	0.00000	0.00000	0.00000	0.00000	0.00000
59 9	H	1S	0.00000	0.00000	0.00000	0.00000	0.00000
60		2S	0.00000	0.00001	0.00003	0.00004	0.00000
61 10	H	1S	0.00000	-0.00002	-0.00011	0.00000	0.00000
62		2S	0.00021	-0.00091	-0.00233	-0.00003	0.00000
63 11	O	1S	0.00000	0.00000	0.00000	0.00000	0.00000
64		2S	0.00000	0.00000	0.00000	0.00000	0.00000
65		2PX	0.00000	0.00000	-0.00001	0.00000	0.00000
66		2PY	0.00000	0.00000	0.00000	0.00000	0.00000

67		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
68		3S	0.00000	-0.00002	-0.00024	0.00000	0.00000
69		3PX	0.00002	-0.00029	-0.00263	0.00000	0.00000
70		3PY	0.00000	0.00000	0.00001	0.00004	0.00000
71		3PZ	0.00000	0.00000	0.00000	0.00000	-0.00011
72	12	O 1S	0.00000	0.00000	0.00000	0.00000	0.00000
73		2S	0.00000	0.00000	0.00000	0.00000	0.00000
74		2PX	0.00000	0.00000	0.00000	0.00000	0.00000
75		2PY	0.00000	0.00000	0.00000	0.00000	0.00000
76		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
77		3S	0.00000	0.00000	0.00000	0.00000	0.00000
78		3PX	0.00000	0.00000	0.00000	0.00000	0.00000
79		3PY	0.00000	0.00000	0.00000	0.00000	0.00000
80		3PZ	0.00000	0.00000	0.00000	0.00000	0.00000
			6	7	8	9	10
6		3S	0.87259				
7		3PX	0.00000	0.08099			
8		3PY	0.00000	0.00000	0.33759		
9		3PZ	0.00000	0.00000	0.00000	0.30222	
10	2	C 1S	0.00481	-0.00001	0.00377	0.00000	2.03869
11		2S	0.00014	0.00803	-0.00123	0.00000	0.01850
12		2PX	0.03843	0.01027	0.02695	0.00000	0.00000
13		2PY	0.01445	0.01190	-0.00708	0.00000	0.00000
14		2PZ	0.00000	0.00000	0.00000	0.01207	0.00000
15		3S	-0.09760	0.02680	-0.03433	0.00000	-0.08015
16		3PX	-0.03171	0.00049	0.00053	0.00000	0.00000
17		3PY	-0.00893	0.00003	-0.02533	0.00000	0.00000
18		3PZ	0.00000	0.00000	0.00000	0.01204	0.00000
19	3	C 1S	-0.00005	0.00014	-0.00006	0.00000	0.00000
20		2S	-0.00065	-0.00065	-0.00194	0.00000	-0.00017
21		2PX	-0.00052	-0.00006	-0.00050	0.00000	0.00000
22		2PY	-0.00529	-0.00230	-0.00856	0.00000	-0.00105
23		2PZ	0.00000	0.00000	0.00000	-0.00057	0.00000
24		3S	-0.01459	-0.01004	-0.00972	0.00000	0.00499
25		3PX	-0.00352	-0.00007	-0.00357	0.00000	0.00000
26		3PY	-0.02108	-0.00966	-0.00896	0.00000	0.00572
27		3PZ	0.00000	0.00000	0.00000	-0.00102	0.00000
28	4	C 1S	0.00002	0.00000	0.00004	0.00000	0.00000
29		2S	0.00007	0.00000	0.00031	0.00000	0.00000
30		2PX	0.00000	-0.00004	0.00000	0.00000	0.00000
31		2PY	-0.00004	0.00000	0.00008	0.00000	0.00000
32		2PZ	0.00000	0.00000	0.00000	-0.00077	0.00000
33		3S	0.00374	0.00000	0.00690	0.00000	-0.00005
34		3PX	0.00000	-0.00009	0.00000	0.00000	0.00014

35		3PY	0.00690	0.00000	0.00856	0.00000	-0.00006
36		3PZ	0.00000	0.00000	0.00000	-0.01048	0.00000
37 5	C	1S	-0.00003	0.00008	0.00006	0.00000	0.00000
38		2S	-0.00081	-0.00045	-0.00234	0.00000	0.00000
39		2PX	-0.00023	-0.00013	-0.00013	0.00000	0.00000
40		2PY	-0.00249	-0.00163	-0.00608	0.00000	0.00000
41		2PZ	0.00000	0.00000	0.00000	-0.00036	0.00000
42		3S	-0.00681	-0.00466	-0.01513	0.00000	0.00004
43		3PX	-0.00429	-0.00009	-0.00341	0.00000	0.00007
44		3PY	-0.01186	-0.00760	-0.01679	0.00000	0.00002
45		3PZ	0.00000	0.00000	0.00000	-0.00675	0.00000
46 6	C	1S	0.00293	0.00024	0.00127	0.00000	0.00000
47		2S	0.00898	0.00713	0.00690	0.00000	0.00000
48		2PX	0.02419	0.01110	0.01133	0.00000	0.00000
49		2PY	0.01175	0.01006	-0.00785	0.00000	0.00000
50		2PZ	0.00000	0.00000	0.00000	0.03716	0.00000
51		3S	-0.06255	0.03463	-0.00067	0.00000	-0.00012
52		3PX	-0.00417	0.00107	-0.00583	0.00000	-0.00007
53		3PY	0.00872	0.00465	-0.02758	0.00000	0.00000
54		3PZ	0.00000	0.00000	0.00000	0.12723	0.00000
55 7	H	1S	0.06782	0.00000	0.09291	0.00000	0.00000
56		2S	0.05904	0.00000	0.06478	0.00000	0.00034
57 8	H	1S	0.00000	0.00000	0.00000	0.00000	0.00000
58		2S	-0.00005	0.00000	-0.00023	0.00000	0.00000
59 9	H	1S	0.00002	0.00004	0.00006	0.00000	0.00000
60		2S	0.00039	0.00044	0.00107	0.00000	0.00000
61 10	H	1S	-0.00147	-0.00412	0.00022	0.00000	0.00000
62		2S	-0.00733	-0.00800	0.00031	0.00000	0.00000
63 11	O	1S	0.00015	-0.00014	0.00000	0.00000	0.00000
64		2S	-0.00023	0.00027	0.00000	0.00000	0.00000
65		2PX	-0.00322	-0.00288	0.00003	0.00000	-0.00002
66		2PY	0.00002	0.00001	0.00012	0.00000	-0.00001
67		2PZ	0.00000	0.00000	0.00000	-0.00045	0.00000
68		3S	-0.00475	0.00474	0.00005	0.00000	-0.00030
69		3PX	-0.03154	-0.01989	0.00025	0.00000	-0.00406
70		3PY	0.00015	0.00011	0.00172	0.00000	-0.00141
71		3PZ	0.00000	0.00000	0.00000	-0.00529	0.00000
72 12	O	1S	0.00000	0.00000	0.00000	0.00000	0.00000
73		2S	0.00000	0.00000	0.00000	0.00000	0.00000
74		2PX	0.00000	0.00000	0.00000	0.00000	0.00000
75		2PY	0.00001	0.00001	0.00004	0.00000	0.00000
76		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
77		3S	0.00010	0.00004	0.00022	0.00000	0.00000
78		3PX	0.00012	0.00009	0.00015	0.00000	0.00000

79		3PY	0.00045	0.00019	0.00104	0.00000	0.00002
80		3PZ	0.00000	0.00000	0.00000	0.00009	0.00000
			11	12	13	14	15
11		2S	0.13181				
12		2PX	0.00000	0.30929			
13		2PY	0.00000	0.00000	0.33884		
14		2PZ	0.00000	0.00000	0.00000	0.17823	
15		3S	0.19469	0.00000	0.00000	0.00000	0.95281
16		3PX	0.00000	0.05862	0.00000	0.00000	0.00000
17		3PY	0.00000	0.00000	0.07830	0.00000	0.00000
18		3PZ	0.00000	0.00000	0.00000	0.11323	0.00000
19 3	C	1S	-0.00017	0.00000	-0.00105	0.00000	0.00499
20		2S	0.00316	0.00000	0.01346	0.00000	0.00323
21		2PX	0.00000	0.00115	0.00000	0.00000	0.00000
22		2PY	0.01346	0.00000	0.06282	0.00000	0.05225
23		2PZ	0.00000	0.00000	0.00000	0.00350	0.00000
24		3S	0.00323	0.00000	0.05222	0.00000	-0.15614
25		3PX	0.00000	0.00245	0.00000	0.00000	0.00000
26		3PY	0.00389	0.00000	0.03163	0.00000	-0.07928
27		3PZ	0.00000	0.00000	0.00000	0.00761	0.00000
28 4	C	1S	0.00000	0.00000	0.00000	0.00000	0.00005
29		2S	0.00000	0.00000	-0.00002	0.00000	-0.00128
30		2PX	-0.00001	0.00000	-0.00007	0.00000	-0.00210
31		2PY	-0.00001	0.00000	-0.00009	0.00000	-0.00212
32		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
33		3S	-0.00065	-0.00052	-0.00528	0.00000	-0.01460
34		3PX	-0.00065	-0.00006	-0.00230	0.00000	-0.01005
35		3PY	-0.00194	-0.00050	-0.00855	0.00000	-0.00973
36		3PZ	0.00000	0.00000	0.00000	-0.00057	0.00000
37 5	C	1S	0.00000	0.00000	0.00000	0.00000	0.00002
38		2S	0.00000	0.00000	0.00000	0.00000	0.00007
39		2PX	0.00000	0.00000	0.00000	0.00000	-0.00003
40		2PY	0.00000	0.00000	0.00000	0.00000	-0.00006
41		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
42		3S	-0.00006	0.00012	0.00021	0.00000	0.00075
43		3PX	0.00006	0.00065	0.00042	0.00000	0.00292
44		3PY	-0.00003	0.00005	0.00009	0.00000	0.00015
45		3PZ	0.00000	0.00000	0.00000	-0.00027	0.00000
46 6	C	1S	0.00000	0.00000	0.00000	0.00000	-0.00001
47		2S	0.00000	-0.00001	0.00000	0.00000	-0.00103
48		2PX	-0.00002	-0.00014	0.00000	0.00000	-0.00328
49		2PY	0.00000	0.00000	0.00000	0.00000	0.00000
50		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
51		3S	-0.00027	-0.00493	0.00000	0.00000	0.00002

52		3PX	-0.00200	-0.01144	0.00000	0.00000	-0.01174
53		3PY	0.00000	0.00000	0.00016	0.00000	0.00000
54		3PZ	0.00000	0.00000	0.00000	0.00031	0.00000
55 7	H	1S	-0.00002	-0.00005	-0.00007	0.00000	-0.00180
56		2S	-0.00161	-0.00006	-0.00215	0.00000	-0.01651
57 8	H	1S	0.00000	0.00000	0.00000	0.00000	0.00002
58		2S	0.00001	0.00000	0.00005	0.00000	0.00091
59 9	H	1S	0.00000	0.00000	0.00000	0.00000	0.00000
60		2S	0.00000	0.00000	0.00000	0.00000	-0.00006
61 10	H	1S	0.00000	0.00000	0.00000	0.00000	0.00002
62		2S	0.00001	0.00004	0.00000	0.00000	0.00053
63 11	O	1S	0.00000	-0.00009	-0.00003	0.00000	-0.00022
64		2S	-0.00005	0.00090	0.00029	0.00000	-0.00387
65		2PX	0.00264	0.01352	0.00516	0.00000	0.01595
66		2PY	0.00084	0.00525	0.00094	0.00000	0.00862
67		2PZ	0.00000	0.00000	0.00000	0.00264	0.00000
68		3S	-0.00158	0.00296	0.00034	0.00000	-0.02338
69		3PX	0.02028	0.04879	0.02040	0.00000	0.08084
70		3PY	0.00643	0.02115	-0.00081	0.00000	0.04028
71		3PZ	0.00000	0.00000	0.00000	0.02486	0.00000
72 12	O	1S	0.00000	0.00000	0.00000	0.00000	0.00014
73		2S	0.00000	0.00000	0.00000	0.00000	-0.00018
74		2PX	0.00000	0.00000	0.00000	0.00000	0.00025
75		2PY	0.00000	0.00000	-0.00001	0.00000	-0.00353
76		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
77		3S	-0.00006	-0.00016	-0.00001	0.00000	-0.00547
78		3PX	-0.00001	-0.00005	-0.00003	0.00000	0.00156
79		3PY	-0.00028	-0.00041	-0.00209	0.00000	-0.03390
80		3PZ	0.00000	0.00000	0.00000	0.00007	0.00000
			16	17	18	19	20
16		3PX	0.13857				
17		3PY	0.00000	0.22507			
18		3PZ	0.00000	0.00000	0.28541		
19 3	C	1S	0.00000	0.00572	0.00000	2.03869	
20		2S	0.00000	0.00388	0.00000	0.01850	0.13179
21		2PX	0.00245	0.00000	0.00000	0.00000	0.00000
22		2PY	0.00000	0.03164	0.00000	0.00000	0.00000
23		2PZ	0.00000	0.00000	0.00761	0.00000	0.00000
24		3S	0.00000	-0.07932	0.00000	-0.08015	0.19469
25		3PX	-0.01134	0.00000	0.00000	0.00000	0.00000
26		3PY	0.00000	-0.00929	0.00000	0.00000	0.00000
27		3PZ	0.00000	0.00000	-0.00472	0.00000	0.00000
28 4	C	1S	-0.00004	0.00022	0.00000	0.00000	-0.00015
29		2S	-0.00066	-0.00201	0.00000	-0.00016	0.00274

30		2PX	-0.00054	-0.00321	0.00000	-0.00077	0.01008
31		2PY	-0.00097	-0.00275	0.00000	-0.00026	0.00336
32		2PZ	0.00000	0.00000	-0.00021	0.00000	0.00000
33		3S	-0.00353	-0.02109	0.00000	0.00481	0.00013
34		3PX	-0.00007	-0.00968	0.00000	-0.00001	0.00803
35		3PY	-0.00358	-0.00897	0.00000	0.00377	-0.00123
36		3PZ	0.00000	0.00000	-0.00102	0.00000	0.00000
37 5	C	1S	0.00005	0.00000	0.00000	0.00000	0.00000
38		2S	0.00016	0.00008	0.00000	0.00000	0.00000
39		2PX	0.00008	0.00000	0.00000	0.00000	-0.00002
40		2PY	-0.00011	0.00004	0.00000	0.00000	0.00000
41		2PZ	0.00000	0.00000	-0.00019	0.00000	0.00000
42		3S	0.00182	0.00160	0.00000	-0.00012	-0.00027
43		3PX	0.00326	0.00250	0.00000	-0.00007	-0.00199
44		3PY	0.00077	0.00023	0.00000	0.00000	0.00000
45		3PZ	0.00000	0.00000	-0.00234	0.00000	0.00000
46 6	C	1S	0.00000	0.00000	0.00000	0.00000	0.00000
47		2S	-0.00214	0.00000	0.00000	0.00000	0.00000
48		2PX	-0.00599	0.00000	0.00000	0.00000	0.00000
49		2PY	0.00000	0.00025	0.00000	0.00000	0.00000
50		2PZ	0.00000	0.00000	-0.00033	0.00000	0.00000
51		3S	-0.01007	0.00000	0.00000	0.00004	-0.00006
52		3PX	-0.01898	0.00000	0.00000	0.00007	0.00006
53		3PY	0.00000	0.00194	0.00000	0.00002	-0.00003
54		3PZ	0.00000	0.00000	-0.00375	0.00000	0.00000
55 7	H	1S	-0.00159	-0.00408	0.00000	0.00000	0.00000
56		2S	-0.00267	-0.00381	0.00000	0.00000	0.00001
57 8	H	1S	0.00001	0.00006	0.00000	0.00000	-0.00002
58		2S	0.00028	0.00164	0.00000	0.00033	-0.00161
59 9	H	1S	0.00000	0.00000	0.00000	0.00000	0.00000
60		2S	-0.00005	-0.00003	0.00000	0.00000	0.00001
61 10	H	1S	0.00007	0.00001	0.00000	0.00000	0.00000
62		2S	0.00095	0.00005	0.00000	0.00000	0.00000
63 11	O	1S	0.00626	0.00198	0.00000	0.00000	0.00000
64		2S	-0.00502	-0.00193	0.00000	0.00000	0.00000
65		2PX	-0.00055	0.01202	0.00000	0.00000	0.00000
66		2PY	0.00948	0.00509	0.00000	0.00000	0.00000
67		2PZ	0.00000	0.00000	0.02102	0.00000	0.00000
68		3S	-0.05953	-0.02300	0.00000	0.00000	-0.00006
69		3PX	-0.00167	0.03810	0.00000	0.00000	-0.00001
70		3PY	0.03150	0.03331	0.00000	0.00002	-0.00028
71		3PZ	0.00000	0.00000	0.10750	0.00000	0.00000
72 12	O	1S	-0.00027	0.00012	0.00000	0.00000	0.00000
73		2S	0.00029	-0.00014	0.00000	0.00000	-0.00005

74	2PX	0.00009	0.00034	0.00000	-0.00002	0.00264
75	2PY	0.00132	-0.00532	0.00000	-0.00001	0.00084
76	2PZ	0.00000	0.00000	-0.00033	0.00000	0.00000
77	3S	0.00464	-0.00156	0.00000	-0.00030	-0.00158
78	3PX	0.00035	0.00193	0.00000	-0.00406	0.02029
79	3PY	0.00967	-0.03410	0.00000	-0.00141	0.00642
80	3PZ	0.00000	0.00000	-0.00357	0.00000	0.00000
		21	22	23	24	25
21	2PX	0.30925				
22	2PY	0.00000	0.33883			
23	2PZ	0.00000	0.00000	0.17820		
24	3S	0.00000	0.00000	0.00000	0.95265	
25	3PX	0.05864	0.00000	0.00000	0.00000	0.13858
26	3PY	0.00000	0.07826	0.00000	0.00000	0.00000
27	3PZ	0.00000	0.00000	0.11322	0.00000	0.00000
28 4	C 1S	-0.00074	-0.00029	0.00000	0.00291	0.00338
29	2S	0.00876	0.00345	0.00000	0.01133	0.00889
30	2PX	0.03024	0.01660	0.00000	0.03548	0.01407
31	2PY	0.01391	0.00108	0.00000	0.00746	0.00762
32	2PZ	0.00000	0.00000	0.00456	0.00000	0.00000
33	3S	0.03841	0.01444	0.00000	-0.09747	-0.03164
34	3PX	0.01027	0.01191	0.00000	0.02684	0.00050
35	3PY	0.02694	-0.00707	0.00000	-0.03426	0.00056
36	3PZ	0.00000	0.00000	0.01206	0.00000	0.00000
37 5	C 1S	0.00000	0.00000	0.00000	-0.00001	0.00000
38	2S	-0.00001	0.00000	0.00000	-0.00103	-0.00214
39	2PX	-0.00014	0.00000	0.00000	-0.00328	-0.00598
40	2PY	0.00000	0.00000	0.00000	0.00000	0.00000
41	2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
42	3S	-0.00493	0.00000	0.00000	0.00001	-0.01009
43	3PX	-0.01144	0.00000	0.00000	-0.01175	-0.01900
44	3PY	0.00000	0.00016	0.00000	0.00000	0.00000
45	3PZ	0.00000	0.00000	0.00031	0.00000	0.00000
46 6	C 1S	0.00000	0.00000	0.00000	0.00002	0.00005
47	2S	0.00000	0.00000	0.00000	0.00007	0.00016
48	2PX	0.00000	0.00000	0.00000	-0.00003	0.00008
49	2PY	0.00000	0.00000	0.00000	-0.00006	-0.00011
50	2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	3S	0.00012	0.00021	0.00000	0.00075	0.00182
52	3PX	0.00065	0.00042	0.00000	0.00292	0.00326
53	3PY	0.00005	0.00009	0.00000	0.00015	0.00076
54	3PZ	0.00000	0.00000	-0.00027	0.00000	0.00000
55 7	H 1S	0.00000	0.00000	0.00000	0.00002	0.00001
56	2S	0.00000	0.00005	0.00000	0.00091	0.00028

57	8	H	1S	-0.00005	-0.00007	0.00000	-0.00180	-0.00159
58			2S	-0.00006	-0.00215	0.00000	-0.01650	-0.00267
59	9	H	1S	0.00000	0.00000	0.00000	0.00002	0.00007
60			2S	0.00004	0.00000	0.00000	0.00053	0.00095
61	10	H	1S	0.00000	0.00000	0.00000	0.00000	0.00000
62			2S	0.00000	0.00000	0.00000	-0.00006	-0.00005
63	11	O	1S	0.00000	0.00000	0.00000	0.00014	-0.00027
64			2S	0.00000	0.00000	0.00000	-0.00018	0.00029
65			2PX	0.00000	0.00000	0.00000	0.00025	0.00008
66			2PY	0.00000	-0.00001	0.00000	-0.00353	0.00132
67			2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
68			3S	-0.00016	-0.00001	0.00000	-0.00547	0.00463
69			3PX	-0.00005	-0.00003	0.00000	0.00157	0.00035
70			3PY	-0.00041	-0.00209	0.00000	-0.03390	0.00967
71			3PZ	0.00000	0.00000	0.00007	0.00000	0.00000
72	12	O	1S	-0.00009	-0.00003	0.00000	-0.00022	0.00626
73			2S	0.00090	0.00029	0.00000	-0.00387	-0.00502
74			2PX	0.01352	0.00516	0.00000	0.01595	-0.00054
75			2PY	0.00525	0.00094	0.00000	0.00862	0.00947
76			2PZ	0.00000	0.00000	0.00264	0.00000	0.00000
77			3S	0.00296	0.00035	0.00000	-0.02338	-0.05955
78			3PX	0.04881	0.02040	0.00000	0.08084	-0.00166
79			3PY	0.02114	-0.00082	0.00000	0.04028	0.03146
80			3PZ	0.00000	0.00000	0.02486	0.00000	0.00000
				26	27	28	29	30
26			3PY	0.22500				
27			3PZ	0.00000	0.28539			
28	4	C	1S	0.00059	0.00000	2.03846		
29			2S	-0.00092	0.00000	0.01965	0.12063	
30			2PX	0.00379	0.00000	0.00000	0.00000	0.32161
31			2PY	-0.00307	0.00000	0.00000	0.00000	0.00000
32			2PZ	0.00000	0.01055	0.00000	0.00000	0.00000
33			3S	-0.00894	0.00000	-0.07769	0.17452	0.00000
34			3PX	0.00002	0.00000	0.00000	0.00000	0.07936
35			3PY	-0.02531	0.00000	0.00000	0.00000	0.00000
36			3PZ	0.00000	0.01204	0.00000	0.00000	0.00000
37	5	C	1S	0.00000	0.00000	0.00000	-0.00014	-0.00076
38			2S	0.00000	0.00000	-0.00014	0.00219	0.00909
39			2PX	0.00000	0.00000	-0.00075	0.00932	0.02998
40			2PY	0.00025	0.00000	-0.00025	0.00296	0.01489
41			2PZ	0.00000	-0.00033	0.00000	0.00000	0.00000
42			3S	0.00000	0.00000	0.00285	0.00767	0.03776
43			3PX	0.00000	0.00000	0.00217	0.01367	0.02059
44			3PY	0.00194	0.00000	-0.00045	0.00050	0.00584

45		3PZ	0.00000	-0.00374	0.00000	0.00000	0.00000
46 6	C	1S	0.00000	0.00000	0.00000	0.00000	0.00000
47		2S	0.00008	0.00000	0.00000	0.00000	-0.00001
48		2PX	0.00000	0.00000	0.00000	0.00000	-0.00001
49		2PY	0.00004	0.00000	0.00000	-0.00001	-0.00005
50		2PZ	0.00000	-0.00019	0.00000	0.00000	0.00000
51		3S	0.00160	0.00000	-0.00002	-0.00083	-0.00121
52		3PX	0.00249	0.00000	0.00000	-0.00092	-0.00059
53		3PY	0.00023	0.00000	0.00012	-0.00171	-0.00308
54		3PZ	0.00000	-0.00233	0.00000	0.00000	0.00000
55 7	H	1S	0.00006	0.00000	0.00000	0.00000	0.00000
56		2S	0.00164	0.00000	0.00000	0.00000	0.00000
57 8	H	1S	-0.00408	0.00000	-0.00116	0.01142	0.00000
58		2S	-0.00381	0.00000	-0.00070	0.00778	0.00000
59 9	H	1S	0.00001	0.00000	0.00000	-0.00002	-0.00011
60		2S	0.00005	0.00000	0.00021	-0.00091	-0.00233
61 10	H	1S	0.00000	0.00000	0.00000	0.00000	0.00000
62		2S	-0.00003	0.00000	0.00000	0.00001	0.00003
63 11	O	1S	0.00012	0.00000	0.00000	0.00000	0.00000
64		2S	-0.00014	0.00000	0.00000	0.00000	0.00000
65		2PX	0.00034	0.00000	0.00000	0.00000	0.00000
66		2PY	-0.00532	0.00000	0.00000	0.00000	0.00000
67		2PZ	0.00000	-0.00033	0.00000	0.00000	0.00000
68		3S	-0.00156	0.00000	0.00000	0.00000	0.00000
69		3PX	0.00194	0.00000	0.00000	0.00000	0.00000
70		3PY	-0.03410	0.00000	0.00000	0.00000	0.00000
71		3PZ	0.00000	-0.00357	0.00000	0.00000	0.00000
72 12	O	1S	0.00198	0.00000	0.00000	0.00000	0.00000
73		2S	-0.00192	0.00000	0.00000	0.00000	0.00000
74		2PX	0.01201	0.00000	0.00000	0.00000	-0.00001
75		2PY	0.00509	0.00000	0.00000	0.00000	0.00000
76		2PZ	0.00000	0.02102	0.00000	0.00000	0.00000
77		3S	-0.02297	0.00000	0.00000	-0.00002	-0.00024
78		3PX	0.03808	0.00000	0.00002	-0.00029	-0.00263
79		3PY	0.03336	0.00000	0.00000	0.00000	0.00001
80		3PZ	0.00000	0.10750	0.00000	0.00000	0.00000
			31	32	33	34	35
31		2PY	0.30698				
32		2PZ	0.00000	0.21607			
33		3S	0.00000	0.00000	0.87242		
34		3PX	0.00000	0.00000	0.00000	0.08103	
35		3PY	0.14984	0.00000	0.00000	0.00000	0.33751
36		3PZ	0.00000	0.13302	0.00000	0.00000	0.00000
37 5	C	1S	-0.00025	0.00000	0.00293	0.00024	0.00127

38		2S	0.00323	0.00000	0.00899	0.00713	0.00690
39		2PX	0.01368	0.00000	0.02419	0.01109	0.01133
40		2PY	0.00103	0.00000	0.01176	0.01006	-0.00784
41		2PZ	0.00000	0.00948	0.00000	0.00000	0.00000
42		3S	0.00778	0.00000	-0.06247	0.03463	-0.00067
43		3PX	0.00788	0.00000	-0.00414	0.00106	-0.00583
44		3PY	-0.00347	0.00000	0.00872	0.00466	-0.02757
45		3PZ	0.00000	0.03690	0.00000	0.00000	0.00000
46 6	C	1S	0.00000	0.00000	-0.00003	0.00008	0.00006
47		2S	-0.00001	0.00000	-0.00081	-0.00045	-0.00234
48		2PX	-0.00001	0.00000	-0.00023	-0.00013	-0.00013
49		2PY	-0.00008	0.00000	-0.00249	-0.00163	-0.00608
50		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
51		3S	-0.00181	0.00000	-0.00682	-0.00465	-0.01513
52		3PX	-0.00122	0.00000	-0.00429	-0.00009	-0.00341
53		3PY	-0.00327	0.00000	-0.01187	-0.00760	-0.01679
54		3PZ	0.00000	-0.00061	0.00000	0.00000	0.00000
55 7	H	1S	0.00000	0.00000	0.00000	0.00000	0.00000
56		2S	0.00000	0.00000	-0.00005	0.00000	-0.00023
57 8	H	1S	0.05744	0.00000	0.06781	0.00000	0.09291
58		2S	0.03041	0.00000	0.05901	0.00000	0.06480
59 9	H	1S	0.00000	0.00000	-0.00147	-0.00412	0.00022
60		2S	-0.00003	0.00000	-0.00732	-0.00800	0.00032
61 10	H	1S	0.00000	0.00000	0.00002	0.00004	0.00006
62		2S	0.00004	0.00000	0.00039	0.00044	0.00107
63 11	O	1S	0.00000	0.00000	0.00000	0.00000	0.00000
64		2S	0.00000	0.00000	0.00000	0.00000	0.00000
65		2PX	0.00000	0.00000	0.00000	0.00000	0.00000
66		2PY	0.00000	0.00000	0.00001	0.00001	0.00004
67		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
68		3S	0.00000	0.00000	0.00010	0.00004	0.00022
69		3PX	0.00000	0.00000	0.00012	0.00009	0.00014
70		3PY	0.00000	0.00000	0.00045	0.00019	0.00104
71		3PZ	0.00000	0.00000	0.00000	0.00000	0.00000
72 12	O	1S	0.00000	0.00000	0.00015	-0.00014	0.00000
73		2S	0.00000	0.00000	-0.00023	0.00027	0.00000
74		2PX	0.00000	0.00000	-0.00321	-0.00288	0.00003
75		2PY	0.00000	0.00000	0.00002	0.00001	0.00012
76		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
77		3S	0.00000	0.00000	-0.00475	0.00473	0.00005
78		3PX	0.00000	0.00000	-0.03150	-0.01988	0.00025
79		3PY	0.00004	0.00000	0.00015	0.00011	0.00171
80		3PZ	0.00000	-0.00011	0.00000	0.00000	0.00000
			36	37	38	39	40

36		3PZ	0.30222				
37 5	C	1S	0.00000	2.03847			
38		2S	0.00000	0.01934	0.12301		
39		2PX	0.00000	0.00000	0.00000	0.31398	
40		2PY	0.00000	0.00000	0.00000	0.00000	0.32380
41		2PZ	0.03717	0.00000	0.00000	0.00000	0.00000
42		3S	0.00000	-0.07526	0.17341	0.00000	0.00000
43		3PX	0.00000	0.00000	0.00000	0.14019	0.00000
44		3PY	0.00000	0.00000	0.00000	0.00000	0.10133
45		3PZ	0.12723	0.00000	0.00000	0.00000	0.00000
46 6	C	1S	0.00000	0.00000	-0.00014	0.00000	-0.00100
47		2S	0.00000	-0.00014	0.00237	0.00000	0.01270
48		2PX	0.00000	0.00000	0.00000	0.00070	0.00000
49		2PY	0.00000	-0.00100	0.01270	0.00000	0.06020
50		2PZ	-0.00036	0.00000	0.00000	0.00000	0.00000
51		3S	0.00000	0.00302	0.00758	0.00000	0.04079
52		3PX	0.00000	0.00000	0.00000	-0.00778	0.00000
53		3PY	0.00000	0.00190	0.01388	0.00000	0.03630
54		3PZ	-0.00675	0.00000	0.00000	0.00000	0.00000
55 7	H	1S	0.00000	0.00000	0.00000	0.00000	0.00000
56		2S	0.00000	0.00000	0.00001	0.00001	0.00005
57 8	H	1S	0.00000	0.00000	-0.00002	-0.00004	-0.00008
58		2S	0.00000	0.00019	-0.00081	-0.00101	-0.00155
59 9	H	1S	0.00000	-0.00114	0.01140	0.04359	0.01456
60		2S	0.00000	-0.00068	0.00770	0.02384	0.00848
61 10	H	1S	0.00000	0.00000	-0.00002	-0.00002	-0.00010
62		2S	0.00000	0.00020	-0.00088	-0.00039	-0.00258
63 11	O	1S	0.00000	0.00000	0.00000	0.00000	0.00000
64		2S	0.00000	0.00000	0.00000	0.00000	0.00000
65		2PX	0.00000	0.00000	0.00000	0.00000	0.00000
66		2PY	0.00000	0.00000	0.00000	0.00000	0.00000
67		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
68		3S	0.00000	0.00000	0.00000	0.00000	0.00000
69		3PX	0.00000	0.00000	0.00000	0.00000	0.00000
70		3PY	0.00000	0.00000	0.00000	0.00000	0.00000
71		3PZ	0.00009	0.00000	0.00000	0.00000	0.00000
72 12	O	1S	0.00000	0.00000	0.00000	0.00000	0.00000
73		2S	0.00000	0.00000	0.00000	0.00000	0.00000
74		2PX	0.00000	0.00000	0.00000	0.00000	0.00000
75		2PY	0.00000	0.00000	0.00000	0.00000	0.00000
76		2PZ	-0.00045	0.00000	0.00000	0.00000	0.00000
77		3S	0.00000	0.00000	0.00000	0.00000	0.00000
78		3PX	0.00000	0.00000	0.00000	0.00000	0.00000
79		3PY	0.00000	0.00000	0.00000	0.00000	0.00000

80		3PZ	-0.00529	0.00000	0.00000	0.00000	0.00000
			41	42	43	44	45
41		2PZ	0.19374				
42		3S	0.00000	0.70346			
43		3PX	0.00000	0.00000	0.27256		
44		3PY	0.00000	0.00000	0.00000	0.13523	
45		3PZ	0.11617	0.00000	0.00000	0.00000	0.25265
46 6	C	1S	0.00000	0.00302	0.00000	0.00190	0.00000
47		2S	0.00000	0.00758	0.00000	0.01387	0.00000
48		2PX	0.00000	0.00000	-0.00778	0.00000	0.00000
49		2PY	0.00000	0.04079	0.00000	0.03630	0.00000
50		2PZ	0.00430	0.00000	0.00000	0.00000	0.01227
51		3S	0.00000	-0.04704	0.00000	0.02845	0.00000
52		3PX	0.00000	0.00000	-0.04510	0.00000	0.00000
53		3PY	0.00000	0.02846	0.00000	0.02008	0.00000
54		3PZ	0.01227	0.00000	0.00000	0.00000	0.02672
55 7	H	1S	0.00000	0.00002	0.00001	0.00009	0.00000
56		2S	0.00000	0.00045	0.00027	0.00118	0.00000
57 8	H	1S	0.00000	-0.00212	-0.00048	-0.00417	0.00000
58		2S	0.00000	-0.00906	-0.00255	-0.00755	0.00000
59 9	H	1S	0.00000	0.06039	0.07572	0.02256	0.00000
60		2S	0.00000	0.04627	0.05886	0.01860	0.00000
61 10	H	1S	0.00000	-0.00208	-0.00216	-0.00328	0.00000
62		2S	0.00000	-0.00821	-0.00362	-0.00806	0.00000
63 11	O	1S	0.00000	0.00000	0.00000	0.00000	0.00000
64		2S	0.00000	0.00000	0.00000	0.00000	0.00000
65		2PX	0.00000	0.00000	0.00000	0.00000	0.00000
66		2PY	0.00000	0.00000	0.00000	0.00000	0.00000
67		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
68		3S	0.00000	-0.00001	-0.00003	-0.00001	0.00000
69		3PX	0.00000	-0.00002	-0.00008	-0.00004	0.00000
70		3PY	0.00000	-0.00002	-0.00005	0.00000	0.00000
71		3PZ	0.00000	0.00000	0.00000	0.00000	0.00000
72 12	O	1S	0.00000	0.00000	0.00000	0.00000	0.00000
73		2S	0.00000	0.00000	0.00001	0.00000	0.00000
74		2PX	0.00000	0.00002	0.00006	0.00000	0.00000
75		2PY	0.00000	0.00000	0.00000	0.00000	0.00000
76		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
77		3S	0.00000	0.00010	0.00028	0.00000	0.00000
78		3PX	0.00000	0.00062	0.00175	-0.00001	0.00000
79		3PY	0.00000	-0.00002	-0.00009	0.00000	0.00000
80		3PZ	0.00000	0.00000	0.00000	0.00000	-0.00019
			46	47	48	49	50
46 6	C	1S	2.03847				

47		2S	0.01934	0.12301			
48		2PX	0.00000	0.00000	0.31401		
49		2PY	0.00000	0.00000	0.00000	0.32381	
50		2PZ	0.00000	0.00000	0.00000	0.00000	0.19372
51		3S	-0.07526	0.17342	0.00000	0.00000	0.00000
52		3PX	0.00000	0.00000	0.14018	0.00000	0.00000
53		3PY	0.00000	0.00000	0.00000	0.10134	0.00000
54		3PZ	0.00000	0.00000	0.00000	0.00000	0.11616
55 7	H	1S	0.00000	-0.00002	-0.00004	-0.00008	0.00000
56		2S	0.00019	-0.00081	-0.00101	-0.00155	0.00000
57 8	H	1S	0.00000	0.00000	0.00000	0.00000	0.00000
58		2S	0.00000	0.00001	0.00001	0.00005	0.00000
59 9	H	1S	0.00000	-0.00002	-0.00002	-0.00010	0.00000
60		2S	0.00020	-0.00088	-0.00040	-0.00258	0.00000
61 10	H	1S	-0.00114	0.01141	0.04361	0.01457	0.00000
62		2S	-0.00068	0.00771	0.02383	0.00848	0.00000
63 11	O	1S	0.00000	0.00000	0.00000	0.00000	0.00000
64		2S	0.00000	0.00000	0.00000	0.00000	0.00000
65		2PX	0.00000	0.00000	0.00000	0.00000	0.00000
66		2PY	0.00000	0.00000	0.00000	0.00000	0.00000
67		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
68		3S	0.00000	0.00000	0.00000	0.00000	0.00000
69		3PX	0.00000	0.00000	0.00000	0.00000	0.00000
70		3PY	0.00000	0.00000	0.00000	0.00000	0.00000
71		3PZ	0.00000	0.00000	0.00000	0.00000	0.00000
72 12	O	1S	0.00000	0.00000	0.00000	0.00000	0.00000
73		2S	0.00000	0.00000	0.00000	0.00000	0.00000
74		2PX	0.00000	0.00000	0.00000	0.00000	0.00000
75		2PY	0.00000	0.00000	0.00000	0.00000	0.00000
76		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
77		3S	0.00000	0.00000	0.00000	0.00000	0.00000
78		3PX	0.00000	0.00000	0.00000	0.00000	0.00000
79		3PY	0.00000	0.00000	0.00000	0.00000	0.00000
80		3PZ	0.00000	0.00000	0.00000	0.00000	0.00000
			51	52	53	54	55
51		3S	0.70351				
52		3PX	0.00000	0.27253			
53		3PY	0.00000	0.00000	0.13525		
54		3PZ	0.00000	0.00000	0.00000	0.25265	
55 7	H	1S	-0.00213	-0.00048	-0.00417	0.00000	0.17441
56		2S	-0.00907	-0.00255	-0.00755	0.00000	0.06565
57 8	H	1S	0.00002	0.00001	0.00009	0.00000	0.00000
58		2S	0.00045	0.00027	0.00118	0.00000	0.00000
59 9	H	1S	-0.00207	-0.00216	-0.00328	0.00000	0.00000

60		2S	-0.00821	-0.00363	-0.00806	0.00000	0.00000
61	10	H 1S	0.06041	0.07571	0.02257	0.00000	0.00000
62		2S	0.04627	0.05882	0.01860	0.00000	-0.00027
63	11	O 1S	0.00000	0.00000	0.00000	0.00000	0.00000
64		2S	0.00000	0.00001	0.00000	0.00000	0.00000
65		2PX	0.00002	0.00006	0.00000	0.00000	0.00000
66		2PY	0.00000	0.00000	0.00000	0.00000	0.00000
67		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
68		3S	0.00010	0.00028	0.00000	0.00000	-0.00001
69		3PX	0.00062	0.00175	-0.00001	0.00000	-0.00012
70		3PY	-0.00002	-0.00009	0.00000	0.00000	0.00001
71		3PZ	0.00000	0.00000	0.00000	-0.00019	0.00000
72	12	O 1S	0.00000	0.00000	0.00000	0.00000	0.00000
73		2S	0.00000	0.00000	0.00000	0.00000	0.00000
74		2PX	0.00000	0.00000	0.00000	0.00000	0.00000
75		2PY	0.00000	0.00000	0.00000	0.00000	0.00000
76		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
77		3S	-0.00001	-0.00003	-0.00001	0.00000	0.00000
78		3PX	-0.00002	-0.00008	-0.00004	0.00000	0.00000
79		3PY	-0.00002	-0.00005	0.00000	0.00000	0.00000
80		3PZ	0.00000	0.00000	0.00000	0.00000	0.00000
			56	57	58	59	60
56		2S	0.06907				
57	8	H 1S	0.00000	0.17440			
58		2S	0.00000	0.06565	0.06908		
59	9	H 1S	0.00000	0.00000	-0.00022	0.17747	
60		2S	-0.00002	-0.00027	-0.00076	0.06886	0.06873
61	10	H 1S	-0.00022	0.00000	0.00000	0.00000	-0.00022
62		2S	-0.00077	0.00000	-0.00002	-0.00022	-0.00055
63	11	O 1S	0.00002	0.00000	0.00000	0.00000	0.00000
64		2S	0.00001	0.00000	0.00000	0.00000	0.00000
65		2PX	-0.00028	0.00000	0.00000	0.00000	0.00000
66		2PY	0.00012	0.00000	0.00000	0.00000	0.00000
67		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
68		3S	0.00002	0.00000	0.00000	0.00000	0.00000
69		3PX	-0.00300	0.00000	0.00000	0.00000	0.00000
70		3PY	0.00141	0.00000	0.00000	0.00000	0.00000
71		3PZ	0.00000	0.00000	0.00000	0.00000	0.00000
72	12	O 1S	0.00000	0.00000	0.00002	0.00000	0.00000
73		2S	0.00000	0.00000	0.00001	0.00000	0.00000
74		2PX	0.00000	0.00000	-0.00028	0.00000	0.00000
75		2PY	0.00000	0.00000	0.00012	0.00000	0.00000
76		2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
77		3S	0.00000	-0.00001	0.00002	0.00000	0.00000

78	3PX	0.00000	-0.00012	-0.00300	0.00000	0.00000
79	3PY	0.00000	0.00001	0.00141	0.00000	0.00000
80	3PZ	0.00000	0.00000	0.00000	0.00000	0.00000
		61	62	63	64	65
61 10 H	1S	0.17751				
62	2S	0.06884	0.06869			
63 11 O	1S	0.00000	0.00000	2.06335		
64	2S	0.00000	0.00000	0.01476	0.13931	
65	2PX	0.00000	0.00000	0.00000	0.00000	0.39508
66	2PY	0.00000	0.00000	0.00000	0.00000	0.00000
67	2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
68	3S	0.00000	0.00000	-0.09838	0.30170	0.00000
69	3PX	0.00000	0.00000	0.00000	0.00000	0.21306
70	3PY	0.00000	0.00000	0.00000	0.00000	0.00000
71	3PZ	0.00000	0.00000	0.00000	0.00000	0.00000
72 12 O	1S	0.00000	0.00000	0.00000	0.00000	0.00000
73	2S	0.00000	0.00000	0.00000	0.00000	0.00000
74	2PX	0.00000	0.00000	0.00000	0.00000	0.00000
75	2PY	0.00000	0.00000	0.00000	0.00000	0.00000
76	2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
77	3S	0.00000	0.00000	0.00000	0.00000	0.00000
78	3PX	0.00000	0.00000	0.00000	0.00000	0.00000
79	3PY	0.00000	0.00000	0.00000	0.00000	0.00000
80	3PZ	0.00000	0.00000	0.00000	0.00000	0.00000
		66	67	68	69	70
66	2PY	0.51148				
67	2PZ	0.00000	0.28916			
68	3S	0.00000	0.00000	1.47960		
69	3PX	0.00000	0.00000	0.00000	0.46581	
70	3PY	0.27526	0.00000	0.00000	0.00000	0.59834
71	3PZ	0.00000	0.16972	0.00000	0.00000	0.00000
72 12 O	1S	0.00000	0.00000	0.00000	0.00000	0.00000
73	2S	0.00000	0.00000	0.00000	0.00000	0.00000
74	2PX	0.00000	0.00000	0.00000	0.00000	0.00000
75	2PY	0.00000	0.00000	-0.00001	0.00000	-0.00001
76	2PZ	0.00000	0.00000	0.00000	0.00000	0.00000
77	3S	-0.00001	0.00000	-0.00014	0.00000	-0.00059
78	3PX	0.00000	0.00000	0.00000	-0.00012	0.00000
79	3PY	-0.00001	0.00000	-0.00059	0.00000	0.00019
80	3PZ	0.00000	-0.00001	0.00000	0.00000	0.00000
		71	72	73	74	75
71	3PZ	0.40122				
72 12 O	1S	0.00000	2.06335			
73	2S	0.00000	0.01476	0.13931		

74	2PX	0.00000	0.00000	0.00000	0.39501	
75	2PY	0.00000	0.00000	0.00000	0.00000	0.51153
76	2PZ	-0.00001	0.00000	0.00000	0.00000	0.00000
77	3S	0.00000	-0.09838	0.30170	0.00000	0.00000
78	3PX	0.00000	0.00000	0.00000	0.21302	0.00000
79	3PY	0.00000	0.00000	0.00000	0.00000	0.27528
80	3PZ	-0.00079	0.00000	0.00000	0.00000	0.00000
		76	77	78	79	80
76	2PZ	0.28918				
77	3S	0.00000	1.47959			
78	3PX	0.00000	0.00000	0.46573		
79	3PY	0.00000	0.00000	0.00000	0.59839	
80	3PZ	0.16973	0.00000	0.00000	0.00000	0.40125

Gross orbital populations:

			1
1	1	C 1S	1.98831
2		2S	0.39601
3		2PX	0.61175
4		2PY	0.59243
5		2PZ	0.40890
6		3S	0.89702
7		3PX	0.22038
8		3PY	0.52980
9		3PZ	0.59812
10	2	C 1S	1.98844
11		2S	0.41255
12		2PX	0.57437
13		2PY	0.62291
14		2PZ	0.34624
15		3S	0.85259
16		3PX	0.14455
17		3PY	0.20196
18		3PZ	0.54091
19	3	C 1S	1.98844
20		2S	0.41252
21		2PX	0.57430
22		2PY	0.62288
23		2PZ	0.34619
24		3S	0.85264
25		3PX	0.14463
26		3PY	0.20197
27		3PZ	0.54089
28	4	C 1S	1.98831
29		2S	0.39599

30		2PX	0.61166
31		2PY	0.59238
32		2PZ	0.40887
33		3S	0.89709
34		3PX	0.22048
35		3PY	0.52983
36		3PZ	0.59813
37 5	C	1S	1.98836
38		2S	0.40042
39		2PX	0.60201
40		2PY	0.61529
41		2PZ	0.37224
42		3S	0.90691
43		3PX	0.47823
44		3PY	0.30389
45		3PZ	0.55835
46 6	C	1S	1.98836
47		2S	0.40043
48		2PX	0.60207
49		2PY	0.61530
50		2PZ	0.37222
51		3S	0.90691
52		3PX	0.47816
53		3PY	0.30392
54		3PZ	0.55833
55 7	H	1S	0.45382
56		2S	0.24906
57 8	H	1S	0.45379
58		2S	0.24910
59 9	H	1S	0.46001
60		2S	0.26063
61 10	H	1S	0.46009
62		2S	0.26053
63 11	O	1S	1.98764
64		2S	0.44612
65		2PX	0.65125
66		2PY	0.80972
67		2PZ	0.48175
68		3S	1.57553
69		3PX	0.83057
70		3PY	0.94748
71		3PZ	0.69352
72 12	O	1S	1.98764
73		2S	0.44613

74	2PX	0.65116
75	2PY	0.80977
76	2PZ	0.48179
77	3S	1.57553
78	3PX	0.83051
79	3PY	0.94752
80	3PZ	0.69356

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	5.554628	0.159037	-0.119044	0.014836	-0.107273	0.433981
2	C	0.159037	5.365050	-0.021473	-0.119119	0.013104	-0.073635
3	C	-0.119044	-0.021473	5.364684	0.159276	-0.073660	0.013094
4	C	0.014836	-0.119119	0.159276	5.554327	0.434097	-0.107262
5	C	-0.107273	0.013104	-0.073660	0.434097	5.307211	0.318176
6	C	0.433981	-0.073635	0.013094	-0.107262	0.318176	5.307310
7	H	0.389761	-0.034085	0.002984	-0.000289	0.002091	-0.029259
8	H	-0.000289	0.002986	-0.034085	0.389727	-0.029231	0.002090
9	H	0.002102	-0.000136	0.001674	-0.023577	0.390143	-0.031214
10	H	-0.023589	0.001675	-0.000136	0.002101	-0.031203	0.390165
11	O	-0.063997	0.461817	-0.070694	0.002562	-0.000269	0.002510
12	O	0.002564	-0.070708	0.461830	-0.063943	0.002508	-0.000269
		7	8	9	10	11	12
1	C	0.389761	-0.000289	0.002102	-0.023589	-0.063997	0.002564
2	C	-0.034085	0.002986	-0.000136	0.001675	0.461817	-0.070708
3	C	0.002984	-0.034085	0.001674	-0.000136	-0.070694	0.461830
4	C	-0.000289	0.389727	-0.023577	0.002101	0.002562	-0.063943
5	C	0.002091	-0.029231	0.390143	-0.031203	-0.000269	0.002508
6	C	-0.029259	0.002090	-0.031214	0.390165	0.002510	-0.000269
7	H	0.374777	0.000000	-0.000021	-0.001257	-0.001826	0.000000
8	H	0.000000	0.374784	-0.001256	-0.000021	0.000000	-0.001819
9	H	-0.000021	-0.001256	0.383916	-0.000987	0.000000	-0.000001
10	H	-0.001257	-0.000021	-0.000987	0.383871	-0.000001	0.000000
11	O	-0.001826	0.000000	0.000000	-0.000001	8.095591	-0.002114
12	O	0.000000	-0.001819	-0.000001	0.000000	-0.002114	8.095551

Mulliken atomic charges:

		1
1	C	-0.242718
2	C	0.315488
3	C	0.315550
4	C	-0.242737
5	C	-0.225694
6	C	-0.225688
7	H	0.297122
8	H	0.297114

9 H 0.279357
10 H 0.279383
11 O -0.423580
12 O -0.423598

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

1
1 C 0.054404
2 C 0.315488
3 C 0.315550
4 C 0.054377
5 C 0.053663
6 C 0.053695
7 H 0.000000
8 H 0.000000
9 H 0.000000
10 H 0.000000
11 O -0.423580
12 O -0.423598

Sum of Mulliken charges= 0.00000

Electronic spatial extent (au): $\langle R^2 \rangle = 822.3773$

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -6.6094 Y= 0.0002 Z= -0.0006 Tot= 6.6094

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -48.8785 YY= -44.3409 ZZ= -47.5132
XY= 0.0010 XZ= -0.0023 YZ= 0.0000

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= -1.9676 YY= 2.5700 ZZ= -0.6024
XY= 0.0010 XZ= -0.0023 YZ= 0.0000

Octapole moment (field-independent basis, Debye-Ang²):

XXX= -28.0637 YYY= 0.0012 ZZZ= 0.0027 XYY= -13.8876
XXY= -0.0036 XXZ= 0.0007 XZZ= 10.0117 YZZ= -0.0015
YYZ= 0.0018 XYZ= 0.0006

Hexadecapole moment (field-independent basis, Debye-Ang³):

XXXX= -547.4950 YYYY= -376.4527 ZZZZ= -45.5862 XXXY= -0.0017
XXXZ= -0.0062 YYYX= 0.0089 YYYZ= 0.0032 ZZZX= 0.0038
ZZZY= 0.0026 XXYY= -173.1632 XXZZ= -107.1959 YYZZ= -80.8196
XXYZ= -0.0088 YYXZ= -0.0051 ZZXY= 0.0013

N-N= 3.214918512333D+02 E-N=-1.525353453315D+03 KE= 3.752598574057D+02

Orbital energies and kinetic energies (alpha):

	1	2
24 (A)--O	-0.47819	2.41914
25 (A)--O	-0.46839	2.33118

26	(A)--O	-0.45277	1.44686
27	(A)--O	-0.44920	1.24264
28	(A)--O	-0.33375	1.54624
29	(A)--V	-0.05309	1.77032
30	(A)--V	0.13048	1.45405
31	(A)--V	0.14309	1.53064
32	(A)--V	0.21793	1.06458
33	(A)--V	0.28841	1.01330

Total kinetic energy from orbitals= 3.752598574057D+02

1|1|UNPC-UNK|SP|RHF|3-21G|C6H4O2|PCUSER|26-Feb-2010|0|# HF/3-21G POP=
REGULAR GEOM=CONNECTIVITY||Title Card Required||0,1|C|C,1,1.39516|C,2,
1.39471206,1,120.00863221|C,3,1.39542701,2,119.99416459,1,-0.05684321,
0|C,4,1.39482508,3,119.99399231,2,0.03411439,0|C,1,1.39482907,2,119.99
84568,3,0.03234809,0|H,1,1.09961031,6,120.00431986,5,-179.97984142,0|H
,4,1.09968011,3,119.98114211,2,-179.99643617,0|H,5,1.09976099,4,120.01
134336,3,-180.,0|H,6,1.09960403,1,120.00799702,2,179.98917535,0|O,2,1.
43,1,119.98077039,6,179.95324796,0|O,3,1.43,2,120.01279489,1,179.96185
208,0||Version=x86-Win32-G03RevB.05|State=1-A|HF=-376.9698206|RMSD=2.5
33e-005|Dipole=1.3003202,-0.0019572,-2.2518757|PG=C01 [X(C6H4O2)]||@

THOSE WHO TRY TO PASS CHEMISTRY OFF AS A NEW SCIENCE
SHOW HOW LITTLE KNOWLEDGE THEY HAVE OF THE CHARACTER
AND LITERATURE OF THE ANCIENTS.

-- NICOLAS LEFEVRE

"COURS DE CHYMIE" J.-N.LELOUP, PARIS, 1751

Job cpu time: 0 days 0 hours 0 minutes 8.0 seconds.

File lengths (MBytes): RWF= 11 Int= 0 D2E= 0 Chk= 7 Scr=

1

Normal termination of Gaussian 03 at Fri Feb 26 12:53:52 2010.