Solid-State Absorption and Luminescence Spectroscopy of Nitronyl Nitroxide Radicals

Electronic Supplementary Information

Rémi Beaulac, Guillaume Bussière, Christian Reber*

Département de Chimie, Université de Montréal, Montréal, Québec H3C3J7, Canada

Christophe Lescop‡, Dominique Luneau||*

Laboratoire de Chimie Inorganique et Biologique (UMR 5046), DRFMC, CEA-Grenoble, 17 rue des Martyrs, 38054 Grenoble cedex 09, France.

‡ Present address: Organométalliques et Catalyse : Chimie et Electrochimie Moléculaires, UMR 6509, Institut de Chimie de Rennes, CNRS - Université de Rennes 1, Campus de Beaulieu, 35042 Rennes cedex, France

|| Present address: Université Claude Bernard Lyon 1 - Bât. 305 - 43 avenue du 11 novembre 1918 – 69622 Villeurbanne cedex

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Figure 1S
Absorption spectrum of NITBzImH in CH_2Cl_2 at 295 K

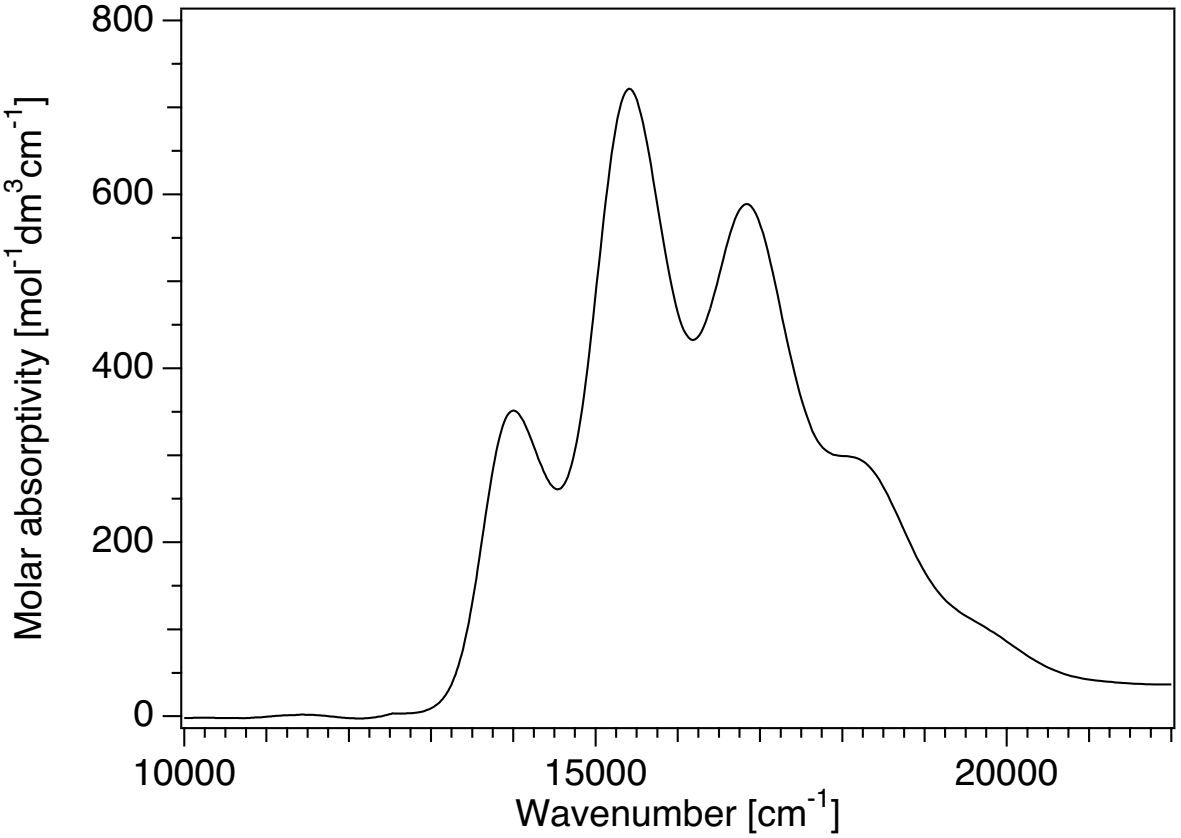


Figure 2S
Raman spectrum of NITBzImH at 77 K (514.5 nm excitation). Vertical arrows denote vibrational frequencies used for the calculation of the luminescence spectrum in Figure 7a.

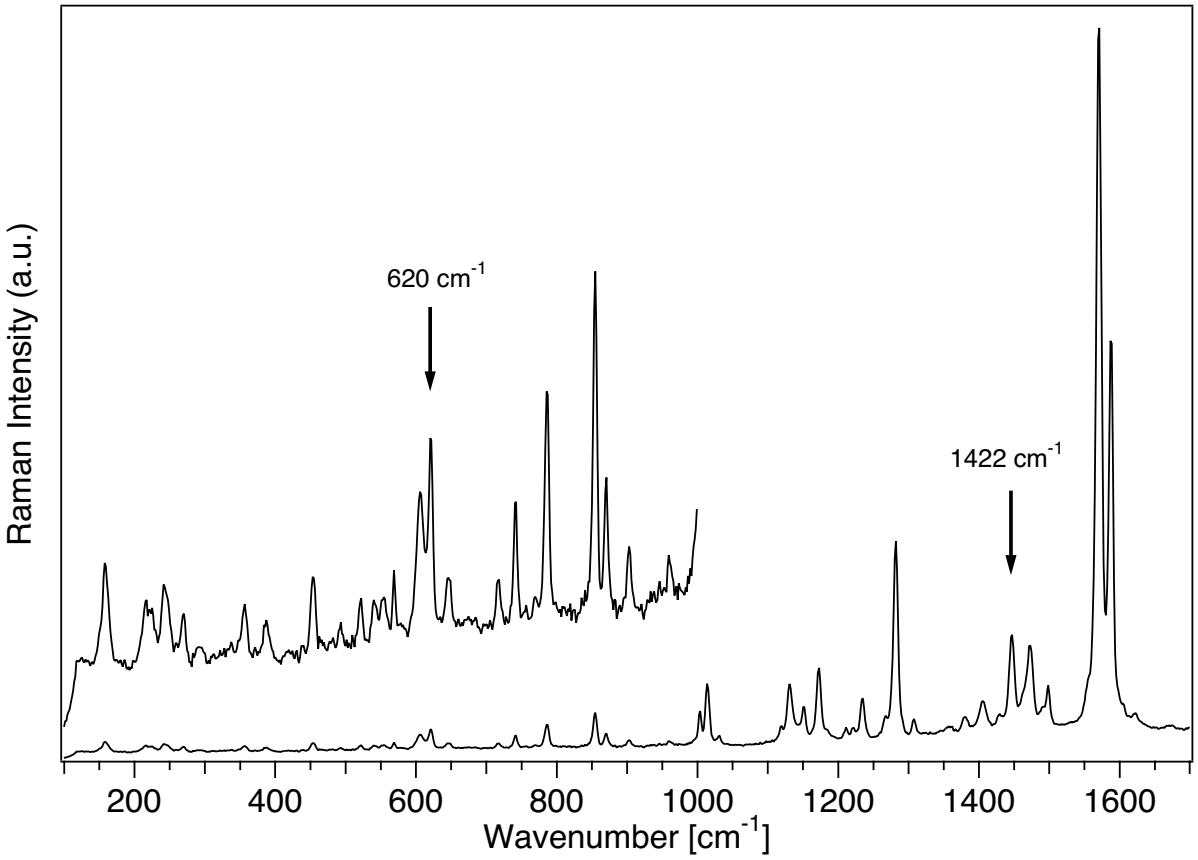


Figure 3S
Raman spectrum of NITCN at 5 K (632.8 nm excitation). Frequencies used for the calculation of the absorption spectrum in Figure 7b are indicated by vertical arrows.

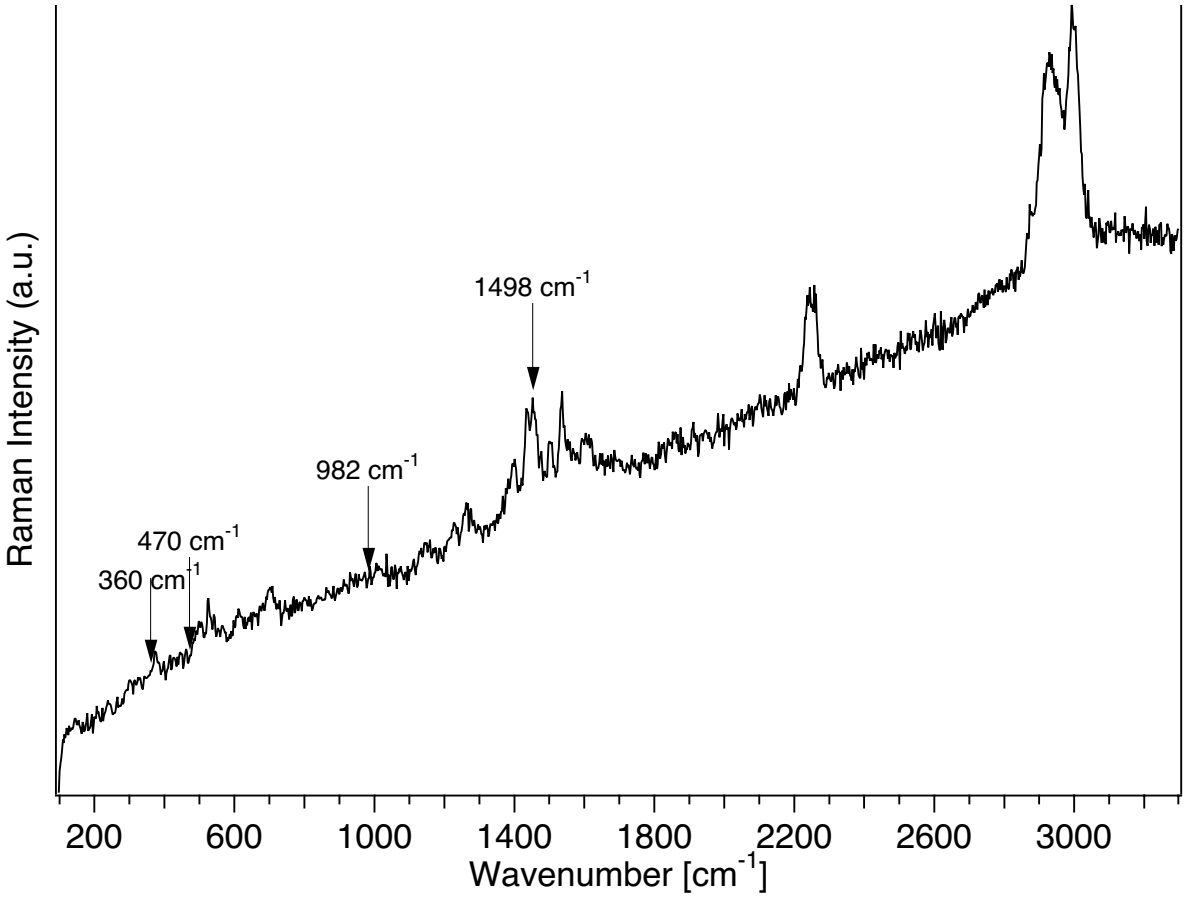


Figure 4S – Calculated molecular orbitals for NITCN. The SOMO-2 and SOMO-3 orbitals are shown top to bottom.

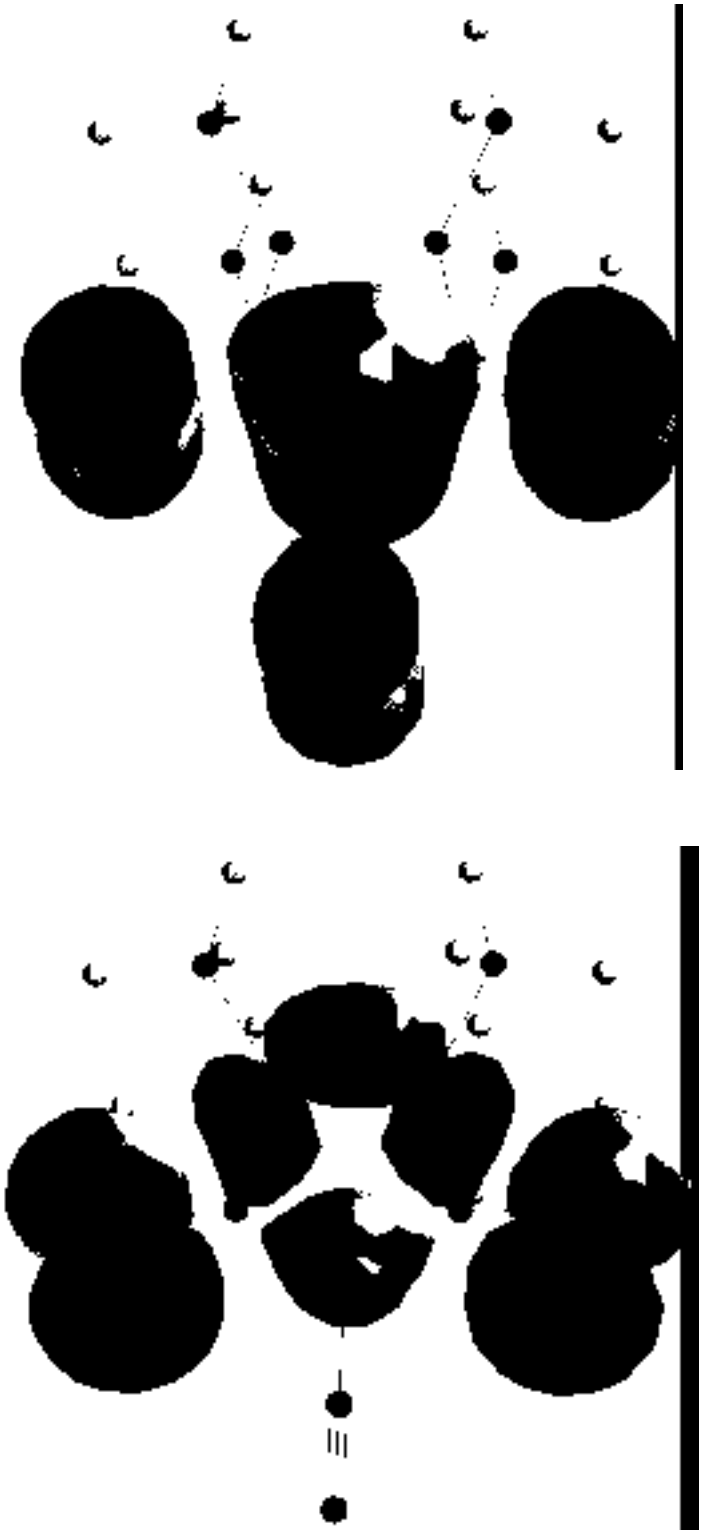
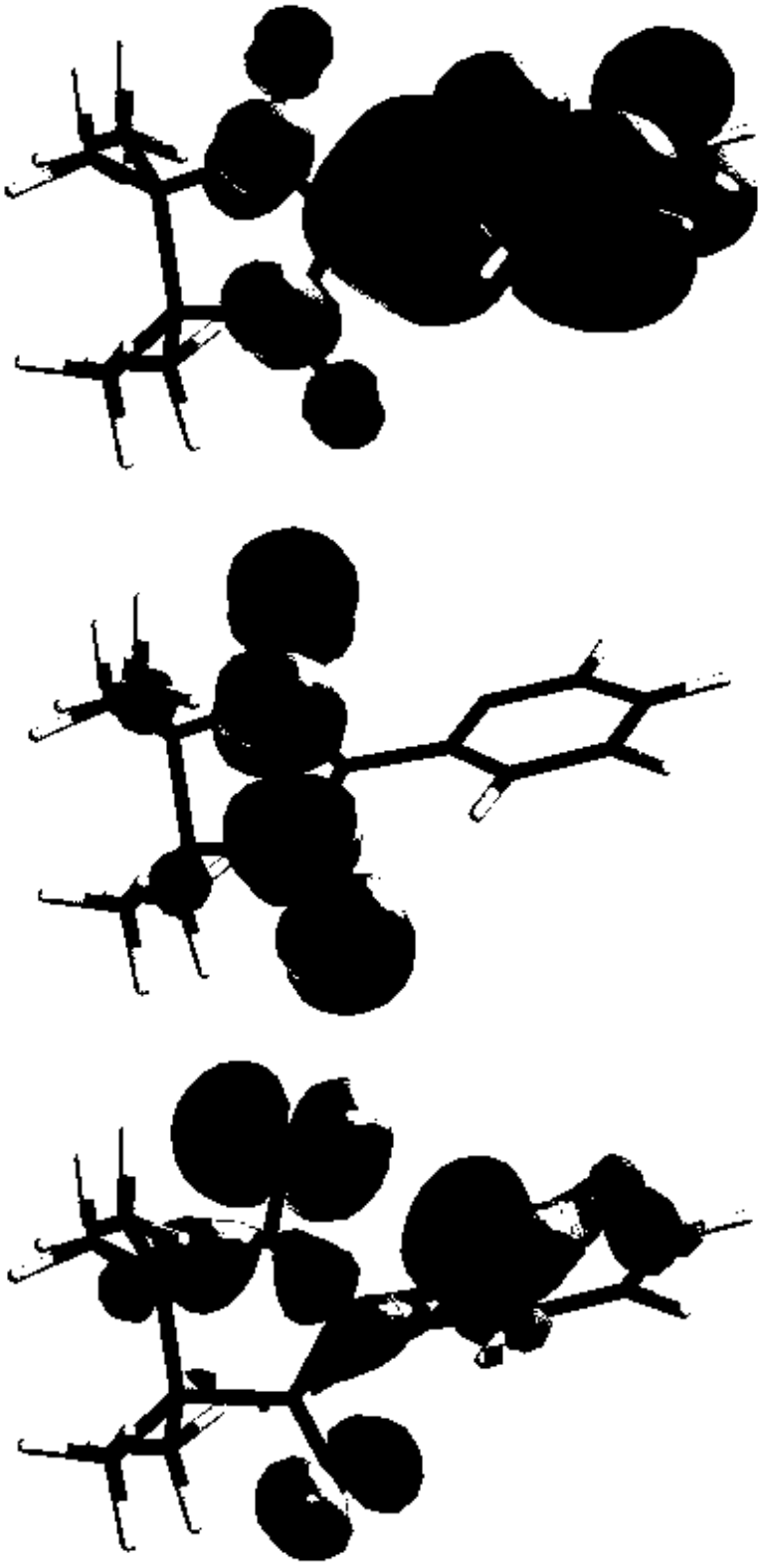


Figure 5S - Calculated molecular orbitals for NITPy. The SOMO+1, SOMO and SOMO-1 orbitals are shown top to bottom.



Output file for NITBzImH's PM3 calculations

```
MacSPARTAN PRO Semi-Empirical Program:  (PowerPC)              Release 1.0.4
   Job run on machine : Orgel(G4/400)

  NITBZIMH.PDB

  Run type: Single point energy
          (Analytical Gradient in FREQ)
          (Numerical Frequency)
  Model: UHF/PM3
  Number of shells:  57
    37 S shells
    20 P shells
  Number of basis functions:  97
  Number of electrons: 105
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2

  Point Group = C1  Order =  1 Nsymop =  1
  This system has 105 degrees of freedom

  Heat of Formation:       70.499 kcal/mol

  Expectation value <S**2> =  1.1444
   Calculating Hessian
  Memory Used:          5.998 Mb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time : 000:10:27.4
  Semi-Empirical Program Wall Time: 000:12:42.9

MacSPARTAN PRO Properties Program:  (PowerPC)                  Release 1.0.4
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:        105

                    Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
    ---------    ------------- ------------- -------------

  1 O  O1           4.6190000     4.1970000     5.5380000
  2 N  N1           3.9650000     3.9150000     4.4770000
  3 C  C1           3.1140000     2.8880000     4.3320000
  4 C  C8           2.7190000     1.9990000     5.4150000
  5 N  N5           3.4860000     1.8620000     6.5320000
  6 C  C9           2.7780000     1.0740000     7.3990000
  7 C  C10          3.0430000     0.6300000     8.6970000
  8 C  C11          2.0700000    -0.1370000     9.2970000
  9 C  C12          0.8840000    -0.4600000     8.6410000
 10 H  H7           0.1480776    -1.0735103     9.1546776
 11 C  C13          0.6190000    -0.0150000     7.3690000
 12 H  H3          -0.3123998    -0.2483469     6.8667267
 13 C  C14          1.5840000     0.7640000     6.7350000
 14 N  N4           1.5640000     1.3660000     5.4820000
 15 H  H6           2.2296203    -0.5104412    10.3055568
 16 H  H4           3.9627729     0.8813411     9.2104059
 17 H  H2           4.2651791     2.4355086     6.8210759
 18 N  N2           2.6310000     2.8730000     3.0800000
 19 C  C3           3.1470000     4.0190000     2.2540000
 20 C  C2           4.0730000     4.7620000     3.2450000
 21 C  C5           5.5450000     4.8020000     2.8670000
 22 H  H12          5.9775678     3.8028033     2.7441680
```

23	H	H14	6.1472949	5.3117665	3.6293934
24	H	H16	5.6943899	5.3551076	1.9330543
25	C	C4	3.5780000	6.1500000	3.6560000
26	H	H18	4.2449498	6.6121207	4.3949586
27	H	H20	2.5803225	6.1308649	4.1086266
28	H	H22	3.5539299	6.8287352	2.7963205
29	C	C6	3.8460000	3.4150000	1.0430000
30	H	H28	4.6308512	2.7032119	1.3223530
31	H	H26	4.2984233	4.1947504	0.4202469
32	H	H5	3.1453505	2.8690624	0.3988229
33	C	C7	1.9260000	4.8080000	1.8080000
34	H	H30	2.2179663	5.7088475	1.2566863
35	H	H32	1.2836121	5.1102747	2.6425790
36	H	H34	1.2917952	4.2241294	1.1286538
37	O	O2	1.8070000	2.0260000	2.5870000

Point Group = C1 Order = 1 Nsymop = 1

Normal Modes and Vibrational Frequencies (cm-1)

	-160.70			-125.03			-99.87		
	A			A			A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.019	-0.021	-0.007	0.060	-0.053	-0.024	-0.037	0.040	0.013
N1	0.014	-0.014	-0.008	0.059	-0.047	-0.025	-0.037	0.040	0.014
C1	-0.013	0.007	0.002	-0.035	0.024	0.009	-0.077	0.071	0.032
C8	-0.008	0.008	0.003	-0.031	0.026	0.009	-0.078	0.076	0.034
N5	-0.075	0.129	0.061	-0.012	0.013	-0.004	-0.034	0.032	-0.001
C9	-0.018	0.036	0.017	-0.001	0.004	-0.002	0.011	-0.027	-0.017
C10	-0.025	0.049	0.024	0.002	0.011	0.000	0.037	-0.044	-0.028
C11	-0.006	0.016	0.008	0.011	0.000	0.001	0.049	-0.051	-0.017
C12	0.014	-0.025	-0.010	0.017	-0.021	0.000	0.035	-0.042	0.004
H7	0.013	-0.024	-0.008	0.029	-0.037	-0.003	0.044	-0.044	0.015
C13	0.035	-0.069	-0.029	0.011	-0.023	0.001	0.010	-0.029	0.014
H3	0.052	-0.104	-0.045	0.017	-0.041	-0.002	-0.003	-0.017	0.034
C14	0.029	-0.058	-0.026	-0.002	-0.005	0.004	-0.004	-0.019	0.006
N4	0.041	-0.089	-0.039	-0.021	0.009	0.011	-0.054	0.037	0.032
H6	-0.011	0.024	0.012	0.013	0.010	0.004	0.069	-0.059	-0.024
H4	-0.045	0.089	0.041	-0.005	0.029	0.003	0.046	-0.046	-0.042
H2	-0.076	0.139	0.049	-0.032	0.041	-0.001	-0.044	0.043	0.005
N2	-0.015	0.011	0.002	-0.055	0.042	0.017	-0.004	0.010	0.005
C3	-0.008	0.008	0.003	0.012	-0.005	-0.005	0.020	-0.012	-0.010
C2	0.017	-0.012	-0.005	0.001	0.000	0.002	0.018	-0.005	-0.012
C5	0.013	-0.041	-0.023	-0.007	0.082	-0.011	0.027	-0.057	0.020
H12	-0.017	-0.050	-0.054	0.045	0.108	-0.036	0.009	-0.073	0.085
H14	0.039	-0.077	-0.019	-0.028	0.096	-0.002	0.020	-0.028	0.007
H16	0.015	-0.023	-0.012	-0.042	0.113	0.002	0.062	-0.110	-0.006
C4	0.050	-0.003	0.006	-0.062	-0.033	0.046	0.045	0.020	-0.065
H18	0.079	-0.017	-0.011	-0.080	-0.019	0.052	0.016	0.009	-0.031
H20	0.061	0.016	0.031	-0.058	-0.095	0.053	0.015	0.063	-0.127
H22	0.044	-0.002	0.007	-0.105	-0.012	0.064	0.122	0.005	-0.078
C6	-0.037	0.004	-0.012	0.050	-0.065	0.045	0.023	-0.039	0.006
H28	-0.065	-0.035	-0.032	0.027	-0.067	0.106	0.004	-0.053	0.023
H26	-0.009	-0.002	0.000	0.091	-0.096	0.036	0.047	-0.055	0.003
H5	-0.064	0.047	-0.018	0.070	-0.077	0.035	0.019	-0.030	0.003
C7	-0.001	0.032	0.027	0.049	0.005	-0.085	0.034	-0.003	-0.032
H30	0.007	0.021	0.013	0.090	-0.019	-0.102	0.051	-0.029	-0.067
H32	0.031	0.057	0.043	0.015	0.043	-0.125	0.048	0.044	-0.038
H34	-0.036	0.045	0.050	0.070	-0.007	-0.095	0.016	-0.014	-0.005
O2	-0.021	0.017	0.002	-0.052	0.041	0.015	0.003	0.001	0.007

-77.46	-33.84	57.31
A	A	A

	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.062	0.054	-0.031	-0.042	0.055	0.017	-0.024	0.024	0.010
N1	0.047	0.027	-0.012	-0.030	0.035	0.016	-0.017	0.016	0.008
C1	0.035	0.031	0.036	0.036	-0.018	-0.002	-0.005	0.006	0.003
C8	0.034	0.046	0.047	0.057	-0.038	-0.010	0.003	-0.002	-0.001
N5	0.006	0.018	0.060	0.047	-0.049	-0.005	0.009	-0.012	-0.006
C9	-0.008	-0.016	0.018	0.026	-0.034	-0.007	0.012	-0.019	-0.009
C10	-0.031	-0.054	0.011	-0.007	-0.005	0.010	0.005	-0.005	-0.003
C11	-0.047	-0.062	-0.026	-0.032	0.026	0.011	-0.004	0.012	0.005
C12	-0.040	-0.031	-0.054	-0.021	0.022	-0.008	-0.003	0.011	0.004
H7	-0.056	-0.036	-0.082	-0.042	0.048	-0.006	-0.013	0.028	0.012
C13	-0.016	0.005	-0.046	0.014	-0.011	-0.026	0.007	-0.009	-0.005
H3	-0.012	0.031	-0.067	0.023	-0.013	-0.042	0.007	-0.009	-0.005
C14	0.002	0.011	-0.011	0.036	-0.034	-0.022	0.013	-0.021	-0.010
N4	0.028	0.049	0.009	0.057	-0.041	-0.025	0.010	-0.015	-0.007
H6	-0.066	-0.093	-0.034	-0.063	0.057	0.027	-0.013	0.030	0.013
H4	-0.037	-0.077	0.033	-0.016	-0.004	0.024	0.004	-0.004	-0.002
H2	0.021	-0.024	0.091	0.047	-0.059	0.010	0.005	-0.010	-0.001
N2	0.014	-0.004	0.043	-0.050	0.039	0.030	-0.018	0.016	0.008
C3	-0.014	-0.018	0.007	-0.008	0.001	0.005	-0.004	0.005	0.002
C2	0.001	0.010	-0.029	-0.007	0.007	-0.002	-0.004	0.006	0.002
C5	-0.010	0.023	-0.068	-0.001	-0.023	0.013	-0.002	-0.033	-0.003
H12	-0.002	0.026	-0.064	-0.007	-0.032	0.066	-0.055	-0.046	-0.088
H14	0.004	0.042	-0.093	-0.008	0.010	-0.003	0.034	-0.124	0.029
H16	-0.043	0.010	-0.081	0.016	-0.068	-0.011	0.013	0.032	0.038
C4	-0.011	0.007	-0.035	0.007	0.022	-0.041	0.032	0.019	0.002
H18	0.023	0.045	-0.089	-0.044	0.000	0.019	0.261	0.141	-0.280
H20	0.018	-0.008	0.030	-0.036	0.051	-0.134	0.198	0.015	0.366
H22	-0.085	-0.015	-0.051	0.105	0.022	-0.044	-0.309	-0.071	-0.058
C6	-0.036	-0.034	0.002	-0.006	-0.059	0.035	0.019	-0.016	0.024
H28	-0.012	-0.009	-0.002	-0.077	-0.125	0.067	0.092	0.077	0.056
H26	-0.072	-0.041	-0.032	0.084	-0.100	0.049	-0.066	-0.014	-0.037
H5	-0.043	-0.067	0.038	-0.027	-0.002	0.009	0.058	-0.126	0.074
C7	-0.031	-0.039	0.014	0.026	0.025	-0.041	0.000	-0.010	-0.037
H30	-0.051	-0.051	-0.017	0.067	-0.065	-0.166	-0.001	0.144	0.215
H32	-0.016	-0.022	0.019	0.090	0.178	-0.047	-0.201	-0.273	-0.098
H34	-0.041	-0.062	0.043	-0.047	-0.015	0.062	0.190	0.073	-0.286
O2	0.015	-0.019	0.065	-0.073	0.055	0.041	-0.025	0.022	0.010

	93.55 A			107.41 A			115.75 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.016	-0.007	-0.005	-0.020	0.005	0.006	0.034	-0.003	-0.010
N1	0.010	-0.004	-0.002	-0.006	-0.003	0.000	0.020	0.002	-0.001
C1	-0.005	0.007	0.005	0.027	-0.029	-0.015	-0.049	0.055	0.030
C8	0.000	0.002	0.002	0.020	-0.019	-0.009	-0.046	0.041	0.018
N5	0.005	-0.008	-0.002	0.033	-0.042	-0.018	0.032	-0.083	-0.048
C9	0.003	-0.007	-0.002	-0.035	0.076	0.037	0.020	-0.060	-0.032
C10	-0.009	0.012	0.007	-0.044	0.085	0.041	-0.024	0.042	0.011
C11	-0.013	0.018	0.008	0.003	-0.013	-0.007	-0.052	0.102	0.045
C12	-0.002	-0.002	-0.002	0.060	-0.117	-0.057	-0.001	-0.002	0.008
H7	-0.003	-0.001	-0.003	0.133	-0.261	-0.125	0.002	-0.003	0.012
C13	0.009	-0.019	-0.011	0.024	-0.039	-0.023	0.033	-0.085	-0.030
H3	0.017	-0.033	-0.019	0.058	-0.104	-0.055	0.066	-0.159	-0.057
C14	0.008	-0.015	-0.007	-0.035	0.080	0.036	0.013	-0.055	-0.022
N4	0.005	-0.008	-0.004	-0.023	0.065	0.028	-0.035	0.025	0.014
H6	-0.025	0.039	0.018	0.007	-0.028	-0.013	-0.109	0.229	0.101
H4	-0.016	0.024	0.014	-0.081	0.150	0.074	-0.049	0.097	0.028
H2	-0.004	0.002	0.004	0.033	-0.038	-0.026	0.007	-0.062	-0.022
N2	-0.011	0.010	0.007	-0.016	0.005	0.001	0.014	0.001	0.006
C3	-0.005	0.004	0.003	-0.005	-0.001	0.000	-0.001	0.006	0.005
C2	0.004	-0.002	-0.001	0.005	-0.009	-0.003	0.010	0.003	-0.003
C5	0.005	-0.009	-0.004	0.008	-0.035	0.001	0.006	0.005	-0.017
H12	0.079	-0.013	0.283	-0.009	-0.042	0.002	-0.001	0.006	-0.046

H14	-0.043	0.246	-0.137	0.014	-0.045	0.003	0.017	-0.017	-0.011
H16	-0.020	-0.262	-0.157	0.020	-0.036	0.002	-0.002	0.027	-0.005
C4	0.007	-0.001	-0.005	0.027	0.000	-0.010	0.011	0.003	0.000
H18	-0.124	-0.088	0.168	0.043	0.000	-0.025	0.044	0.026	-0.045
H20	-0.091	0.026	-0.223	0.034	0.016	0.007	0.036	-0.005	0.055
H22	0.233	0.057	0.034	0.020	-0.008	-0.016	-0.048	-0.012	-0.011
C6	-0.008	0.007	0.002	-0.009	-0.010	0.001	-0.020	0.022	-0.012
H28	0.229	0.273	0.009	-0.024	-0.026	0.003	-0.025	0.007	-0.033
H26	-0.310	0.040	-0.178	0.010	-0.016	0.007	-0.016	0.028	-0.001
H5	0.060	-0.288	0.177	-0.015	0.007	-0.006	-0.032	0.042	-0.016
C7	-0.005	0.005	0.004	0.003	0.010	-0.002	-0.016	0.001	0.032
H30	-0.006	0.116	0.184	0.011	0.021	0.021	-0.033	-0.042	-0.046
H32	-0.117	-0.174	-0.016	-0.011	-0.008	-0.006	0.046	0.069	0.055
H34	0.109	0.074	-0.161	0.014	0.024	-0.024	-0.071	-0.031	0.111
O2	-0.013	0.011	0.009	-0.025	0.013	0.003	0.036	-0.020	0.005

	132.19 A			147.83 A			245.53 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.010	0.009	-0.009	0.011	-0.004	-0.005	0.005	0.028	-0.049
N1	0.005	0.006	-0.005	0.004	-0.001	-0.001	-0.007	0.001	-0.031
C1	-0.004	0.011	0.008	0.000	0.002	-0.001	-0.001	-0.015	-0.003
C8	0.001	0.012	0.010	-0.001	0.003	-0.001	0.004	-0.029	0.022
N5	0.008	-0.008	0.003	0.000	0.003	-0.002	-0.013	-0.041	0.039
C9	0.008	-0.013	-0.002	0.001	0.000	-0.004	-0.017	-0.029	0.054
C10	-0.004	-0.004	0.004	0.001	0.002	-0.003	-0.028	-0.037	0.060
C11	-0.013	0.009	0.006	-0.001	0.004	-0.002	-0.022	-0.044	0.064
C12	-0.007	0.002	-0.002	-0.001	0.005	-0.002	-0.021	-0.042	0.061
H7	-0.012	0.008	-0.003	-0.002	0.007	0.000	-0.023	-0.047	0.053
C13	0.005	-0.010	-0.009	0.000	0.002	-0.003	-0.012	-0.031	0.062
H3	0.010	-0.015	-0.016	0.000	0.001	-0.003	-0.012	-0.030	0.063
C14	0.008	-0.009	-0.004	0.001	0.000	-0.004	-0.012	-0.029	0.052
N4	0.003	0.007	0.005	0.000	0.002	-0.003	0.007	-0.036	0.043
H6	-0.026	0.026	0.014	-0.001	0.006	-0.001	-0.017	-0.049	0.062
H4	-0.007	-0.003	0.009	0.001	0.001	-0.004	-0.030	-0.038	0.064
H2	0.007	-0.011	0.010	-0.001	0.004	-0.002	0.005	-0.078	0.049
N2	-0.001	-0.002	0.007	0.003	-0.002	-0.002	0.013	0.019	-0.019
C3	-0.005	-0.005	0.000	0.000	0.000	-0.001	0.012	0.024	-0.029
C2	-0.001	0.002	-0.008	0.001	0.000	0.000	0.002	0.013	-0.029
C5	-0.004	0.013	-0.014	0.008	0.004	0.017	0.000	0.034	-0.040
H12	-0.053	0.019	-0.230	0.127	0.005	0.431	0.022	0.043	-0.025
H14	0.028	-0.171	0.084	-0.075	0.367	-0.161	-0.005	0.062	-0.055
H16	0.008	0.203	0.100	-0.007	-0.344	-0.191	-0.020	0.022	-0.051
C4	0.007	0.006	-0.015	-0.012	-0.005	0.009	0.012	0.021	-0.043
H18	-0.143	-0.106	0.191	0.052	0.049	-0.082	0.023	0.030	-0.059
H20	-0.109	0.047	-0.275	0.044	-0.029	0.132	0.018	0.035	-0.031
H22	0.285	0.076	0.031	-0.141	-0.030	-0.007	0.007	0.008	-0.055
C6	-0.003	-0.016	0.006	-0.014	-0.009	-0.006	0.014	0.068	-0.052
H28	-0.168	-0.198	0.008	-0.246	-0.272	-0.024	0.010	0.053	-0.083
H26	0.210	-0.043	0.127	0.271	-0.050	0.150	0.016	0.096	-0.016
H5	-0.044	0.182	-0.116	-0.090	0.276	-0.166	0.013	0.100	-0.077
C7	-0.013	-0.007	0.012	-0.008	0.000	0.014	0.033	0.044	-0.056
H30	-0.022	0.180	0.316	-0.019	0.070	0.123	0.067	0.042	-0.044
H32	-0.194	-0.314	-0.014	-0.072	-0.118	0.007	0.013	0.050	-0.075
H34	0.167	0.112	-0.258	0.052	0.046	-0.082	0.044	0.059	-0.079
O2	0.000	-0.004	0.009	0.008	-0.004	-0.005	0.012	0.037	-0.047

	247.85 A			264.58 A			274.67 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.082	0.069	0.035	0.047	0.028	-0.010	-0.063	0.062	0.028
N1	0.014	-0.008	-0.003	0.015	0.024	0.013	0.051	-0.032	-0.017
C1	0.010	-0.006	-0.002	0.023	0.005	0.016	0.034	-0.022	-0.009

C8	-0.008	-0.001	-0.003	-0.026	-0.053	-0.044	-0.015	0.008	-0.001
N5	-0.008	-0.006	-0.005	-0.043	-0.044	-0.039	-0.021	0.008	0.002
C9	-0.006	-0.008	-0.007	-0.071	0.008	-0.023	-0.009	-0.015	-0.013
C10	0.005	-0.004	-0.009	-0.013	0.045	-0.026	0.009	-0.008	-0.015
C11	0.007	0.004	0.003	0.049	-0.010	-0.003	0.007	0.013	0.007
C12	0.005	0.002	0.008	0.030	-0.015	0.033	0.007	0.002	0.011
H7	0.008	0.003	0.014	0.065	-0.037	0.056	0.008	0.012	0.024
C13	-0.004	-0.003	0.008	-0.041	0.002	0.049	0.003	-0.023	0.002
H3	-0.006	-0.010	0.016	-0.077	0.004	0.115	0.006	-0.047	0.009
C14	-0.010	-0.001	-0.002	-0.065	-0.016	-0.020	-0.013	-0.009	-0.009
N4	-0.013	0.006	0.000	-0.024	-0.071	-0.055	-0.020	0.015	0.001
H6	0.011	0.011	0.005	0.110	-0.037	-0.023	0.005	0.039	0.017
H4	0.010	-0.001	-0.018	-0.009	0.103	-0.062	0.019	-0.010	-0.033
H2	-0.002	-0.017	-0.002	-0.036	-0.059	-0.035	-0.023	0.004	0.012
N2	0.013	-0.007	-0.003	0.018	0.011	0.026	0.022	-0.013	-0.004
C3	0.011	-0.006	-0.002	0.007	0.005	0.022	0.045	-0.032	-0.015
C2	0.012	-0.007	-0.003	0.010	0.024	0.002	0.054	-0.036	-0.020
C5	-0.020	0.029	-0.097	0.002	0.054	-0.032	0.062	0.050	0.020
H12	0.000	0.041	-0.114	0.027	0.066	-0.034	0.121	0.080	-0.006
H14	0.020	0.060	-0.150	0.007	0.077	-0.052	0.009	0.053	0.060
H16	-0.112	0.019	-0.118	-0.039	0.053	-0.040	0.059	0.095	0.047
C4	0.021	-0.025	0.094	0.040	0.048	-0.044	-0.033	-0.062	-0.035
H18	0.035	-0.084	0.121	0.051	0.058	-0.061	-0.057	0.003	-0.055
H20	0.027	-0.048	0.106	0.040	0.092	-0.044	-0.026	-0.128	-0.020
H22	0.016	0.043	0.148	0.060	0.015	-0.071	-0.096	-0.079	-0.048
C6	-0.051	-0.078	-0.009	0.016	-0.033	0.047	0.002	0.021	-0.060
H28	-0.056	-0.085	-0.012	0.005	-0.033	0.081	0.030	0.030	-0.120
H26	-0.061	-0.125	-0.074	0.033	-0.058	0.028	-0.043	0.056	-0.049
H5	-0.097	-0.093	0.053	0.019	-0.045	0.053	-0.015	0.028	-0.047
C7	0.064	0.073	0.010	-0.017	-0.024	0.041	0.008	-0.034	0.067
H30	0.134	0.077	0.053	-0.053	-0.019	0.030	-0.044	0.002	0.099
H32	0.071	0.078	0.013	-0.004	-0.033	0.056	0.032	-0.094	0.110
H34	0.039	0.141	-0.024	-0.020	-0.042	0.059	-0.005	-0.016	0.062
O2	0.047	-0.033	-0.016	0.015	0.005	0.041	-0.084	0.066	0.038

	294.24 A			311.06 A			323.23 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.036	0.028	0.013	0.042	0.057	0.013	0.050	0.005	-0.020
N1	0.017	-0.014	-0.008	0.028	0.014	0.031	-0.015	0.022	0.016
C1	0.025	-0.022	-0.011	0.010	0.034	0.033	0.098	-0.069	-0.025
C8	-0.005	0.006	0.001	-0.007	-0.002	-0.006	0.015	-0.028	-0.018
N5	-0.015	0.014	0.007	-0.005	-0.024	-0.013	-0.057	0.036	0.028
C9	-0.002	-0.010	-0.007	-0.025	-0.002	-0.014	-0.041	-0.008	-0.013
C10	0.010	-0.015	-0.011	-0.011	0.037	-0.006	0.037	-0.058	-0.047
C11	-0.001	0.015	0.007	0.026	-0.008	-0.009	0.003	0.053	0.029
C12	0.002	0.004	0.005	0.018	-0.004	0.004	0.012	0.019	0.027
H7	0.000	0.013	0.013	0.033	-0.016	0.011	0.017	0.036	0.055
C13	0.008	-0.021	-0.005	-0.022	0.021	0.019	0.025	-0.087	-0.014
H3	0.018	-0.050	-0.010	-0.053	0.054	0.062	0.079	-0.244	-0.041
C14	-0.006	-0.001	-0.003	-0.018	-0.012	-0.020	-0.052	0.023	-0.008
N4	-0.016	0.024	0.008	0.004	-0.030	-0.032	-0.044	0.065	0.009
H6	-0.010	0.040	0.018	0.054	-0.030	-0.022	-0.011	0.126	0.058
H4	0.023	-0.031	-0.026	-0.026	0.095	-0.008	0.117	-0.165	-0.138
H2	-0.007	0.002	0.008	-0.009	-0.030	0.007	0.016	-0.058	0.008
N2	0.004	-0.006	-0.003	0.027	0.026	0.022	0.018	-0.001	0.004
C3	-0.011	0.008	0.006	0.003	0.007	-0.010	-0.006	0.008	0.005
C2	-0.008	0.005	0.003	-0.001	-0.011	0.007	-0.024	0.016	0.011
C5	-0.028	-0.028	-0.091	-0.002	-0.099	0.006	-0.019	-0.023	0.030
H12	-0.041	-0.040	-0.048	-0.083	-0.135	-0.002	-0.053	-0.040	0.032
H14	0.024	0.021	-0.167	0.038	-0.149	0.007	-0.008	-0.046	0.037
H16	-0.082	-0.090	-0.138	0.043	-0.110	0.008	0.012	-0.030	0.031
C4	0.064	0.006	0.076	-0.073	-0.053	0.050	-0.029	0.020	-0.009
H18	0.070	-0.090	0.133	-0.125	-0.052	0.096	-0.032	0.029	-0.012

H20	0.048	0.042	0.039	-0.091	-0.135	0.011	-0.031	0.023	-0.013
H22	0.139	0.062	0.120	-0.085	-0.010	0.085	-0.024	0.010	-0.017
C6	0.088	0.067	0.033	-0.031	0.053	-0.057	-0.017	-0.013	0.006
H28	0.060	0.048	0.066	-0.037	0.022	-0.126	-0.018	-0.013	0.005
H26	0.145	0.098	0.112	-0.040	0.084	-0.025	-0.023	-0.026	-0.014
H5	0.147	0.105	-0.061	-0.060	0.102	-0.068	-0.031	-0.020	0.024
C7	-0.056	-0.087	-0.035	0.015	-0.007	-0.080	0.019	0.028	-0.024
H30	-0.113	-0.121	-0.118	0.042	-0.015	-0.080	0.057	0.026	-0.009
H32	-0.053	-0.044	-0.050	-0.041	0.001	-0.128	0.000	0.036	-0.042
H34	-0.040	-0.183	0.030	0.060	-0.025	-0.107	0.027	0.047	-0.047
O2	-0.036	0.025	0.011	0.023	0.012	0.060	0.015	-0.003	0.013

	352.58 A			355.09 A			368.74 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.015	-0.065	0.073	0.030	0.070	-0.072	-0.034	0.019	0.040
N1	0.003	-0.004	0.044	-0.010	0.007	-0.026	0.077	-0.047	-0.012
C1	0.000	0.001	0.012	-0.005	-0.003	-0.009	-0.025	0.029	0.015
C8	-0.003	-0.002	0.001	0.000	0.007	0.002	0.005	-0.016	-0.009
N5	0.006	0.004	-0.005	-0.003	0.000	0.004	0.016	-0.021	-0.013
C9	0.003	0.011	-0.002	0.004	-0.014	-0.003	-0.030	0.062	0.032
C10	0.008	0.002	-0.008	-0.007	0.008	0.008	0.019	-0.042	-0.014
C11	0.001	0.007	-0.012	0.001	-0.005	0.004	-0.003	-0.004	0.004
C12	0.000	0.009	-0.011	0.003	-0.009	0.002	-0.019	0.030	0.020
H7	-0.001	0.013	-0.010	0.005	-0.014	-0.001	-0.031	0.048	0.025
C13	0.003	0.001	-0.014	-0.005	0.008	0.009	0.017	-0.031	-0.010
H3	0.010	-0.007	-0.023	-0.020	0.036	0.024	0.083	-0.161	-0.073
C14	0.003	0.007	-0.003	0.004	-0.010	-0.002	-0.020	0.042	0.025
N4	-0.003	0.001	-0.004	0.002	0.002	0.003	0.012	-0.027	-0.012
H6	-0.001	0.003	-0.013	0.000	-0.001	0.006	0.015	-0.038	-0.011
H4	0.012	-0.011	-0.011	-0.022	0.038	0.019	0.080	-0.165	-0.064
H2	-0.013	0.040	-0.015	0.015	-0.035	0.014	-0.025	0.033	-0.004
N2	-0.001	-0.017	0.013	-0.005	-0.006	-0.014	-0.047	0.073	0.025
C3	0.004	-0.018	0.025	0.003	0.001	0.001	-0.029	0.045	0.016
C2	-0.005	-0.020	0.027	-0.012	-0.001	-0.017	0.038	-0.017	-0.006
C5	-0.048	-0.013	-0.100	-0.010	-0.081	-0.018	0.041	-0.028	-0.014
H12	-0.050	-0.012	-0.117	-0.078	-0.115	-0.005	0.036	-0.029	-0.020
H14	0.020	0.017	-0.177	0.022	-0.112	-0.024	0.036	-0.035	-0.006
H16	-0.151	-0.034	-0.131	0.033	-0.104	-0.024	0.051	-0.020	-0.007
C4	-0.050	-0.009	-0.094	-0.078	-0.031	0.009	-0.014	-0.036	-0.044
H18	-0.072	0.085	-0.137	-0.103	-0.009	0.016	-0.063	0.025	-0.041
H20	-0.054	-0.006	-0.103	-0.079	-0.107	0.010	-0.028	-0.081	-0.072
H22	-0.067	-0.091	-0.161	-0.125	-0.008	0.029	-0.035	-0.067	-0.069
C6	0.048	0.064	0.015	0.088	-0.017	0.066	-0.023	0.003	0.047
H28	0.051	0.059	-0.007	0.088	0.015	0.160	-0.037	0.002	0.092
H26	0.052	0.115	0.077	0.120	-0.033	0.069	0.007	-0.022	0.038
H5	0.077	0.098	-0.043	0.151	-0.057	0.036	-0.007	-0.011	0.042
C7	0.060	0.056	0.019	0.002	0.047	0.100	-0.061	0.002	-0.008
H30	0.130	0.061	0.061	-0.013	0.072	0.134	-0.109	-0.002	-0.037
H32	0.050	0.059	0.011	0.072	0.019	0.168	-0.086	-0.007	-0.024
H34	0.052	0.119	-0.025	-0.056	0.103	0.110	-0.025	-0.054	0.004
O2	-0.010	-0.025	0.046	-0.007	0.022	-0.059	0.071	0.008	-0.055

	369.18 A			376.52 A			462.43 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.014	-0.061	0.056	-0.027	-0.012	0.034	-0.008	-0.011	0.001
N1	-0.026	0.036	0.052	0.050	-0.039	-0.008	0.010	-0.009	-0.009
C1	0.009	0.009	0.005	0.068	-0.053	-0.024	0.041	-0.031	-0.016
C8	-0.001	0.006	0.004	0.009	0.010	0.008	-0.010	0.055	0.034
N5	0.000	0.000	0.005	-0.034	0.033	0.034	0.025	-0.043	0.002
C9	0.005	-0.005	0.006	0.033	-0.107	-0.049	-0.042	0.027	0.014
C10	-0.006	0.000	0.012	-0.015	0.035	0.010	-0.035	0.064	0.021

C11	-0.005	-0.003	0.010	0.012	0.007	0.009	0.055	-0.087	-0.028
C12	0.000	-0.009	0.003	0.032	-0.035	-0.010	-0.029	0.085	0.044
H7	-0.002	-0.010	-0.001	0.054	-0.068	-0.018	-0.141	0.305	0.146
C13	0.005	-0.002	0.005	-0.027	0.045	0.029	0.028	-0.060	-0.023
H3	0.000	0.011	0.008	-0.116	0.197	0.122	0.041	-0.117	-0.022
C14	0.006	-0.004	0.004	0.012	-0.052	-0.038	0.014	-0.060	-0.045
N4	0.001	0.005	0.006	-0.021	0.057	0.014	-0.009	0.055	0.004
H6	-0.009	0.000	0.012	-0.017	0.076	0.039	0.169	-0.284	-0.119
H4	-0.011	0.004	0.019	-0.094	0.212	0.065	-0.079	0.177	0.045
H2	0.000	0.009	-0.005	0.005	-0.024	0.038	-0.030	0.008	0.055
N2	0.073	0.021	-0.018	-0.029	0.034	0.012	0.008	-0.017	-0.007
C3	0.051	0.012	-0.008	-0.033	0.034	0.018	-0.010	0.002	0.004
C2	0.000	0.025	0.025	0.010	-0.005	0.006	-0.010	0.005	0.002
C5	-0.028	-0.018	-0.047	0.014	-0.005	0.006	-0.009	-0.004	0.009
H12	-0.081	-0.039	-0.071	0.018	-0.003	0.005	-0.015	-0.008	0.013
H14	0.044	-0.035	-0.097	0.005	-0.006	0.014	-0.010	-0.008	0.013
H16	-0.077	-0.038	-0.068	0.022	-0.001	0.010	0.004	-0.007	0.009
C4	-0.044	0.016	-0.003	-0.003	-0.005	-0.043	0.001	0.011	-0.002
H18	-0.070	0.041	0.004	-0.025	0.038	-0.052	0.006	0.008	-0.005
H20	-0.054	-0.009	-0.025	-0.012	-0.004	-0.062	0.001	0.022	-0.002
H22	-0.047	0.005	-0.012	0.001	-0.046	-0.077	0.007	0.005	-0.007
C6	-0.023	-0.067	-0.027	-0.027	0.007	0.039	-0.006	-0.001	0.008
H28	-0.042	-0.095	-0.045	-0.036	0.008	0.069	-0.007	0.000	0.015
H26	-0.028	-0.125	-0.101	-0.009	-0.010	0.031	-0.001	-0.005	0.007
H5	-0.092	-0.067	0.044	-0.017	-0.004	0.037	-0.003	-0.003	0.007
C7	-0.011	-0.064	0.015	-0.037	0.017	-0.025	-0.001	0.010	-0.005
H30	-0.093	-0.048	0.000	-0.038	0.007	-0.043	0.016	0.005	-0.006
H32	-0.007	-0.101	0.034	-0.069	0.024	-0.054	-0.004	0.019	-0.012
H34	0.001	-0.108	0.039	-0.004	-0.014	-0.031	-0.001	0.016	-0.010
O2	0.009	0.123	-0.081	0.043	-0.005	-0.039	-0.009	0.002	-0.013

	476.38 A			485.53 A			517.75 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.007	-0.019	0.002	0.070	0.096	-0.008	0.020	-0.012	-0.009
N1	-0.023	0.009	0.006	0.007	-0.027	0.058	-0.099	0.071	0.043
C1	-0.053	0.040	0.025	-0.009	-0.029	0.027	-0.017	0.008	0.005
C8	0.076	0.034	0.054	-0.028	-0.021	0.004	0.040	-0.080	-0.042
N5	0.013	-0.039	0.085	0.001	0.012	-0.013	-0.031	0.028	0.010
C9	-0.085	-0.031	-0.004	0.026	0.012	0.002	0.016	-0.015	-0.005
C10	0.012	0.001	-0.021	0.023	0.017	0.000	-0.006	0.022	0.016
C11	0.038	0.028	0.030	0.002	0.012	-0.039	0.010	-0.018	-0.014
C12	0.060	0.017	-0.008	-0.006	0.016	-0.028	-0.014	0.024	0.003
H7	0.101	-0.032	-0.007	-0.009	0.029	-0.017	-0.046	0.088	0.034
C13	-0.022	0.005	-0.003	-0.006	0.005	-0.027	0.008	-0.019	-0.013
H3	-0.045	-0.054	0.068	0.005	0.020	-0.053	0.016	-0.024	-0.025
C14	-0.067	0.020	-0.063	0.018	-0.003	0.016	0.014	-0.017	-0.004
N4	0.069	0.031	-0.060	-0.030	-0.014	0.020	-0.029	0.041	0.033
H6	0.038	0.056	0.040	-0.010	-0.007	-0.044	0.030	-0.075	-0.038
H4	0.060	0.014	-0.114	0.010	0.013	0.023	-0.038	0.077	0.047
H2	0.040	-0.129	0.177	0.010	0.010	-0.036	0.122	-0.140	-0.084
N2	-0.041	-0.018	0.009	-0.020	-0.038	0.023	-0.078	0.070	0.031
C3	0.000	-0.032	0.010	-0.009	-0.043	0.062	0.019	-0.006	-0.012
C2	-0.001	-0.021	0.001	-0.020	-0.058	0.054	0.050	-0.034	-0.020
C5	-0.003	0.010	0.002	-0.040	0.019	0.014	0.053	0.025	-0.037
H12	0.026	0.025	-0.004	0.027	0.055	-0.016	0.101	0.050	-0.059
H14	-0.016	0.025	0.003	-0.044	0.056	-0.007	0.040	0.046	-0.042
H16	-0.024	0.022	0.005	-0.127	0.048	0.016	-0.002	0.052	-0.031
C4	0.014	-0.019	0.005	0.032	-0.029	-0.018	0.007	-0.068	0.012
H18	0.024	-0.030	0.003	0.051	-0.008	-0.047	-0.012	-0.064	0.027
H20	0.016	-0.005	0.012	0.030	0.056	-0.023	0.007	-0.127	0.015
H22	0.018	-0.015	0.008	0.080	-0.092	-0.071	-0.034	-0.033	0.042
C6	0.003	0.012	-0.008	-0.039	0.024	0.020	0.017	0.010	-0.020
H28	0.016	0.017	-0.040	-0.019	0.018	-0.060	0.025	0.017	-0.030

H26	-0.018	0.050	0.022	-0.079	0.080	0.059	0.004	0.032	-0.003
H5	0.009	0.026	-0.027	-0.054	0.059	0.006	0.024	0.013	-0.029
C7	0.017	-0.015	0.004	0.034	-0.028	-0.011	-0.005	-0.022	0.013
H30	0.039	-0.018	0.009	0.109	-0.058	-0.022	-0.058	-0.006	0.013
H32	0.015	-0.005	-0.001	-0.014	0.017	-0.067	0.001	-0.047	0.029
H34	0.011	0.000	-0.003	0.060	-0.026	-0.039	-0.002	-0.040	0.024
O2	-0.019	-0.002	-0.064	-0.018	0.025	-0.101	0.031	-0.019	0.004

	556.15			568.81			570.57		
	A			A			A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.027	0.009	0.000	0.025	0.009	0.030	0.034	0.026	0.045
N1	0.073	-0.073	-0.036	-0.015	-0.007	0.049	0.045	-0.005	0.029
C1	-0.076	0.046	0.037	0.004	0.006	0.013	0.023	0.017	-0.031
C8	0.055	-0.102	-0.035	-0.004	0.007	0.011	0.013	0.022	-0.033
N5	-0.039	0.014	0.033	-0.001	-0.009	0.012	0.020	0.021	-0.032
C9	0.007	-0.027	0.007	-0.007	-0.003	0.010	0.006	0.010	-0.030
C10	0.026	0.023	0.023	0.011	0.001	0.009	-0.066	-0.030	-0.024
C11	0.021	0.002	-0.024	0.005	0.005	0.000	-0.024	-0.038	0.052
C12	0.004	0.037	-0.025	0.011	0.008	-0.014	-0.018	-0.035	0.060
H7	-0.003	0.073	0.006	0.012	0.008	-0.012	-0.049	-0.034	0.019
C13	-0.014	-0.011	-0.032	-0.004	0.003	-0.012	0.053	0.008	0.052
H3	0.000	-0.034	-0.047	-0.009	0.007	-0.006	0.051	0.000	0.059
C14	-0.001	-0.004	0.002	-0.001	0.000	-0.003	0.009	0.014	-0.023
N4	-0.020	0.028	0.034	0.003	-0.001	-0.003	0.011	0.029	-0.035
H6	0.009	-0.051	-0.042	-0.009	0.002	0.001	0.023	-0.003	0.058
H4	0.001	0.074	0.041	0.018	-0.004	0.000	-0.075	-0.017	-0.014
H2	0.166	-0.227	-0.067	-0.006	-0.010	0.026	-0.066	0.129	0.000
N2	0.010	0.021	0.007	0.065	0.016	-0.027	-0.093	0.053	0.005
C3	0.025	-0.008	-0.023	-0.052	0.016	-0.082	0.019	-0.039	-0.038
C2	-0.048	0.023	0.012	-0.046	-0.083	-0.018	-0.039	-0.011	0.021
C5	-0.063	-0.020	0.027	-0.059	0.019	0.027	-0.062	-0.009	0.024
H12	-0.100	-0.040	0.042	0.052	0.069	0.023	-0.061	-0.009	0.021
H14	-0.048	-0.032	0.024	-0.134	0.067	0.058	-0.056	-0.007	0.020
H16	-0.031	-0.042	0.020	-0.090	0.062	0.047	-0.070	-0.007	0.025
C4	-0.003	0.058	-0.007	0.045	-0.090	-0.018	0.014	0.018	0.005
H18	0.025	0.041	-0.022	0.102	-0.130	-0.040	0.048	-0.002	-0.013
H20	0.001	0.120	-0.001	0.057	-0.005	0.011	0.019	0.086	0.017
H22	0.034	0.035	-0.027	0.082	-0.097	-0.025	0.046	0.001	-0.010
C6	0.022	-0.017	-0.042	0.045	-0.028	-0.026	0.033	-0.017	-0.071
H28	0.021	-0.024	-0.057	0.034	0.006	0.103	0.045	-0.011	-0.093
H26	0.017	-0.021	-0.051	0.102	-0.068	-0.034	0.017	0.010	-0.050
H5	0.005	-0.010	-0.028	0.118	-0.084	-0.054	0.040	-0.010	-0.082
C7	0.020	-0.010	0.017	-0.079	0.071	-0.023	0.016	-0.022	0.031
H30	-0.004	0.004	0.030	-0.094	0.090	-0.001	-0.017	0.000	0.053
H32	0.052	-0.029	0.051	-0.018	0.054	0.031	0.067	-0.048	0.084
H34	-0.007	0.005	0.030	-0.133	0.112	-0.004	-0.029	0.009	0.046
O2	0.016	0.015	0.020	0.023	0.038	0.030	0.001	-0.033	-0.022

	577.58			617.12			638.52		
	A			A			A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.018	-0.016	-0.032	0.005	0.003	0.007	0.018	0.000	0.053
N1	-0.025	-0.014	-0.017	0.005	0.003	0.008	0.034	0.022	0.021
C1	0.055	-0.077	0.005	0.023	-0.012	-0.020	0.042	0.008	-0.037
C8	-0.055	0.044	0.066	-0.069	0.038	-0.009	-0.019	0.085	0.025
N5	0.017	-0.035	0.013	-0.080	-0.042	-0.010	-0.021	0.011	-0.006
C9	-0.009	0.001	0.023	-0.006	-0.014	0.066	0.000	0.025	-0.002
C10	0.059	0.015	0.002	0.018	-0.033	0.093	0.018	0.022	-0.012
C11	0.015	0.036	-0.050	0.010	-0.030	0.089	-0.002	0.027	-0.053
C12	0.012	0.018	-0.044	0.064	0.052	-0.052	-0.033	-0.024	0.007
H7	0.053	-0.007	-0.015	0.005	0.046	-0.144	0.017	-0.041	0.059
C13	-0.055	0.002	-0.033	0.060	0.055	-0.046	-0.047	-0.030	0.015

H3	-0.054	0.008	-0.038	0.057	0.060	-0.043	-0.038	-0.024	-0.004
C14	-0.012	-0.016	0.028	0.036	0.034	-0.037	-0.009	-0.020	0.039
N4	-0.004	-0.045	0.019	-0.038	-0.018	-0.067	0.045	-0.047	0.039
H6	-0.026	0.042	-0.041	-0.092	-0.087	0.085	0.026	0.014	-0.063
H4	0.067	-0.002	-0.005	0.035	-0.066	0.078	0.037	-0.034	-0.019
H2	-0.143	0.144	0.103	0.087	-0.229	-0.111	0.396	-0.488	-0.181
N2	-0.065	0.087	0.055	-0.021	0.007	-0.006	-0.034	-0.008	-0.021
C3	0.037	-0.013	-0.024	0.005	0.000	-0.001	-0.010	-0.007	-0.023
C2	-0.023	0.003	-0.009	0.005	0.006	0.007	0.005	0.014	0.001
C5	-0.032	-0.006	0.002	0.004	0.001	0.000	0.010	0.003	0.001
H12	-0.040	-0.010	0.006	-0.005	-0.003	-0.003	-0.008	-0.007	0.007
H14	-0.032	-0.011	0.006	0.015	-0.003	-0.007	0.018	-0.007	0.002
H16	-0.025	-0.006	0.003	0.000	-0.003	-0.003	0.031	-0.008	-0.002
C4	0.002	0.016	0.004	-0.003	0.008	0.002	-0.007	0.015	0.004
H18	0.026	-0.008	-0.002	-0.009	0.015	0.003	-0.011	0.015	0.009
H20	0.009	0.044	0.018	-0.005	0.004	-0.003	-0.006	0.002	0.004
H22	0.010	0.024	0.009	-0.003	0.003	-0.002	-0.011	0.024	0.012
C6	0.027	-0.004	-0.057	0.002	0.000	-0.004	0.013	-0.009	-0.020
H28	0.033	-0.008	-0.088	0.001	-0.002	-0.009	0.015	0.001	0.002
H26	0.011	0.014	-0.047	-0.001	-0.001	-0.007	0.019	-0.012	-0.020
H5	0.016	0.008	-0.053	-0.003	0.001	0.000	0.031	-0.021	-0.029
C7	0.023	-0.022	0.032	0.003	-0.005	0.002	-0.017	0.006	-0.006
H30	-0.024	-0.001	0.042	-0.008	-0.002	0.003	-0.026	0.016	0.006
H32	0.055	-0.053	0.069	0.003	-0.010	0.005	0.005	-0.001	0.015
H34	0.004	-0.018	0.046	0.004	-0.009	0.004	-0.037	0.024	-0.001
O2	0.056	0.013	0.012	-0.006	-0.016	-0.001	-0.028	-0.035	-0.025

	664.90 A			691.33 A			704.22 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.050	-0.028	-0.059	-0.003	-0.007	-0.001	-0.007	-0.034	0.047
N1	-0.032	-0.025	-0.040	-0.004	0.007	-0.003	0.041	0.065	-0.023
C1	0.000	-0.032	0.036	0.009	-0.003	0.003	0.043	0.031	0.040
C8	-0.018	0.037	0.031	-0.016	0.025	0.012	-0.003	-0.029	-0.018
N5	0.022	0.036	-0.010	-0.012	0.017	0.004	-0.017	-0.004	-0.016
C9	0.007	0.043	-0.032	0.067	-0.117	-0.056	0.005	0.003	0.008
C10	-0.054	-0.004	-0.043	-0.007	0.006	0.002	0.008	0.005	0.013
C11	-0.016	-0.007	0.013	0.013	-0.029	-0.011	-0.002	0.007	0.002
C12	-0.012	-0.026	0.029	-0.020	0.036	0.018	-0.001	0.003	-0.002
H7	-0.033	-0.029	-0.007	0.002	-0.016	-0.011	0.012	-0.028	-0.021
C13	0.054	0.015	0.029	0.006	0.005	0.003	-0.002	0.003	0.000
H3	0.044	0.043	0.035	0.183	-0.344	-0.163	-0.002	0.012	-0.005
C14	0.017	0.010	-0.034	-0.063	0.135	0.061	0.010	-0.013	0.001
N4	-0.005	-0.005	-0.038	0.023	-0.051	-0.030	-0.025	-0.001	0.004
H6	0.046	0.008	0.008	0.042	-0.082	-0.035	0.000	-0.038	-0.015
H4	-0.026	-0.056	-0.066	-0.151	0.279	0.128	0.025	-0.044	0.004
H2	0.308	-0.286	-0.166	-0.004	-0.003	0.019	-0.055	0.063	-0.040
N2	0.030	0.025	0.051	0.006	-0.003	0.007	0.002	-0.030	0.071
C3	0.007	-0.011	0.035	-0.005	-0.007	0.003	-0.067	-0.095	0.002
C2	-0.027	-0.029	-0.013	-0.004	-0.002	-0.009	-0.030	0.020	-0.109
C5	-0.041	-0.001	0.011	-0.003	0.000	0.000	0.006	0.003	-0.011
H12	0.000	0.017	0.014	0.002	0.002	0.005	0.007	-0.008	0.073
H14	-0.075	0.017	0.027	-0.013	0.001	0.008	-0.106	-0.017	0.098
H16	-0.048	0.014	0.019	0.008	0.002	0.003	0.211	-0.001	0.022
C4	0.009	-0.038	-0.012	0.001	-0.005	-0.001	-0.004	0.011	-0.006
H18	0.042	-0.067	-0.022	0.008	-0.016	0.001	0.057	-0.127	0.032
H20	0.017	0.007	0.006	0.004	-0.003	0.005	0.027	-0.021	0.064
H22	0.033	-0.042	-0.015	0.000	0.006	0.008	-0.036	0.166	0.121
C6	-0.014	0.015	0.031	-0.003	0.001	0.004	-0.004	-0.008	0.002
H28	-0.004	0.010	-0.015	0.002	0.005	0.001	0.054	0.053	-0.011
H26	-0.041	0.049	0.053	-0.005	0.011	0.014	-0.036	0.128	0.145
H5	-0.029	0.036	0.028	0.004	0.002	-0.004	0.105	0.000	-0.116
C7	0.030	-0.021	0.013	0.001	-0.001	0.001	-0.005	-0.008	0.002
H30	0.071	-0.035	0.010	0.019	-0.005	0.004	0.186	-0.033	0.057

H32	0.004	0.000	-0.016	0.000	0.006	-0.002	0.030	0.070	-0.001
H34	0.047	-0.022	-0.003	-0.001	0.008	-0.004	-0.074	0.129	-0.043
O2	0.057	0.060	0.027	0.003	0.008	0.000	0.014	0.040	-0.043

	729.13 A			812.47 A			838.31 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.000	-0.003	0.003	-0.011	-0.014	-0.004	0.001	0.000	0.000
N1	0.002	0.005	-0.002	0.018	0.043	-0.028	-0.003	0.001	0.001
C1	0.000	0.005	0.004	0.021	0.058	-0.064	0.001	-0.001	0.000
C8	-0.001	0.000	0.000	0.025	0.043	-0.066	0.002	-0.003	-0.001
N5	0.000	-0.003	-0.002	-0.053	-0.018	-0.039	0.004	-0.003	-0.003
C9	-0.018	0.034	0.017	-0.009	-0.012	0.020	-0.035	0.066	0.029
C10	0.028	-0.051	-0.022	0.031	-0.002	0.038	0.040	-0.082	-0.037
C11	0.025	-0.048	-0.023	0.004	0.000	0.001	0.016	-0.032	-0.011
C12	0.022	-0.044	-0.020	-0.008	-0.004	0.001	-0.026	0.056	0.024
H7	-0.225	0.431	0.194	0.022	-0.010	0.039	0.179	-0.339	-0.154
C13	0.019	-0.037	-0.016	-0.042	-0.021	0.000	-0.033	0.060	0.026
H3	-0.104	0.210	0.096	-0.046	-0.028	0.010	0.142	-0.297	-0.133
C14	-0.024	0.046	0.022	-0.002	-0.014	0.022	0.036	-0.072	-0.034
N4	0.005	-0.013	-0.008	0.060	0.020	0.027	-0.008	0.016	0.011
H6	-0.232	0.447	0.200	-0.039	-0.016	0.003	-0.109	0.206	0.097
H4	-0.162	0.314	0.140	0.025	-0.010	0.055	-0.195	0.375	0.162
H2	0.024	-0.026	-0.022	-0.107	0.030	0.007	0.033	-0.026	-0.035
N2	0.000	-0.002	0.006	0.003	0.030	-0.045	0.004	-0.003	-0.001
C3	-0.005	-0.008	0.001	0.029	0.022	0.029	-0.001	-0.001	0.000
C2	-0.002	0.001	-0.009	-0.027	-0.017	-0.031	0.000	0.000	0.000
C5	0.001	0.001	-0.002	-0.079	-0.006	0.018	0.001	0.000	0.000
H12	0.001	-0.001	0.006	-0.048	0.004	0.046	0.000	0.000	0.000
H14	-0.008	-0.002	0.008	-0.149	0.005	0.069	0.004	0.001	-0.002
H16	0.019	-0.001	0.001	-0.034	0.011	0.037	-0.001	0.000	-0.001
C4	-0.001	0.000	-0.001	0.021	-0.075	-0.022	-0.001	0.000	0.000
H18	0.005	-0.012	0.003	0.073	-0.146	-0.021	0.000	-0.002	0.000
H20	0.002	-0.002	0.005	0.036	-0.045	0.014	0.000	0.001	0.000
H22	-0.003	0.014	0.011	0.037	-0.037	0.009	0.000	0.002	0.001
C6	-0.001	0.000	0.001	-0.033	0.031	0.067	0.000	0.000	0.001
H28	0.004	0.004	-0.002	-0.049	-0.001	0.029	0.001	0.000	0.000
H26	-0.004	0.012	0.014	-0.050	0.010	0.030	-0.001	0.000	0.001
H5	0.008	0.001	-0.009	-0.102	0.052	0.120	0.000	0.000	0.001
C7	0.000	-0.002	0.000	0.064	-0.039	0.029	-0.001	0.000	-0.001
H30	0.018	-0.005	0.005	0.030	-0.048	-0.003	0.003	0.000	0.001
H32	0.003	0.005	0.000	0.024	-0.053	0.003	0.000	0.001	0.000
H34	-0.005	0.010	-0.004	0.119	-0.108	0.033	-0.004	0.004	-0.002
O2	0.002	0.003	-0.003	0.007	0.000	0.017	-0.001	0.001	0.000

	883.58 A			887.04 A			918.29 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.009	-0.006	-0.012	-0.022	-0.008	-0.040	0.000	0.000	0.000
N1	-0.001	0.004	-0.006	-0.005	0.009	-0.024	0.000	0.000	-0.001
C1	0.003	0.011	0.004	0.005	0.022	-0.029	0.000	0.000	0.000
C8	0.004	0.002	-0.008	0.017	0.034	-0.042	-0.001	0.002	0.001
N5	-0.055	-0.049	0.031	-0.027	0.001	-0.039	0.002	-0.001	-0.001
C9	-0.006	-0.017	0.044	-0.003	-0.003	0.000	-0.007	0.015	0.008
C10	0.090	0.028	0.035	0.000	-0.005	0.016	0.043	-0.079	-0.035
C11	-0.022	0.040	-0.118	0.005	-0.008	0.023	-0.039	0.072	0.033
C12	-0.089	-0.069	0.060	0.009	0.006	-0.006	-0.020	0.039	0.019
H7	-0.064	-0.087	0.079	0.021	0.010	0.017	0.100	-0.192	-0.083
C13	0.083	0.020	0.054	-0.035	-0.015	-0.007	0.042	-0.087	-0.041
H3	0.122	0.072	-0.038	-0.046	-0.030	0.018	-0.200	0.393	0.182
C14	0.025	0.021	-0.028	-0.004	-0.008	0.013	-0.016	0.029	0.014
N4	-0.012	0.034	-0.076	0.049	0.014	0.023	0.003	-0.005	-0.005
H6	0.012	0.067	-0.116	-0.026	-0.023	0.023	0.175	-0.338	-0.152

H4	0.056	-0.021	0.126	0.004	-0.011	0.013	-0.170	0.329	0.148
H2	-0.093	-0.044	0.106	-0.044	0.018	-0.030	0.006	-0.002	-0.008
N2	0.001	-0.001	0.002	0.014	0.026	-0.011	-0.001	0.001	0.000
C3	-0.006	-0.008	0.000	-0.051	-0.072	0.005	0.000	0.000	0.000
C2	0.005	-0.003	0.017	0.024	-0.016	0.081	0.000	0.000	0.001
C5	0.004	-0.003	0.008	0.032	-0.013	0.031	0.000	0.000	0.000
H12	0.009	0.003	-0.017	0.060	0.014	-0.079	-0.001	0.000	0.000
H14	0.036	0.006	-0.024	0.171	0.027	-0.111	0.002	0.000	-0.001
H16	-0.059	0.000	0.000	-0.235	0.003	-0.006	-0.001	0.000	0.000
C4	0.002	0.000	0.009	-0.001	0.015	0.045	0.000	-0.001	0.000
H18	-0.017	0.042	-0.002	-0.076	0.199	-0.009	0.000	0.001	-0.001
H20	-0.008	0.010	-0.011	-0.040	0.068	-0.042	0.000	0.001	0.000
H22	0.010	-0.045	-0.027	0.044	-0.185	-0.117	0.001	-0.003	-0.002
C6	0.002	-0.006	-0.005	-0.011	-0.044	-0.010	0.000	0.000	0.000
H28	0.009	0.000	-0.010	0.068	0.029	-0.052	0.000	0.000	0.000
H26	-0.002	0.010	0.011	-0.062	0.141	0.179	0.000	0.001	0.001
H5	0.015	-0.004	-0.021	0.128	-0.023	-0.172	0.000	0.000	-0.001
C7	-0.008	0.001	-0.002	-0.042	-0.023	0.001	0.000	0.000	0.000
H30	0.013	-0.002	0.004	0.222	-0.063	0.069	0.001	0.000	0.001
H32	-0.006	0.011	-0.004	-0.016	0.090	-0.022	0.000	0.000	0.000
H34	-0.016	0.018	-0.008	-0.123	0.158	-0.071	-0.001	0.001	0.000
O2	0.000	0.002	-0.001	0.033	0.035	0.019	0.000	0.000	0.000

	954.65 A			961.28 A			963.91 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.027	0.023	0.022	-0.005	-0.006	-0.004	0.003	0.003	0.002
N1	-0.030	-0.073	0.059	0.007	0.016	-0.013	-0.007	-0.008	0.009
C1	-0.050	-0.036	-0.053	0.012	0.008	0.013	-0.009	-0.004	-0.008
C8	-0.004	0.012	0.001	0.002	0.000	-0.002	0.000	0.000	-0.001
N5	-0.006	-0.013	0.019	0.000	0.006	-0.006	-0.005	-0.005	0.004
C9	-0.014	-0.006	0.001	0.005	0.001	-0.001	-0.005	-0.001	0.000
C10	-0.007	0.003	-0.015	0.001	0.003	0.008	-0.004	0.001	-0.006
C11	-0.001	0.003	-0.009	0.004	-0.008	-0.001	0.001	0.000	-0.002
C12	-0.005	-0.002	0.001	-0.003	0.008	0.004	-0.001	0.001	0.000
H7	-0.018	-0.008	-0.026	0.023	-0.028	0.000	-0.007	-0.003	-0.015
C13	0.025	0.011	0.000	-0.006	-0.011	-0.003	0.009	0.004	0.000
H3	0.043	0.047	-0.048	-0.027	0.003	0.030	0.016	0.018	-0.020
C14	0.009	0.003	0.003	-0.004	0.001	-0.001	0.003	0.001	0.003
N4	0.017	0.001	0.014	-0.001	0.001	-0.006	0.004	-0.001	0.007
H6	0.044	0.023	-0.010	-0.030	0.018	0.014	0.014	0.010	0.000
H4	0.012	0.030	-0.063	0.002	-0.025	0.021	0.005	0.011	-0.029
H2	-0.011	-0.057	0.110	0.010	0.009	-0.037	-0.008	-0.015	0.029
N2	0.014	0.060	-0.082	-0.002	-0.015	0.020	-0.001	0.011	-0.011
C3	-0.013	-0.010	-0.014	-0.018	0.020	0.011	-0.025	0.014	0.011
C2	-0.009	-0.024	-0.020	0.022	-0.027	-0.010	-0.017	0.018	0.008
C5	0.030	-0.024	-0.047	-0.027	-0.072	0.017	0.025	0.057	-0.014
H12	0.211	0.052	-0.005	0.329	0.103	-0.087	-0.250	-0.080	0.070
H14	-0.165	0.026	0.079	-0.192	0.096	0.040	0.144	-0.075	-0.024
H16	0.145	0.055	0.018	-0.293	0.106	0.076	0.243	-0.082	-0.059
C4	-0.028	0.065	-0.020	0.028	0.053	-0.007	-0.030	-0.046	0.006
H18	0.020	-0.067	0.022	-0.121	0.128	0.075	0.097	-0.109	-0.063
H20	0.004	0.038	0.051	0.011	-0.230	-0.043	-0.013	0.217	0.039
H22	-0.069	0.233	0.115	-0.139	0.150	0.077	0.128	-0.134	-0.071
C6	-0.048	-0.003	0.034	-0.005	0.025	-0.060	-0.019	0.018	-0.065
H28	-0.011	0.062	0.096	-0.078	0.051	0.235	-0.081	0.073	0.278
H26	-0.046	0.097	0.160	0.166	-0.159	-0.162	0.169	-0.142	-0.123
H5	0.068	-0.019	-0.073	0.097	-0.106	-0.056	0.139	-0.130	-0.105
C7	0.021	-0.053	0.010	0.007	-0.001	0.054	0.006	-0.023	0.076
H30	0.176	-0.065	0.071	0.130	-0.098	-0.043	0.283	-0.163	-0.014
H32	0.082	-0.010	0.041	-0.190	0.107	-0.144	-0.222	0.163	-0.178
H34	-0.050	0.066	-0.023	0.180	-0.121	-0.011	0.174	-0.083	-0.034
O2	0.022	0.013	0.034	-0.005	-0.001	-0.007	0.002	0.002	0.005

	969.59			970.72			981.31		
	A			A			A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.002	0.002	0.001	0.008	0.008	0.006	0.005	0.005	0.003
N1	-0.002	-0.004	0.003	-0.010	-0.019	0.011	-0.003	-0.009	0.007
C1	-0.003	-0.002	-0.002	-0.013	-0.010	-0.006	-0.009	-0.008	-0.010
C8	0.000	0.001	0.003	0.002	0.001	0.011	-0.007	-0.013	0.017
N5	0.012	0.009	-0.001	0.068	0.046	-0.011	0.026	0.007	0.018
C9	0.019	-0.018	-0.008	0.039	0.012	0.011	0.006	0.001	0.001
C10	-0.020	0.054	0.038	0.057	-0.015	0.073	0.003	0.000	0.004
C11	0.046	-0.093	-0.040	-0.017	0.012	0.005	-0.002	0.000	-0.004
C12	-0.052	0.098	0.047	0.007	-0.026	0.004	0.001	0.001	0.000
H7	0.202	-0.351	-0.125	0.075	0.048	0.198	0.011	-0.001	0.013
C13	0.023	-0.081	-0.033	-0.083	-0.027	0.012	-0.003	-0.002	0.000
H3	-0.156	0.216	0.158	-0.147	-0.256	0.233	-0.013	-0.020	0.028
C14	-0.021	0.028	0.006	-0.035	-0.008	-0.044	-0.005	0.000	-0.007
N4	-0.003	0.001	-0.019	-0.026	0.030	-0.091	-0.024	-0.005	-0.015
H6	-0.194	0.305	0.145	-0.132	-0.141	-0.030	-0.011	-0.004	-0.004
H4	0.081	-0.197	-0.018	-0.048	-0.133	0.326	-0.006	-0.019	0.030
H2	0.019	0.016	-0.026	0.115	0.089	-0.192	0.038	0.000	0.008
N2	0.000	0.003	-0.003	0.002	0.009	-0.014	0.001	0.016	-0.020
C3	0.001	-0.001	-0.001	-0.002	0.001	-0.005	-0.012	-0.001	-0.025
C2	-0.003	0.000	0.000	-0.011	-0.010	-0.002	0.033	0.048	0.003
C5	0.004	0.005	-0.006	0.021	-0.002	-0.016	-0.053	0.050	0.035
H12	-0.018	-0.007	0.010	0.052	0.009	-0.002	-0.334	-0.079	0.056
H14	0.002	-0.008	0.005	-0.018	0.000	0.014	0.128	-0.046	-0.050
H16	0.045	-0.006	-0.006	0.068	0.007	-0.003	-0.024	-0.073	-0.032
C4	-0.004	-0.002	0.003	-0.025	0.010	0.002	0.090	-0.021	-0.028
H18	0.011	-0.007	-0.008	0.041	-0.051	-0.018	-0.130	0.132	0.067
H20	-0.003	0.034	0.005	-0.010	0.117	0.034	0.050	-0.467	-0.111
H22	0.016	-0.018	-0.010	0.030	0.016	0.005	-0.150	0.056	0.042
C6	-0.002	-0.003	0.005	-0.010	0.004	0.005	-0.037	0.024	0.005
H28	0.007	0.000	-0.016	-0.013	0.015	0.041	-0.060	0.065	0.190
H26	-0.016	0.020	0.024	0.004	0.002	0.013	0.048	-0.024	0.009
H5	-0.001	0.006	-0.005	0.012	-0.009	-0.007	0.054	-0.041	-0.035
C7	0.002	0.001	-0.004	0.008	-0.010	0.002	0.008	-0.058	-0.020
H30	-0.018	0.010	0.001	0.025	-0.010	0.011	0.170	-0.031	0.106
H32	0.018	-0.013	0.014	0.021	-0.009	0.011	0.165	-0.035	0.097
H34	-0.009	0.003	0.004	-0.005	0.006	0.000	-0.151	0.162	-0.049
O2	0.001	0.000	0.002	0.005	0.003	0.007	-0.001	-0.003	0.004

	984.81			987.40			990.06		
	A			A			A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.006	0.008	-0.001	-0.001	0.001	0.001	0.000	0.000	0.001
N1	-0.012	-0.028	0.021	0.007	-0.006	-0.003	0.004	-0.002	-0.002
C1	-0.021	-0.015	-0.020	0.000	0.000	0.000	0.001	0.000	0.000
C8	0.001	0.008	-0.003	0.000	0.002	-0.002	-0.002	-0.002	0.003
N5	0.004	0.003	-0.001	-0.002	-0.002	-0.003	0.003	0.001	0.003
C9	0.002	0.000	0.002	0.000	-0.002	-0.001	0.001	0.000	0.000
C10	0.006	-0.001	0.008	-0.001	0.002	0.001	0.000	0.000	-0.001
C11	-0.002	0.001	-0.001	0.002	-0.003	-0.001	0.000	0.001	0.000
C12	-0.001	-0.003	0.002	-0.002	0.003	0.002	0.001	0.000	-0.001
H7	0.012	-0.001	0.023	0.004	-0.011	-0.006	-0.001	0.002	0.000
C13	-0.007	-0.003	0.001	0.002	-0.002	-0.001	0.000	0.001	0.000
H3	-0.015	-0.023	0.027	-0.004	0.015	0.001	0.001	-0.003	0.000
C14	-0.003	0.000	-0.005	0.000	0.002	0.002	0.000	0.000	-0.001
N4	0.007	0.007	-0.008	0.003	0.001	0.002	-0.004	-0.002	-0.001
H6	-0.013	-0.010	-0.003	-0.004	0.010	0.005	0.001	-0.002	-0.001
H4	-0.003	-0.016	0.034	0.006	-0.007	-0.007	-0.002	0.001	0.002
H2	0.008	-0.003	0.002	-0.009	0.005	0.002	0.007	-0.002	0.001
N2	0.006	0.019	-0.028	-0.006	0.004	0.003	0.007	-0.004	-0.004
C3	0.014	-0.006	0.053	0.009	-0.005	0.001	-0.006	0.001	-0.009

C2	0.016	0.019	-0.004	-0.012	0.000	0.002	0.005	0.005	0.001
C5	-0.031	0.024	-0.004	0.043	-0.003	0.062	0.008	0.012	0.050
H12	-0.142	-0.033	0.052	0.009	0.004	-0.103	-0.101	-0.025	-0.044
H14	-0.024	-0.027	0.025	0.309	0.020	-0.175	0.237	0.004	-0.135
H16	0.091	-0.024	-0.011	-0.349	-0.021	-0.016	-0.230	-0.037	-0.021
C4	0.034	0.000	-0.038	-0.043	-0.005	-0.067	-0.013	-0.002	-0.042
H18	-0.034	-0.036	0.047	0.173	-0.369	-0.020	0.080	-0.199	0.005
H20	0.041	-0.238	-0.024	0.038	0.073	0.112	0.028	-0.016	0.048
H22	-0.101	0.158	0.094	-0.023	0.303	0.180	-0.033	0.187	0.112
C6	0.063	-0.068	-0.005	0.033	0.036	0.014	-0.065	-0.045	-0.010
H28	0.152	-0.116	-0.399	-0.036	-0.062	-0.040	0.033	0.111	0.120
H26	-0.133	0.121	0.084	0.035	-0.123	-0.180	-0.047	0.191	0.291
H5	-0.056	0.081	-0.006	-0.157	0.058	0.192	0.256	-0.086	-0.309
C7	-0.063	0.044	0.052	-0.038	-0.026	-0.006	0.053	0.047	0.007
H30	0.094	-0.078	-0.069	0.191	-0.052	0.069	-0.311	0.085	-0.115
H32	-0.330	0.205	-0.220	0.007	0.068	-0.008	-0.020	-0.097	0.004
H34	0.133	-0.080	-0.031	-0.138	0.151	-0.059	0.204	-0.244	0.103
O2	0.002	-0.002	0.011	0.002	-0.001	0.000	-0.001	0.001	0.000

	1059.81			1081.45			1094.47		
		A			A			A	
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.004	0.007	-0.021	0.002	0.003	0.000	0.001	0.001	0.002
N1	-0.035	-0.070	0.045	-0.005	-0.008	0.002	0.000	0.000	-0.001
C1	-0.026	-0.039	0.035	-0.004	-0.004	0.001	-0.001	-0.001	-0.001
C8	0.026	0.052	-0.041	0.004	0.003	0.005	0.003	0.001	0.003
N5	-0.074	-0.008	-0.074	0.031	0.025	-0.011	0.014	0.011	-0.007
C9	-0.007	-0.002	-0.004	0.004	-0.009	0.012	-0.008	-0.002	-0.009
C10	0.007	-0.002	0.010	0.058	0.009	0.050	0.055	0.023	0.013
C11	-0.001	-0.002	0.004	0.023	-0.023	0.076	-0.007	-0.004	0.000
C12	-0.005	-0.005	0.005	-0.061	-0.048	0.031	-0.022	-0.010	-0.001
H7	0.014	-0.007	0.032	-0.070	-0.047	0.031	-0.340	0.012	-0.420
C13	-0.006	-0.005	0.003	-0.078	-0.026	-0.028	0.027	-0.003	0.036
H3	-0.024	-0.033	0.051	0.081	0.248	-0.467	-0.077	-0.181	0.315
C14	0.004	0.004	-0.002	-0.010	-0.006	-0.001	-0.014	-0.003	-0.006
N4	0.100	0.044	0.016	-0.006	0.023	-0.056	0.001	-0.006	0.012
H6	-0.039	-0.023	0.003	0.141	0.036	0.085	-0.442	-0.222	-0.015
H4	-0.006	-0.021	0.043	0.211	0.250	-0.329	0.196	0.255	-0.348
H2	-0.092	0.040	-0.137	0.063	0.082	-0.185	0.020	0.018	-0.026
N2	-0.009	-0.050	0.074	-0.001	-0.002	0.002	0.000	0.001	-0.002
C3	-0.006	-0.018	0.018	0.000	-0.001	0.001	0.001	0.001	-0.001
C2	-0.004	-0.020	0.022	-0.001	-0.002	0.002	0.000	0.000	0.000
C5	0.013	0.030	-0.024	0.001	0.002	-0.002	0.000	0.000	0.000
H12	-0.096	-0.028	0.038	-0.007	-0.002	0.003	0.001	0.000	0.000
H14	0.021	-0.035	0.013	0.001	-0.003	0.002	0.000	0.000	0.000
H16	0.182	-0.030	-0.031	0.017	-0.003	-0.003	-0.002	0.001	0.000
C4	0.010	0.031	-0.023	0.001	0.003	-0.002	0.000	0.000	0.000
H18	-0.023	-0.008	0.031	-0.002	-0.001	0.003	0.000	0.000	0.000
H20	0.017	-0.106	-0.007	0.001	-0.009	-0.001	0.000	0.000	0.000
H22	-0.082	0.151	0.077	-0.007	0.013	0.007	0.001	-0.002	-0.001
C6	0.007	0.021	-0.031	0.000	0.001	-0.001	0.000	-0.001	0.001
H28	-0.037	0.013	0.083	-0.002	0.001	0.004	0.001	0.000	-0.002
H26	0.087	-0.099	-0.120	0.004	-0.004	-0.005	-0.002	0.002	0.003
H5	0.010	-0.034	0.011	0.001	-0.002	0.000	0.000	0.000	-0.001
C7	0.001	0.024	-0.030	0.000	0.001	-0.001	0.000	-0.001	0.000
H30	-0.155	0.079	-0.020	-0.006	0.003	-0.001	0.003	-0.001	0.001
H32	0.062	-0.056	0.049	0.002	-0.002	0.002	0.000	0.001	0.000
H34	-0.031	-0.002	0.022	-0.001	0.000	0.001	0.000	0.000	-0.001
O2	0.021	0.027	0.003	0.002	0.002	0.001	0.000	0.000	0.001

	1132.40			1170.91			1179.79		
		A			A			A	
	X	Y	Z	X	Y	Z	X	Y	Z

O1	-0.001	-0.001	-0.001	-0.003	-0.003	-0.004	0.020	0.007	0.034
N1	0.001	0.001	0.001	0.001	0.001	0.003	-0.010	-0.012	0.002
C1	0.001	0.001	0.000	0.000	0.002	-0.007	-0.020	-0.011	-0.027
C8	-0.003	-0.001	-0.004	0.007	0.005	-0.009	-0.002	0.001	-0.001
N5	0.002	0.001	0.001	0.022	0.019	-0.013	0.006	0.000	0.006
C9	-0.011	0.003	-0.015	-0.031	0.011	-0.054	-0.002	-0.001	0.001
C10	-0.022	-0.007	-0.010	0.034	0.026	-0.021	0.001	0.000	0.002
C11	-0.010	0.002	-0.015	0.048	0.015	0.022	-0.001	0.000	-0.001
C12	0.019	0.009	0.001	0.029	-0.001	0.033	-0.001	0.000	-0.001
H7	0.385	-0.020	0.490	-0.222	0.021	-0.301	0.002	-0.001	0.002
C13	0.021	0.003	0.017	-0.015	-0.026	0.041	0.002	0.001	0.000
H3	0.097	0.129	-0.174	0.141	0.246	-0.383	0.001	-0.002	0.004
C14	0.016	0.006	0.006	-0.052	-0.025	-0.006	0.000	0.000	-0.001
N4	-0.006	-0.004	0.002	-0.004	-0.006	0.009	-0.002	-0.001	0.000
H6	-0.602	-0.299	-0.032	-0.281	-0.152	0.015	0.006	0.003	-0.001
H4	0.042	0.108	-0.190	-0.132	-0.248	0.412	0.002	0.002	-0.002
H2	-0.003	-0.039	0.090	0.014	-0.076	0.192	0.008	-0.012	0.028
N2	0.000	-0.001	0.001	-0.002	-0.003	0.002	-0.008	0.003	-0.024
C3	0.000	-0.001	0.001	-0.004	-0.009	0.007	-0.074	-0.085	-0.061
C2	0.000	0.000	0.001	0.001	-0.006	0.011	-0.056	-0.057	-0.094
C5	0.000	0.000	0.000	0.000	0.002	-0.003	0.041	0.026	0.033
H12	0.000	0.000	0.000	-0.005	-0.001	0.006	-0.089	-0.023	-0.047
H14	0.000	0.000	0.000	-0.005	-0.004	0.005	0.233	-0.018	-0.100
H16	0.001	0.000	0.000	0.023	-0.001	-0.001	-0.074	-0.056	-0.037
C4	0.000	0.000	0.000	0.000	0.003	-0.003	0.021	0.044	0.042
H18	0.000	0.000	0.000	0.000	-0.006	0.003	-0.114	0.227	0.038
H20	0.000	0.000	0.000	0.002	-0.005	0.003	-0.028	-0.030	-0.065
H22	0.000	0.001	0.000	-0.006	0.018	0.010	-0.041	-0.068	-0.047
C6	0.000	0.000	-0.001	0.001	0.003	-0.003	0.022	0.040	0.045
H28	-0.001	0.000	0.001	-0.004	-0.001	0.006	-0.043	-0.059	-0.031
H26	0.002	-0.002	-0.003	0.011	-0.014	-0.017	-0.024	-0.050	-0.096
H5	0.000	-0.001	0.001	-0.001	-0.004	0.005	-0.160	0.079	0.198
C7	0.000	0.001	-0.001	0.000	0.003	-0.003	0.044	0.022	0.033
H30	-0.004	0.002	-0.001	-0.022	0.009	-0.004	-0.086	-0.008	-0.079
H32	0.001	-0.001	0.001	0.003	-0.006	0.003	-0.075	-0.038	-0.039
H34	0.000	-0.001	0.001	-0.001	-0.004	0.004	0.185	-0.169	0.053
O2	0.000	0.000	0.000	0.005	0.005	0.003	0.030	0.032	0.017

	1198.35 A			1233.58 A			1238.87 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.022	0.014	0.032	0.008	0.003	0.013	-0.006	0.001	-0.013
N1	-0.019	-0.023	-0.008	-0.006	-0.018	0.008	0.019	0.041	-0.032
C1	-0.015	-0.032	0.032	-0.016	-0.016	-0.002	0.006	0.026	-0.043
C8	0.017	-0.002	0.049	-0.003	0.007	-0.015	0.004	-0.016	0.040
N5	-0.032	-0.020	0.001	-0.001	0.006	-0.014	0.010	-0.017	0.045
C9	-0.037	-0.029	0.005	0.010	0.010	-0.006	-0.030	-0.031	0.018
C10	-0.008	0.005	-0.019	0.006	0.000	0.006	-0.015	-0.001	-0.012
C11	0.003	0.011	-0.022	0.002	-0.004	0.010	-0.006	0.010	-0.030
C12	0.020	0.007	0.008	-0.008	-0.004	0.000	0.020	0.012	-0.002
H7	-0.010	0.010	-0.037	-0.002	-0.005	0.010	0.009	0.013	-0.024
C13	0.030	0.007	0.018	-0.010	-0.003	-0.005	0.030	0.009	0.014
H3	0.076	0.083	-0.096	-0.019	-0.017	0.016	0.053	0.045	-0.040
C14	-0.031	-0.006	-0.016	0.008	0.003	0.001	-0.024	-0.008	-0.004
N4	0.047	0.011	0.023	0.002	0.004	-0.006	-0.010	-0.015	0.016
H6	-0.090	-0.036	-0.028	0.012	0.001	0.012	-0.020	0.003	-0.034
H4	-0.047	-0.062	0.077	0.009	0.007	-0.001	-0.022	-0.014	-0.001
H2	-0.003	0.243	-0.568	-0.011	-0.077	0.169	0.040	0.202	-0.433
N2	0.007	0.002	0.009	-0.002	-0.016	0.012	-0.004	0.021	-0.054
C3	0.029	0.072	-0.044	-0.101	0.083	0.035	-0.083	-0.064	0.053
C2	-0.013	0.040	-0.078	-0.120	0.113	0.005	-0.021	-0.005	0.114
C5	0.005	-0.011	0.019	0.057	-0.024	-0.005	0.011	0.003	-0.024
H12	0.027	0.008	-0.039	0.226	0.061	-0.064	0.058	0.015	0.027
H14	0.039	0.023	-0.035	0.081	0.031	-0.055	-0.029	-0.018	0.029

H16	-0.131	0.006	0.005	-0.003	0.037	0.016	0.147	0.009	0.004
C4	0.003	-0.012	0.020	0.032	-0.052	-0.010	0.009	-0.010	-0.029
H18	-0.007	0.051	-0.015	0.018	-0.046	-0.008	0.018	-0.089	0.016
H20	-0.017	0.022	-0.025	0.010	-0.171	-0.057	0.026	-0.087	0.015
H22	0.034	-0.114	-0.065	-0.001	-0.110	-0.056	-0.034	0.087	0.054
C6	-0.008	-0.018	0.017	0.031	-0.031	-0.030	0.019	0.010	-0.019
H28	0.029	0.006	-0.037	0.059	-0.052	-0.177	-0.016	-0.037	-0.034
H26	-0.061	0.086	0.104	-0.012	-0.017	-0.050	0.043	-0.089	-0.122
H5	0.011	0.022	-0.034	0.033	0.001	-0.064	-0.008	-0.018	0.026
C7	-0.002	-0.021	0.017	0.048	-0.027	0.004	0.027	0.009	-0.009
H30	0.136	-0.055	0.029	0.055	-0.008	0.042	-0.112	0.042	-0.021
H32	-0.011	0.035	-0.013	0.138	-0.080	0.095	0.046	-0.073	0.040
H34	0.009	0.021	-0.026	0.058	-0.056	0.027	0.024	-0.055	0.043
O2	-0.018	-0.020	-0.008	0.005	0.006	0.003	0.018	0.018	0.013

	1271.27 A			1304.58 A			1324.52 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.039	-0.021	-0.055	-0.008	-0.003	-0.012	0.014	0.005	0.025
N1	0.010	-0.009	0.039	0.004	-0.012	0.013	0.010	0.045	-0.057
C1	0.081	0.055	0.096	0.013	0.007	0.019	-0.022	-0.005	-0.046
C8	0.001	-0.002	-0.001	-0.001	0.000	0.000	0.005	0.000	0.001
N5	-0.010	-0.001	-0.008	-0.003	0.000	-0.002	0.006	0.000	0.004
C9	0.010	0.007	-0.002	0.002	0.001	0.000	-0.005	-0.002	0.000
C10	-0.003	0.002	-0.008	0.000	0.001	-0.003	0.000	-0.003	0.007
C11	0.002	0.000	0.004	0.000	0.000	0.001	0.000	0.001	-0.003
C12	0.003	0.000	0.003	0.001	0.000	0.001	-0.002	0.001	-0.005
H7	-0.010	0.001	-0.013	-0.003	0.000	-0.003	0.008	0.001	0.007
C13	-0.008	-0.004	0.000	-0.002	-0.001	-0.001	0.005	0.001	0.003
H3	-0.008	-0.002	-0.003	-0.002	-0.002	-0.001	0.006	0.002	0.002
C14	0.005	-0.001	0.008	0.001	0.000	0.002	-0.002	0.001	-0.004
N4	0.002	0.003	-0.004	0.003	0.003	-0.002	-0.014	-0.009	0.004
H6	-0.018	-0.011	0.003	-0.005	-0.003	0.001	0.014	0.009	-0.003
H4	-0.007	-0.004	0.001	-0.002	-0.001	0.001	0.004	0.005	-0.004
H2	-0.014	0.009	-0.024	-0.004	0.000	-0.002	0.005	-0.004	0.020
N2	0.051	0.069	-0.001	0.009	0.024	0.000	-0.060	-0.100	0.038
C3	-0.047	0.054	-0.066	0.111	-0.104	-0.063	0.037	0.091	-0.110
C2	-0.048	-0.092	0.045	-0.110	0.088	0.049	-0.045	-0.077	0.090
C5	0.020	0.022	-0.009	0.022	-0.021	-0.015	0.002	0.013	-0.016
H12	-0.018	0.000	-0.011	0.223	0.067	-0.043	0.039	0.017	0.020
H14	0.084	-0.021	-0.030	0.076	0.009	-0.066	0.066	-0.042	-0.023
H16	0.146	-0.037	-0.026	0.122	0.027	0.020	0.154	-0.018	-0.011
C4	0.008	0.025	-0.008	0.029	-0.020	-0.007	0.008	0.011	-0.017
H18	-0.040	0.050	0.019	0.031	-0.069	0.014	-0.032	-0.001	0.028
H20	-0.002	-0.027	-0.022	0.015	-0.187	-0.047	0.017	-0.055	0.010
H22	-0.076	0.111	0.061	-0.007	-0.080	-0.047	-0.049	0.082	0.044
C6	0.010	-0.009	0.016	-0.028	0.021	0.014	-0.007	-0.020	0.018
H28	0.006	-0.038	-0.062	-0.074	0.058	0.227	0.031	0.026	0.001
H26	-0.064	0.057	0.048	-0.016	0.073	0.103	-0.071	0.089	0.104
H5	-0.036	0.023	0.035	-0.089	0.007	0.104	-0.048	0.056	0.004
C7	0.021	-0.017	0.018	-0.021	0.027	0.016	-0.010	-0.017	0.020
H30	0.130	-0.057	0.019	-0.109	0.011	-0.070	0.120	-0.061	0.010
H32	0.031	-0.046	0.032	-0.187	0.091	-0.132	-0.009	0.051	-0.012
H34	0.073	-0.074	0.021	-0.041	0.072	-0.020	0.055	-0.008	-0.043
O2	-0.059	-0.059	-0.041	-0.012	-0.013	-0.009	0.042	0.045	0.022

	1358.14 A			1369.12 A			1386.36 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.002	0.004	-0.003	0.002	0.000	0.004	0.000	0.000	-0.001
N1	-0.013	-0.020	0.006	-0.002	0.003	-0.010	0.000	-0.002	0.001
C1	-0.005	-0.015	0.017	0.002	-0.008	0.014	0.000	-0.001	0.000
C8	0.000	0.000	0.003	0.024	0.016	0.000	0.000	0.000	0.000

N5	-0.009	0.001	-0.011	0.028	0.029	-0.039	0.000	0.001	-0.001
C9	0.005	0.005	-0.003	-0.063	-0.005	-0.060	0.000	0.000	0.000
C10	0.003	0.002	-0.002	0.052	-0.010	0.083	0.001	0.000	0.000
C11	0.002	-0.002	0.006	0.009	-0.008	0.028	0.000	0.000	0.000
C12	-0.004	-0.003	0.002	-0.072	-0.018	-0.043	-0.001	0.000	0.000
H7	-0.002	-0.003	0.006	0.075	-0.032	0.159	0.000	0.000	0.002
C13	-0.003	0.000	-0.004	0.059	0.031	-0.003	0.000	0.000	0.000
H3	-0.007	-0.006	0.005	0.045	0.005	0.044	0.000	0.000	0.000
C14	0.003	0.002	-0.001	-0.053	0.037	-0.130	0.000	0.000	-0.001
N4	0.009	0.005	-0.002	-0.015	-0.065	0.116	0.000	0.000	0.001
H6	-0.005	-0.005	0.007	0.107	0.038	0.035	0.001	0.000	0.000
H4	0.000	-0.003	0.006	0.065	0.005	0.073	0.001	0.000	0.001
H2	-0.012	-0.018	0.028	0.009	0.017	0.047	0.001	-0.002	0.000
N2	0.003	-0.008	0.024	0.015	0.019	0.002	0.000	-0.001	0.002
C3	-0.083	-0.033	-0.134	-0.002	-0.005	0.004	-0.001	-0.010	-0.013
C2	0.107	0.099	0.058	-0.002	-0.004	0.005	0.020	0.005	0.004
C5	-0.013	-0.020	-0.023	0.000	0.001	0.000	-0.019	-0.004	-0.038
H12	-0.049	-0.042	0.136	0.001	0.001	-0.003	0.072	-0.018	0.397
H14	-0.167	0.016	0.081	0.000	-0.002	0.001	0.140	-0.161	-0.020
H16	-0.115	0.123	0.056	0.008	-0.006	-0.003	-0.089	0.234	0.114
C4	-0.023	-0.027	-0.026	0.001	0.001	-0.001	0.018	0.009	0.052
H18	-0.003	-0.063	0.001	-0.003	-0.005	0.006	0.305	-0.156	-0.163
H20	0.063	0.019	0.158	0.001	-0.001	0.001	-0.225	0.075	-0.493
H22	0.150	0.008	0.002	-0.007	0.001	0.000	-0.351	-0.013	0.018
C6	0.024	0.013	0.026	0.002	0.001	-0.003	-0.005	0.013	0.008
H28	-0.085	-0.095	0.023	-0.014	-0.010	0.013	-0.025	-0.043	-0.057
H26	-0.141	0.070	-0.011	-0.006	0.010	0.005	0.021	-0.007	0.007
H5	-0.080	0.046	0.097	-0.002	-0.010	0.011	0.034	-0.066	0.024
C7	0.022	0.019	0.026	0.001	0.003	-0.001	-0.025	0.008	0.003
H30	0.106	-0.103	-0.110	0.008	-0.002	-0.003	0.037	-0.029	-0.029
H32	-0.057	-0.160	0.019	-0.008	-0.020	0.001	0.100	0.014	0.083
H34	0.084	-0.090	0.045	-0.010	-0.004	0.014	0.136	-0.046	-0.087
O2	0.001	0.004	-0.005	-0.010	-0.010	-0.006	0.000	0.001	0.000

	1387.06 A			1389.53 A			1393.58 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.000	0.000	0.000	-0.002	0.000	-0.003	0.001	0.000	0.004
N1	-0.001	-0.001	0.000	0.004	-0.001	0.004	-0.002	0.000	-0.006
C1	0.000	0.000	0.002	0.000	0.002	-0.005	0.002	-0.001	0.008
C8	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.001
N5	0.000	0.000	-0.001	0.001	0.000	0.001	-0.001	0.000	-0.001
C9	0.000	0.000	-0.001	-0.001	-0.001	0.001	0.001	0.001	-0.001
C10	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000
C11	0.000	0.000	0.001	-0.001	0.000	-0.001	0.001	0.000	0.001
C12	-0.001	0.000	0.000	0.001	0.001	0.000	-0.001	-0.001	0.000
H7	0.001	-0.001	0.001	0.000	0.001	-0.001	0.000	-0.001	0.003
C13	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	-0.001
H3	0.000	-0.001	0.000	0.001	0.001	0.000	-0.001	-0.001	0.001
C14	0.000	0.001	0.000	-0.001	-0.001	0.000	0.000	0.001	-0.002
N4	0.001	0.000	0.001	-0.001	-0.001	0.000	0.001	0.000	0.001
H6	0.000	0.000	0.001	0.001	0.001	-0.001	0.000	-0.001	0.002
H4	0.000	0.000	0.001	0.000	0.001	-0.001	0.000	-0.001	0.002
H2	-0.003	0.001	0.003	0.003	0.002	-0.005	-0.002	-0.001	0.001
N2	0.001	0.001	0.001	-0.002	-0.007	0.000	0.008	0.010	-0.003
C3	-0.003	-0.006	-0.010	-0.009	0.009	0.003	-0.017	0.009	0.005
C2	0.014	-0.001	0.002	-0.023	0.022	0.010	-0.016	-0.018	-0.004
C5	-0.012	0.008	0.008	0.049	-0.009	-0.008	0.020	-0.007	-0.049
H12	0.051	0.036	-0.062	-0.162	-0.080	-0.016	-0.050	-0.088	0.459
H14	-0.002	-0.047	0.033	-0.155	0.112	0.053	0.113	-0.104	-0.027
H16	0.023	-0.092	-0.047	-0.110	0.054	0.011	-0.164	0.324	0.146
C4	-0.025	0.027	0.006	0.050	-0.089	-0.012	-0.018	0.013	-0.018
H18	0.096	-0.046	-0.062	-0.172	0.219	0.017	-0.099	0.060	0.048
H20	0.011	-0.181	0.042	-0.045	0.431	-0.122	0.097	-0.116	0.221

H22	0.163	-0.047	-0.049	-0.301	0.207	0.193	0.210	-0.013	-0.030
C6	0.034	0.029	0.008	0.035	-0.012	-0.030	-0.011	-0.024	-0.022
H28	-0.301	-0.315	0.058	-0.126	-0.077	0.195	0.174	0.199	0.016
H26	-0.301	0.123	-0.085	-0.184	0.143	0.031	0.183	-0.026	0.109
H5	0.156	-0.135	-0.036	-0.071	0.034	0.049	-0.170	0.085	0.101
C7	-0.025	-0.040	-0.012	0.029	-0.033	0.003	0.024	-0.043	-0.005
H30	-0.129	0.198	0.281	-0.153	0.105	0.104	-0.163	0.166	0.208
H32	0.217	0.446	0.000	-0.049	0.187	-0.116	0.014	0.290	-0.112
H34	0.225	-0.135	-0.108	-0.065	0.058	0.011	-0.007	-0.016	0.014
O2	0.000	0.000	-0.001	0.002	0.003	0.002	-0.005	-0.005	-0.003

	1397.29			1401.06			1401.70		
	A			A			A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.005	-0.001	-0.009	0.004	0.001	0.009	-0.001	0.000	-0.003
N1	0.002	-0.007	0.015	0.001	0.007	-0.014	0.003	0.000	0.010
C1	0.003	0.003	0.001	-0.005	-0.005	-0.002	-0.010	-0.006	-0.012
C8	0.000	0.000	0.000	0.000	0.000	0.000	-0.003	0.000	-0.001
N5	0.002	0.002	-0.001	-0.001	-0.001	0.001	0.003	0.001	0.002
C9	-0.003	-0.001	-0.001	0.002	0.001	0.001	-0.002	-0.003	0.002
C10	0.002	0.000	0.003	-0.001	0.000	-0.002	0.000	0.000	0.001
C11	-0.001	-0.001	0.001	0.000	0.000	0.000	-0.002	0.000	-0.002
C12	-0.002	0.000	-0.001	0.001	0.000	0.001	0.003	0.001	0.001
H7	0.003	-0.001	0.006	-0.002	0.001	-0.003	0.001	0.001	-0.002
C13	0.003	0.002	-0.001	-0.002	-0.001	0.000	0.001	0.000	0.000
H3	0.002	0.001	0.001	-0.001	0.000	-0.001	0.002	0.002	-0.002
C14	-0.003	0.000	-0.004	0.002	0.000	0.002	-0.002	-0.002	0.002
N4	0.001	-0.002	0.004	0.000	0.001	-0.003	0.002	0.002	-0.001
H6	0.004	0.002	0.001	-0.003	-0.001	-0.001	0.002	0.002	-0.003
H4	0.002	0.000	0.003	-0.002	0.000	-0.002	0.001	0.001	-0.002
H2	0.003	0.003	-0.005	0.000	-0.003	0.003	0.005	0.003	-0.006
N2	-0.002	-0.001	0.005	0.002	0.006	-0.004	0.001	-0.001	0.002
C3	0.020	-0.038	-0.052	0.052	-0.002	0.037	-0.014	-0.004	0.029
C2	0.001	0.042	0.015	-0.049	-0.019	-0.015	0.039	0.013	-0.021
C5	-0.007	-0.014	0.009	0.002	0.000	-0.030	-0.086	-0.013	0.028
H12	0.016	0.014	-0.107	0.068	-0.013	0.306	0.218	0.111	-0.059
H14	-0.024	0.098	-0.053	0.183	-0.139	-0.051	0.246	0.013	-0.216
H16	0.078	0.000	0.018	-0.054	0.184	0.087	0.258	0.012	0.067
C4	0.015	-0.062	-0.015	0.014	-0.027	-0.030	-0.009	-0.036	0.002
H18	-0.115	0.190	-0.024	-0.260	0.175	0.127	-0.014	0.187	-0.111
H20	0.021	0.190	0.041	0.109	0.097	0.225	-0.006	0.086	0.009
H22	-0.010	0.144	0.125	0.062	0.059	0.041	0.095	0.127	0.106
C6	-0.068	0.033	0.071	0.001	0.042	0.012	0.029	-0.022	-0.072
H28	0.185	0.098	-0.351	-0.240	-0.287	-0.089	-0.015	0.056	0.205
H26	0.290	-0.244	-0.063	-0.123	0.043	-0.051	0.042	0.167	0.217
H5	0.137	-0.071	-0.079	0.267	-0.274	-0.058	-0.236	-0.012	0.255
C7	-0.046	0.002	-0.005	-0.030	0.039	-0.012	-0.035	0.027	-0.032
H30	0.022	0.058	0.113	0.150	-0.098	-0.107	0.178	0.026	0.120
H32	0.185	0.203	0.081	-0.009	-0.223	0.085	0.106	-0.065	0.102
H34	0.253	-0.165	-0.097	-0.046	-0.006	0.038	0.092	-0.225	0.099
O2	0.000	0.001	-0.001	-0.003	-0.004	0.001	0.002	0.001	0.002

	1403.60			1410.75			1416.92		
	A			A			A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.002	0.000	-0.004	-0.001	0.000	-0.003	0.011	0.005	0.017
N1	-0.002	-0.006	0.010	0.000	-0.001	0.005	-0.011	0.002	-0.029
C1	0.001	0.000	0.004	0.001	0.002	-0.001	-0.007	-0.015	0.015
C8	0.000	0.000	0.001	0.000	0.000	0.000	0.001	-0.001	0.005
N5	-0.001	0.000	-0.002	0.001	0.000	0.000	-0.010	-0.004	-0.004
C9	0.000	0.000	-0.001	-0.001	0.000	0.000	0.008	0.006	-0.002
C10	0.002	0.001	0.000	0.000	0.000	0.001	0.003	0.005	-0.009
C11	0.000	-0.001	0.002	0.000	0.000	0.000	0.004	-0.002	0.008

C12	-0.002	-0.001	0.000	0.000	0.000	0.000	-0.005	-0.005	0.004
H7	0.001	-0.001	0.004	0.000	0.000	0.000	-0.005	-0.005	0.007
C13	0.001	0.001	-0.002	0.000	0.000	0.000	-0.004	0.001	-0.008
H3	-0.001	-0.001	0.002	0.001	0.000	0.000	-0.010	-0.008	0.006
C14	-0.001	0.001	-0.002	0.000	0.000	0.000	0.005	0.003	-0.001
N4	0.001	0.000	0.002	-0.001	-0.001	0.000	0.005	0.004	-0.002
H6	0.000	-0.001	0.002	0.001	0.001	-0.001	-0.012	-0.010	0.009
H4	0.001	-0.001	0.003	0.000	0.000	-0.001	-0.004	-0.006	0.009
H2	-0.002	0.000	0.002	0.001	0.001	-0.002	-0.012	-0.013	0.016
N2	0.000	-0.004	0.003	-0.002	-0.006	0.001	0.015	0.021	-0.003
C3	-0.035	0.017	-0.025	-0.027	0.019	-0.004	-0.014	-0.010	0.013
C2	0.049	0.012	-0.010	0.025	-0.009	-0.006	0.017	0.009	0.004
C5	-0.094	0.008	0.014	-0.021	-0.037	0.021	-0.027	0.033	-0.002
H12	0.321	0.150	0.050	-0.122	-0.043	-0.106	0.201	0.095	0.033
H14	0.280	-0.198	-0.103	0.029	0.334	-0.251	0.066	-0.305	0.149
H16	0.185	-0.061	0.005	0.205	0.191	0.159	-0.065	-0.214	-0.138
C4	-0.004	-0.023	0.001	0.005	0.027	-0.007	0.029	0.002	-0.031
H18	-0.013	0.088	-0.051	-0.047	-0.167	0.148	-0.228	-0.159	0.302
H20	-0.014	0.098	-0.016	0.022	0.033	0.051	0.073	0.200	0.148
H22	0.012	0.077	0.066	-0.103	-0.118	-0.098	-0.224	-0.125	-0.098
C6	-0.003	0.006	0.040	-0.003	0.027	-0.028	0.010	-0.018	-0.020
H28	0.013	-0.033	-0.105	-0.075	-0.140	-0.158	0.051	0.091	0.102
H26	-0.072	-0.094	-0.161	0.163	0.090	0.216	0.011	0.021	0.030
H5	0.112	0.060	-0.158	0.032	-0.330	0.244	-0.121	0.103	0.040
C7	0.079	-0.046	0.026	0.027	-0.032	0.036	-0.027	-0.007	0.024
H30	-0.232	0.046	-0.024	-0.198	-0.057	-0.175	-0.101	-0.076	-0.169
H32	-0.222	0.083	-0.219	0.023	0.076	-0.013	0.212	0.081	0.141
H34	-0.237	0.229	0.039	0.020	0.234	-0.212	0.232	0.092	-0.295
O2	0.001	0.001	-0.001	0.002	0.003	0.001	-0.009	-0.010	-0.004

	1419.24 A			1419.99 A			1432.04 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.021	-0.009	-0.034	0.008	0.003	0.013	-0.040	-0.015	-0.069
N1	0.017	-0.009	0.058	-0.007	0.003	-0.021	0.030	-0.027	0.120
C1	0.017	0.028	-0.016	-0.006	-0.011	0.007	0.033	0.059	-0.039
C8	-0.003	0.002	-0.010	0.001	-0.001	0.004	-0.008	0.006	-0.027
N5	0.017	0.007	0.006	-0.007	-0.003	-0.002	0.042	0.022	0.006
C9	-0.015	-0.010	0.002	0.006	0.004	-0.001	-0.038	-0.025	0.006
C10	-0.003	-0.008	0.016	0.001	0.004	-0.007	-0.020	-0.035	0.055
C11	-0.007	0.002	-0.013	0.003	-0.001	0.005	-0.018	0.011	-0.046
C12	0.008	0.007	-0.007	-0.003	-0.003	0.003	0.028	0.028	-0.027
H7	0.009	0.008	-0.009	-0.004	-0.003	0.004	0.022	0.032	-0.049
C13	0.008	-0.001	0.012	-0.003	0.001	-0.005	0.017	-0.015	0.051
H3	0.018	0.014	-0.010	-0.008	-0.005	0.004	0.056	0.046	-0.039
C14	-0.010	-0.005	0.000	0.004	0.002	0.000	-0.020	-0.015	0.009
N4	-0.007	-0.006	0.005	0.003	0.002	-0.002	-0.014	-0.008	0.001
H6	0.022	0.017	-0.014	-0.009	-0.007	0.006	0.067	0.056	-0.050
H4	0.008	0.010	-0.013	-0.003	-0.004	0.006	0.022	0.037	-0.056
H2	0.022	0.024	-0.031	-0.009	-0.009	0.011	0.054	0.045	-0.046
N2	-0.016	-0.019	-0.004	0.007	0.010	0.001	-0.038	-0.054	0.009
C3	0.013	0.003	0.019	0.004	-0.012	-0.007	0.003	0.016	-0.018
C2	-0.007	0.000	-0.027	0.018	-0.002	0.004	0.007	0.027	-0.037
C5	-0.005	-0.029	0.003	-0.026	-0.025	0.009	0.002	0.014	-0.003
H12	-0.068	-0.044	0.047	-0.031	-0.013	-0.020	0.073	0.029	0.041
H14	0.070	0.190	-0.183	0.066	0.183	-0.182	0.003	-0.150	0.100
H16	0.097	0.219	0.150	0.164	0.153	0.124	-0.115	-0.086	-0.068
C4	-0.009	-0.001	0.001	0.029	0.032	-0.016	0.010	0.014	-0.006
H18	-0.012	0.071	-0.031	-0.131	-0.292	0.305	-0.079	-0.119	0.148
H20	0.020	-0.032	0.054	0.030	0.129	0.049	0.027	0.061	0.058
H22	0.105	0.021	0.015	-0.299	-0.217	-0.171	-0.094	-0.126	-0.097
C6	0.022	-0.034	0.018	0.003	-0.007	0.028	-0.004	0.006	-0.007
H28	0.024	0.089	0.203	0.013	0.030	0.051	-0.008	-0.025	-0.048
H26	-0.261	-0.053	-0.249	-0.128	-0.071	-0.174	0.058	0.037	0.089

H5	-0.033	0.348	-0.260	0.030	0.168	-0.167	-0.002	-0.090	0.079
C7	-0.029	0.003	0.025	-0.006	0.012	-0.039	0.003	0.001	-0.010
H30	-0.062	-0.120	-0.225	0.154	0.131	0.282	0.061	0.036	0.092
H32	0.156	-0.006	0.135	-0.056	0.017	-0.057	-0.038	0.005	-0.034
H34	0.173	0.126	-0.273	-0.071	-0.239	0.266	-0.039	-0.067	0.094
O2	0.009	0.009	0.005	-0.004	-0.004	-0.002	0.022	0.024	0.009

	1454.61 A			1482.26 A			1562.05 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.024	-0.009	-0.040	0.007	0.001	0.015	0.000	0.000	0.000
N1	0.028	0.001	0.066	0.000	0.016	-0.027	0.009	0.014	-0.002
C1	0.016	0.031	-0.027	-0.016	-0.024	0.005	-0.021	-0.017	-0.020
C8	-0.012	-0.012	0.007	-0.045	-0.019	-0.020	-0.063	-0.016	-0.041
N5	-0.009	-0.020	0.036	0.043	0.058	-0.053	0.051	0.026	0.017
C9	0.013	-0.001	0.016	-0.044	-0.046	0.043	-0.143	-0.063	-0.033
C10	0.066	0.082	-0.106	0.049	0.023	0.007	0.009	0.008	-0.008
C11	-0.018	-0.041	0.072	-0.133	-0.055	-0.032	0.074	0.023	0.034
C12	-0.030	-0.047	0.065	0.080	0.021	0.046	-0.077	-0.014	-0.056
H7	-0.008	-0.055	0.116	0.057	0.027	0.005	0.006	-0.025	0.059
C13	0.014	0.064	-0.123	0.051	0.042	-0.034	0.027	0.021	-0.015
H3	-0.066	-0.071	0.077	0.055	0.034	-0.022	-0.014	-0.059	0.111
C14	-0.015	0.000	-0.013	-0.088	-0.065	0.041	0.079	-0.010	0.107
N4	-0.001	-0.016	0.030	0.044	0.027	-0.007	0.027	0.030	-0.033
H6	-0.082	-0.077	0.083	0.087	0.060	-0.028	-0.014	-0.025	0.037
H4	-0.015	-0.064	0.119	0.064	0.038	-0.017	-0.034	-0.062	0.103
H2	0.000	0.025	-0.081	0.080	-0.065	0.123	0.092	0.030	-0.049
N2	-0.030	-0.034	-0.013	0.023	0.020	0.021	0.024	0.014	0.035
C3	0.005	0.009	-0.002	-0.003	-0.001	-0.004	-0.002	0.001	-0.005
C2	-0.002	0.007	-0.018	-0.002	-0.008	0.010	-0.003	-0.005	0.003
C5	0.003	0.003	0.000	0.001	0.000	0.000	0.001	0.000	0.000
H12	0.012	0.003	0.015	-0.009	-0.003	-0.004	-0.003	-0.002	0.000
H14	0.002	-0.033	0.023	-0.005	0.007	-0.001	-0.002	0.001	0.001
H16	-0.038	-0.013	-0.012	0.009	0.000	0.001	0.001	0.000	0.000
C4	0.001	0.004	0.001	0.000	0.000	0.000	0.000	0.001	0.000
H18	-0.016	-0.022	0.031	0.005	0.000	-0.004	0.000	-0.001	0.001
H20	0.007	0.006	0.016	-0.002	-0.006	-0.006	-0.001	-0.002	-0.002
H22	-0.009	-0.034	-0.025	-0.004	0.007	0.005	-0.003	0.000	0.000
C6	0.000	0.000	-0.003	0.000	0.001	0.002	0.000	0.001	0.001
H28	-0.004	-0.008	-0.007	0.000	-0.001	-0.002	0.001	0.000	-0.002
H26	0.007	0.014	0.024	-0.003	-0.005	-0.009	-0.001	-0.002	-0.004
H5	0.000	-0.021	0.016	0.003	0.004	-0.006	0.002	0.003	-0.003
C7	-0.001	0.000	-0.002	0.002	-0.001	0.001	0.001	0.000	0.001
H30	0.022	0.002	0.017	-0.009	-0.001	-0.007	-0.004	0.000	-0.004
H32	-0.007	-0.005	-0.004	-0.002	0.000	-0.002	-0.001	0.000	-0.002
H34	-0.009	-0.014	0.019	-0.001	0.007	-0.004	0.000	0.004	-0.002
O2	0.017	0.019	0.009	-0.014	-0.014	-0.008	-0.012	-0.012	-0.007

	1603.89 A			1632.73 A			1686.76 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.020	0.008	0.034	0.021	0.011	0.030	0.005	0.004	0.005
N1	-0.082	-0.079	-0.055	-0.070	-0.065	-0.046	-0.018	-0.020	-0.006
C1	0.109	0.091	0.092	0.039	0.050	-0.007	-0.004	0.016	-0.041
C8	0.022	-0.007	0.028	-0.046	0.054	-0.158	0.013	0.032	-0.043
N5	-0.001	0.017	-0.035	0.052	-0.017	0.095	-0.013	-0.046	0.077
C9	-0.041	-0.014	-0.016	-0.002	-0.017	0.030	0.048	0.054	-0.063
C10	0.021	0.014	-0.006	-0.019	-0.011	0.003	0.067	0.051	-0.038
C11	-0.013	-0.014	0.016	0.005	0.015	-0.027	-0.076	-0.063	0.054
C12	-0.014	0.006	-0.029	0.033	-0.013	0.064	-0.028	0.038	-0.114
H7	0.028	0.003	0.026	-0.043	-0.008	-0.031	0.098	0.034	0.037
C13	0.021	0.010	0.002	-0.023	0.004	-0.033	0.026	-0.028	0.091
H3	0.015	-0.009	0.034	-0.032	-0.003	-0.029	0.071	0.033	0.008

C14	0.007	-0.022	0.056	0.008	0.026	-0.043	-0.042	-0.040	0.039
N4	-0.016	0.000	-0.018	-0.011	-0.025	0.038	-0.014	0.001	-0.019
H6	0.024	0.004	0.020	-0.032	-0.002	-0.033	0.080	0.011	0.070
H4	0.008	-0.011	0.036	-0.012	0.004	-0.025	0.049	0.004	0.046
H2	0.005	-0.017	0.029	0.079	0.061	-0.063	-0.017	0.036	-0.080
N2	-0.068	-0.043	-0.091	0.018	0.000	0.051	0.024	0.009	0.045
C3	0.008	-0.002	0.018	0.001	0.000	0.002	-0.001	0.000	-0.001
C2	0.010	0.015	0.001	0.003	0.003	0.004	-0.001	-0.002	0.000
C5	-0.004	-0.001	-0.001	-0.001	0.000	-0.002	0.001	0.000	-0.001
H12	0.007	0.004	-0.001	0.000	0.001	-0.002	0.000	0.000	0.000
H14	0.003	0.005	-0.009	0.001	0.005	-0.007	0.001	0.000	-0.002
H16	0.010	0.005	0.002	0.010	0.003	0.000	0.002	0.001	0.000
C4	-0.001	-0.003	-0.003	-0.001	0.000	-0.002	0.000	0.001	0.000
H18	0.000	0.007	-0.008	0.000	0.006	-0.006	0.000	0.002	-0.001
H20	0.001	0.005	0.001	0.000	0.000	-0.002	0.000	-0.001	0.000
H22	0.004	0.010	0.005	0.000	0.009	0.004	0.001	0.002	0.000
C6	-0.001	-0.002	-0.003	0.001	0.000	-0.001	0.001	0.001	0.000
H28	-0.001	0.001	0.006	0.001	0.001	0.001	0.000	0.001	0.000
H26	0.003	0.004	0.009	0.001	-0.001	-0.004	0.001	-0.001	-0.003
H5	-0.003	-0.007	0.005	0.002	0.002	-0.003	0.002	0.002	-0.002
C7	-0.004	0.000	-0.002	-0.001	0.001	-0.001	0.000	0.001	0.000
H30	0.009	-0.001	0.007	-0.002	0.001	-0.003	-0.002	0.001	-0.002
H32	0.003	-0.003	0.005	0.001	0.000	0.001	0.001	0.001	0.000
H34	-0.002	-0.009	0.005	0.000	0.003	-0.002	0.001	0.003	-0.002
O2	0.029	0.031	0.015	-0.008	-0.006	-0.009	-0.009	-0.009	-0.007

	1715.98 A			1788.68 A			1853.37 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.004	-0.004	-0.003	-0.010	-0.007	-0.011	-0.001	-0.001	0.000
N1	0.019	0.026	-0.004	0.047	0.054	0.014	0.005	0.008	0.000
C1	0.015	-0.017	0.066	-0.032	-0.095	0.122	-0.004	-0.019	0.030
C8	-0.161	-0.075	-0.032	0.021	0.055	-0.077	0.000	0.019	-0.040
N5	0.009	-0.017	0.050	0.010	-0.010	0.033	0.029	0.035	-0.038
C9	0.059	0.044	-0.028	-0.054	-0.011	-0.040	0.022	-0.076	0.188
C10	-0.010	-0.016	0.024	0.038	0.023	-0.007	-0.009	0.041	-0.102
C11	0.030	0.013	0.007	-0.075	-0.038	-0.003	0.030	0.004	0.027
C12	-0.027	-0.001	-0.027	0.043	0.014	0.019	-0.048	0.011	-0.080
H7	0.005	-0.005	0.015	0.012	0.020	-0.029	0.026	0.006	0.015
C13	0.012	-0.002	0.018	-0.040	-0.033	0.027	-0.001	-0.034	0.074
H3	0.023	0.014	-0.006	-0.025	-0.001	-0.026	0.037	0.024	-0.009
C14	-0.058	-0.009	-0.044	0.089	0.049	-0.006	-0.023	0.013	-0.055
N4	0.114	0.053	0.014	-0.020	-0.014	0.009	-0.004	-0.005	0.008
H6	0.001	-0.003	0.008	0.031	0.016	0.000	-0.010	-0.018	0.029
H4	0.007	0.011	-0.016	0.030	0.001	0.031	-0.056	-0.028	-0.005
H2	0.019	-0.014	0.023	0.017	0.032	-0.057	0.043	-0.008	0.058
N2	-0.037	-0.018	-0.059	-0.037	-0.010	-0.078	-0.007	-0.002	-0.013
C3	0.002	0.002	0.001	0.000	0.002	-0.005	0.000	0.000	-0.001
C2	0.002	0.002	0.002	0.003	0.005	-0.001	0.001	0.001	0.000
C5	-0.001	0.000	0.001	-0.001	-0.001	0.001	0.000	0.000	0.000
H12	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000
H14	-0.002	0.000	0.002	-0.003	-0.002	0.004	-0.001	0.000	0.000
H16	-0.002	-0.001	0.001	-0.004	-0.001	0.001	0.000	0.000	0.000
C4	0.000	-0.001	0.000	0.000	-0.002	0.000	0.000	0.000	0.000
H18	0.001	-0.002	0.001	0.002	-0.005	0.002	0.000	-0.001	0.000
H20	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000
H22	-0.001	-0.001	0.000	0.001	-0.004	-0.001	0.000	0.000	0.000
C6	-0.001	-0.001	0.000	-0.001	0.000	0.002	0.000	0.000	0.000
H28	0.000	-0.001	0.000	0.000	0.000	-0.001	0.000	0.000	0.000
H26	-0.001	0.002	0.004	-0.001	0.001	0.005	0.000	0.000	0.001
H5	-0.002	-0.002	0.002	-0.003	-0.001	0.004	-0.001	0.000	0.001
C7	-0.001	-0.001	0.000	0.000	-0.002	0.001	0.000	0.000	0.000
H30	0.004	-0.002	0.002	0.004	-0.002	0.003	0.001	0.000	0.000
H32	-0.001	-0.002	0.000	-0.001	0.000	0.000	0.000	0.000	0.000

H34	-0.001	-0.004	0.003	0.001	-0.005	0.002	0.000	-0.001	0.001
O2	0.014	0.014	0.009	0.013	0.011	0.011	0.002	0.002	0.002

	1860.32 A			3091.31 A			3092.23 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	-0.004	-0.002	-0.005	0.000	0.000	0.000	0.000	0.000	0.000
N1	0.020	0.023	0.007	0.000	0.000	0.000	0.000	0.001	0.000
C1	-0.024	-0.058	0.067	0.000	0.000	0.000	0.000	0.000	0.000
C8	0.074	0.082	-0.076	0.000	0.000	0.000	0.000	0.000	0.000
N5	0.005	-0.008	0.019	0.000	0.000	0.000	0.000	0.000	0.000
C9	0.044	0.019	0.008	0.000	0.000	0.000	0.000	0.000	0.000
C10	-0.038	-0.033	0.029	0.000	0.000	0.000	0.000	0.000	0.000
C11	0.070	0.038	-0.005	0.000	0.000	0.000	0.000	0.000	0.000
C12	-0.032	-0.014	-0.006	0.000	0.000	0.000	0.000	0.000	0.000
H7	-0.011	-0.018	0.028	0.001	0.000	0.000	0.001	0.001	-0.001
C13	0.059	0.056	-0.056	0.000	0.000	0.000	0.000	0.000	0.000
H3	0.032	-0.004	0.042	0.000	0.000	0.000	0.001	0.000	0.000
C14	-0.112	-0.094	0.075	0.000	0.000	0.000	0.000	0.000	0.000
N4	-0.045	-0.012	-0.023	0.000	0.000	0.000	0.000	0.000	0.000
H6	-0.026	-0.009	-0.009	0.000	0.000	0.001	0.000	-0.001	0.002
H4	-0.021	0.004	-0.033	0.000	0.000	0.000	0.001	0.000	0.001
H2	0.005	0.023	-0.030	0.001	0.000	0.000	0.001	0.000	0.000
N2	-0.013	-0.002	-0.031	0.000	0.000	0.000	0.000	0.000	0.000
C3	-0.001	0.001	-0.003	0.000	0.000	0.000	0.000	-0.001	0.000
C2	0.002	0.003	-0.001	-0.001	0.000	0.000	0.000	0.000	0.000
C5	-0.001	0.000	0.000	0.000	0.000	-0.001	0.000	-0.005	-0.002
H12	0.001	0.000	0.000	0.001	-0.001	-0.001	-0.019	0.044	0.004
H14	-0.001	-0.001	0.002	0.005	0.004	0.006	0.018	0.016	0.026
H16	-0.001	0.000	0.000	-0.001	-0.005	0.008	0.001	0.000	-0.005
C4	0.000	-0.001	0.000	-0.016	-0.002	-0.009	0.065	0.006	0.050
H18	0.001	-0.002	0.001	0.095	0.065	0.106	-0.449	-0.308	-0.494
H20	0.000	0.001	0.001	0.099	0.002	-0.055	-0.353	-0.012	0.198
H22	0.001	-0.002	0.000	-0.007	-0.049	0.058	0.026	0.251	-0.303
C6	0.000	0.000	0.001	-0.005	0.001	-0.003	-0.003	-0.001	-0.001
H28	0.000	0.000	0.000	0.038	-0.036	0.014	0.014	-0.015	0.006
H26	0.000	0.000	0.002	-0.003	0.000	-0.001	0.002	0.007	-0.006
H5	-0.001	0.000	0.001	0.029	0.023	0.025	0.018	0.014	0.016
C7	0.000	-0.001	0.000	0.023	0.066	0.045	0.007	0.015	0.008
H30	0.001	-0.001	0.001	-0.107	-0.302	0.227	-0.028	-0.079	0.056
H32	0.000	0.000	0.000	0.257	-0.082	-0.309	0.040	-0.011	-0.049
H34	0.001	-0.002	0.000	-0.420	-0.391	-0.454	-0.095	-0.089	-0.105
O2	0.004	0.003	0.004	0.000	0.000	0.000	0.000	0.000	0.000

	3093.90 A			3094.34 A			3106.18 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C8	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N5	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C9	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C10	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C11	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C12	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H7	0.000	0.000	0.000	-0.001	0.000	0.001	0.000	0.000	0.000
C13	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H3	0.001	0.000	0.000	-0.002	0.000	-0.001	-0.001	0.000	0.000
C14	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H6	0.000	0.000	0.000	0.000	0.000	-0.001	0.000	0.000	0.001
H4	0.001	0.000	0.000	-0.002	0.000	-0.001	0.000	0.000	0.000

H2	0.000	0.000	0.000	-0.001	-0.001	-0.001	0.000	0.000	0.000
N2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C3	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C2	0.000	0.000	-0.001	0.000	0.000	0.000	0.000	0.000	0.000
C5	-0.007	-0.023	-0.036	-0.014	-0.035	-0.063	-0.010	0.047	-0.027
H12	-0.095	0.209	0.007	-0.141	0.313	0.008	0.162	-0.388	-0.062
H14	0.204	0.173	0.261	0.357	0.306	0.456	0.011	0.040	0.006
H16	-0.027	-0.113	0.152	-0.049	-0.206	0.287	-0.055	-0.210	0.381
C4	0.000	0.001	-0.001	-0.002	0.001	-0.005	-0.009	-0.008	0.017
H18	0.003	0.003	0.003	0.024	0.018	0.026	-0.025	-0.018	-0.013
H20	-0.010	0.000	0.004	-0.004	0.000	-0.001	0.140	0.002	-0.056
H22	0.001	-0.009	0.011	0.000	-0.025	0.031	-0.007	0.106	-0.139
C6	0.066	0.024	0.023	-0.037	-0.016	-0.013	-0.006	0.050	-0.027
H28	-0.257	0.275	-0.100	0.131	-0.142	0.052	0.316	-0.263	0.110
H26	-0.104	-0.233	0.198	0.067	0.145	-0.122	-0.202	-0.333	0.255
H5	-0.414	-0.322	-0.377	0.245	0.189	0.223	-0.039	0.000	-0.046
C7	0.003	0.005	0.000	-0.002	-0.004	-0.001	-0.013	-0.011	0.018
H30	-0.012	-0.036	0.023	0.009	0.028	-0.018	0.057	0.170	-0.098
H32	-0.002	0.004	0.005	-0.004	-0.001	0.004	0.102	-0.056	-0.138
H34	-0.022	-0.019	-0.025	0.023	0.021	0.026	0.007	0.009	0.026
O2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	3107.53 A			3111.39 A			3113.82 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N1	0.000	-0.001	0.000	0.000	0.000	0.000	0.000	-0.001	0.000
C1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C8	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N5	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C9	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C10	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C11	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001
C12	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	-0.001
H7	0.000	0.000	0.000	-0.003	-0.002	0.002	-0.008	-0.007	0.006
C13	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C14	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H6	0.000	0.000	0.001	-0.001	0.002	-0.005	-0.002	0.005	-0.013
H4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N2	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000
C3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C5	-0.004	0.021	-0.010	-0.009	0.052	-0.027	-0.002	0.015	-0.005
H12	0.073	-0.174	-0.027	0.177	-0.428	-0.069	0.050	-0.122	-0.018
H14	-0.007	0.008	-0.012	-0.006	0.028	-0.016	-0.014	-0.003	-0.019
H16	-0.022	-0.082	0.153	-0.057	-0.218	0.402	-0.014	-0.050	0.095
C4	0.026	0.019	-0.038	-0.007	-0.007	0.014	0.036	0.025	-0.046
H18	0.028	0.020	-0.006	-0.017	-0.012	-0.007	0.013	0.010	-0.033
H20	-0.362	-0.006	0.150	0.116	0.002	-0.046	-0.472	-0.010	0.193
H22	0.020	-0.238	0.312	-0.006	0.086	-0.114	0.028	-0.297	0.393
C6	-0.005	0.019	-0.012	0.010	-0.049	0.029	0.005	-0.012	0.008
H28	0.134	-0.114	0.048	-0.333	0.277	-0.118	-0.089	0.076	-0.032
H26	-0.076	-0.120	0.092	0.203	0.330	-0.251	0.047	0.074	-0.056
H5	0.002	0.014	-0.002	0.014	-0.021	0.024	-0.010	-0.015	-0.006
C7	0.033	0.021	-0.048	0.007	0.006	-0.009	-0.027	-0.016	0.042
H30	-0.133	-0.405	0.228	-0.031	-0.091	0.052	0.113	0.343	-0.190
H32	-0.272	0.146	0.368	-0.049	0.028	0.068	0.235	-0.128	-0.323
H34	0.013	0.007	-0.032	-0.006	-0.007	-0.016	-0.028	-0.022	0.009
O2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	3115.54 A			3128.65 A			3161.93 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C8	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N5	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C9	0.000	0.000	0.001	0.000	0.000	0.000	-0.001	0.000	0.000
C10	0.005	0.001	0.005	-0.008	-0.001	-0.007	0.011	0.003	0.006
C11	-0.007	0.022	-0.057	0.010	-0.018	0.051	-0.002	0.000	-0.003
C12	-0.035	-0.031	0.027	-0.043	-0.035	0.028	0.010	0.010	-0.011
H7	0.423	0.355	-0.300	0.469	0.388	-0.322	-0.121	-0.103	0.090
C13	0.007	0.002	0.002	0.013	0.004	0.004	0.070	0.017	0.039
H3	-0.078	-0.021	-0.038	-0.158	-0.042	-0.081	-0.792	-0.200	-0.426
C14	0.000	0.000	-0.001	0.000	0.000	0.000	-0.002	-0.002	0.002
N4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H6	0.101	-0.244	0.656	-0.095	0.209	-0.572	0.006	-0.009	0.028
H4	-0.075	-0.019	-0.046	0.119	0.031	0.070	-0.125	-0.034	-0.070
H2	0.001	0.001	0.001	0.001	0.001	0.000	-0.003	-0.002	-0.001
N2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C5	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H12	0.002	-0.005	-0.001	0.000	-0.001	0.000	0.000	0.000	0.000
H14	0.000	0.000	0.000	0.000	0.000	0.000	-0.001	0.000	-0.001
H16	-0.001	-0.003	0.005	0.000	0.000	0.000	0.000	0.001	-0.002
C4	0.001	0.000	-0.001	0.000	0.000	0.000	0.000	0.000	0.000
H18	0.001	0.001	0.000	0.000	0.000	0.000	-0.001	0.000	-0.001
H20	-0.008	0.000	0.003	0.000	0.000	0.000	0.000	0.000	0.000
H22	0.000	-0.006	0.007	0.000	0.000	0.000	0.000	0.001	-0.001
C6	0.000	-0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H28	-0.004	0.003	-0.001	0.000	0.000	0.000	-0.001	0.001	0.000
H26	0.003	0.004	-0.003	0.000	0.000	0.000	-0.001	-0.001	0.001
H5	0.000	0.000	0.000	0.000	0.000	0.000	-0.001	-0.001	-0.001
C7	-0.001	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000
H30	0.002	0.007	-0.004	0.000	0.000	0.000	-0.001	-0.002	0.001
H32	0.004	-0.002	-0.006	0.000	0.000	0.000	0.000	0.000	0.000
H34	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000
O2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	3168.06 A			3207.10 A			3207.78 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C8	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N5	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C9	0.000	0.001	-0.003	0.000	0.000	0.000	0.000	0.000	0.000
C10	0.070	0.020	0.038	0.000	0.000	0.000	0.000	0.000	0.000
C11	0.000	-0.007	0.015	0.000	0.000	0.000	0.000	0.000	0.000
C12	-0.006	-0.004	0.003	0.000	0.000	0.000	0.000	0.000	0.000
H7	0.049	0.041	-0.034	0.000	0.000	0.000	0.000	0.000	0.000
C13	-0.010	-0.002	-0.005	0.000	0.000	0.000	0.000	0.000	0.000
H3	0.110	0.028	0.059	0.000	0.000	0.000	0.000	0.000	0.000
C14	0.000	0.000	-0.001	0.000	0.000	0.000	0.000	0.000	0.000
N4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H6	-0.020	0.058	-0.152	0.000	0.000	0.000	0.000	0.000	0.000
H4	-0.787	-0.215	-0.439	0.000	0.000	0.000	0.000	0.000	0.000
H2	0.001	0.000	0.001	-0.001	-0.001	-0.001	-0.001	-0.001	0.000
N2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C3	0.000	0.000	0.000	0.000	0.000	-0.001	-0.001	0.001	0.000
C2	0.000	0.000	0.000	0.001	0.001	0.000	-0.001	0.001	0.000

C5	0.000	0.000	0.000	0.024	0.003	-0.005	-0.013	-0.002	0.002
H12	0.000	0.000	0.000	-0.105	0.285	0.032	0.056	-0.152	-0.017
H14	0.000	0.000	0.000	-0.171	-0.160	-0.247	0.093	0.088	0.135
H16	0.000	0.001	-0.001	-0.025	-0.160	0.274	0.013	0.087	-0.148
C4	0.000	0.000	0.000	-0.004	0.017	0.005	-0.007	0.029	0.009
H18	0.000	0.000	0.000	-0.159	-0.093	-0.168	-0.277	-0.162	-0.291
H20	0.000	0.000	0.000	0.205	0.016	-0.089	0.354	0.027	-0.154
H22	0.000	0.001	-0.001	0.004	-0.134	0.192	0.006	-0.231	0.332
C6	0.000	0.000	0.000	0.010	-0.011	-0.024	-0.007	0.007	0.015
H28	0.000	0.000	0.000	-0.248	0.222	-0.108	0.159	-0.142	0.069
H26	0.000	-0.001	0.001	-0.145	-0.271	0.189	0.093	0.173	-0.121
H5	-0.001	0.000	-0.001	0.264	0.188	0.214	-0.170	-0.120	-0.137
C7	0.000	0.000	0.000	-0.011	0.006	-0.005	-0.017	0.009	-0.008
H30	0.000	-0.001	0.001	-0.054	-0.136	0.081	-0.084	-0.211	0.126
H32	0.000	0.000	0.000	0.090	-0.042	-0.130	0.138	-0.065	-0.200
H34	0.000	0.000	0.000	0.099	0.105	0.112	0.154	0.165	0.175
O2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	3210.25 A			3211.64 A			3228.22 A		
	X	Y	Z	X	Y	Z	X	Y	Z
O1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.001	0.001
N1	0.000	0.000	0.000	0.000	0.000	0.000	-0.001	-0.001	-0.001
C1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C8	0.000	0.000	0.000	0.000	0.000	0.000	-0.003	0.000	-0.004
N5	0.000	0.000	0.000	0.000	0.000	0.000	0.059	0.041	0.021
C9	0.000	0.000	0.000	0.000	0.000	0.000	-0.003	-0.003	0.003
C10	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C11	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C12	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H7	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.002	-0.001
C13	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H3	-0.001	0.000	0.000	0.001	0.000	0.000	0.003	0.001	0.002
C14	0.000	0.000	0.000	0.000	0.000	0.000	-0.001	0.000	0.000
N4	0.000	0.000	0.000	0.000	0.000	0.000	-0.001	0.000	0.000
H6	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H4	-0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.001
H2	0.002	0.002	0.001	-0.002	-0.001	-0.001	-0.745	-0.525	-0.285
N2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C3	0.000	0.000	0.001	-0.001	0.001	0.000	0.000	0.000	0.000
C2	0.001	0.000	0.000	0.001	-0.001	0.000	0.000	0.000	0.000
C5	0.032	0.003	-0.007	0.008	0.001	-0.002	0.000	0.000	0.000
H12	-0.140	0.384	0.045	-0.036	0.098	0.012	0.000	0.000	0.000
H14	-0.218	-0.206	-0.317	-0.056	-0.054	-0.082	-0.001	-0.001	-0.001
H16	-0.032	-0.209	0.359	-0.008	-0.053	0.091	0.000	0.000	0.000
C4	-0.002	0.005	0.001	0.006	-0.022	-0.007	0.000	0.000	0.000
H18	-0.043	-0.025	-0.045	0.205	0.119	0.214	0.000	0.000	-0.001
H20	0.063	0.005	-0.027	-0.280	-0.022	0.119	0.000	0.000	0.000
H22	0.001	-0.038	0.055	-0.005	0.174	-0.250	0.000	0.000	0.000
C6	-0.011	0.011	0.022	-0.003	0.003	0.007	0.000	0.000	0.000
H28	0.245	-0.216	0.107	0.074	-0.065	0.032	0.001	-0.001	0.000
H26	0.139	0.258	-0.180	0.042	0.078	-0.054	0.000	0.001	0.000
H5	-0.246	-0.174	-0.199	-0.077	-0.054	-0.062	-0.001	-0.001	-0.001
C7	0.009	-0.005	0.003	-0.029	0.016	-0.012	0.000	0.000	0.000
H30	0.043	0.109	-0.064	-0.142	-0.357	0.212	0.000	0.001	-0.001
H32	-0.073	0.035	0.108	0.241	-0.117	-0.356	-0.001	0.001	0.002
H34	-0.077	-0.081	-0.087	0.254	0.272	0.290	-0.001	-0.001	-0.002
O2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

```
 Reason for exit: Successful completion
 Properties Program CPU Time : 000:00:02.9
 Properties Program Wall Time: 000:00:04.0
```

Output file for NITCN's PM3 calculation

```
MacSPARTAN PRO Density Functional Program:  (PowerPC)    Release 1.0


begin on orgel(G4/400)

nitcn.1

run type:                  FREQ
model:             LSDA/VWN/DN*
number of shells:           102
  63 S shells
  26 P shells
  13 D shells
number of valence orbitals: 206
point group symmetry used:   CS
spin multiplicity:            2

                      cartesian coordinates (angstroms)
        atom           x              y              z

       C6     1      1.4182841     -1.2338086      1.5747391
       C1     2      0.7796596      0.0000000      0.9850763
       C5     3      1.4182841      1.2338086      1.5747391
       H2     4      2.5053542      1.1776515      1.4026311
       H4     5      1.2355460      1.2858433      2.6592484
       H6     6      1.0525967      2.1607439      1.1075806
       C2     7     -0.7798874      0.0000000      0.9841933
       C7     8     -1.4186011      1.2330845      1.5746323
       H3     9     -1.2314147      1.2868817      2.6590736
       H9    10     -2.5069936      1.1766339      1.4066109
       H10   11     -1.0545654      2.1597670      1.1044514
       C8    12     -1.4186011     -1.2330845      1.5746323
       H5    13     -1.2314147     -1.2868817      2.6590736
       H11   14     -1.0545654     -2.1597670      1.1044514
       H12   15     -2.5069936     -1.1766339      1.4066109
       N1    16     -1.1164416      0.0000000     -0.4742317
       C3    17      0.0009760      0.0000000     -1.2272838
       N2    18      1.1176183      0.0000000     -0.4738283
       O1    19      2.3009419      0.0000000     -0.8764513
       C4    20      0.0001910      0.0000000     -2.6240318
       N3    21     -0.0034628      0.0000000     -3.7863289
       O2    22     -2.2993012      0.0000000     -0.8783799
       H1    23      2.5053542     -1.1776515      1.4026311
       H7    24      1.0525967     -2.1607439      1.1075806
       H8    25      1.2355460     -1.2858433      2.6592484

stoichiometry:        O2N3C8H12

molecular charge            0.0
number of electrons        97.0

integration mesh:          FINE
integration points and checksum: 101278      97.000005


  <S*S>  =           0.757

  E(DFT) =        -621.64894    VWN
                  -626.85744    pBP86


estimating force constant matrix by central differences
```

```
 force constant matrix estimation completed

 total time:     1415 min.  23.95 sec.

 end

  Reason for exit: Successful completion
  DFT Engine CPU Time : 023:35:24.0
  DFT Engine Wall Time: 026:17:34.3

MacSPARTAN PRO Properties Program:  (PowerPC)                    Release 1.0.4

  Molecule (CS ) and archive (C1 ) have different symmetry
  Use of molecular symmetry enabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          0

                    Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
     ---------    ------------- ------------- -------------

  1 C  C6           1.4182841    -1.2338086     1.5747390
  2 C  C1           0.7796597     0.0000000     0.9850763
  3 C  C5           1.4182841     1.2338086     1.5747390
  4 H  H2           2.5053542     1.1776515     1.4026311
  5 H  H4           1.2355460     1.2858433     2.6592484
  6 H  H6           1.0525968     2.1607439     1.1075806
  7 C  C2          -0.7798874     0.0000000     0.9841933
  8 C  C7          -1.4186010     1.2330845     1.5746323
  9 H  H3          -1.2314147     1.2868817     2.6590736
 10 H  H9          -2.5069936     1.1766339     1.4066109
 11 H  H10         -1.0545654     2.1597670     1.1044513
 12 C  C8          -1.4186010    -1.2330845     1.5746323
 13 H  H5          -1.2314147    -1.2868817     2.6590736
 14 H  H11         -1.0545654    -2.1597670     1.1044513
 15 H  H12         -2.5069936    -1.1766339     1.4066109
 16 N  N1          -1.1164416     0.0000000    -0.4742317
 17 C  C3           0.0009760     0.0000000    -1.2272839
 18 N  N2           1.1176183     0.0000000    -0.4738283
 19 O  O1           2.3009419     0.0000000    -0.8764513
 20 C  C4           0.0001910     0.0000000    -2.6240318
 21 N  N3          -0.0034628     0.0000000    -3.7863290
 22 O  O2          -2.2993012     0.0000000    -0.8783799
 23 H  H1           2.5053542    -1.1776515     1.4026311
 24 H  H7           1.0525968    -2.1607439     1.1075806
 25 H  H8           1.2355460    -1.2858433     2.6592484

  Point Group = CS  Order =  1 Nsymop =  2

  Normal Modes and Vibrational Frequencies (cm-1)

                   -83.63                  90.61                  136.16
                     A"                      A"                     A'
               X      Y      Z         X      Y      Z         X      Y      Z
 C6        -0.025 -0.063 -0.069     0.000 -0.024 -0.052    -0.009  0.001  0.033
 C1         0.000 -0.015  0.000     0.000  0.002  0.000     0.006  0.000  0.016
 C5         0.025 -0.063  0.069     0.000 -0.024  0.052    -0.009 -0.001  0.033
 H2         0.021 -0.064  0.040     0.000 -0.016  0.047    -0.006  0.004  0.051
 H4         0.054 -0.139  0.078     0.003 -0.073  0.054    -0.027 -0.009  0.031
 H6         0.024 -0.026  0.145    -0.001 -0.004  0.094    -0.005  0.001  0.033
 C2         0.000  0.015  0.000     0.000  0.001  0.000     0.006  0.000 -0.016
 C7         0.025  0.063 -0.069    -0.001 -0.025  0.051    -0.009  0.001 -0.033
```

H3	0.051	0.137	-0.077	-0.001	-0.071	0.054	-0.026	0.009	-0.031
H9	0.021	0.066	-0.043	-0.001	-0.018	0.049	-0.006	-0.004	-0.051
H10	0.026	0.027	-0.142	-0.001	-0.004	0.091	-0.005	-0.001	-0.034
C8	-0.025	0.063	0.069	0.001	-0.025	-0.051	-0.009	-0.001	-0.033
H5	-0.051	0.137	0.077	0.001	-0.071	-0.054	-0.026	-0.009	-0.031
H11	-0.026	0.027	0.142	0.001	-0.004	-0.091	-0.005	0.001	-0.034
H12	-0.021	0.066	0.043	0.001	-0.018	-0.049	-0.006	0.004	-0.051
N1	0.000	-0.047	0.000	0.000	0.049	0.000	0.042	0.000	-0.019
C3	0.000	0.000	0.000	0.000	0.011	0.000	0.055	0.000	0.000
N2	0.000	0.047	0.000	0.000	0.049	0.000	0.042	0.000	0.019
O1	0.000	0.090	0.000	0.000	0.094	0.000	0.055	0.000	0.054
C4	0.000	0.000	0.000	0.000	-0.066	0.000	-0.015	0.000	0.000
N3	0.000	0.000	0.000	0.000	-0.160	0.000	-0.212	0.000	0.000
O2	0.000	-0.090	0.000	0.000	0.095	0.000	0.055	0.000	-0.054
H1	-0.021	-0.064	-0.040	0.000	-0.016	-0.047	-0.006	-0.004	0.051
H7	-0.024	-0.026	-0.145	0.001	-0.004	-0.094	-0.005	-0.001	0.033
H8	-0.054	-0.139	-0.078	-0.003	-0.073	-0.054	-0.027	0.009	0.031

	138.66 A"			184.18 A"			185.13 A"		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	-0.022	-0.013	0.024	0.041	-0.006	-0.014	0.037	0.008	-0.084
C1	0.000	-0.015	0.000	0.000	-0.019	0.000	0.000	0.030	0.000
C5	0.022	-0.013	-0.024	-0.041	-0.006	0.014	-0.037	0.008	0.084
H2	0.048	-0.139	0.194	-0.021	-0.021	0.148	-0.018	0.009	0.197
H4	-0.191	0.145	-0.068	-0.174	0.044	-0.011	-0.145	-0.022	0.068
H6	0.211	-0.033	-0.215	0.022	-0.023	-0.069	0.012	0.025	0.080
C2	0.000	0.012	0.000	0.000	-0.032	0.000	0.000	0.016	0.000
C7	0.025	0.013	0.024	-0.032	-0.009	-0.083	-0.041	0.005	-0.018
H3	-0.164	-0.133	0.065	-0.113	0.035	-0.072	-0.171	-0.038	0.006
H9	0.048	0.130	-0.170	-0.018	-0.017	-0.167	-0.022	0.018	-0.150
H10	0.200	0.030	0.197	0.000	-0.029	-0.099	0.020	0.020	0.058
C8	-0.025	0.013	-0.024	0.032	-0.009	0.083	0.041	0.005	0.018
H5	0.164	-0.133	-0.065	0.113	0.035	0.072	0.171	-0.038	-0.006
H11	-0.200	0.030	-0.197	0.000	-0.029	0.099	-0.020	0.020	-0.058
H12	-0.048	0.130	0.170	0.018	-0.017	0.167	0.022	0.018	0.150
N1	0.000	0.016	0.000	0.000	-0.060	0.000	0.000	0.014	0.000
C3	0.000	0.000	0.000	0.000	-0.083	0.000	0.000	0.080	0.000
N2	0.000	-0.016	0.000	0.000	-0.018	0.000	0.000	0.059	0.000
O1	0.000	0.069	0.000	0.000	0.037	0.000	0.000	-0.137	0.000
C4	0.000	0.000	0.000	0.000	-0.028	0.000	0.000	0.028	0.000
N3	0.000	-0.001	0.000	0.000	0.042	0.000	0.000	-0.041	0.000
O2	0.000	-0.065	0.000	0.000	0.140	0.000	0.000	-0.028	0.000
H1	-0.048	-0.139	-0.194	0.021	-0.021	-0.148	0.018	0.009	-0.197
H7	-0.211	-0.033	0.215	-0.022	-0.023	0.069	-0.012	0.025	-0.080
H8	0.191	0.145	0.068	0.174	0.044	0.011	0.145	-0.022	-0.068

	221.35 A'			246.15 A"			266.70 A"		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.009	0.014	0.017	0.046	-0.008	0.011	-0.038	-0.025	0.058
C1	-0.014	0.000	0.012	0.000	-0.038	0.000	0.000	-0.031	0.000
C5	0.009	-0.014	0.017	-0.046	-0.008	-0.011	0.038	-0.025	-0.058
H2	-0.027	0.081	-0.253	-0.019	-0.052	0.177	0.019	-0.021	-0.186
H4	0.274	-0.176	0.069	-0.226	0.113	-0.048	0.156	-0.018	-0.039
H6	-0.175	0.019	0.229	0.057	-0.046	-0.168	-0.019	-0.033	-0.031
C2	-0.014	0.000	-0.010	0.000	-0.039	0.000	0.000	-0.031	0.000
C7	0.003	0.012	-0.018	0.048	-0.008	-0.008	-0.039	-0.025	-0.059
H3	0.236	0.158	-0.065	0.256	0.126	-0.052	-0.169	-0.024	-0.037
H9	-0.028	-0.073	0.219	0.018	-0.062	0.208	-0.019	-0.017	-0.199
H10	-0.162	-0.017	-0.206	-0.075	-0.048	-0.184	0.026	-0.032	-0.024
C8	0.003	-0.012	-0.018	-0.048	-0.008	0.008	0.039	-0.025	0.059
H5	0.236	-0.158	-0.065	-0.256	0.126	0.052	0.169	-0.024	0.037

H11	-0.162	0.017	-0.206	0.075	-0.048	0.184	-0.026	-0.032	0.024
H12	-0.028	0.073	0.219	-0.018	-0.062	-0.208	0.019	-0.017	0.199
N1	-0.007	0.000	-0.009	0.000	-0.002	0.000	0.000	-0.009	0.000
C3	0.000	0.000	0.000	0.000	0.096	0.000	0.000	0.125	0.000
N2	-0.007	0.000	0.010	0.000	-0.002	0.000	0.000	-0.009	0.000
O1	-0.006	0.000	0.014	0.000	0.002	0.000	0.000	0.024	0.000
C4	0.011	0.000	0.000	0.000	0.076	0.000	0.000	0.109	0.000
N3	0.004	0.000	0.000	0.000	-0.060	0.000	0.000	-0.077	0.000
O2	-0.005	0.000	-0.015	0.000	0.001	0.000	0.000	0.024	0.000
H1	-0.027	-0.081	-0.253	0.019	-0.052	-0.177	-0.019	-0.021	0.186
H7	-0.175	-0.019	0.229	-0.057	-0.046	0.168	0.019	-0.033	0.031
H8	0.274	0.176	0.069	0.226	0.113	0.048	-0.156	-0.018	0.039

	284.16 A'			284.60 A'			318.22 A'		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.044	-0.008	-0.061	-0.047	-0.033	-0.072	0.016	-0.034	-0.077
C1	-0.005	0.000	0.010	-0.023	0.000	-0.020	-0.002	0.000	0.009
C5	0.044	0.008	-0.061	-0.047	0.033	-0.072	0.016	0.034	-0.077
H2	0.010	0.052	-0.295	-0.040	0.028	-0.019	0.014	0.003	-0.075
H4	0.265	-0.030	-0.022	-0.101	0.135	-0.087	0.010	0.157	-0.084
H6	-0.087	0.005	0.036	-0.035	-0.014	-0.178	0.029	-0.013	-0.182
C2	-0.016	0.000	0.023	-0.017	0.000	0.001	0.002	0.000	0.009
C7	-0.064	-0.027	0.035	0.016	-0.021	0.086	-0.016	0.034	-0.079
H3	-0.245	-0.150	0.073	0.199	-0.025	0.055	-0.006	0.160	-0.087
H9	-0.038	0.008	-0.152	-0.011	-0.062	0.281	-0.014	0.002	-0.074
H10	0.029	0.017	0.194	-0.102	0.001	0.038	-0.031	-0.013	-0.188
C8	-0.064	0.027	0.035	0.016	0.021	0.086	-0.016	-0.034	-0.079
H5	-0.245	0.150	0.073	0.199	0.025	0.055	-0.006	-0.160	-0.087
H11	0.029	-0.017	0.194	-0.102	-0.001	0.038	-0.031	0.013	-0.188
H12	-0.038	-0.008	-0.152	-0.011	0.062	0.281	-0.014	-0.002	-0.074
N1	0.007	0.000	0.005	0.003	0.000	-0.009	0.003	0.000	0.030
C3	0.013	0.000	0.011	0.021	0.000	-0.006	0.000	0.000	0.024
N2	0.001	0.000	0.009	0.007	0.000	0.001	-0.004	0.000	0.030
O1	0.009	0.000	0.033	0.029	0.000	0.066	0.016	0.000	0.092
C4	0.011	0.000	0.012	0.021	0.000	-0.007	0.000	0.000	0.031
N3	-0.003	0.000	0.013	-0.005	0.000	-0.007	0.000	0.000	0.032
O2	0.023	0.000	-0.038	0.021	0.000	-0.061	-0.017	0.000	0.093
H1	0.010	-0.052	-0.295	-0.040	-0.028	-0.019	0.014	-0.003	-0.075
H7	-0.087	-0.005	0.036	-0.035	0.014	-0.178	0.029	0.013	-0.182
H8	0.265	0.030	-0.022	-0.101	-0.135	-0.087	0.010	-0.157	-0.084

	346.47 A"			352.02 A'			360.73 A'		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.096	0.013	0.003	-0.063	-0.034	-0.001	-0.025	0.019	0.012
C1	0.000	-0.037	0.000	0.026	0.000	-0.006	-0.021	0.000	-0.026
C5	-0.096	0.013	-0.003	-0.063	0.034	-0.001	-0.025	-0.019	0.012
H2	-0.106	0.158	-0.112	-0.057	0.151	-0.008	-0.030	0.008	-0.030
H4	0.002	-0.068	0.017	-0.062	0.006	0.001	0.014	-0.103	0.022
H6	-0.248	-0.008	0.083	-0.172	-0.001	0.015	-0.058	0.008	0.094
C2	0.000	-0.036	0.000	0.026	0.000	0.005	0.021	0.000	-0.026
C7	0.095	0.014	-0.003	-0.060	-0.033	0.001	0.026	-0.018	0.012
H3	-0.011	-0.071	0.019	-0.059	-0.007	0.000	-0.016	-0.105	0.024
H9	0.105	0.160	-0.120	-0.054	-0.147	0.010	0.032	0.012	-0.034
H10	0.250	-0.006	0.088	-0.167	0.001	-0.014	0.064	0.008	0.097
C8	-0.095	0.014	0.003	-0.060	0.033	0.001	0.026	0.018	0.012
H5	0.011	-0.071	-0.019	-0.059	0.007	0.000	-0.016	0.105	0.024
H11	-0.250	-0.006	-0.088	-0.167	-0.001	-0.014	0.064	-0.008	0.097
H12	-0.105	0.160	0.120	-0.054	0.147	0.010	0.032	-0.012	-0.034
N1	0.000	-0.016	0.000	0.057	0.000	0.035	0.004	0.000	-0.020
C3	0.000	0.009	0.000	0.037	0.000	-0.001	0.000	0.000	-0.074
N2	0.000	-0.018	0.000	0.057	0.000	-0.035	-0.005	0.000	-0.019

O1	0.000	0.006	0.000	0.041	0.000	-0.098	0.038	0.000	0.117
C4	0.000	0.023	0.000	0.008	0.000	-0.001	-0.001	0.000	-0.096
N3	0.000	-0.012	0.000	0.003	0.000	-0.001	0.000	0.000	-0.103
O2	0.000	0.006	0.000	0.040	0.000	0.100	-0.039	0.000	0.115
H1	0.106	0.158	0.112	-0.057	-0.151	-0.008	-0.030	-0.008	-0.030
H7	0.248	-0.008	-0.083	-0.172	0.001	0.015	-0.058	-0.008	0.094
H8	-0.002	-0.068	-0.017	-0.062	-0.006	0.001	0.014	0.103	0.022

	371.60			416.94			418.72		
	A"			A'			A'		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.062	-0.048	0.010	0.089	0.037	0.014	0.007	-0.009	-0.002
C1	0.000	-0.064	0.000	0.013	0.000	0.004	-0.003	0.000	0.016
C5	-0.062	-0.048	-0.010	0.089	-0.037	0.014	0.007	0.009	-0.002
H2	-0.056	0.047	0.007	0.099	-0.172	0.124	0.005	-0.003	-0.010
H4	-0.091	-0.074	-0.013	-0.008	0.016	-0.004	0.013	0.040	-0.003
H6	-0.145	-0.077	-0.002	0.236	-0.007	-0.049	0.012	-0.002	-0.027
C2	0.000	0.065	0.000	-0.013	0.000	0.005	-0.004	0.000	-0.016
C7	-0.064	0.048	0.010	-0.090	-0.037	0.015	0.002	-0.011	0.003
H3	-0.090	0.076	0.013	0.010	0.021	-0.005	0.013	-0.041	0.003
H9	-0.058	-0.049	-0.004	-0.100	-0.174	0.129	0.000	-0.005	0.015
H10	-0.149	0.077	0.001	-0.242	-0.008	-0.053	0.001	0.001	0.026
C8	0.064	0.048	-0.010	-0.090	0.037	0.015	0.002	0.011	0.003
H5	0.090	0.076	-0.013	0.010	-0.021	-0.005	0.013	0.041	0.003
H11	0.149	0.077	-0.001	-0.242	0.008	-0.053	0.001	-0.001	0.026
H12	0.058	-0.049	0.004	-0.100	0.174	0.129	0.000	0.005	0.015
N1	0.000	0.114	0.000	0.004	0.000	-0.007	-0.025	0.000	-0.036
C3	0.000	0.000	0.000	0.000	0.000	-0.026	0.015	0.000	-0.001
N2	0.000	-0.114	0.000	-0.001	0.000	-0.009	-0.025	0.000	0.035
O1	0.000	0.034	0.000	0.007	0.000	0.016	-0.051	0.000	-0.039
C4	0.000	0.000	0.000	-0.005	0.000	-0.040	0.244	0.000	-0.001
N3	0.000	0.000	0.000	0.002	0.000	-0.043	-0.071	0.000	-0.001
O2	0.000	-0.034	0.000	-0.004	0.000	0.015	-0.051	0.000	0.040
H1	0.056	0.047	-0.007	0.099	0.172	0.124	0.005	0.003	-0.010
H7	0.145	-0.077	0.002	0.236	0.007	-0.049	0.012	0.002	-0.027
H8	0.091	-0.074	0.013	-0.008	-0.016	-0.004	0.013	-0.040	-0.003

	504.96			523.40			544.20		
	A"			A'			A"		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.013	-0.024	0.030	0.007	-0.053	0.022	-0.031	0.056	-0.044
C1	0.000	-0.034	0.000	-0.002	0.000	0.094	0.000	0.055	0.000
C5	-0.013	-0.024	-0.030	0.007	0.053	0.022	0.031	0.056	0.044
H2	-0.017	-0.019	-0.060	0.003	0.072	-0.015	0.034	0.013	0.072
H4	0.011	0.033	-0.029	0.041	0.149	0.024	0.020	-0.027	0.047
H6	-0.028	-0.053	-0.074	-0.030	0.005	-0.046	0.086	0.114	0.119
C2	0.000	-0.034	0.000	0.004	0.000	0.092	0.000	-0.055	0.000
C7	0.013	-0.024	-0.030	-0.007	0.051	0.021	0.031	-0.056	-0.044
H3	-0.011	0.033	-0.029	-0.039	0.144	0.022	0.021	0.026	-0.047
H9	0.017	-0.019	-0.060	-0.003	0.069	-0.015	0.034	-0.013	-0.072
H10	0.028	-0.053	-0.074	0.029	0.004	-0.045	0.086	-0.114	-0.118
C8	-0.013	-0.024	0.030	-0.007	-0.051	0.021	-0.031	-0.056	0.044
H5	0.011	0.033	0.029	-0.039	-0.144	0.022	-0.021	0.026	0.047
H11	-0.028	-0.053	0.074	0.029	-0.004	-0.045	-0.086	-0.114	0.118
H12	-0.017	-0.019	0.060	-0.003	-0.069	-0.015	-0.034	-0.013	0.072
N1	0.000	0.086	0.000	0.042	0.000	0.019	0.000	0.126	0.000
C3	0.000	0.107	0.000	0.000	0.000	-0.041	0.000	0.000	0.000
N2	0.000	0.086	0.000	-0.042	0.000	0.021	0.000	-0.126	0.000
O1	0.000	-0.009	0.000	-0.068	0.000	-0.015	0.000	0.021	0.000
C4	0.000	-0.187	0.000	0.000	0.000	-0.096	0.000	0.000	0.000
N3	0.000	0.069	0.000	0.000	0.000	-0.109	0.000	0.000	0.000
O2	0.000	-0.009	0.000	0.066	0.000	-0.015	0.000	-0.020	0.000
H1	0.017	-0.019	0.060	0.003	-0.072	-0.015	-0.034	0.013	-0.072

H7	0.028	-0.053	0.074	-0.030	-0.005	-0.046	-0.086	0.114	-0.119
H8	-0.011	0.033	0.029	0.041	-0.149	0.024	-0.020	-0.027	-0.047

	544.42			610.66			612.66		
	A'			A'			A"		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.025	-0.080	0.031	0.025	-0.052	0.024	0.010	-0.021	0.020
C1	0.075	0.000	0.043	0.049	0.000	0.021	0.000	-0.021	0.000
C5	0.025	0.080	0.031	0.025	0.052	0.024	-0.010	-0.021	-0.020
H2	0.030	0.177	0.029	0.030	0.115	0.025	-0.014	-0.021	-0.048
H4	0.016	0.126	0.028	0.024	0.077	0.024	0.013	0.037	-0.020
H6	-0.070	0.021	-0.014	-0.027	0.023	0.005	-0.018	-0.046	-0.063
C2	0.074	0.000	-0.046	-0.050	0.000	0.021	0.000	-0.021	0.000
C7	0.024	-0.082	-0.031	-0.025	0.053	0.025	0.010	-0.021	-0.020
H3	0.018	-0.129	-0.028	-0.024	0.078	0.024	-0.012	0.037	-0.020
H9	0.029	-0.178	-0.027	-0.029	0.116	0.025	0.014	-0.021	-0.049
H10	-0.071	-0.021	0.016	0.028	0.023	0.005	0.018	-0.046	-0.064
C8	0.024	0.082	-0.031	-0.025	-0.053	0.025	-0.010	-0.021	0.020
H5	0.018	0.129	-0.028	-0.024	-0.078	0.024	0.012	0.037	0.020
H11	-0.071	0.021	0.016	0.028	-0.023	0.005	-0.018	-0.046	0.064
H12	0.029	0.178	-0.027	-0.029	-0.116	0.025	-0.014	-0.021	0.049
N1	-0.027	0.000	-0.048	-0.080	0.000	-0.028	0.000	0.128	0.000
C3	-0.030	0.000	0.000	0.000	0.000	0.002	0.000	-0.161	0.000
N2	-0.025	0.000	0.047	0.080	0.000	-0.029	0.000	0.127	0.000
O1	-0.039	0.000	0.027	0.115	0.000	-0.019	0.000	-0.023	0.000
C4	-0.053	0.000	0.001	0.000	0.000	-0.017	0.000	0.093	0.000
N3	0.009	0.000	0.001	0.000	0.000	-0.021	0.000	-0.028	0.000
O2	-0.042	0.000	-0.026	-0.115	0.000	-0.020	0.000	-0.023	0.000
H1	0.030	-0.177	0.029	0.030	-0.115	0.025	0.014	-0.021	0.048
H7	-0.070	-0.021	-0.014	-0.027	-0.023	0.005	0.018	-0.046	0.063
H8	0.016	-0.126	0.028	0.024	-0.077	0.024	-0.013	0.037	0.020

	647.04			772.64			884.11		
	A'			A'			A'		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.002	0.011	-0.018	-0.042	0.049	0.000	0.004	-0.065	0.024
C1	0.082	0.000	-0.101	-0.073	0.000	0.087	-0.046	0.000	-0.012
C5	0.002	-0.011	-0.018	-0.042	-0.049	0.000	0.004	0.065	0.024
H2	0.026	0.131	0.101	-0.067	-0.186	-0.117	-0.002	-0.036	0.007
H4	-0.139	-0.177	-0.034	0.085	0.095	0.014	0.069	0.052	0.038
H6	-0.083	0.003	0.077	0.031	-0.067	-0.092	0.114	0.136	0.074
C2	0.081	0.000	0.100	0.075	0.000	0.088	-0.045	0.000	0.011
C7	0.001	0.012	0.018	0.042	-0.049	0.000	0.004	-0.063	-0.023
H3	-0.137	0.177	0.034	-0.086	0.097	0.014	0.068	-0.052	-0.037
H9	0.024	-0.127	-0.100	0.066	-0.188	-0.118	-0.002	0.034	-0.007
H10	-0.082	-0.003	-0.076	-0.032	-0.068	-0.092	0.110	-0.131	-0.071
C8	0.001	-0.012	0.018	0.042	0.049	0.000	0.004	0.063	-0.023
H5	-0.137	-0.177	0.034	-0.086	-0.097	0.014	0.068	0.052	-0.037
H11	-0.082	0.003	-0.076	-0.032	0.068	-0.092	0.110	0.131	-0.071
H12	0.024	0.127	-0.100	0.066	0.188	-0.118	-0.002	-0.034	-0.007
N1	-0.032	0.000	0.036	-0.037	0.000	-0.005	-0.018	0.000	0.118
C3	-0.044	0.000	0.000	-0.001	0.000	0.010	-0.069	0.000	-0.001
N2	-0.032	0.000	-0.036	0.037	0.000	-0.007	-0.019	0.000	-0.120
O1	-0.010	0.000	0.050	0.049	0.000	-0.027	0.032	0.000	0.019
C4	0.053	0.000	0.000	0.001	0.000	-0.013	0.052	0.000	0.001
N3	-0.011	0.000	0.000	0.000	0.000	-0.017	-0.008	0.000	0.001
O2	-0.008	0.000	-0.049	-0.049	0.000	-0.028	0.033	0.000	-0.018
H1	0.026	-0.131	0.101	-0.067	0.186	-0.117	-0.002	0.036	0.007
H7	-0.083	-0.003	0.077	0.031	0.067	-0.092	0.114	-0.136	0.074
H8	-0.139	0.177	-0.034	0.085	-0.095	0.014	0.069	-0.052	0.038

924.32	925.00	941.22

	A'			A"			A"	
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.007	0.059	-0.022	0.054	-0.004	0.056	0.040	-0.004	0.058
C1	0.068	0.000	0.008	0.000	0.040	0.000	0.000	0.043	0.000
C5	0.007	-0.059	-0.022	-0.054	-0.004	-0.056	-0.040	-0.004	-0.058
H2	0.019	0.097	0.015	-0.056	-0.231	0.000	-0.035	-0.187	0.033
H4	-0.081	-0.050	-0.039	-0.012	-0.238	-0.037	-0.044	-0.248	-0.046
H6	-0.129	-0.135	-0.063	0.165	0.170	0.123	0.129	0.152	0.123
C2	-0.070	0.000	0.008	0.000	-0.037	0.000	0.000	0.047	0.000
C7	-0.007	-0.060	-0.023	-0.050	0.004	0.051	0.044	-0.004	-0.062
H3	0.083	-0.053	-0.040	-0.010	0.218	0.034	0.044	-0.265	-0.048
H9	-0.019	0.098	0.016	-0.052	0.214	0.001	0.040	-0.207	0.032
H10	0.130	-0.136	-0.064	0.153	-0.157	-0.113	-0.142	0.165	0.132
C8	-0.007	0.060	-0.023	0.050	0.004	-0.051	-0.044	-0.004	0.062
H5	0.083	0.053	-0.040	0.010	0.218	-0.034	-0.044	-0.265	0.048
H11	0.130	0.136	-0.064	-0.153	-0.157	0.113	0.142	0.165	-0.132
H12	-0.019	-0.098	0.016	0.052	0.214	-0.001	-0.040	-0.207	-0.032
N1	-0.028	0.000	0.095	0.000	-0.009	0.000	0.000	0.011	0.000
C3	-0.001	0.000	0.071	0.000	0.000	0.000	0.000	0.001	0.000
N2	0.027	0.000	0.091	0.000	0.010	0.000	0.000	0.011	0.000
O1	0.008	0.000	-0.017	0.000	-0.001	0.000	0.000	-0.001	0.000
C4	0.001	0.000	-0.049	0.000	0.000	0.000	0.000	0.000	0.000
N3	0.000	0.000	-0.077	0.000	0.000	0.000	0.000	0.000	0.000
O2	-0.007	0.000	-0.018	0.000	0.001	0.000	0.000	-0.001	0.000
H1	0.019	-0.097	0.015	0.056	-0.231	0.000	0.035	-0.187	-0.033
H7	-0.129	0.135	-0.063	-0.165	0.170	-0.123	-0.129	0.152	-0.123
H8	-0.081	0.050	-0.039	0.012	-0.238	0.037	0.044	-0.248	0.046

	970.16			977.14			979.89		
	A'			A"			A"		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	-0.002	-0.059	-0.028	0.071	0.002	-0.063	0.023	0.015	-0.018
C1	-0.041	0.000	-0.060	0.000	0.002	0.000	0.000	-0.009	0.000
C5	-0.002	0.059	-0.028	-0.071	0.002	0.063	-0.023	0.015	0.018
H2	0.005	-0.047	0.051	-0.123	-0.286	-0.215	-0.041	-0.134	-0.068
H4	-0.024	-0.147	-0.021	0.253	0.259	0.100	0.093	0.064	0.035
H6	0.131	0.198	0.144	0.152	-0.003	-0.125	0.087	0.042	-0.015
C2	-0.040	0.000	0.058	0.000	-0.007	0.000	0.000	-0.004	0.000
C7	-0.001	-0.056	0.027	-0.027	0.010	-0.026	0.070	0.011	0.060
H3	-0.027	0.143	0.021	0.087	-0.115	-0.037	-0.254	0.241	0.100
H9	0.007	0.039	-0.053	-0.045	0.074	0.083	0.121	-0.308	-0.211
H10	0.123	-0.190	-0.140	0.026	0.036	0.068	-0.173	0.024	-0.106
C8	-0.001	0.056	0.027	0.027	0.010	0.026	-0.070	0.011	-0.060
H5	-0.027	-0.143	0.021	-0.087	-0.115	0.037	0.254	0.241	-0.100
H11	0.123	0.190	-0.140	-0.026	0.036	-0.068	0.173	0.024	0.106
H12	0.007	-0.039	-0.053	0.045	0.074	-0.083	-0.121	-0.308	0.211
N1	0.014	0.000	-0.074	0.000	0.012	0.000	0.000	-0.023	0.000
C3	0.077	0.000	0.003	0.000	0.000	0.000	0.000	0.000	0.000
N2	0.016	0.000	0.081	0.000	-0.025	0.000	0.000	-0.005	0.000
O1	-0.013	0.000	-0.021	0.000	0.002	0.000	0.000	0.001	0.000
C4	-0.031	0.000	-0.001	0.000	0.001	0.000	0.000	0.001	0.000
N3	0.005	0.000	-0.002	0.000	0.000	0.000	0.000	0.000	0.000
O2	-0.014	0.000	0.019	0.000	0.000	0.000	0.000	0.002	0.000
H1	0.005	0.047	0.051	0.123	-0.286	0.215	0.041	-0.134	0.068
H7	0.131	-0.198	0.144	-0.152	-0.003	0.125	-0.087	0.042	0.015
H8	-0.024	0.147	-0.021	-0.253	0.259	-0.100	-0.093	0.064	-0.035

	993.40			1118.94			1127.33		
	A'			A'			A'		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.023	0.045	0.004	-0.052	-0.001	0.030	-0.005	0.015	0.061
C1	0.018	0.000	0.061	0.089	0.000	-0.084	0.033	0.000	-0.103
C5	0.023	-0.045	0.004	-0.052	0.001	0.030	-0.005	-0.015	0.061

H2	0.035	0.144	0.034	-0.080	-0.145	-0.130	-0.029	0.013	-0.123
H4	-0.065	0.046	-0.013	0.134	0.067	0.053	0.106	0.215	0.063
H6	-0.152	-0.148	-0.061	0.120	0.008	-0.091	-0.004	-0.110	-0.136
C2	-0.021	0.000	0.064	0.083	0.000	0.070	-0.046	0.000	-0.112
C7	-0.023	-0.049	0.006	-0.051	-0.004	-0.021	0.012	-0.015	0.064
H3	0.063	0.055	-0.013	0.118	-0.037	-0.044	-0.123	0.222	0.070
H9	-0.034	0.146	0.030	-0.075	0.147	0.113	0.039	-0.009	-0.140
H10	0.160	-0.160	-0.071	0.121	-0.024	0.071	-0.012	-0.108	-0.147
C8	-0.023	0.049	0.006	-0.051	0.004	-0.021	0.012	0.015	0.064
H5	0.063	-0.055	-0.013	0.118	0.037	-0.044	-0.123	-0.222	0.070
H11	0.160	0.160	-0.071	0.121	0.024	0.071	-0.012	0.108	-0.147
H12	-0.034	-0.146	0.030	-0.075	-0.147	0.113	0.039	0.009	-0.140
N1	0.027	0.000	-0.097	-0.006	0.000	-0.049	0.005	0.000	0.010
C3	0.003	0.000	-0.076	-0.082	0.000	-0.001	0.006	0.000	-0.011
N2	-0.026	0.000	-0.093	-0.007	0.000	0.049	-0.004	0.000	0.004
O1	-0.009	0.000	0.020	0.026	0.000	-0.006	-0.016	0.000	0.008
C4	-0.001	0.000	0.038	0.005	0.000	0.000	0.000	0.000	0.002
N3	0.000	0.000	0.064	-0.001	0.000	0.000	0.000	0.000	0.004
O2	0.008	0.000	0.021	0.028	0.000	0.008	0.012	0.000	0.007
H1	0.035	-0.144	0.034	-0.080	0.145	-0.130	-0.029	-0.013	-0.123
H7	-0.152	0.148	-0.061	0.120	-0.008	-0.091	-0.004	0.110	-0.136
H8	-0.065	-0.046	-0.013	0.134	-0.067	0.053	0.106	-0.215	0.063

	1159.24 A"			1197.05 A'			1224.61 A'		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.017	-0.061	-0.002	-0.042	-0.005	-0.027	-0.001	0.007	0.038
C1	0.000	0.160	0.000	0.092	0.000	0.089	-0.010	0.000	-0.095
C5	-0.017	-0.061	0.002	-0.042	0.005	-0.027	-0.001	-0.007	0.038
H2	-0.031	-0.015	-0.080	-0.038	-0.145	0.024	-0.011	0.052	-0.058
H4	-0.045	0.031	-0.011	0.055	-0.112	-0.006	0.056	0.140	0.037
H6	-0.089	-0.140	-0.098	0.067	0.066	0.021	0.019	-0.040	-0.054
C2	0.000	0.158	0.000	0.091	0.000	-0.089	-0.010	0.000	0.096
C7	0.017	-0.061	0.002	-0.041	-0.006	0.028	0.000	0.007	-0.038
H3	0.044	0.032	-0.011	0.054	0.112	0.005	0.056	-0.142	-0.038
H9	0.031	-0.014	-0.080	-0.038	0.146	-0.024	-0.011	-0.052	0.060
H10	0.089	-0.139	-0.098	0.067	-0.066	-0.023	0.018	0.041	0.054
C8	-0.017	-0.061	-0.002	-0.041	0.006	0.028	0.000	-0.007	-0.038
H5	-0.044	0.032	0.011	0.054	-0.112	0.005	0.056	0.142	-0.038
H11	-0.089	-0.139	0.098	0.067	0.066	-0.023	0.018	-0.041	0.054
H12	-0.031	-0.014	0.080	-0.038	-0.146	-0.024	-0.011	0.052	0.060
N1	0.000	-0.017	0.000	0.015	0.000	0.056	0.012	0.000	0.045
C3	0.000	0.004	0.000	0.079	0.000	0.000	0.169	0.000	0.000
N2	0.000	-0.018	0.000	0.015	0.000	-0.056	0.012	0.000	-0.045
O1	0.000	0.001	0.000	-0.058	0.000	0.024	-0.068	0.000	0.016
C4	0.000	0.003	0.000	-0.006	0.000	0.000	-0.019	0.000	0.000
N3	0.000	-0.001	0.000	0.001	0.000	0.000	0.004	0.000	0.000
O2	0.000	0.001	0.000	-0.058	0.000	-0.024	-0.068	0.000	-0.017
H1	0.031	-0.015	0.080	-0.038	0.145	0.024	-0.011	-0.052	-0.058
H7	0.089	-0.140	0.098	0.067	-0.066	0.021	0.019	0.040	-0.054
H8	0.045	0.031	0.011	0.055	0.112	-0.006	0.056	-0.140	0.037

	1238.29 A"			1268.45 A'			1346.71 A"		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	-0.010	-0.039	-0.002	-0.050	0.000	-0.014	-0.029	0.066	-0.030
C1	0.000	0.166	0.000	0.153	0.000	0.047	0.000	-0.054	0.000
C5	0.010	-0.039	0.002	-0.050	0.000	-0.014	0.029	0.066	0.030
H2	-0.008	-0.046	-0.085	-0.044	-0.108	0.018	-0.018	-0.245	-0.145
H4	-0.111	-0.025	-0.024	0.124	-0.089	0.019	-0.154	-0.211	0.008
H6	-0.120	-0.133	-0.078	0.108	0.043	-0.042	-0.136	-0.091	-0.139
C2	0.000	-0.167	0.000	-0.153	0.000	0.047	0.000	0.051	0.000
C7	0.009	0.040	-0.002	0.051	0.001	-0.014	0.024	-0.058	-0.026

H3	-0.111	0.024	0.025	-0.124	-0.089	0.020	-0.124	0.179	-0.008
H9	-0.008	0.045	0.086	0.044	-0.111	0.016	-0.015	0.213	0.117
H10	-0.121	0.134	0.079	-0.108	0.043	-0.042	-0.114	0.075	0.118
C8	-0.009	0.040	0.002	0.051	-0.001	-0.014	-0.024	-0.058	0.026
H5	0.111	0.024	-0.025	-0.124	0.089	0.020	0.124	0.179	0.008
H11	0.121	0.134	-0.079	-0.108	-0.043	-0.042	0.114	0.075	-0.118
H12	0.008	0.045	-0.086	0.044	0.111	0.016	0.015	0.213	-0.117
N1	0.000	0.013	0.000	0.005	0.000	-0.026	0.000	-0.003	0.000
C3	0.000	0.000	0.000	0.000	0.000	-0.026	0.000	0.000	0.000
N2	0.000	-0.013	0.000	-0.005	0.000	-0.026	0.000	0.003	0.000
O1	0.000	0.001	0.000	-0.013	0.000	0.013	0.000	0.000	0.000
C4	0.000	0.000	0.000	0.000	0.000	0.004	0.000	0.000	0.000
N3	0.000	0.000	0.000	0.000	0.000	0.011	0.000	0.000	0.000
O2	0.000	-0.001	0.000	0.013	0.000	0.013	0.000	0.000	0.000
H1	0.008	-0.046	0.085	-0.044	0.108	0.018	0.018	-0.245	0.145
H7	0.120	-0.133	0.078	0.108	-0.043	-0.042	0.136	-0.091	0.139
H8	0.111	-0.025	0.024	0.124	0.089	0.019	0.154	-0.211	-0.008

	1356.03 A"			1360.68 A'			1374.07 A'		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	-0.028	0.046	-0.027	-0.031	0.051	-0.034	0.021	-0.043	0.026
C1	0.000	-0.013	0.000	0.002	0.000	0.003	0.012	0.000	0.005
C5	0.028	0.046	0.027	-0.031	-0.051	-0.034	0.021	0.043	0.026
H2	-0.018	-0.183	-0.161	0.023	0.223	0.203	-0.023	-0.184	-0.169
H4	-0.178	-0.184	-0.002	0.209	0.187	0.001	-0.171	-0.198	0.000
H6	-0.120	-0.096	-0.128	0.129	0.102	0.136	-0.099	-0.094	-0.142
C2	0.000	-0.021	0.000	0.004	0.000	-0.004	-0.012	0.000	0.005
C7	-0.032	0.056	0.032	-0.029	0.045	0.030	-0.025	0.049	0.030
H3	0.200	-0.217	-0.001	0.189	-0.163	-0.002	0.195	-0.218	0.000
H9	0.019	-0.218	-0.180	0.019	-0.199	-0.182	0.025	-0.208	-0.192
H10	0.139	-0.110	-0.151	0.116	-0.091	-0.119	0.112	-0.106	-0.157
C8	0.032	0.056	-0.032	-0.029	-0.045	0.030	-0.025	-0.049	0.030
H5	-0.200	-0.217	0.001	0.189	0.163	-0.002	0.195	0.218	0.000
H11	-0.139	-0.110	0.151	0.116	0.091	-0.119	0.112	0.106	-0.157
H12	-0.019	-0.218	0.180	0.019	0.199	-0.182	0.025	0.208	-0.192
N1	0.000	0.002	0.000	0.011	0.000	-0.011	0.018	0.000	0.013
C3	0.000	-0.001	0.000	-0.025	0.000	0.003	-0.001	0.000	-0.048
N2	0.000	0.002	0.000	0.013	0.000	0.009	-0.017	0.000	0.014
O1	0.000	-0.001	0.000	-0.003	0.000	0.002	0.014	0.000	-0.007
C4	0.000	-0.001	0.000	0.002	0.000	0.000	0.000	0.000	0.004
N3	0.000	0.000	0.000	-0.001	0.000	-0.001	0.000	0.000	0.015
O2	0.000	-0.001	0.000	-0.001	0.000	-0.001	-0.015	0.000	-0.007
H1	0.018	-0.183	0.161	0.023	-0.223	0.203	-0.023	0.184	-0.169
H7	0.120	-0.096	0.128	0.129	-0.102	0.136	-0.099	0.094	-0.142
H8	0.178	-0.184	0.002	0.209	-0.187	0.001	-0.171	0.198	0.000

	1399.49 A"			1420.75 A"			1426.26 A"		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.019	0.014	-0.001	0.006	-0.011	-0.026	-0.018	-0.019	0.001
C1	0.000	0.022	0.000	0.000	-0.006	0.000	0.000	-0.008	0.000
C5	-0.019	0.014	0.001	-0.006	-0.011	0.026	0.018	-0.019	-0.001
H2	0.019	0.090	0.187	-0.031	0.241	-0.249	-0.019	-0.061	-0.191
H4	0.247	-0.231	0.056	-0.145	-0.121	-0.001	-0.254	0.224	-0.057
H6	0.040	-0.104	-0.265	0.270	0.039	-0.112	-0.019	0.105	0.255
C2	0.000	-0.022	0.000	0.000	0.006	0.000	0.000	-0.008	0.000
C7	-0.019	-0.013	-0.001	-0.005	0.010	-0.025	-0.019	-0.019	-0.001
H3	0.244	0.223	-0.056	-0.144	0.117	0.002	0.258	0.229	-0.059
H9	0.019	-0.088	-0.186	-0.030	-0.234	0.245	0.018	-0.064	-0.193
H10	0.038	0.102	0.258	0.264	-0.038	0.107	0.022	0.107	0.261
C8	0.019	-0.013	0.001	0.005	0.010	0.025	0.019	-0.019	0.001
H5	-0.244	0.223	0.056	0.144	0.117	-0.002	-0.258	0.229	0.059

H11	-0.038	0.102	-0.258	-0.264	-0.038	-0.107	-0.022	0.107	-0.261
H12	-0.019	-0.088	0.186	0.030	-0.234	-0.245	-0.018	-0.064	0.193
N1	0.000	0.001	0.000	0.000	-0.001	0.000	0.000	0.000	0.000
C3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N2	0.000	-0.001	0.000	0.000	0.001	0.000	0.000	0.000	0.000
O1	0.000	0.000	0.000	0.000	-0.001	0.000	0.000	0.000	0.000
C4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O2	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000
H1	-0.019	0.090	-0.187	0.031	0.241	0.249	0.019	-0.061	0.191
H7	-0.040	-0.104	0.265	-0.270	0.039	0.112	0.019	0.105	-0.255
H8	-0.247	-0.231	-0.056	0.145	-0.121	0.001	0.254	0.224	0.057

	1427.70 A'			1450.06 A'			1451.46 A"		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	-0.009	-0.023	0.005	0.009	-0.016	-0.016	0.009	-0.013	-0.022
C1	-0.032	0.000	-0.008	0.002	0.000	-0.035	0.000	-0.006	0.000
C5	-0.009	0.023	0.005	0.009	0.016	-0.016	-0.009	-0.013	0.022
H2	0.027	0.078	0.186	0.026	-0.268	0.214	-0.026	0.250	-0.213
H4	0.229	-0.237	0.058	0.127	0.123	0.006	-0.111	-0.111	0.002
H6	0.013	-0.112	-0.266	-0.281	-0.052	0.095	0.292	0.050	-0.110
C2	-0.031	0.000	0.008	0.002	0.000	0.034	0.000	-0.006	0.000
C7	-0.009	-0.023	-0.005	0.009	-0.015	0.016	0.009	-0.013	0.022
H3	0.226	0.234	-0.059	0.123	-0.122	-0.006	0.112	-0.116	0.002
H9	0.026	-0.075	-0.184	0.025	0.259	-0.208	0.026	0.255	-0.217
H10	0.012	0.112	0.263	-0.271	0.049	-0.094	-0.300	0.050	-0.114
C8	-0.009	0.023	-0.005	0.009	0.015	0.016	-0.009	-0.013	-0.022
H5	0.226	-0.234	-0.059	0.123	0.122	-0.006	-0.112	-0.116	-0.002
H11	0.012	-0.112	0.263	-0.271	-0.049	-0.094	0.300	0.050	0.114
H12	0.026	0.075	-0.184	0.025	-0.259	-0.208	-0.026	0.255	0.217
N1	-0.003	0.000	0.001	0.006	0.000	-0.007	0.000	0.001	0.000
C3	0.004	0.000	0.000	-0.004	0.000	0.005	0.000	0.000	0.000
N2	-0.003	0.000	-0.001	0.008	0.000	0.003	0.000	0.001	0.000
O1	0.004	0.000	-0.002	-0.005	0.000	0.001	0.000	-0.001	0.000
C4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N3	0.000	0.000	0.000	0.000	0.000	-0.001	0.000	0.000	0.000
O2	0.004	0.000	0.002	-0.002	0.000	0.000	0.000	-0.001	0.000
H1	0.027	-0.078	0.186	0.026	0.268	0.214	0.026	0.250	0.213
H7	0.013	0.112	-0.266	-0.281	0.052	0.095	-0.292	0.050	0.110
H8	0.229	0.237	0.058	0.127	-0.123	0.006	0.111	-0.111	-0.002

	1453.84 A'			1458.54 A'			1481.32 A'		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.008	-0.010	0.008	-0.004	-0.023	0.001	-0.010	0.011	0.018
C1	0.008	0.000	-0.001	-0.047	0.000	-0.015	-0.021	0.000	0.016
C5	0.008	0.010	0.008	-0.004	0.023	0.001	-0.010	-0.011	0.018
H2	-0.006	-0.078	-0.051	0.034	0.028	0.227	-0.018	0.269	-0.156
H4	-0.060	0.001	-0.003	0.247	-0.185	0.054	-0.064	-0.151	0.010
H6	-0.051	-0.014	0.005	-0.061	-0.122	-0.223	0.278	0.028	-0.150
C2	-0.008	0.000	-0.002	0.047	0.000	-0.016	0.021	0.000	0.017
C7	-0.008	0.011	0.007	0.004	0.024	0.001	0.010	-0.011	0.019
H3	0.055	0.007	-0.003	-0.251	-0.185	0.056	0.065	-0.156	0.010
H9	0.005	-0.091	-0.042	-0.034	0.024	0.233	0.018	0.276	-0.160
H10	0.064	-0.016	0.010	0.065	-0.125	-0.224	-0.286	0.028	-0.153
C8	-0.008	-0.011	0.007	0.004	-0.024	0.001	0.010	0.011	0.019
H5	0.055	-0.007	-0.003	-0.251	0.185	0.056	0.065	0.156	0.010
H11	0.064	0.016	0.010	0.065	0.125	-0.224	-0.286	-0.028	-0.153
H12	0.005	0.091	-0.042	-0.034	-0.024	0.233	0.018	-0.276	-0.160
N1	-0.034	0.000	-0.093	-0.013	0.000	-0.005	0.008	0.000	-0.015
C3	0.000	0.000	0.206	0.000	0.000	0.022	0.000	0.000	0.038
N2	0.035	0.000	-0.093	0.013	0.000	-0.005	-0.008	0.000	-0.015

O1	-0.046	0.000	0.027	-0.007	0.000	0.002	0.003	0.000	0.001
C4	0.000	0.000	-0.011	0.000	0.000	-0.001	0.000	0.000	-0.002
N3	0.000	0.000	-0.057	0.000	0.000	-0.007	0.000	0.000	-0.010
O2	0.045	0.000	0.027	0.007	0.000	0.002	-0.003	0.000	0.001
H1	-0.006	0.078	-0.051	0.034	-0.028	0.227	-0.018	-0.269	-0.156
H7	-0.051	0.014	0.005	-0.061	0.122	-0.223	0.278	-0.028	-0.150
H8	-0.060	-0.001	-0.003	0.247	0.185	0.054	-0.064	0.151	0.010

	1549.59			1557.35			2305.59		
	A'			A'			A'		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.004	-0.004	0.003	-0.003	0.001	0.000	0.000	0.000	0.000
C1	-0.021	0.000	-0.014	0.011	0.000	-0.003	0.000	0.000	-0.001
C5	0.004	0.004	0.003	-0.003	-0.001	0.000	0.000	0.000	0.000
H2	0.001	0.001	-0.026	0.001	-0.015	0.036	0.000	0.000	0.000
H4	-0.021	-0.021	0.000	0.037	0.024	0.006	0.000	0.000	0.000
H6	-0.001	-0.008	-0.020	-0.020	-0.005	0.007	0.000	0.000	0.000
C2	-0.023	0.000	0.014	-0.008	0.000	-0.005	0.000	0.000	-0.001
C7	0.005	-0.004	-0.003	0.002	0.000	0.000	0.000	0.000	0.000
H3	-0.027	0.025	0.001	-0.033	0.020	0.006	0.000	0.000	0.000
H9	0.001	-0.003	0.031	-0.001	-0.014	0.032	0.000	0.000	0.000
H10	0.002	0.007	0.021	0.020	-0.007	0.004	0.000	0.000	0.000
C8	0.005	0.004	-0.003	0.002	0.000	0.000	0.000	0.000	0.000
H5	-0.027	-0.025	0.001	-0.033	-0.020	0.006	0.000	0.000	0.000
H11	0.002	-0.007	0.021	0.020	0.007	0.004	0.000	0.000	0.000
H12	0.001	0.003	0.031	-0.001	0.014	0.032	0.000	0.000	0.000
N1	0.158	0.000	0.000	0.139	0.000	-0.010	-0.003	0.000	0.001
C3	-0.124	0.000	0.007	0.010	0.000	0.096	0.000	0.000	0.039
N2	0.134	0.000	-0.001	-0.163	0.000	-0.011	0.003	0.000	0.001
O1	-0.065	0.000	0.022	0.086	0.000	-0.021	-0.002	0.000	0.001
C4	0.012	0.000	-0.001	-0.001	0.000	-0.006	-0.001	0.000	-0.228
N3	-0.003	0.000	-0.001	0.000	0.000	-0.019	0.000	0.000	0.160
O2	-0.079	0.000	-0.025	-0.075	0.000	-0.017	0.002	0.000	0.001
H1	0.001	-0.001	-0.026	0.001	0.015	0.036	0.000	0.000	0.000
H7	-0.001	0.008	-0.020	-0.020	0.005	0.007	0.000	0.000	0.000
H8	-0.021	0.021	0.000	0.037	-0.024	0.006	0.000	0.000	0.000

	2969.82			2971.96			2976.78		
	A"			A'			A"		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.004	-0.009	0.004	0.005	-0.010	0.004	0.017	-0.025	0.014
C1	0.000	0.001	0.000	-0.001	0.000	0.000	0.000	0.001	0.000
C5	-0.004	-0.009	-0.004	0.005	0.010	0.004	-0.017	-0.025	-0.014
H2	0.121	-0.009	-0.020	-0.132	0.010	0.021	0.386	-0.026	-0.062
H4	-0.022	0.005	0.125	0.023	-0.005	-0.134	-0.068	0.013	0.380
H6	-0.045	0.108	-0.056	0.048	-0.118	0.061	-0.128	0.300	-0.157
C2	0.000	-0.002	0.000	-0.001	0.000	0.000	0.000	0.000	0.000
C7	-0.016	0.025	0.014	0.016	-0.026	-0.014	0.007	-0.007	-0.005
H3	-0.069	-0.014	-0.382	0.068	0.014	0.377	0.024	0.004	0.129
H9	0.382	0.026	0.060	-0.377	-0.026	-0.058	-0.135	-0.008	-0.021
H10	-0.128	-0.302	0.159	0.126	0.302	-0.158	0.040	0.091	-0.048
C8	0.016	0.025	-0.014	0.016	0.026	-0.014	-0.007	-0.007	0.005
H5	0.069	-0.014	0.382	0.068	-0.014	0.377	-0.024	0.004	-0.129
H11	0.128	-0.302	-0.159	0.126	-0.302	-0.158	-0.040	0.091	0.048
H12	-0.382	0.026	-0.060	-0.377	0.026	-0.058	0.135	-0.008	0.021
N1	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.000
C3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H1	-0.121	-0.009	0.020	-0.132	-0.010	0.021	-0.386	-0.026	0.062

H7	0.045	0.108	0.056	0.048	0.118	0.061	0.128	0.300	0.157
H8	0.022	0.005	-0.125	0.023	0.005	-0.134	0.068	0.013	-0.380

	2979.23			3060.84			3064.29		
	A'			A"			A'		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	0.016	-0.025	0.014	-0.010	-0.005	0.000	0.005	0.004	0.004
C1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001
C5	0.016	0.025	0.014	0.010	-0.005	0.000	0.005	-0.004	0.004
H2	-0.380	0.025	0.060	-0.096	0.004	0.015	-0.039	0.001	0.007
H4	0.067	-0.013	-0.376	-0.002	0.000	0.016	0.006	-0.002	-0.032
H6	0.127	-0.299	0.155	-0.023	0.058	-0.030	-0.020	0.050	-0.025
C2	-0.001	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.000
C7	-0.007	0.008	0.006	0.054	0.022	0.019	0.055	0.026	0.013
H3	-0.026	-0.005	-0.141	-0.041	-0.008	-0.276	-0.031	-0.005	-0.226
H9	0.144	0.008	0.022	-0.525	-0.027	-0.078	-0.528	-0.025	-0.079
H10	-0.043	-0.099	0.052	-0.085	-0.228	0.123	-0.105	-0.273	0.144
C8	-0.007	-0.008	0.006	-0.054	0.022	-0.019	0.055	-0.026	0.013
H5	-0.026	0.005	-0.141	0.041	-0.008	0.276	-0.031	0.005	-0.226
H11	-0.043	0.099	0.052	0.085	-0.228	-0.123	-0.105	0.273	0.144
H12	0.144	-0.008	0.022	0.525	-0.027	0.078	-0.528	0.025	-0.079
N1	0.000	0.000	-0.001	0.000	0.000	0.000	0.000	0.000	0.000
C3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N2	0.001	0.000	-0.001	0.000	0.000	0.000	0.000	0.000	0.000
O1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H1	-0.380	-0.025	0.060	0.096	0.004	-0.015	-0.039	-0.001	0.007
H7	0.127	0.299	0.155	0.023	0.058	0.030	-0.020	-0.050	-0.025
H8	0.067	0.013	-0.376	0.002	0.000	-0.016	0.006	0.002	-0.032

	3066.90			3068.94			3069.20		
	A"			A'			A"		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	-0.051	-0.025	0.010	0.035	0.025	0.009	-0.018	0.005	0.032
C1	0.000	0.000	0.000	0.002	0.000	0.001	0.000	0.000	0.000
C5	0.051	-0.025	-0.010	0.035	-0.025	0.009	0.018	0.005	-0.032
H2	-0.482	0.024	0.076	-0.319	0.013	0.053	-0.206	0.013	0.026
H4	-0.024	0.004	0.186	0.008	-0.005	-0.011	-0.053	0.014	0.315
H6	-0.104	0.271	-0.143	-0.115	0.289	-0.148	0.039	-0.087	0.039
C2	0.000	0.000	0.000	0.000	0.000	-0.001	0.000	-0.001	0.000
C7	-0.006	0.007	-0.023	-0.004	0.018	-0.041	-0.007	-0.026	0.043
H3	0.038	0.010	0.215	0.065	0.020	0.361	-0.066	-0.019	-0.352
H9	0.087	0.007	0.009	0.083	0.009	0.004	0.014	-0.004	0.011
H10	-0.045	-0.105	0.050	-0.102	-0.243	0.120	0.140	0.340	-0.169
C8	0.006	0.007	0.023	-0.004	-0.018	-0.041	0.007	-0.026	-0.043
H5	-0.038	0.010	-0.215	0.065	-0.020	0.361	0.066	-0.019	0.352
H11	0.045	-0.105	-0.050	-0.102	0.243	0.120	-0.140	0.340	0.169
H12	-0.087	0.007	-0.009	0.083	-0.009	0.004	-0.014	-0.004	-0.011
N1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H1	0.482	0.024	-0.076	-0.319	-0.013	0.053	0.206	0.013	-0.026
H7	0.104	0.271	0.143	-0.115	-0.289	-0.148	-0.039	-0.087	-0.039
H8	0.024	0.004	-0.186	0.008	0.005	-0.011	0.053	0.014	-0.315

3071.17	3079.16	3079.88

	A'			A"			A'		
	X	Y	Z	X	Y	Z	X	Y	Z
C6	-0.042	-0.011	0.029	-0.007	-0.028	-0.047	-0.003	-0.027	-0.049
C1	-0.002	0.000	0.000	0.000	-0.001	0.000	0.000	0.000	-0.002
C5	-0.042	0.011	0.029	0.007	-0.028	0.047	-0.003	0.027	-0.049
H2	0.426	-0.023	-0.062	-0.007	-0.004	0.010	-0.031	0.007	-0.005
H4	0.052	-0.012	-0.338	0.072	-0.021	-0.389	-0.075	0.023	0.413
H6	0.032	-0.090	0.051	-0.154	0.368	-0.182	0.148	-0.352	0.175
C2	0.000	0.000	-0.001	0.000	0.000	0.000	0.000	0.000	-0.001
C7	0.001	0.017	-0.030	-0.006	-0.016	0.024	0.004	0.015	-0.024
H3	0.047	0.014	0.254	-0.037	-0.011	-0.191	0.036	0.012	0.193
H9	0.025	0.005	-0.003	0.021	-0.001	0.007	-0.009	0.002	-0.006
H10	-0.091	-0.217	0.109	0.087	0.208	-0.104	-0.083	-0.198	0.099
C8	0.001	-0.017	-0.030	0.006	-0.016	-0.024	0.004	-0.015	-0.024
H5	0.047	-0.014	0.254	0.037	-0.011	0.191	0.036	-0.012	0.193
H11	-0.091	0.217	0.109	-0.087	0.208	0.104	-0.083	0.198	0.099
H12	0.025	-0.005	-0.003	-0.021	-0.001	-0.007	-0.009	-0.002	-0.006
N1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
N3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H1	0.426	0.023	-0.062	0.007	-0.004	-0.010	-0.031	-0.007	-0.005
H7	0.032	0.090	0.051	0.154	0.368	0.182	0.148	0.352	0.175
H8	0.052	0.012	-0.338	-0.072	-0.021	0.389	-0.075	-0.023	0.413

```
 Reason for exit: Successful completion
 Properties Program CPU Time : 000:00:02.7
 Properties Program Wall Time: 000:00:04.3
```

Output file for NITPy's DFT calculation

```
MacSPARTAN PRO Density Functional Program:  (PowerPC)    Release 1.0


 begin on I101174-CHIMI(G4/400)

 NITPY.PDB

 run type:                ENERGY
 model:              LSDA/VWN/DN*
 number of shells:            134
   83 S shells
   34 P shells
   17 D shells
 number of valence orbitals: 270
 point group symmetry used:   C1
 spin multiplicity:            2

                      cartesian coordinates (angstroms)
         atom           x              y              z

       H10    1      2.1890463     -4.1998782      2.7473155
       C2     2      1.7858078     -3.3343446      2.2279674
       C1     3      2.6138078     -2.3723446      1.7129674
       C9     4      2.0508078     -1.2923446      1.0669674
       C8     5      0.6768078     -1.2353446      0.9529674
       C1     6      0.0388078     -0.1473446      0.1969674
       N1     7      0.3738078      1.1546554      0.2719674
       C2     8     -0.5411922      2.0196554     -0.5650326
       C3     9     -1.0911922      0.9556554     -1.5600326
       C6    10     -0.2381922      0.7796554     -2.8120326
       H24   11     -0.5736894     -0.0813162     -3.4021345
       H20   12      0.8143908      0.5981871     -2.5670558
       H22   13     -0.2939757      1.6598232     -3.4612240
       C7    14     -2.5561922      1.1076554     -1.9210326
       H8    15     -2.8710635      0.3396744     -2.6372832
       H9    16     -2.7488267      2.0825731     -2.3813402
       H12   17     -3.2114372      0.9988505     -1.0506707
       N2    18     -0.8931922     -0.3023446     -0.7550326
       O2    19     -1.4131922     -1.4083446     -1.1300326
       C5    20     -1.5931922      2.5736554      0.3919674
       H2    21     -1.1297560      3.1878405      1.1731121
       H4    22     -2.1354663      1.7738103      0.9086021
       H5    23     -2.3204347      3.2041497     -0.1302073
       C4    24      0.2548078      3.1556554     -1.1850326
       H14   25     -0.3537719      3.7144946     -1.9038470
       H18   26      0.5985376      3.8642656     -0.4225084
       H16   27      1.1536729      2.7972149     -1.6972124
       O1    28      1.2468078      1.6586554      1.0649674
       N3    29     -0.1551922     -2.1553446      1.4549674
       C3    30      0.4028078     -3.1923446      2.0909674
       H15   31     -0.2795296     -3.9358475      2.4948827
       H3    32      2.7004429     -0.5309792      0.6457098
       H7    33      3.6928103     -2.4612983      1.8154154

 stoichiometry:       O2N3C12H16

 molecular charge            0.0
 number of electrons       125.0

 integration mesh:          FINE
 integration points and checksum: 132470     125.000042
```

```
   <S*S>  =           0.757

   E(DFT) =        -775.14404    VWN
                   -781.75710    pBP86


 total time:       20 min.  34.02 sec.

 end

  Reason for exit: Successful completion
  DFT Engine CPU Time : 000:20:34.1
  DFT Engine Wall Time: 000:21:48.9

MacSPARTAN PRO Properties Program:  (PowerPC)                    Release 1.0.4
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          0

                     Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
     ---------    ------------ ------------ ------------

  1 H  H10          2.1890463    -4.1998781     2.7473155
  2 C  C2           1.7858078    -3.3343446     2.2279674
  3 C  C1           2.6138078    -2.3723446     1.7129674
  4 C  C9B          2.0508078    -1.2923446     1.0669674
  5 C  C8B          0.6768078    -1.2353446     0.9529674
  6 C  C1B          0.0388078    -0.1473446     0.1969674
  7 N  N1B          0.3738078     1.1546554     0.2719674
  8 C  C2B         -0.5411922     2.0196554    -0.5650326
  9 C  C3B         -1.0911922     0.9556553    -1.5600326
 10 C  C6B         -0.2381922     0.7796554    -2.8120326
 11 H  H24         -0.5736894    -0.0813162    -3.4021345
 12 H  H20          0.8143908     0.5981871    -2.5670558
 13 H  H22         -0.2939757     1.6598231    -3.4612240
 14 C  C7B         -2.5561922     1.1076554    -1.9210326
 15 H  H8          -2.8710635     0.3396744    -2.6372832
 16 H  H9          -2.7488266     2.0825731    -2.3813403
 17 H  H12         -3.2114373     0.9988505    -1.0506707
 18 N  N2B         -0.8931922    -0.3023446    -0.7550326
 19 O  O2B         -1.4131922    -1.4083446    -1.1300326
 20 C  C5B         -1.5931922     2.5736554     0.3919674
 21 H  H2          -1.1297560     3.1878405     1.1731121
 22 H  H4          -2.1354663     1.7738103     0.9086021
 23 H  H5          -2.3204347     3.2041497    -0.1302073
 24 C  C4B          0.2548078     3.1556554    -1.1850326
 25 H  H14         -0.3537719     3.7144946    -1.9038470
 26 H  H18          0.5985376     3.8642656    -0.4225084
 27 H  H16          1.1536729     2.7972149    -1.6972124
 28 O  O1B          1.2468078     1.6586554     1.0649674
 29 N  N3B         -0.1551922    -2.1553446     1.4549674
 30 C  C3           0.4028078    -3.1923446     2.0909674
 31 H  H15         -0.2795296    -3.9358475     2.4948826
 32 H  H3           2.7004429    -0.5309792     0.6457098
 33 H  H7           3.6928103    -2.4612983     1.8154154

  Point Group = C1  Order =  1 Nsymop =  1
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:02.0
  Properties Program Wall Time: 000:00:04.1
```

Output file for NITCN's DFT calculation

```
MacSPARTAN PRO Density Functional Program:  (PowerPC)    Release 1.0


 begin on I101174-CHIMI(G4/400)

 NITCN DFT SWVN DN*

 run type:                ENERGY
 model:             LSDA/VWN/DN*
 number of shells:           102
   63 S shells
   26 P shells
   13 D shells
 number of valence orbitals: 206
 point group symmetry used:   C1
 spin multiplicity:            2

                      cartesian coordinates (angstroms)
         atom           x              y              z

        O1     1      1.6154536      1.6150001      0.9169178
        N1     2      0.7794536      0.7790001      0.4819178
        C2     3      0.0004536      0.0000000      1.2269178
        N1     4     -0.7795464     -0.7789999      0.4819178
        C3     5     -0.5495464     -0.5500000     -0.9970821
        C3     6      0.5494536      0.5500001     -0.9970821
        C4     7      0.1314535      1.8790001     -1.5880821
        H18    8     -0.1178729      1.7882140     -2.6505599
        H10    9     -0.7262861      2.3121124     -1.0624040
        H8    10      0.9342655      2.6225427     -1.5114632
        C4    11      1.8784536      0.1320001     -1.5880821
        H6    12      2.6219712      0.9348534     -1.5115848
        H3    13      2.3117015     -0.7257016     -1.0624426
        H1    14      1.7876347     -0.1173494     -2.6505564
        C4    15     -0.1315464     -1.8789999     -1.5880821
        H20   16     -0.9343607     -2.6225429     -1.5114854
        H2    17      0.7261907     -2.3121175     -1.0624035
        H24   18      0.1177898     -1.7882073     -2.6505573
        C4    19     -1.8785464     -0.1319999     -1.5880821
        H16   20     -2.6220681     -0.9348457     -1.5115382
        H14   21     -1.7877394      0.1173184     -2.6505643
        H12   22     -2.3117796      0.7257180     -1.0624574
        O1    23     -1.6145464     -1.6149999      0.9169178
        C1    24     -0.0005464      0.0000000      2.6429178
        N2    25     -0.0005464      0.0000000      3.7629178

 stoichiometry:        O2N3C8H12

 molecular charge            0.0
 number of electrons        97.0

 integration mesh:          FINE
 integration points and checksum: 103882      97.000003


   <S*S>  =           0.757

   E(DFT) =        -621.64114    VWN
                   -626.85163    pBP86


 total time:        9 min.  55.40 sec.
```

```
 end

  Reason for exit: Successful completion
  DFT Engine CPU Time : 000:09:55.5
  DFT Engine Wall Time: 000:10:39.6

MacSPARTAN PRO Properties Program:  (PowerPC)                    Release 1.0.4
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          0

                    Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
     ---------    ------------- ------------- -------------

   1 O  O1           1.6154536     1.6150000     0.9169178
   2 N  N1           0.7794536     0.7790001     0.4819178
   3 C  C2           0.0004536     0.0000001     1.2269178
   4 N  N1A         -0.7795464    -0.7789999     0.4819178
   5 C  C3A         -0.5495465    -0.5500000    -0.9970821
   6 C  C3           0.5494536     0.5500001    -0.9970821
   7 C  C4A          0.1314535     1.8790001    -1.5880821
   8 H  H18         -0.1178730     1.7882140    -2.6505599
   9 H  H10         -0.7262861     2.3121124    -1.0624040
  10 H  H8           0.9342654     2.6225427    -1.5114632
  11 C  C4           1.8784536     0.1320001    -1.5880821
  12 H  H6           2.6219712     0.9348535    -1.5115848
  13 H  H3           2.3117015    -0.7257015    -1.0624426
  14 H  H1           1.7876346    -0.1173494    -2.6505564
  15 C  C4C         -0.1315464    -1.8789999    -1.5880821
  16 H  H20         -0.9343606    -2.6225429    -1.5114854
  17 H  H2           0.7261907    -2.3121176    -1.0624035
  18 H  H24          0.1177898    -1.7882072    -2.6505573
  19 C  C4B         -1.8785464    -0.1319999    -1.5880821
  20 H  H16         -2.6220681    -0.9348457    -1.5115382
  21 H  H14         -1.7877394     0.1173184    -2.6505643
  22 H  H12         -2.3117796     0.7257179    -1.0624574
  23 O  O1A         -1.6145464    -1.6149999     0.9169178
  24 C  C1          -0.0005464     0.0000001     2.6429179
  25 N  N2          -0.0005464     0.0000001     3.7629178

  Point Group = C1  Order =  1 Nsymop =  1
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:01.3
  Properties Program Wall Time: 000:00:02.9
```

Output file for NITBzImH's DFT calculations
A) Spartan calculation

```
MacSPARTAN PRO Density Functional Program:  (PowerPC)    Release 1.0


 begin on I101174-CHIMI(G4/400)

 NITBZIMH.PDB

 run type:                ENERGY
 model:             LSDA/VWN/DN*
 number of shells:           154
   94 S shells
   40 P shells
   20 D shells
 number of valence orbitals: 314
 point group symmetry used:   C1
 spin multiplicity:            2

                      cartesian coordinates (angstroms)
         atom           x              y              z

        O1     1      1.7091148      1.5197653      0.6574220
        N1     2      1.0551148      1.2377653     -0.4035780
        C1     3      0.2041148      0.2107653     -0.5485780
        C8     4     -0.1908852     -0.6782347      0.5344220
        N4     5     -1.3458852     -1.3112347      0.6014220
        C14    6     -1.3258852     -1.9132347      1.8544220
        C13    7     -2.2908852     -2.6922347      2.4884220
        H34    8     -3.2212945     -2.9353492      1.9870373
        C12    9     -2.0258852     -3.1372347      3.7604220
        H32   10     -2.7641224     -3.7503622      4.2760398
        C11   11     -0.8398852     -2.8142347      4.4164220
        H30   12     -0.6813913     -3.1854968      5.4286695
        C10   13      0.1331148     -2.0472347      3.8164220
        H28   14      1.0534771     -1.7997200      4.3353775
        C9    15     -0.1318852     -1.6032347      2.5184220
        N3    16      0.5761148     -0.8152347      1.6514220
        H26   17      1.4676432     -0.3780936      1.8521407
        N2    18     -0.2788852      0.1957653     -1.8005780
        C3    19      0.2371148      1.3417653     -2.6265780
        C2    20      1.1631148      2.0847653     -1.6355780
        C5    21      2.6351148      2.1247653     -2.0135780
        H2    22      3.0609960      1.1210956     -2.1166139
        H6    23      2.7922181      2.6722650     -2.9486882
        H4    24      3.2312758      2.6301322     -1.2443027
        C4    25      0.6681148      3.4727653     -1.2245780
        H8    26     -0.3218783      3.4385991     -0.7576270
        H12   27      0.6368115      4.1561199     -2.0793741
        H10   28      1.3362116      3.9253765     -0.4816876
        C6    29      0.9361148      0.7377653     -3.8375780
        H20   30      0.2311613      0.1879469     -4.4727196
        H22   31      1.3941233      1.5109026     -4.4631961
        H24   32      1.7071114      0.0162456     -3.5470054
        C7    33     -0.9838852      2.1307653     -3.0725780
        H14   34     -1.6270197      2.4122345     -2.2320710
        H16   35     -0.7002467      3.0352360     -3.6208078
        H18   36     -1.6157756      1.5389048     -3.7461923
        O2    37     -1.1028852     -0.6512347     -2.2935780

 stoichiometry:       O2N4C14H17

 molecular charge            0.0
```

```
 number of electrons       145.0

 integration mesh:          FINE
 integration points and checksum: 148948     145.000000


   <S*S>  =           0.757

   E(DFT) =        -905.67047    VWN
                   -913.38698    pBP86


 total time:       30 min.  50.40 sec.

 end

  Reason for exit: Successful completion
  DFT Engine CPU Time : 000:30:50.6
  DFT Engine Wall Time: 000:32:33.3

MacSPARTAN PRO Properties Program:  (PowerPC)                    Release 1.0.4
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          0

                    Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
     ---------    ------------- ------------- -------------

   1 O  O1           1.7091148     1.5197653     0.6574220
   2 N  N1           1.0551149     1.2377653    -0.4035780
   3 C  C1           0.2041148     0.2107653    -0.5485780
   4 C  C8          -0.1908852    -0.6782347     0.5344220
   5 N  N4          -1.3458852    -1.3112347     0.6014220
   6 C  C14         -1.3258851    -1.9132347     1.8544221
   7 C  C13         -2.2908852    -2.6922347     2.4884220
   8 H  H34         -3.2212945    -2.9353492     1.9870374
   9 C  C12         -2.0258851    -3.1372347     3.7604220
  10 H  H32         -2.7641224    -3.7503622     4.2760398
  11 C  C11         -0.8398852    -2.8142347     4.4164220
  12 H  H30         -0.6813913    -3.1854967     5.4286695
  13 C  C10          0.1331148    -2.0472347     3.8164220
  14 H  H28          1.0534771    -1.7997200     4.3353775
  15 C  C9          -0.1318851    -1.6032346     2.5184220
  16 N  N3           0.5761148    -0.8152347     1.6514220
  17 H  H26          1.4676433    -0.3780936     1.8521407
  18 N  N2          -0.2788852     0.1957653    -1.8005780
  19 C  C3           0.2371148     1.3417653    -2.6265780
  20 C  C2           1.1631149     2.0847653    -1.6355779
  21 C  C5           2.6351148     2.1247654    -2.0135780
  22 H  H2           3.0609960     1.1210956    -2.1166139
  23 H  H6           2.7922182     2.6722650    -2.9486882
  24 H  H4           3.2312758     2.6301321    -1.2443027
  25 C  C4           0.6681149     3.4727653    -1.2245780
  26 H  H8          -0.3218783     3.4385991    -0.7576269
  27 H  H12          0.6368115     4.1561199    -2.0793741
  28 H  H10          1.3362116     3.9253765    -0.4816877
  29 C  C6           0.9361149     0.7377653    -3.8375780
  30 H  H20          0.2311613     0.1879469    -4.4727196
  31 H  H22          1.3941233     1.5109026    -4.4631961
  32 H  H24          1.7071114     0.0162456    -3.5470054
  33 C  C7          -0.9838851     2.1307653    -3.0725780
  34 H  H14         -1.6270197     2.4122345    -2.2320710
  35 H  H16         -0.7002467     3.0352360    -3.6208078
```

```
36 H  H18         -1.6157756     1.5389048    -3.7461923
37 O  O2          -1.1028851    -0.6512346    -2.2935780

 Point Group = C1  Order =  1 Nsymop =  1
 Reason for exit: Successful completion
 Properties Program CPU Time : 000:00:02.8
 Properties Program Wall Time: 000:00:05.7
```

B) Gaussian-99 calculation

```
Entering Gaussian System, Link 0=g99
 Input=/export/home/cours/remi/nit/nitbzimh.com
 Output=/export/home/cours/remi/nit/nitbzimh.log
 Initial command:
 /export/local/gauss/g99/l1.exe /tmp/3260.master.cluster.umontreal.ca/Gau-17691.inp -
scrdir=/tmp/3260.master.cluster.umontreal.ca/
 Entering Link 1 = /export/local/gauss/g99/l1.exe PID=     17692.

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M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr.,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, C. Adamo, J. Jaramillo, R. Cammi,
C. Pomelli, J. Ochterski, G. A. Petersson, P. Y. Ayala, K. Morokuma,
D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman,
J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski,
B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez,
M. Head-Gordon, E. S. Replogle, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 2000.

******************************************
Gaussian 99:  x86-Linux-G99RevB.08+ 22-May-2000
                10-Nov-2002
******************************************
%chk=nitbzimh
%nproc=1
Will use up to    1 processors via shared memory.
%mem=100MB
----------------------------------------------------------------------
#p PBE1PBE/6-311+g(3df,2p) geom=connectivity TD(NState=2,50-50) test
----------------------------------------------------------------------
1/38=1,57=2/1;
2/17=6,18=5,40=1/2;
3/5=4,6=6,7=216,11=2,25=1,30=1/1,2,8,3;
4//1;
5/5=2,38=4,42=-13/2;
8/6=1,10=1,23=2/1;
9/41=2,42=1,48=2/14;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;
Leave Link    1 at Sun Nov 10 16:40:14 2002, MaxMem=   13107200 cpu:       0.1
(Enter /export/local/gauss/g99/l101.exe)
-----------------------------------------
Energies d'excitation de NITBzImH (PBE1PBE)
-----------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 2
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
N                     1    B6       2    A5       3    D4       0
C                     7    B7       1    A6       2    D5       0
N                     2    B8       1    A7       6    D6       0
H                     3    B9       2    A8       1    D7       0
H                     4    B10      3    A9       2    D8       0
H                     5    B11      4    A10      3    D9       0
```

```
H                  6    B12      1    A11      2    D10      0
H                  7    B13      1    A12      2    D11      0
C                  8    B14      7    A13      1    D12      0
N                 15    B15      8    A14      7    D13      0
C                 16    B16     15    A15      8    D14      0
C                 17    B17     16    A16     15    D15      0
N                 15    B18      8    A17      7    D16      0
H                 17    B19     16    A18     15    D17      0
H                 17    B20     16    A19     15    D18      0
H                 18    B21     17    A20     16    D19      0
H                 18    B22     17    A21     16    D20      0
O                 16    B23     15    A22      8    D21      0
O                 19    B24     15    A23      8    D22      0
     Variables:
 B1                    1.33093
 B2                    1.35025
 B3                    1.40873
 B4                    1.41328
 B5                    1.34727
 B6                    1.43996
 B7                    1.3337
 B8                    1.31515
 B9                    1.07
 B10                   1.07
 B11                   1.07
 B12                   1.07
 B13                   1.
 B14                   1.54
 B15                   1.47317
 B16                   1.47775
 B17                   1.53765
 B18                   1.3103
 B19                   1.07
 B20                   1.07
 B21                   1.07
 B22                   1.07
 B23                   1.36
 B24                   1.36
 A1                  121.93599
 A2                  118.00161
 A3                  119.53585
 A4                  123.80464
 A5                  106.49471
 A6                  105.19041
 A7                  110.59346
 A8                  120.9992
 A9                  120.23207
 A10                 120.36888
 A11                 121.27017
 A12                 127.4048
 A13                 125.10939
 A14                 124.80455
 A15                 104.82374
 A16                 103.83012
 A17                 124.97647
 A18                 105.17377
 A19                 116.95215
 A20                 111.88797
 A21                 109.48012
 A22                 118.06225
 A23                 126.32205
 D1                   -0.00001
 D2                   0.
 D3                    0.00001
 D4                 -180.
```

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 D5                    -0.00002
 D6                  -179.99999
 D7                   180.
 D8                   180.
 D9                  -179.99999
 D10                  180.
 D11                  179.99998
 D12                 -179.99997
 D13                  178.88554
 D14                  160.71815
 D15                    2.75682
 D16                    1.1145
 D17                  125.39424
 D18                 -113.34301
 D19                  142.36782
 D20                  -96.72837
 D21                   35.77404
 D22                   26.70251
Leave Link  101 at Sun Nov 10 16:40:14 2002, MaxMem=   13107200 cpu:       0.1
(Enter /export/local/gauss/g99/l202.exe)
```

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.330934(1)					
3	3	C	2	1.350248(2)	1	121.936(25)			
4	4	C	3	1.408727(3)	2	118.002(26)	1	0.000(48)	0
5	5	C	4	1.413281(4)	3	119.536(27)	2	0.000(49)	0
6	6	C	1	1.347269(5)	2	123.805(28)	3	0.000(50)	0
7	7	N	1	1.439962(6)	2	106.495(29)	3	-180.000(51)	0
8	8	C	7	1.333695(7)	1	105.190(30)	2	0.000(52)	0
9	9	N	2	1.315146(8)	1	110.593(31)	6	-180.000(53)	0
10	10	H	3	1.070000(9)	2	120.999(32)	1	180.000(54)	0
11	11	H	4	1.070000(10)	3	120.232(33)	2	180.000(55)	0
12	12	H	5	1.070000(11)	4	120.369(34)	3	-180.000(56)	0
13	13	H	6	1.070000(12)	1	121.270(35)	2	180.000(57)	0
14	14	H	7	1.000000(13)	1	127.405(36)	2	180.000(58)	0
15	15	C	8	1.540000(14)	7	125.109(37)	1	-180.000(59)	0
16	16	N	15	1.473173(15)	8	124.805(38)	7	178.886(60)	0
17	17	C	16	1.477753(16)	15	104.824(39)	8	160.718(61)	0
18	18	C	17	1.537652(17)	16	103.830(40)	15	2.757(62)	0
19	19	N	15	1.310301(18)	8	124.976(41)	7	1.115(63)	0
20	20	H	17	1.070000(19)	16	105.174(42)	15	125.394(64)	0
21	21	H	17	1.070000(20)	16	116.952(43)	15	-113.343(65)	0
22	22	H	18	1.070000(21)	17	111.888(44)	16	142.368(66)	0
23	23	H	18	1.070000(22)	17	109.480(45)	16	-96.728(67)	0
24	24	O	16	1.360000(23)	15	118.062(46)	8	35.774(68)	0
25	25	O	19	1.360000(24)	15	126.322(47)	8	26.703(69)	0

Z-Matrix 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	1.330934
3	6	0	1.145874	0.000000	2.045177
4	6	0	2.365099	0.000000	1.339485
5	6	0	2.352112	0.000000	-0.073736
6	6	0	1.119499	0.000000	-0.749571
7	7	0	-1.380702	0.000000	-0.408844
8	6	0	-2.081226	0.000000	0.726061
9	7	0	-1.231108	0.000000	1.793517
10	1	0	1.128380	0.000000	3.115034

11	1	0	3.294484	0.000000	1.869716
12	1	0	3.270285	-0.000001	-0.623152
13	1	0	1.072183	0.000000	-1.818524
14	1	0	-1.737604	0.000000	-1.342985
15	6	0	-3.618476	-0.000001	0.818044
16	7	0	-4.385595	-0.023528	2.075507
17	6	0	-5.733112	0.457049	1.705378
18	6	0	-5.645198	0.662071	0.183993
19	7	0	-4.432368	-0.020884	-0.208617
20	1	0	-6.404586	-0.304612	2.042860
21	1	0	-6.039874	1.399221	2.109245
22	1	0	-6.551909	0.380562	-0.309491
23	1	0	-5.439933	1.690961	-0.026131
24	8	0	-3.886672	0.656887	3.142143
25	8	0	-4.165018	-0.536929	-1.438179

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.330934	0.000000			
3	C	2.344307	1.350248	0.000000		
4	C	2.718072	2.365115	1.408727	0.000000	
5	C	2.353267	2.739622	2.438196	1.413281	0.000000
6	C	1.347269	2.362578	2.794872	2.432216	1.405733
7	N	1.439962	2.221073	3.522187	4.133725	3.747825
8	C	2.204238	2.167342	3.486293	4.488440	4.504904
9	N	2.175392	1.315146	2.390267	3.624755	4.040556
10	H	3.313107	2.110984	1.070000	2.163804	3.415519
11	H	3.788068	3.338250	2.155762	1.070000	2.159878
12	H	3.329126	3.809621	3.410733	2.161320	1.070000
13	H	2.111067	3.326960	3.864403	3.412426	2.163909
14	H	2.196105	3.188905	4.449055	4.901819	4.282145
15	C	3.709793	3.654645	4.919846	6.006253	6.036820
16	N	4.851981	4.448413	5.531602	6.790740	7.072233
17	C	5.998815	5.763478	6.902522	8.119347	8.291259
18	C	5.686867	5.798454	7.072552	8.120244	8.028806
19	N	4.437324	4.692179	6.016378	6.971558	6.785852
20	H	6.729398	6.451229	7.556603	8.803119	9.014018
21	H	6.548802	6.248493	7.320990	8.555345	8.783430
22	H	6.570246	6.764860	8.058856	9.076177	8.915267
23	H	5.696745	5.856095	7.107919	8.102024	7.973555
24	O	5.040911	4.337995	5.192433	6.539551	7.049525
25	O	4.438922	5.030274	6.373981	7.116610	6.680043

		6	7	8	9	10
6	C	0.000000				
7	N	2.523311	0.000000			
8	C	3.524504	1.333695	0.000000		
9	N	3.463040	2.207435	1.364611	0.000000	
10	H	3.864614	4.325876	4.001095	2.704365	0.000000
11	H	3.404588	5.200884	5.496017	4.526233	2.498564
12	H	2.154498	4.655921	5.518971	5.109092	4.308340
13	H	1.070000	2.829106	4.052024	4.283922	4.933878
14	H	2.918078	1.000000	2.097386	3.177135	5.299793
15	C	4.990574	2.552036	1.540000	2.578968	5.273406
16	N	6.187703	3.898966	2.670520	3.167153	5.611157
17	C	7.293418	4.860278	3.808442	4.526003	7.019693
18	C	6.860831	4.356113	3.665252	4.744797	7.410175
19	N	5.578198	3.058299	2.530203	3.775850	6.478349
20	H	8.031333	5.598487	4.529701	5.188433	7.614980
21	H	7.835003	5.477817	4.420624	5.018141	7.372469
22	H	7.693439	5.186144	4.604802	5.733969	8.417781
23	H	6.812405	4.413975	3.834847	4.887195	7.474557
24	O	6.374848	4.395554	3.086842	3.049970	5.057963
25	O	5.356173	3.016660	3.051953	4.397724	7.002864

		11	12	13	14	15

```
   11  H    0.000000
   12  H    2.492985   0.000000
   13  H    4.306011   2.502112   0.000000
   14  H    5.970206   5.059359   2.849744   0.000000
   15  C    6.992498   7.037903   5.380871   2.864913   0.000000
   16  N    7.682871   8.117623   6.704578   4.324176   1.473173
   17  C    9.040652   9.310859   7.677162   5.046335   2.338363
   18  C    9.121289   8.976394   7.040712   4.247269   2.224401
   19  N    8.001509   7.713828   5.735182   2.923864   1.310301
   20  H    9.705397  10.040097   8.420520   5.773860   3.058655
   21  H    9.441686   9.803207   8.244182   5.690803   3.080291
   22  H   10.091840   9.834567   7.781310   4.938671   3.165627
   23  H    9.096352   8.892900   6.962735   4.277931   2.624821
   24  O    7.322539   8.113630   7.044854   5.016609   2.429993
   25  O    8.177691   7.499086   5.278374   2.487909   2.382759
                 16         17         18         19         20
   16  N    0.000000
   17  C    1.477753   0.000000
   18  C    2.373704   1.537652   0.000000
   19  N    2.284605   2.362992   1.446211   0.000000
   20  H    2.038726   1.070000   2.228572   3.006542   0.000000
   21  H    2.182200   1.070000   2.098988   3.158047   1.743695
   22  H    3.247218   2.176230   1.070000   2.159581   2.454532
   23  H    2.909980   2.146302   1.070000   1.994719   3.032094
   24  O    1.360000   2.348099   3.441379   3.461900   2.910807
   25  O    3.557840   3.650871   2.501995   1.360000   4.145753
                 21         22         23         24         25
   21  H    0.000000
   22  H    2.673973   0.000000
   23  H    2.237156   1.741818   0.000000
   24  O    2.500843   4.369625   3.676939   0.000000
   25  O    4.455107   2.795170   2.929639   4.741521   0.000000
                      Interatomic angles:
      C1-C2-C3=121.936        C2-C3-C4=118.0016       C3-C4-C5=119.5358
      C2-C1-C6=123.8046       C2-C1-N7=106.4947       C6-C1-N7=129.7007
      C1-N7-C8=105.1904       C1-C2-N9=110.5935       C3-C2-N9=127.4705
    C2-C3-H10=120.9992      C4-C3-H10=120.9992      C3-C4-H11=120.2321
    C5-C4-H11=120.2321      C4-C5-H12=120.3689      C1-C6-H13=121.2702
    C1-N7-H14=127.4048      C8-N7-H14=127.4048      N7-C8-C15=125.1094
   C8-C15-N16=124.8046    C15-N16-C17=104.8237    N16-C17-C18=103.8301
   C8-C15-N19=124.9765    N16-C15-N19=110.1879    N16-C17-H20=105.1738
  C18-C17-H20=116.2864    N16-C17-H21=116.9522    C18-C17-H21=105.8094
  H20-C17-H21=109.1373    C17-C18-H22=111.888     C17-C18-H23=109.4801
  H22-C18-H23=108.9641    C15-N16-O24=118.0622    C17-N16-O24=111.6083
  C15-N19-O25=126.322
Stoichiometry    C10H9N4O2(2)
Framework group  C1[X(C10H9N4O2)]
Deg. of freedom   69
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0        2.003250    0.659580    0.070646
   2          6             0        1.941579   -0.660886   -0.084117
   3          6             0        3.052021   -1.428056   -0.123339
   4          6             0        4.301460   -0.790208    0.005357
   5          6             0        4.353983    0.612562    0.169191
   6          6             0        3.155200    1.346058    0.200629
   7          7             0        0.644308    1.135752    0.065373
   8          6             0       -0.107376    0.045565   -0.093391
   9          7             0        0.691546   -1.056930   -0.184998
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   10          1              0        2.984988   -2.488605   -0.248412
   11          1              0        5.204380   -1.363752   -0.020749
   12          1              0        5.295742    1.110745    0.268199
   13          1              0        3.157512    2.409021    0.323118
   14          1              0        0.331419    2.080781    0.160345
   15          6              0       -1.645754    0.032847   -0.162890
   16          7              0       -2.468543   -1.172844   -0.361803
   17          6              0       -3.817255   -0.791695    0.106655
   18          6              0       -3.668023    0.689804    0.490407
   19          7              0       -2.409497    1.095403   -0.095367
   20          1              0       -4.469568   -1.005179   -0.714206
   21          1              0       -4.183459   -1.284375    0.983046
   22          1              0       -4.537663    1.257902    0.233715
   23          1              0       -3.498599    0.770215    1.543844
   24          8              0       -2.049927   -2.334334    0.208551
   25          8              0       -2.063068    2.360604   -0.454330
 ---------------------------------------------------------------------
 TstSym:  Max error for IOp=  1 IAt=   13 Err= 2.07D-15
 Rotational constants (GHZ):      1.3744576      0.3122816      0.2584302
 Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,N-14,C-12,N-14,H-1,H-1,H-1,H-1,H-1,C-12,
 N-14,C-12,C-12,N-14,H-1,H-1,H-1,H-1,O-16,O-16
 Leave Link  202 at Sun Nov 10 16:40:15 2002, MaxMem=   13107200 cpu:       0.1
 (Enter /export/local/gauss/g99/l301.exe)
 Standard basis: 6-311+G(3df,2p) (5D, 7F)
 There are   705 symmetry adapted basis functions of A   symmetry.
 Crude estimate of integral set expansion from redundant integrals=1.000.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   705 basis functions     1027 primitive gaussians
    57 alpha electrons       56 beta electrons
       nuclear repulsion energy      1046.6459735087 Hartrees.
 Leave Link  301 at Sun Nov 10 16:40:16 2002, MaxMem=   13107200 cpu:       0.1
 (Enter /export/local/gauss/g99/l302.exe)
 One-electron integrals computed using PRISM.
 Error in orthogonal basis= 1.47D-09 with   705 functions, increasing threshold to
2.00D-04.
 NBasis=   705 RedAO= T  NBF=   705
 NBsUse=   703 2.00D-04 NBFU=   703
 Leave Link  302 at Sun Nov 10 16:40:48 2002, MaxMem=   13107200 cpu:      31.9
 (Enter /export/local/gauss/g99/l308.exe)
 Leave Link  308 at Sun Nov 10 16:40:51 2002, MaxMem=   13107200 cpu:       2.4
 (Enter /export/local/gauss/g99/l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Sun Nov 10 16:40:52 2002, MaxMem=   13107200 cpu:       0.7
 (Enter /export/local/gauss/g99/l401.exe)
 Projected INDO guess.
 Initial guess orbital symmetries:
 Alpha Orbitals:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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The electronic state of the initial guess is 2-A.
<S**2> of initial guess= 1.2025
Leave Link  401 at Sun Nov 10 16:42:34 2002, MaxMem=   13107200 cpu:      101.2
(Enter /export/local/gauss/g99/l502.exe)
IExCor=1009 DFT=T Ex=PBE+HF Corr=PBE ExCW=0 ScaHFX= 0.2500
ScaDFX=  0.7500  0.7500  1.0000  1.0000
IRadAn=      0 IRanWt=     -1 IRanGd=            0 ICorTp=0
Using DIIS extrapolation.
UHF open shell SCF:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Level shift goal  0.100 maximum shift  0.100.
No special actions if energy rises.
Dynamic level shift is on during FON iterations.
Integral symmetry usage will be decided dynamically.
IEnd=   2109381 IEndB=   2109381 NGot=  13107200 MDV=  11656862
LenX=  11656862
Fock matrices will be formed incrementally for  20 cycles.

Cycle   1  Pass 1  IDiag  1:
Petite list used in FoFDir.
MinBra= 0 MaxBra= 3 Meth= 1.
IRaf=       0 NMat=   1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 1 JSym2E=1.
E= -751.217928630314
DIIS: error= 5.58D-01 at cycle   1.
Coeff: 0.100D+01
Gap=     0.158 Goal=     0.100 Shift=    0.000
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T= 3000. Gap= 0.076 NK=0 IS=    1 IE=  703
         NO(<0.9)=   0  NV(>0.1)=   0  56.98e < EF 0.02e >EF  Err=4.1D-11
Gap=     0.152 Goal=     0.100 Shift=    0.000
T= 3000. Gap= 0.107 NK=0 IS=    1 IE=  703
         NO(<0.9)=   0  NV(>0.1)=   0  56.00e < EF 0.00e >EF  Err=3.1D-11
RMSDP=2.09D-02 MaxDP=3.80D+00

Cycle   2  Pass 1  IDiag  1:
RMSU=  1.48D-02    CP:  6.65D-01
E= -754.574994521004     Delta-E=       -3.357065890689 Rises=F
DIIS: error= 1.08D-01 at cycle   2.
Coeff: 0.423D-01 0.958D+00
Gap=     0.521 Goal=     0.100 Shift=    0.000
T= 2700. Gap= 0.144 NK=0 IS=    1 IE=  703
         NO(<0.9)=   0  NV(>0.1)=   0  57.00e < EF 0.00e >EF  Err=7.3D-11
Gap=     0.509 Goal=     0.100 Shift=    0.000
T= 2700. Gap= 0.072 NK=0 IS=    1 IE=  703
         NO(<0.9)=   0  NV(>0.1)=   0  55.99e < EF 0.01e >EF  Err=7.8D-11
RMSDP=1.12D-02 MaxDP=2.29D+00

Cycle   3  Pass 1  IDiag  1:
RMSU=  9.41D-03    CP:  7.77D-01  7.57D-01
E= -753.418557952772     Delta-E=        1.156436568232 Rises=F
DIIS: error= 2.55D-01 at cycle   3.
Coeff: 0.449D-02 0.659D+00 0.336D+00
Gap=     0.247 Goal=     0.100 Shift=    0.000
T= 2700. Gap= 0.131 NK=3 IS=   47 IE=   79
         NO(<0.9)=   0  NV(>0.1)=   0  56.94e < EF 0.06e >EF  Err=0.0D+00
Gap=     0.081 Goal=     0.100 Shift=    0.019
T= 2700. Gap= 0.109 NK=3 IS=   46 IE=   77
         NO(<0.9)=   0  NV(>0.1)=   0  55.90e < EF 0.10e >EF  Err=7.1D-15
RMSDP=7.91D-03 MaxDP=2.00D+00

Cycle   4  Pass 1  IDiag  1:
RMSU=  2.25D-03    CP:  6.59D-01  8.18D-01  4.22D-01
E= -755.060710362160     Delta-E=       -1.642152409388 Rises=F
DIIS: error= 2.42D-02 at cycle   4.
Coeff:-0.200D-02 0.225D+00 0.569D-01 0.721D+00
Gap=     0.169 Goal=     0.100 Shift=    0.000
T= 2371. Gap= 0.144 NK=4 IS=   48 IE=   79
         NO(<0.9)=   0  NV(>0.1)=   0  57.00e < EF 0.00e >EF  Err=0.0D+00
Gap=     0.128 Goal=     0.100 Shift=    0.000
T= 2371. Gap= 0.105 NK=3 IS=   48 IE=   73
         NO(<0.9)=   0  NV(>0.1)=   0  56.00e < EF 0.00e >EF  Err=0.0D+00
RMSDP=3.58D-03 MaxDP=1.17D+00

Cycle   5  Pass 1  IDiag  1:
RMSU=  1.85D-03    CP:  6.03D-01  8.16D-01  2.50D-01  6.94D-01
E= -755.090933375248     Delta-E=       -0.030223013087 Rises=F
DIIS: error= 3.56D-02 at cycle   5.
Coeff:-0.205D-02 0.830D-01-0.126D-01 0.560D+00 0.372D+00
Gap=     0.160 Goal=     0.100 Shift=    0.000
T= 2247. Gap= 0.148 NK=4 IS=   46 IE=   79
         NO(<0.9)=   0  NV(>0.1)=   0  57.00e < EF 0.00e >EF  Err=7.1D-15
Gap=     0.119 Goal=     0.100 Shift=    0.000
T= 2247. Gap= 0.115 NK=3 IS=   48 IE=   75
         NO(<0.9)=   0  NV(>0.1)=   0  56.00e < EF 0.00e >EF  Err=0.0D+00
RMSDP=1.17D-03 MaxDP=2.01D-01

Cycle   6  Pass 1  IDiag  1:
RMSU=  8.11D-04    CP:  6.09D-01  8.27D-01  2.42D-01  8.30D-01  6.22D-01
E= -755.131075098303     Delta-E=       -0.040141723055 Rises=F
DIIS: error= 3.67D-03 at cycle   6.
Coeff:-0.953D-03 0.356D-01-0.149D-01 0.287D+00 0.192D+00 0.502D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
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T= 1286. Gap= 0.144 NK=4 IS=   56 IE=   79
         NO(<0.9)=   0  NV(>0.1)=   0  57.00e < EF 0.00e >EF  Err=7.1D-15
Gap=     0.110 Goal=     0.100 Shift=    0.000
T= 1286. Gap= 0.109 NK=3 IS=   55 IE=   76
         NO(<0.9)=   0  NV(>0.1)=   0  56.00e < EF 0.00e >EF  Err=7.1D-15
RMSDP=3.68D-04 MaxDP=9.31D-02

Cycle   7  Pass 1  IDiag  1:
RMSU=  2.34D-04    CP:  6.05D-01  8.17D-01  2.39D-01  8.68D-01  6.58D-01
                   CP:  9.56D-01
E= -755.132353500676     Delta-E=       -0.001278402373 Rises=F
DIIS: error= 1.93D-03 at cycle   7.
Coeff:-0.663D-04 0.325D-02-0.482D-02 0.408D-01 0.391D-02 0.291D+00
Coeff: 0.666D+00
Gap=     0.145 Goal=     0.100 Shift=    0.000
T= 1027. Gap= 0.145 NK=4 IS=   46 IE=   79
         NO(<0.9)=   0  NV(>0.1)=   0  57.00e < EF 0.00e >EF  Err=0.0D+00
Gap=     0.112 Goal=     0.100 Shift=    0.000
T= 1027. Gap= 0.111 NK=3 IS=   48 IE=   76
         NO(<0.9)=   0  NV(>0.1)=   0  56.00e < EF 0.00e >EF  Err=7.1D-15
RMSDP=3.30D-04 MaxDP=9.68D-02

Cycle   8  Pass 1  IDiag  1:
RMSU=  1.34D-04    CP:  6.10D-01  8.23D-01  2.47D-01  8.59D-01  5.95D-01
                   CP:  1.07D+00  6.95D-01
E= -755.132661832019     Delta-E=       -0.000308331343 Rises=F
DIIS: error= 1.09D-03 at cycle   8.
Coeff: 0.321D-04-0.745D-03-0.167D-02-0.388D-02-0.187D-01 0.990D-01
Coeff: 0.396D+00 0.530D+00
Gap=     0.145 Goal=     0.100 Shift=    0.000
Gap=     0.113 Goal=     0.100 Shift=    0.000
RMSDP=6.48D-05 MaxDP=9.37D-03

Cycle   9  Pass 1  IDiag  1:
RMSU=  5.02D-05    CP:  6.09D-01  8.23D-01  2.44D-01  8.60D-01  5.95D-01
                   CP:  1.08D+00  7.46D-01  1.03D+00
E= -755.132753650815     Delta-E=       -0.000091818796 Rises=F
DIIS: error= 5.17D-04 at cycle   9.
Coeff: 0.315D-04-0.944D-03 0.768D-03-0.222D-01-0.167D-01-0.501D-01
Coeff:-0.124D-01 0.221D+00 0.881D+00
Gap=     0.145 Goal=     0.100 Shift=    0.000
Gap=     0.112 Goal=     0.100 Shift=    0.000
RMSDP=4.19D-05 MaxDP=6.71D-03

Cycle  10  Pass 1  IDiag  1:
RMSU=  2.73D-05    CP:  6.09D-01  8.23D-01  2.43D-01  8.61D-01  5.93D-01
                   CP:  1.11D+00  8.03D-01  1.12D+00  1.14D+00
E= -755.132800698257     Delta-E=       -0.000047047442 Rises=F
DIIS: error= 2.97D-04 at cycle  10.
Coeff: 0.129D-05 0.194D-03 0.666D-03-0.883D-02-0.182D-02-0.584D-01
Coeff:-0.139D+00-0.598D-01 0.499D+00 0.768D+00
Gap=     0.145 Goal=     0.100 Shift=    0.000
Gap=     0.112 Goal=     0.100 Shift=    0.000
RMSDP=2.98D-05 MaxDP=5.14D-03

Cycle  11  Pass 1  IDiag  1:
RMSU=  1.57D-05    CP:  6.09D-01  8.24D-01  2.42D-01  8.59D-01  5.93D-01
                   CP:  1.12D+00  8.03D-01  1.20D+00  1.27D+00  1.58D+00
E= -755.132825385961     Delta-E=       -0.000024687703 Rises=F
DIIS: error= 2.15D-04 at cycle  11.
Coeff: 0.340D-06 0.264D-03 0.211D-03 0.118D-02 0.353D-02-0.129D-01
Coeff:-0.737D-01-0.124D+00-0.104D+00 0.490D+00 0.820D+00
Gap=     0.145 Goal=     0.100 Shift=    0.000
Gap=     0.112 Goal=     0.100 Shift=    0.000
RMSDP=2.37D-05 MaxDP=3.74D-03
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Cycle  12  Pass 1  IDiag  1:
RMSU=  8.77D-06    CP:  6.09D-01  8.24D-01  2.42D-01  8.58D-01  5.93D-01
                   CP:  1.13D+00  8.20D-01  1.24D+00  1.39D+00  2.18D+00
                   CP:  1.37D+00
E= -755.132839699415     Delta-E=       -0.000014313454 Rises=F
DIIS: error= 1.38D-04 at cycle  12.
Coeff: 0.121D-05 0.425D-04 0.585D-04 0.252D-02 0.274D-02 0.766D-02
Coeff:-0.192D-02-0.520D-01-0.243D+00 0.718D-01 0.469D+00 0.743D+00
Gap=     0.145 Goal=     0.100 Shift=    0.000
Gap=     0.112 Goal=     0.100 Shift=    0.000
RMSDP=1.47D-05 MaxDP=1.69D-03

Cycle  13  Pass 1  IDiag  1:
RMSU=  7.26D-06    CP:  6.09D-01  8.24D-01  2.42D-01  8.58D-01  5.93D-01
                   CP:  1.13D+00  8.27D-01  1.27D+00  1.50D+00  2.50D+00
                   CP:  1.64D+00  1.39D+00
E= -755.132845812309     Delta-E=       -0.000006112894 Rises=F
DIIS: error= 1.10D-04 at cycle  13.
Coeff: 0.976D-06-0.297D-04-0.593D-04 0.801D-03 0.122D-02 0.788D-02
Coeff: 0.351D-01 0.313D-01-0.959D-01-0.154D+00-0.167D+00 0.427D+00
Coeff: 0.913D+00
Gap=     0.145 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=1.40D-05 MaxDP=2.56D-03

Cycle  14  Pass 1  IDiag  1:
RMSU=  4.69D-06    CP:  6.09D-01  8.24D-01  2.42D-01  8.58D-01  5.95D-01
                   CP:  1.13D+00  8.34D-01  1.27D+00  1.52D+00  2.76D+00
                   CP:  1.89D+00  1.98D+00  1.65D+00
E= -755.132849165911     Delta-E=       -0.000003353602 Rises=F
DIIS: error= 5.87D-05 at cycle  14.
Coeff: 0.137D-05-0.648D-05-0.567D-04-0.119D-02 0.272D-03-0.159D-02
Coeff: 0.233D-01 0.399D-01 0.445D-01-0.102D+00-0.326D+00-0.791D-01
Coeff: 0.481D+00 0.921D+00
Gap=     0.145 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=1.03D-05 MaxDP=1.68D-03

Cycle  15  Pass 1  IDiag  1:
RMSU=  2.49D-06    CP:  6.09D-01  8.24D-01  2.42D-01  8.58D-01  5.96D-01
                   CP:  1.13D+00  8.41D-01  1.28D+00  1.58D+00  2.90D+00
                   CP:  2.07D+00  2.47D+00  2.33D+00  1.49D+00
E= -755.132850705390     Delta-E=       -0.000001539480 Rises=F
DIIS: error= 4.56D-05 at cycle  15.
Coeff:-0.566D-06 0.612D-04-0.216D-04-0.123D-02 0.153D-03-0.541D-02
Coeff: 0.311D-02 0.110D-01 0.586D-01 0.671D-02-0.137D+00-0.206D+00
Coeff:-0.116D+00 0.582D+00 0.804D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=8.10D-06 MaxDP=1.83D-03

Cycle  16  Pass 1  IDiag  1:
RMSU=  1.92D-06    CP:  6.09D-01  8.24D-01  2.42D-01  8.57D-01  5.97D-01
                   CP:  1.13D+00  8.46D-01  1.29D+00  1.59D+00  2.99D+00
                   CP:  2.20D+00  2.81D+00  2.69D+00  1.96D+00  1.29D+00
E= -755.132851218807     Delta-E=       -0.000000513417 Rises=F
DIIS: error= 2.20D-05 at cycle  16.
Coeff: 0.159D-06 0.225D-04 0.248D-04-0.683D-03-0.113D-03-0.242D-02
Coeff:-0.894D-03-0.210D-02 0.110D-01 0.228D-01 0.167D-01-0.546D-01
Coeff:-0.170D+00-0.762D-03 0.314D+00 0.866D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=4.37D-06 MaxDP=1.08D-03
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Cycle  17  Pass 1  IDiag  1:
RMSU=  1.19D-06    CP:  6.09D-01  8.24D-01  2.41D-01  8.57D-01  5.98D-01
                   CP:  1.13D+00  8.50D-01  1.29D+00  1.60D+00  3.00D+00
                   CP:  2.24D+00  2.93D+00  2.87D+00  2.18D+00  1.60D+00
                   CP:  1.30D+00
E= -755.132851320178     Delta-E=       -0.000000101370 Rises=F
DIIS: error= 9.95D-06 at cycle  17.
Coeff: 0.187D-06 0.801D-05 0.870D-05 0.133D-05 0.728D-04-0.330D-04
Coeff:-0.995D-03-0.407D-02-0.911D-02 0.905D-02 0.417D-01 0.237D-01
Coeff:-0.555D-01-0.138D+00-0.626D-01 0.416D+00 0.779D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=1.64D-06 MaxDP=4.00D-04

Cycle  18  Pass 1  IDiag  1:
RMSU=  5.07D-07    CP:  6.09D-01  8.23D-01  2.41D-01  8.57D-01  5.98D-01
                   CP:  1.13D+00  8.51D-01  1.29D+00  1.60D+00  3.00D+00
                   CP:  2.26D+00  2.98D+00  2.93D+00  2.27D+00  1.76D+00
                   CP:  1.51D+00  1.23D+00
E= -755.132851346778     Delta-E=       -0.000000026600 Rises=F
DIIS: error= 5.49D-06 at cycle  18.
Coeff: 0.831D-07 0.200D-05-0.251D-05 0.143D-03 0.669D-04 0.462D-03
Coeff:-0.287D-03-0.104D-02-0.567D-02-0.223D-02 0.116D-01 0.221D-01
Coeff: 0.241D-01-0.526D-01-0.112D+00-0.743D-01 0.299D+00 0.891D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=7.76D-07 MaxDP=1.64D-04

Cycle  19  Pass 1  IDiag  1:
RMSU=  2.71D-07    CP:  6.09D-01  8.23D-01  2.41D-01  8.57D-01  5.98D-01
                   CP:  1.13D+00  8.52D-01  1.28D+00  1.60D+00  3.00D+00
                   CP:  2.27D+00  3.00D+00  2.95D+00  2.31D+00  1.83D+00
                   CP:  1.66D+00  1.44D+00  1.24D+00
E= -755.132851355302     Delta-E=       -0.000000008523 Rises=F
DIIS: error= 3.88D-06 at cycle  19.
Coeff:-0.588D-07 0.122D-05-0.226D-05 0.223D-04-0.348D-04 0.127D-03
Coeff: 0.251D-03 0.144D-02 0.173D-02-0.438D-02-0.130D-01-0.290D-03
Coeff: 0.355D-01 0.302D-01-0.261D-01-0.207D+00-0.164D+00 0.498D+00
Coeff: 0.848D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=4.60D-07 MaxDP=1.08D-04

Cycle  20  Pass 1  IDiag  1:
Restarting incremental Fock formation.
E= -755.132851358927     Delta-E=       -0.000000003625 Rises=F
DIIS: error= 1.77D-06 at cycle  20.
Coeff:-0.769D-07 0.277D-05-0.114D-05-0.480D-04-0.461D-04-0.118D-03
Coeff: 0.351D-03 0.105D-02 0.271D-02-0.106D-02-0.980D-02-0.885D-02
Coeff: 0.569D-02 0.290D-01 0.373D-01-0.454D-01-0.182D+00-0.154D+00
Coeff: 0.323D+00 0.100D+01
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=1.04D-06 MaxDP=1.26D-04

Cycle  21  Pass 1  IDiag  1:
RMSU=  9.91D-07    CP:  1.00D+00
E= -755.132851360144     Delta-E=       -0.000000001217 Rises=F
DIIS: error= 1.11D-06 at cycle  21.
Coeff: 0.148D-05-0.247D-06-0.302D-04-0.631D-05-0.129D-03-0.299D-05
Coeff:-0.822D-04 0.682D-03 0.871D-03 0.609D-04-0.340D-02-0.775D-02
Coeff: 0.184D-02 0.229D-01 0.429D-01-0.335D-01-0.209D+00-0.966D-01
Coeff: 0.440D+00 0.842D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
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RMSDP=3.19D-07 MaxDP=2.61D-05

Cycle  22  Pass 1  IDiag  1:
RMSU=  7.86D-08    CP:  1.00D+00  1.31D+00
E= -755.132851360428     Delta-E=       -0.000000000284 Rises=F
DIIS: error= 4.84D-07 at cycle  22.
Coeff:-0.933D-06-0.344D-05 0.927D-05 0.955D-06 0.203D-04-0.255D-03
Coeff:-0.541D-03 0.422D-03 0.276D-02 0.898D-03-0.570D-02-0.732D-02
Coeff: 0.431D-03 0.371D-01 0.405D-01-0.601D-01-0.154D+00-0.110D+00
Coeff: 0.429D+00 0.826D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=1.32D-07 MaxDP=9.74D-06

Cycle  23  Pass 1  IDiag  1:
RMSU=  9.48D-08    CP:  1.00D+00  1.22D+00  1.30D+00
E= -755.132851360506     Delta-E=       -0.000000000078 Rises=F
DIIS: error= 2.26D-07 at cycle  23.
Coeff: 0.101D-04 0.110D-04 0.279D-04-0.744D-05-0.109D-03-0.365D-03
Coeff: 0.516D-04 0.117D-02 0.955D-03-0.919D-03-0.326D-02-0.457D-02
Coeff: 0.690D-02 0.259D-01 0.118D-01-0.503D-01-0.125D+00 0.295D-01
Coeff: 0.343D+00 0.765D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=1.43D-07 MaxDP=1.44D-05

Cycle  24  Pass 1  IDiag  1:
RMSU=  4.19D-08    CP:  1.00D+00  1.09D+00  1.50D+00  1.35D+00
E= -755.132851360524     Delta-E=       -0.000000000018 Rises=F
DIIS: error= 1.40D-07 at cycle  24.
Coeff: 0.872D-06-0.833D-05-0.244D-04 0.422D-04 0.178D-03 0.444D-04
Coeff:-0.559D-03-0.458D-03 0.650D-03 0.204D-02-0.514D-04-0.738D-02
Coeff:-0.264D-02 0.162D-01 0.224D-01-0.134D-01-0.114D+00-0.101D+00
Coeff: 0.453D+00 0.744D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=6.10D-08 MaxDP=6.46D-06

Cycle  25  Pass 1  IDiag  1:
RMSU=  1.97D-08    CP:  1.00D+00  1.04D+00  1.52D+00  1.48D+00  1.38D+00
E= -755.132851360543     Delta-E=       -0.000000000020 Rises=F
DIIS: error= 7.46D-08 at cycle  25.
Coeff:-0.550D-05-0.216D-04 0.205D-05 0.267D-04 0.506D-04-0.194D-03
Coeff:-0.109D-04 0.456D-03 0.665D-03-0.327D-03-0.430D-02-0.273D-02
Coeff: 0.801D-02 0.150D-01 0.597D-02-0.544D-01-0.106D+00 0.518D-01
Coeff: 0.352D+00 0.735D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=1.70D-08 MaxDP=3.71D-06

Cycle  26  Pass 1  IDiag  1:
RMSU=  7.49D-09    CP:  1.00D+00  1.05D+00  1.52D+00  1.50D+00  1.41D+00
                   CP:  1.22D+00
E= -755.132851360548     Delta-E=       -0.000000000005 Rises=F
DIIS: error= 4.90D-08 at cycle  26.
Coeff: 0.706D-06-0.455D-06-0.229D-04 0.136D-04-0.217D-04 0.763D-04
Coeff: 0.601D-04 0.742D-05-0.607D-05-0.615D-03-0.141D-02 0.234D-03
Coeff: 0.344D-02 0.738D-02 0.704D-03-0.330D-01-0.818D-01 0.258D-02
Coeff: 0.329D+00 0.774D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=1.82D-08 MaxDP=1.65D-06

Cycle  27  Pass 1  IDiag  1:
RMSU=  4.16D-09    CP:  1.00D+00  1.07D+00  1.51D+00  1.49D+00  1.34D+00
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                   CP:  1.22D+00  1.44D+00
E= -755.132851360557     Delta-E=       -0.000000000009 Rises=F
DIIS: error= 1.96D-08 at cycle  27.
Coeff:-0.339D-06 0.592D-05 0.139D-04-0.520D-05-0.186D-04-0.564D-04
Coeff: 0.177D-04 0.157D-03 0.322D-04-0.110D-02-0.111D-02 0.115D-02
Coeff: 0.521D-02 0.902D-02-0.318D-02-0.544D-01-0.682D-01-0.246D-01
Coeff: 0.317D+00 0.820D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=1.06D-08 MaxDP=1.02D-06

Cycle  28  Pass 1  IDiag  1:
RMSU=  5.00D-09    CP:  1.00D+00  1.08D+00  1.52D+00  1.49D+00  1.25D+00
                   CP:  1.10D+00  1.49D+00  1.66D+00
E= -755.132851360369     Delta-E=        0.000000000188 Rises=F
DIIS: error= 9.44D-09 at cycle  28.
Coeff: 0.343D-05 0.639D-06 0.431D-06-0.187D-04-0.421D-04 0.189D-04
Coeff: 0.949D-04 0.326D-03 0.113D-03-0.580D-03-0.937D-03-0.807D-03
Coeff: 0.401D-02 0.742D-02 0.829D-03-0.206D-01-0.741D-01-0.505D-01
Coeff: 0.275D+00 0.860D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=9.80D-09 MaxDP=2.35D-06

Cycle  29  Pass 1  IDiag  1:
RMSU=  3.66D-09    CP:  1.00D+00  1.08D+00  1.55D+00  1.47D+00  1.19D+00
                   CP:  1.04D+00  1.39D+00  2.62D+00  1.75D+00
E= -755.132851360261     Delta-E=        0.000000000109 Rises=F
DIIS: error= 3.06D-09 at cycle  29.
Coeff:-0.603D-06 0.167D-05-0.377D-05-0.131D-04 0.264D-05 0.160D-04
Coeff: 0.150D-03 0.231D-03-0.855D-04-0.625D-03-0.113D-02 0.839D-03
Coeff: 0.376D-02 0.704D-02-0.114D-02-0.315D-01-0.590D-01 0.346D-01
Coeff: 0.394D+00 0.653D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=8.44D-09 MaxDP=2.06D-06

Cycle  30  Pass 1  IDiag  1:
RMSU=  3.03D-09    CP:  1.00D+00  1.08D+00  1.57D+00  1.46D+00  1.19D+00
                   CP:  1.05D+00  1.37D+00  3.00D+00  2.49D+00  1.96D+00
E= -755.132851360136     Delta-E=        0.000000000124 Rises=F
DIIS: error= 1.91D-09 at cycle  30.
Coeff: 0.925D-06-0.216D-06-0.212D-05-0.276D-05-0.974D-05 0.213D-04
Coeff: 0.104D-03 0.415D-04-0.184D-03-0.455D-03-0.210D-03 0.111D-02
Coeff: 0.415D-02 0.211D-02-0.901D-02-0.287D-01-0.273D-01 0.816D-01
Coeff: 0.326D+00 0.651D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=1.14D-08 MaxDP=2.63D-06

Cycle  31  Pass 1  IDiag  1:
RMSU=  2.98D-09    CP:  1.00D+00  1.08D+00  1.58D+00  1.44D+00  1.17D+00
                   CP:  1.10D+00  1.45D+00  3.00D+00  3.00D+00  3.00D+00
                   CP:  2.92D+00
E= -755.132851359921     Delta-E=        0.000000000215 Rises=F
DIIS: error= 1.30D-09 at cycle  31.
Coeff:-0.205D-06-0.299D-06-0.121D-05-0.113D-04 0.922D-05 0.968D-04
Coeff: 0.549D-04-0.159D-03-0.427D-03-0.297D-03 0.949D-03 0.431D-02
Coeff: 0.261D-02-0.837D-02-0.304D-01-0.339D-01 0.737D-01 0.367D+00
Coeff: 0.800D+00-0.175D+00
Gap=     0.144 Goal=     0.100 Shift=    0.000
Gap=     0.111 Goal=     0.100 Shift=    0.000
RMSDP=2.83D-09 MaxDP=4.16D-07

SCF Done:  E(UPBE+HF-PBE) =  -755.132851360     A.U. after   31 cycles
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            Convg  =    0.2826D-08             -V/T =  2.0040
            S**2   =   0.8196
KE= 7.520871466376D+02 PE=-3.856023948294D+03 EE= 1.302157976787D+03
Annihilation of the first spin contaminant:
S**2 before annihilation     0.8196,   after     0.7510
Leave Link  502 at Wed Nov 13 02:31:11 2002, MaxMem=   13107200 cpu:  208084.7
(Enter /export/local/gauss/g99/l801.exe)
Range of M.O.s used for correlation:    17   703
NBasis=   705 NAE=    57 NBE=    56 NFC=    16 NFV=     0
NROrb=    687 NOA=    41 NOB=    40 NVA=   646 NVB=   647

**** Warning!!: The largest alpha MO coefficient is  0.32090582D+03


**** Warning!!: The largest beta MO coefficient is  0.33436933D+03

Leave Link  801 at Wed Nov 13 02:31:11 2002, MaxMem=   13107200 cpu:       0.4
(Enter /export/local/gauss/g99/l914.exe)
UHF ground state
MDV=  13107200 DFT=T DoStab=F Mixed=T DoRPA=T DoScal=F NonHer=T
Making orbital integer symmetry assigments:
Orbital symmetries:
Alpha Orbitals:
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Symmetry not used in FoFDir.
MinBra= 0 MaxBra= 3 Meth= 1.
IRaf=       0 NMat=   2 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 JSym2E=0.
    8 initial guesses have been made.
Convergence on wavefunction:    0.000100000000000
Davidson Disk Diagonalization:  ConvIn= 1.00D-04 SkipCon=T Conv= 1.00D-04.
Max sub-space:   200 roots to seek:     8 dimension of matrix:  52366
Iteration     1 Dimension     8
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   3 NMax=   3.
CISAX will form   3 AO SS matrices at one time.
NMat=  3 NSing=  3.
NMat=  3 NSing=  3.
NMat=  2 NSing=  2.
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   3 NMax=   3.
CISAX will form   3 AO SS matrices at one time.
NMat=  3 NSing=  3.
NMat=  3 NSing=  3.
NMat=  2 NSing=  2.
Excitation Energies [eV] at current iteration:
Root      1 :     2.176600919357994
Root      2 :     2.853216075231499
Iteration     2 Dimension    12
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Root      1 not converged, maximum delta is    0.171164327258943
Root      2 not converged, maximum delta is    0.102569720489540
Excitation Energies [eV] at current iteration:
Root      1 :     1.733699920148450   Change is   -0.442900999209544
Root      2 :     2.527612906485791   Change is   -0.325603168745707
Iteration     3 Dimension    16
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Root      1 not converged, maximum delta is    0.071651921220748
Root      2 not converged, maximum delta is    0.121746708805069
Excitation Energies [eV] at current iteration:
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Root      1 :     1.581831715732621   Change is   -0.151868204415829
Root      2 :     2.453872355544780   Change is   -0.073740550941011
Iteration     4 Dimension    20
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Root      1 not converged, maximum delta is    0.021041550768105
Root      2 not converged, maximum delta is    0.190835304803194
Excitation Energies [eV] at current iteration:
Root      1 :     1.562101454774631   Change is   -0.019730260957989
Root      2 :     2.414453216494582   Change is   -0.039419139050198
Iteration     5 Dimension    24
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Root      1 not converged, maximum delta is    0.122114985015686
New state      2 was old state      1
Root      2 not converged, maximum delta is    0.516233983686732
Excitation Energies [eV] at current iteration:
Root      1 :     1.548136508383307   Change is   -0.013964946391325
Root      2 :     1.840013114201777   Change is    0.277911659427145
Iteration     6 Dimension    28
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Root      1 not converged, maximum delta is    0.471073024504509
New state      2 was old state      1
Root      2 not converged, maximum delta is    0.111848986489484
Excitation Energies [eV] at current iteration:
Root      1 :     1.457295708868557   Change is   -0.090840799514750
Root      2 :     1.582595964337266   Change is    0.034459455953959
Iteration     7 Dimension    32
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Root      1 not converged, maximum delta is    0.065021596273123
Root      2 not converged, maximum delta is    0.064690417115200
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Excitation Energies [eV] at current iteration:
Root      1 :     1.430605162794342   Change is   -0.026690546074215
Root      2 :     1.576902873979556   Change is   -0.005693090357710
Iteration     8 Dimension    36
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Root      1 not converged, maximum delta is    0.009476737939926
Root      2 not converged, maximum delta is    0.008576434269276
Excitation Energies [eV] at current iteration:
Root      1 :     1.426838967886410   Change is   -0.003766194907932
Root      2 :     1.576230729355172   Change is   -0.000672144624384
Iteration     9 Dimension    40
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Root      1 not converged, maximum delta is    0.003147396031235
Root      2 not converged, maximum delta is    0.001496841582145
Excitation Energies [eV] at current iteration:
Root      1 :     1.426218701379538   Change is   -0.000620266506873
Root      2 :     1.576117514665059   Change is   -0.000113214690112
Iteration    10 Dimension    44
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Root      1 not converged, maximum delta is    0.000643575016481
Root      2 not converged, maximum delta is    0.000469965745529
Excitation Energies [eV] at current iteration:
Root      1 :     1.426105576078415   Change is   -0.000113125301122
Root      2 :     1.576096816536748   Change is   -0.000020698128311
Iteration    11 Dimension    48
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Root      1 not converged, maximum delta is    0.000324049980968
Root      2 not converged, maximum delta is    0.000146864944721
Excitation Energies [eV] at current iteration:
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Root      1 :     1.426086305916433   Change is   -0.000019270161982
Root      2 :     1.576093049929668   Change is   -0.000003766607080
Iteration    12 Dimension    52
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Root      1 not converged, maximum delta is    0.000207342526733
Root      2 not converged, maximum delta is    0.000103405777952
Excitation Energies [eV] at current iteration:
Root      1 :     1.426082776836404   Change is   -0.000003529080029
Root      2 :     1.576092267662776   Change is   -0.000000782266892
Iteration    13 Dimension    56
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Cannot handle 2e integral symmetry, ISym2E=1.
CISAX:  IP=  1 NPass=   2 NMax=   2.
CISAX will form   2 AO SS matrices at one time.
NMat=  2 NSing=  2.
NMat=  2 NSing=  2.
Root      1 has converged.
Root      2 has converged.
Excitation Energies [eV] at current iteration:
Root      1 :     1.426082039047649   Change is   -0.000000737788755
Root      2 :     1.576092094424559   Change is   -0.000000173238217
Convergence achieved on expansion vectors.
*********************************************************************
Excited states from <AA,BB:AA,BB> singles matrix:
*********************************************************************

1PDM for each excited state written to RWF  633
Ground to excited state Transition electric dipole moments (Au):
      state          X           Y           Z          Osc.
        1        -0.0521      0.1115      0.0141      0.0005
        2        -0.0187      0.5434     -0.0959      0.0118
Ground to excited state transition velocity dipole Moments (Au):
      state          X           Y           Z          Osc.
        1         0.0029     -0.0057     -0.0004      0.0005
        2         0.0011     -0.0315      0.0055      0.0118
Ground to excited state transition magnetic dipole Moments (Au):
      state          X           Y           Z
        1         0.1706     -0.7043      0.3127
        2        -0.0275      0.1617      0.1461
<0|del|b> * <b|rxdel|0>  (Au), Rotatory Strengths (R) in
cgs (10**-40 erg-esu-cm/Gauss)
      state          X           Y           Z     R(velocity)
        1         0.0005      0.0040     -0.0001     19.6391
        2         0.0000     -0.0051      0.0008    -17.5768
<0|r|b> * <b|rxdel|0>  (Au), Rotatory Strengths (R) in
cgs (10**-40 erg-esu-cm/Gauss)
      state          X           Y           Z     R(length)
        1        -0.0089     -0.0785      0.0044     19.5645
        2         0.0005      0.0879     -0.0140    -17.5279
 <0|del|b> * <b|r|0>  (Au)
      state          X           Y           Z       Osc.(frdel)
        1        -0.0002     -0.0006      0.0000      0.0005
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        2         0.0000     -0.0171     -0.0005      0.0118
Ground to excited state transition densities written to RWF  633

Excitation energies and oscillator strengths:

Excited State   1:   ?Spin  -A      1.4261 eV  869.40 nm  f=0.0005
    56A -> 58A        0.10016
    57A -> 58A       -0.10236
    51B -> 57B       -0.54869
    51B -> 58B        0.19388
    52B -> 57B       -0.23091
    54B -> 57B       -0.75078
    54B -> 58B        0.21473
    55B -> 57B       -0.17281
    56B -> 57B        0.17208
This state for optimization and/or second-order correction.
Total Energy, E(RPA) =  -755.080443447
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State   2:   ?Spin  -A      1.5761 eV  786.65 nm  f=0.0118
    51A -> 58A        0.15756
    55A -> 58A       -0.19081
    56A -> 58A        0.41998
    56A -> 59A       -0.10512
    57A -> 58A       -0.50830
    51B -> 57B        0.14354
    53B -> 57B        0.25883
    53B -> 58B        0.11361
    54B -> 57B        0.12473
    54B -> 58B       -0.10115
    55B -> 57B       -0.26375
    55B -> 58B       -0.14968
    56B -> 57B        0.73906
    56B -> 58B        0.39829
Leave Link  914 at Wed Nov 20 12:12:18 2002, MaxMem=   13107200 cpu:  639585.9
(Enter /export/local/gauss/g99/l601.exe)
Copying SCF densities to generalized density rwf, ISCF=1 IROHF=0.

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

           Population analysis using the SCF density.

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Orbital symmetries:
Alpha Orbitals:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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The electronic state is 2-A.
Alpha  occ. eigenvalues --  -19.25002 -19.22033 -14.54065 -14.52469 -14.44843
Alpha  occ. eigenvalues --  -14.36938 -10.34972 -10.32945 -10.29999 -10.29406
Alpha  occ. eigenvalues --  -10.26363 -10.23710 -10.23511 -10.23425 -10.23194
Alpha  occ. eigenvalues --  -10.22372  -1.14746  -1.11186  -1.06622  -0.97192
Alpha  occ. eigenvalues --   -0.92116  -0.88773  -0.85072  -0.83271  -0.78237
Alpha  occ. eigenvalues --   -0.77068  -0.69561  -0.68762  -0.66241  -0.62713
Alpha  occ. eigenvalues --   -0.61762  -0.57643  -0.57151  -0.55658  -0.53591
Alpha  occ. eigenvalues --   -0.51284  -0.50892  -0.49298  -0.48377  -0.48117
Alpha  occ. eigenvalues --   -0.47874  -0.45994  -0.45928  -0.43980  -0.43674
Alpha  occ. eigenvalues --   -0.39724  -0.38910  -0.38115  -0.37634  -0.33157
Alpha  occ. eigenvalues --   -0.31825  -0.31200  -0.29716  -0.28138  -0.27081
Alpha  occ. eigenvalues --   -0.25535  -0.23647
Alpha virt. eigenvalues --   -0.09203  -0.01149  -0.00111   0.00966   0.01192
Alpha virt. eigenvalues --    0.01928   0.02357   0.02995   0.03533   0.04026
Alpha virt. eigenvalues --    0.04865   0.05398   0.05801   0.06655   0.06745
Alpha virt. eigenvalues --    0.07220   0.07632   0.07806   0.08486   0.09294
Alpha virt. eigenvalues --    0.09770   0.10180   0.11062   0.11114   0.11629
Alpha virt. eigenvalues --    0.12434   0.12814   0.13432   0.13908   0.14264
Alpha virt. eigenvalues --    0.14735   0.14909   0.15397   0.15540   0.16128
Alpha virt. eigenvalues --    0.16583   0.16657   0.17726   0.18500   0.18775
Alpha virt. eigenvalues --    0.18935   0.19266   0.19372   0.19590   0.20036
Alpha virt. eigenvalues --    0.20243   0.20670   0.21140   0.21663   0.21789
Alpha virt. eigenvalues --    0.22244   0.22531   0.23319   0.23332   0.23603
Alpha virt. eigenvalues --    0.24101   0.24264   0.24569   0.25087   0.25425
Alpha virt. eigenvalues --    0.25843   0.26219   0.26461   0.26747   0.27493
Alpha virt. eigenvalues --    0.28482   0.29193   0.29624   0.29897   0.30025
Alpha virt. eigenvalues --    0.30812   0.31187   0.31290   0.32010   0.32593
Alpha virt. eigenvalues --    0.33151   0.33485   0.34045   0.34338   0.34815
Alpha virt. eigenvalues --    0.35285   0.35826   0.36189   0.36720   0.37596
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Alpha virt. eigenvalues --    0.38432   0.39172   0.40311   0.41363   0.41929
Alpha virt. eigenvalues --    0.42145   0.42578   0.43262   0.43507   0.44791
Alpha virt. eigenvalues --    0.44960   0.45733   0.46507   0.47226   0.47435
Alpha virt. eigenvalues --    0.48039   0.48848   0.49848   0.50084   0.50641
Alpha virt. eigenvalues --    0.50749   0.51992   0.52378   0.53019   0.53641
Alpha virt. eigenvalues --    0.54641   0.55052   0.55780   0.56115   0.56553
Alpha virt. eigenvalues --    0.57287   0.57916   0.58199   0.58737   0.58989
Alpha virt. eigenvalues --    0.59617   0.60361   0.60877   0.61029   0.61521
Alpha virt. eigenvalues --    0.62138   0.62785   0.63555   0.63907   0.64096
Alpha virt. eigenvalues --    0.64937   0.65480   0.65737   0.66301   0.66561
Alpha virt. eigenvalues --    0.67163   0.68126   0.68627   0.68956   0.69926
Alpha virt. eigenvalues --    0.70595   0.71128   0.71531   0.73281   0.73714
Alpha virt. eigenvalues --    0.73845   0.74714   0.75446   0.75829   0.76466
Alpha virt. eigenvalues --    0.77207   0.78213   0.78693   0.79158   0.79950
Alpha virt. eigenvalues --    0.81016   0.81724   0.82927   0.83319   0.83831
Alpha virt. eigenvalues --    0.84767   0.85681   0.86495   0.87525   0.88256
Alpha virt. eigenvalues --    0.88563   0.89538   0.90453   0.93170   0.93211
Alpha virt. eigenvalues --    0.93545   0.94954   0.95715   0.96435   0.96787
Alpha virt. eigenvalues --    0.97708   0.99192   0.99912   1.00638   1.01928
Alpha virt. eigenvalues --    1.03295   1.03761   1.04644   1.05243   1.06315
Alpha virt. eigenvalues --    1.06827   1.07613   1.08009   1.08740   1.09504
Alpha virt. eigenvalues --    1.09882   1.10594   1.10793   1.11080   1.12265
Alpha virt. eigenvalues --    1.12999   1.13280   1.13928   1.14112   1.15319
Alpha virt. eigenvalues --    1.16048   1.16845   1.17900   1.18114   1.18905
Alpha virt. eigenvalues --    1.19189   1.20357   1.20420   1.21649   1.22641
Alpha virt. eigenvalues --    1.22909   1.23374   1.24507   1.25075   1.25467
Alpha virt. eigenvalues --    1.26086   1.26264   1.27125   1.28314   1.28998
Alpha virt. eigenvalues --    1.29807   1.30746   1.32448   1.32669   1.33026
Alpha virt. eigenvalues --    1.33964   1.34315   1.34554   1.35268   1.36389
Alpha virt. eigenvalues --    1.36675   1.37575   1.38997   1.39826   1.40485
Alpha virt. eigenvalues --    1.41345   1.41447   1.42225   1.43450   1.44331
Alpha virt. eigenvalues --    1.44817   1.45259   1.46382   1.46994   1.47445
Alpha virt. eigenvalues --    1.47940   1.48358   1.49016   1.49722   1.50094
Alpha virt. eigenvalues --    1.51284   1.51389   1.52398   1.53046   1.55273
Alpha virt. eigenvalues --    1.56458   1.59230   1.60866   1.61199   1.61864
Alpha virt. eigenvalues --    1.62390   1.63480   1.64588   1.66654   1.67415
Alpha virt. eigenvalues --    1.68436   1.68966   1.70518   1.71908   1.73423
Alpha virt. eigenvalues --    1.74605   1.76298   1.77466   1.79080   1.79483
Alpha virt. eigenvalues --    1.81985   1.82436   1.84797   1.85945   1.87696
Alpha virt. eigenvalues --    1.88841   1.90429   1.91416   1.92035   1.93273
Alpha virt. eigenvalues --    1.94817   1.95928   1.97616   2.00116   2.01518
Alpha virt. eigenvalues --    2.02001   2.03407   2.03989   2.04339   2.04705
Alpha virt. eigenvalues --    2.05281   2.06299   2.09229   2.10279   2.10782
Alpha virt. eigenvalues --    2.12453   2.14141   2.14766   2.17142   2.17352
Alpha virt. eigenvalues --    2.20811   2.22898   2.24717   2.27560   2.28536
Alpha virt. eigenvalues --    2.33274   2.34161   2.36304   2.37390   2.41870
Alpha virt. eigenvalues --    2.42337   2.42507   2.43965   2.45108   2.46295
Alpha virt. eigenvalues --    2.49183   2.49958   2.51739   2.52621   2.53533
Alpha virt. eigenvalues --    2.55161   2.56698   2.58400   2.60655   2.62515
Alpha virt. eigenvalues --    2.64017   2.66517   2.67610   2.67750   2.69205
Alpha virt. eigenvalues --    2.71365   2.73509   2.74684   2.75995   2.77147
Alpha virt. eigenvalues --    2.78364   2.79644   2.80621   2.82091   2.82918
Alpha virt. eigenvalues --    2.84880   2.86437   2.87901   2.88444   2.88861
Alpha virt. eigenvalues --    2.89388   2.90353   2.90989   2.92190   2.92496
Alpha virt. eigenvalues --    2.95371   2.96259   2.96737   2.97874   3.00004
Alpha virt. eigenvalues --    3.00937   3.02245   3.02736   3.04204   3.06045
Alpha virt. eigenvalues --    3.07286   3.07470   3.09567   3.10335   3.12238
Alpha virt. eigenvalues --    3.14608   3.15202   3.15959   3.17452   3.18146
Alpha virt. eigenvalues --    3.19900   3.21736   3.22553   3.23343   3.24836
Alpha virt. eigenvalues --    3.25059   3.28129   3.28711   3.29445   3.31071
Alpha virt. eigenvalues --    3.32502   3.33676   3.34011   3.36176   3.37451
Alpha virt. eigenvalues --    3.37957   3.38511   3.40988   3.43117   3.44983
Alpha virt. eigenvalues --    3.45387   3.47097   3.47455   3.49426   3.50250
Alpha virt. eigenvalues --    3.50479   3.52573   3.53225   3.53698   3.55630
Alpha virt. eigenvalues --    3.55737   3.57275   3.57482   3.59182   3.59627
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Alpha virt. eigenvalues --    3.60445   3.60824   3.62854   3.66009   3.67535
Alpha virt. eigenvalues --    3.67816   3.71028   3.72684   3.72886   3.74993
Alpha virt. eigenvalues --    3.75487   3.77204   3.79940   3.81096   3.81991
Alpha virt. eigenvalues --    3.83038   3.84453   3.85457   3.87563   3.88341
Alpha virt. eigenvalues --    3.89815   3.91095   3.91917   3.94433   3.95581
Alpha virt. eigenvalues --    3.96999   3.98314   4.00303   4.01816   4.03577
Alpha virt. eigenvalues --    4.05179   4.06134   4.08140   4.08858   4.11470
Alpha virt. eigenvalues --    4.12149   4.15914   4.18952   4.20178   4.21440
Alpha virt. eigenvalues --    4.22997   4.25368   4.26166   4.27833   4.28850
Alpha virt. eigenvalues --    4.29944   4.31554   4.32147   4.32874   4.35249
Alpha virt. eigenvalues --    4.36430   4.37562   4.38597   4.40232   4.40958
Alpha virt. eigenvalues --    4.41496   4.41688   4.43280   4.44427   4.45061
Alpha virt. eigenvalues --    4.45643   4.46343   4.48069   4.50213   4.52628
Alpha virt. eigenvalues --    4.52992   4.54261   4.56976   4.59040   4.60718
Alpha virt. eigenvalues --    4.63556   4.63871   4.65122   4.66672   4.68932
Alpha virt. eigenvalues --    4.70747   4.73396   4.74200   4.77945   4.80723
Alpha virt. eigenvalues --    4.81014   4.82517   4.83567   4.83856   4.85342
Alpha virt. eigenvalues --    4.88380   4.90727   4.94758   4.97566   4.99149
Alpha virt. eigenvalues --    5.00277   5.01890   5.06065   5.07151   5.07744
Alpha virt. eigenvalues --    5.09406   5.10913   5.13682   5.14677   5.18999
Alpha virt. eigenvalues --    5.19786   5.22955   5.24554   5.27692   5.29644
Alpha virt. eigenvalues --    5.33062   5.34214   5.35375   5.36536   5.41014
Alpha virt. eigenvalues --    5.44590   5.46847   5.49684   5.51983   5.58504
Alpha virt. eigenvalues --    5.67364   5.69302   5.74149   5.78857   5.80110
Alpha virt. eigenvalues --    5.82816   5.85252   5.87303   5.94528   5.97243
Alpha virt. eigenvalues --    6.02573   6.04777   6.05540   6.08312   6.12632
Alpha virt. eigenvalues --    6.20897   6.25654   6.28728   6.40639   6.54204
Alpha virt. eigenvalues --    6.67782   6.73008   6.94572   7.05892   7.11776
Alpha virt. eigenvalues --    7.14358   7.15625   7.19079   7.22010   7.24182
Alpha virt. eigenvalues --    7.25970   7.31775   7.32436   7.33107   7.37034
Alpha virt. eigenvalues --    7.38430   7.39896   7.41100   7.42420   7.47666
Alpha virt. eigenvalues --    7.47835   7.52471   7.56392   7.56812   7.57499
Alpha virt. eigenvalues --    7.58635   7.60663   7.66141   7.67923   7.68267
Alpha virt. eigenvalues --    7.69580   7.72383   7.77207   7.83277   7.90537
Alpha virt. eigenvalues --    7.91960   7.93171   7.98530   8.01153   8.02618
Alpha virt. eigenvalues --    8.05145   8.07954   8.14135   8.20018   8.25256
Alpha virt. eigenvalues --    8.34918   8.40216   8.41018   8.41701   8.48402
Alpha virt. eigenvalues --    8.59646   8.65897   8.68823   8.73074   9.46847
Alpha virt. eigenvalues --   10.43314  10.47006  10.49351  10.51456  10.54064
Alpha virt. eigenvalues --   10.57745  10.61831  10.65729  10.73090  10.77830
Alpha virt. eigenvalues --   10.83406  10.93271  11.08798  11.21115  11.24435
Alpha virt. eigenvalues --   11.26423  11.28532  11.37079  11.60841  12.01720
Alpha virt. eigenvalues --   14.35823  14.38147  14.38969  14.42944  14.51595
Alpha virt. eigenvalues --   14.55683  14.58026  14.63126  15.08492  15.11347
Alpha virt. eigenvalues --   24.24526  24.47718  24.57874  24.89136  25.07148
Alpha virt. eigenvalues --   25.16857  25.25263  25.59772  25.81459  26.32462
Alpha virt. eigenvalues --   35.96314  36.22980  36.32215  36.54586  50.38895
Alpha virt. eigenvalues --   50.47163
 Beta  occ. eigenvalues --  -19.23209 -19.21468 -14.53668 -14.51771 -14.44849
 Beta  occ. eigenvalues --  -14.37043 -10.35295 -10.32872 -10.30007 -10.29371
 Beta  occ. eigenvalues --  -10.26390 -10.23692 -10.23542 -10.23411 -10.23181
 Beta  occ. eigenvalues --  -10.22401  -1.13623  -1.09062  -1.06649  -0.95816
 Beta  occ. eigenvalues --   -0.92197  -0.88834  -0.84164  -0.82087  -0.78228
 Beta  occ. eigenvalues --   -0.77051  -0.69095  -0.68631  -0.66265  -0.62712
 Beta  occ. eigenvalues --   -0.61527  -0.57345  -0.56350  -0.54768  -0.53383
 Beta  occ. eigenvalues --   -0.51133  -0.50412  -0.48532  -0.48109  -0.47593
 Beta  occ. eigenvalues --   -0.46812  -0.45983  -0.44907  -0.43139  -0.42604
 Beta  occ. eigenvalues --   -0.38933  -0.38134  -0.37468  -0.36502  -0.33293
 Beta  occ. eigenvalues --   -0.30367  -0.29514  -0.28024  -0.27720  -0.25425
 Beta  occ. eigenvalues --   -0.23096
 Beta virt. eigenvalues --   -0.11970  -0.07995  -0.01212   0.00006   0.00977
 Beta virt. eigenvalues --    0.01149   0.01977   0.02454   0.03055   0.03595
 Beta virt. eigenvalues --    0.04050   0.05014   0.05421   0.05836   0.06606
 Beta virt. eigenvalues --    0.06890   0.07408   0.07785   0.07899   0.08478
 Beta virt. eigenvalues --    0.09449   0.09868   0.10370   0.11126   0.11189
```

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Beta virt. eigenvalues --    0.11652   0.12558   0.12886   0.13678   0.13990
Beta virt. eigenvalues --    0.14324   0.14837   0.14974   0.15439   0.15701
Beta virt. eigenvalues --    0.16204   0.16671   0.16754   0.17825   0.18615
Beta virt. eigenvalues --    0.18800   0.18994   0.19339   0.19392   0.19705
Beta virt. eigenvalues --    0.20058   0.20278   0.20702   0.21221   0.21725
Beta virt. eigenvalues --    0.21911   0.22256   0.22599   0.23369   0.23405
Beta virt. eigenvalues --    0.23626   0.24265   0.24387   0.24653   0.25162
Beta virt. eigenvalues --    0.25447   0.25905   0.26330   0.26641   0.26837
Beta virt. eigenvalues --    0.27597   0.28703   0.29284   0.29776   0.29964
Beta virt. eigenvalues --    0.30138   0.30863   0.31367   0.31684   0.32255
Beta virt. eigenvalues --    0.32707   0.33189   0.33526   0.34271   0.34425
Beta virt. eigenvalues --    0.34893   0.35342   0.35938   0.36262   0.36844
Beta virt. eigenvalues --    0.37721   0.38490   0.39240   0.40441   0.41397
Beta virt. eigenvalues --    0.42025   0.42240   0.42623   0.43330   0.43513
Beta virt. eigenvalues --    0.44820   0.45032   0.45797   0.46541   0.47287
Beta virt. eigenvalues --    0.47562   0.48095   0.48970   0.49939   0.50166
Beta virt. eigenvalues --    0.50718   0.50786   0.52135   0.52501   0.53065
Beta virt. eigenvalues --    0.53685   0.54716   0.55102   0.55892   0.56141
Beta virt. eigenvalues --    0.56589   0.57271   0.57950   0.58238   0.58768
Beta virt. eigenvalues --    0.59022   0.59642   0.60376   0.60891   0.61047
Beta virt. eigenvalues --    0.61564   0.62200   0.62779   0.63580   0.63941
Beta virt. eigenvalues --    0.64220   0.65019   0.65509   0.65686   0.66259
Beta virt. eigenvalues --    0.66599   0.67218   0.68362   0.68670   0.69048
Beta virt. eigenvalues --    0.69927   0.70699   0.71223   0.71582   0.73331
Beta virt. eigenvalues --    0.73721   0.73912   0.74805   0.75506   0.75871
Beta virt. eigenvalues --    0.76602   0.77341   0.78250   0.78728   0.79207
Beta virt. eigenvalues --    0.80054   0.81212   0.81814   0.83053   0.83433
Beta virt. eigenvalues --    0.83994   0.84897   0.85776   0.86587   0.87623
Beta virt. eigenvalues --    0.88309   0.88675   0.89674   0.90596   0.93222
Beta virt. eigenvalues --    0.93299   0.93768   0.95073   0.95944   0.96667
Beta virt. eigenvalues --    0.96918   0.97849   0.99306   1.00168   1.00701
Beta virt. eigenvalues --    1.02290   1.03522   1.03989   1.04940   1.05469
Beta virt. eigenvalues --    1.06837   1.06974   1.08477   1.08824   1.09421
Beta virt. eigenvalues --    1.09670   1.10085   1.10895   1.11170   1.11762
Beta virt. eigenvalues --    1.12521   1.13191   1.13607   1.14230   1.14364
Beta virt. eigenvalues --    1.15419   1.16423   1.17053   1.17994   1.18260
Beta virt. eigenvalues --    1.19030   1.19281   1.20508   1.20635   1.21688
Beta virt. eigenvalues --    1.22784   1.22919   1.23633   1.24629   1.25474
Beta virt. eigenvalues --    1.25667   1.26161   1.26446   1.27357   1.28361
Beta virt. eigenvalues --    1.29136   1.30081   1.30946   1.32506   1.32714
Beta virt. eigenvalues --    1.33267   1.34028   1.34440   1.34712   1.35343
Beta virt. eigenvalues --    1.36530   1.36788   1.37715   1.39042   1.40180
Beta virt. eigenvalues --    1.40488   1.41363   1.41508   1.42301   1.43545
Beta virt. eigenvalues --    1.44401   1.44858   1.45327   1.46409   1.47045
Beta virt. eigenvalues --    1.47502   1.47998   1.48581   1.49012   1.49789
Beta virt. eigenvalues --    1.50134   1.51337   1.51454   1.52459   1.53130
Beta virt. eigenvalues --    1.55313   1.56654   1.59270   1.61182   1.61372
Beta virt. eigenvalues --    1.62010   1.62446   1.63551   1.64715   1.66831
Beta virt. eigenvalues --    1.67408   1.68773   1.69119   1.70612   1.72093
Beta virt. eigenvalues --    1.73449   1.74827   1.76372   1.77464   1.79164
Beta virt. eigenvalues --    1.79531   1.82086   1.82555   1.84831   1.86217
Beta virt. eigenvalues --    1.87812   1.88911   1.90445   1.91512   1.92090
Beta virt. eigenvalues --    1.93273   1.94820   1.95935   1.97627   2.00259
Beta virt. eigenvalues --    2.01566   2.02028   2.03514   2.04039   2.04403
Beta virt. eigenvalues --    2.04834   2.05340   2.06350   2.09238   2.10288
Beta virt. eigenvalues --    2.10750   2.12536   2.14061   2.14834   2.17206
Beta virt. eigenvalues --    2.17446   2.20903   2.22942   2.24936   2.27616
Beta virt. eigenvalues --    2.29009   2.33303   2.34156   2.36516   2.37874
Beta virt. eigenvalues --    2.42019   2.42526   2.42645   2.44095   2.45617
Beta virt. eigenvalues --    2.46521   2.49380   2.50029   2.52044   2.52692
Beta virt. eigenvalues --    2.53570   2.55288   2.57027   2.58672   2.61088
Beta virt. eigenvalues --    2.62518   2.64018   2.66727   2.67612   2.67830
Beta virt. eigenvalues --    2.69523   2.71429   2.73597   2.75033   2.76137
Beta virt. eigenvalues --    2.77373   2.78478   2.79860   2.80599   2.82126
Beta virt. eigenvalues --    2.82953   2.84914   2.86552   2.87851   2.88542
```

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Beta virt. eigenvalues --    2.88973   2.89404   2.90408   2.90998   2.92236
Beta virt. eigenvalues --    2.92546   2.95397   2.96294   2.96864   2.97792
Beta virt. eigenvalues --    3.00157   3.00992   3.02322   3.02814   3.04140
Beta virt. eigenvalues --    3.05741   3.07292   3.07452   3.09534   3.10858
Beta virt. eigenvalues --    3.12582   3.14818   3.15361   3.16054   3.17576
Beta virt. eigenvalues --    3.18215   3.19987   3.21854   3.22557   3.23599
Beta virt. eigenvalues --    3.24996   3.25084   3.28199   3.28896   3.29456
Beta virt. eigenvalues --    3.31200   3.32501   3.33856   3.34453   3.36363
Beta virt. eigenvalues --    3.37671   3.38253   3.38661   3.41228   3.44019
Beta virt. eigenvalues --    3.45459   3.45990   3.47557   3.48368   3.49607
Beta virt. eigenvalues --    3.50762   3.51451   3.53303   3.53965   3.55182
Beta virt. eigenvalues --    3.56029   3.57116   3.57492   3.58586   3.59565
Beta virt. eigenvalues --    3.59886   3.60620   3.61129   3.63599   3.66426
Beta virt. eigenvalues --    3.68054   3.68127   3.71568   3.72807   3.73722
Beta virt. eigenvalues --    3.75431   3.75750   3.77318   3.80284   3.81282
Beta virt. eigenvalues --    3.82192   3.83118   3.84551   3.85510   3.87605
Beta virt. eigenvalues --    3.88403   3.90007   3.91328   3.92105   3.94722
Beta virt. eigenvalues --    3.95998   3.97131   3.98436   4.00424   4.02667
Beta virt. eigenvalues --    4.03917   4.05459   4.06259   4.08400   4.09515
Beta virt. eigenvalues --    4.11822   4.12945   4.16505   4.19164   4.20288
Beta virt. eigenvalues --    4.21617   4.23576   4.25772   4.26342   4.28039
Beta virt. eigenvalues --    4.29068   4.30193   4.31653   4.32327   4.33439
Beta virt. eigenvalues --    4.35281   4.36799   4.37819   4.38698   4.40264
Beta virt. eigenvalues --    4.41114   4.41606   4.41964   4.43391   4.44646
Beta virt. eigenvalues --    4.45176   4.45654   4.46560   4.48201   4.50434
Beta virt. eigenvalues --    4.52788   4.53156   4.54456   4.57277   4.59215
Beta virt. eigenvalues --    4.61018   4.63585   4.64108   4.65459   4.67079
Beta virt. eigenvalues --    4.69288   4.70884   4.73657   4.74295   4.78297
Beta virt. eigenvalues --    4.80856   4.81429   4.82558   4.83868   4.83999
Beta virt. eigenvalues --    4.85561   4.88594   4.90874   4.94902   4.97770
Beta virt. eigenvalues --    4.99481   5.00429   5.01827   5.06289   5.09997
Beta virt. eigenvalues --    5.11009   5.11241   5.11831   5.14412   5.15651
Beta virt. eigenvalues --    5.19401   5.19806   5.24488   5.28551   5.29658
Beta virt. eigenvalues --    5.31996   5.33735   5.34685   5.36506   5.38092
Beta virt. eigenvalues --    5.41642   5.46109   5.47305   5.50328   5.52106
Beta virt. eigenvalues --    5.58863   5.67589   5.69826   5.75075   5.79677
Beta virt. eigenvalues --    5.80286   5.83091   5.85583   5.87669   5.94747
Beta virt. eigenvalues --    5.97775   6.02574   6.05023   6.07523   6.09009
Beta virt. eigenvalues --    6.13057   6.21420   6.25706   6.28768   6.40666
Beta virt. eigenvalues --    6.54278   6.67795   6.73004   6.94601   7.06880
Beta virt. eigenvalues --    7.11725   7.14338   7.15554   7.18969   7.21970
Beta virt. eigenvalues --    7.24280   7.25821   7.31722   7.32206   7.33039
Beta virt. eigenvalues --    7.37012   7.38406   7.39391   7.40821   7.42409
Beta virt. eigenvalues --    7.47634   7.47804   7.52422   7.56312   7.56758
Beta virt. eigenvalues --    7.57138   7.58608   7.60574   7.65932   7.67881
Beta virt. eigenvalues --    7.68196   7.69525   7.71906   7.76807   7.83245
Beta virt. eigenvalues --    7.90500   7.92034   7.93199   7.98534   8.01144
Beta virt. eigenvalues --    8.02626   8.05133   8.07946   8.14127   8.20008
Beta virt. eigenvalues --    8.25350   8.34963   8.40215   8.41020   8.41713
Beta virt. eigenvalues --    8.48384   8.59757   8.65888   8.68818   8.73072
Beta virt. eigenvalues --    9.46837  10.43362  10.48566  10.50564  10.51880
Beta virt. eigenvalues --   10.56003  10.58149  10.63028  10.66732  10.74223
Beta virt. eigenvalues --   10.77526  10.85051  10.93807  11.09252  11.21352
Beta virt. eigenvalues --   11.24647  11.26766  11.28535  11.37112  11.61222
Beta virt. eigenvalues --   12.01694  14.41079  14.42602  14.45163  14.45371
Beta virt. eigenvalues --   14.57591  14.58845  14.58953  14.63381  15.11154
Beta virt. eigenvalues --   15.12140  24.24517  24.47742  24.57880  24.88900
Beta virt. eigenvalues --   25.07150  25.16858  25.25247  25.59761  25.81455
Beta virt. eigenvalues --   26.32459  35.96944  36.23248  36.32291  36.54501
Beta virt. eigenvalues --   50.40078  50.48043
        Condensed to atoms (all electrons):
             1          2          3          4          5          6
   1  C   13.365055  -2.414237  -1.777967  -0.326620  -0.345482  -0.306348
   2  C   -2.414237  14.787229  -2.620564  -0.395543  -0.565602  -1.197607
   3  C   -1.777967  -2.620564  14.568328   0.145987   1.099852  -0.592707
```

4	C	-0.326620	-0.395543	0.145987	6.339235	-0.101808	-0.003553
5	C	-0.345482	-0.565602	1.099852	-0.101808	6.754908	-0.081221
6	C	-0.306348	-1.197607	-0.592707	-0.003553	-0.081221	7.255768
7	N	0.285660	0.081504	0.024287	0.000526	-0.026803	-0.331206
8	C	0.179114	0.324146	-3.132676	0.004402	-0.502974	0.226091
9	N	0.353012	-0.117005	-0.604020	-0.063453	-0.019186	-0.036092
10	H	0.000045	-0.210578	0.547574	-0.025089	0.014073	-0.004589
11	H	0.003662	0.086479	-0.226715	0.586749	-0.119799	0.001922
12	H	0.008863	0.041482	-0.063292	-0.070362	0.539243	-0.121928
13	H	-0.228464	-0.035851	-0.049310	0.023552	-0.062283	0.668683
14	H	-0.157519	0.098949	0.015265	0.000468	-0.003501	-0.022030
15	C	-2.935096	-2.282224	-1.269897	0.139698	-0.186997	0.020929
16	N	0.029795	-0.048498	-0.014762	-0.000130	-0.001265	0.000503
17	C	0.024264	0.000923	0.006855	-0.000101	-0.000281	0.000556
18	C	-0.091719	-0.030898	-0.013865	0.001498	-0.001443	-0.000578
19	N	-0.006822	0.016533	-0.001782	-0.000312	0.000031	0.000148
20	H	-0.001007	-0.001357	-0.000118	0.000005	-0.000004	0.000002
21	H	0.002289	0.000090	0.000122	-0.000009	0.000008	-0.000004
22	H	-0.000025	0.000555	0.000005	-0.000001	0.000000	0.000000
23	H	0.001245	0.002196	0.000254	-0.000005	0.000013	0.000002
24	O	0.045696	-0.010725	0.012593	-0.001486	0.000892	-0.000101
25	O	0.019652	0.039759	0.006480	0.000084	-0.000188	0.000142

		7	8	9	10	11	12
1	C	0.285660	0.179114	0.353012	0.000045	0.003662	0.008863
2	C	0.081504	0.324146	-0.117005	-0.210578	0.086479	0.041482
3	C	0.024287	-3.132676	-0.604020	0.547574	-0.226715	-0.063292
4	C	0.000526	0.004402	-0.063453	-0.025089	0.586749	-0.070362
5	C	-0.026803	-0.502974	-0.019186	0.014073	-0.119799	0.539243
6	C	-0.331206	0.226091	-0.036092	-0.004589	0.001922	-0.121928
7	N	7.949789	-0.027022	-0.262553	-0.002398	-0.000551	0.000531
8	C	-0.027022	23.667426	0.652338	0.025720	0.017845	0.015878
9	N	-0.262553	0.652338	8.399344	0.003068	0.000741	-0.000307
10	H	-0.002398	0.025720	0.003068	0.523240	-0.003355	-0.000174
11	H	-0.000551	0.017845	0.000741	-0.003355	0.548860	-0.002806
12	H	0.000531	0.015878	-0.000307	-0.000174	-0.002806	0.548381
13	H	-0.004432	0.037686	-0.000394	0.000010	-0.000245	-0.003699
14	H	0.397550	0.030513	0.010903	0.000001	0.000000	-0.000011
15	C	0.048696	-15.839845	-0.132128	0.011636	0.001143	0.000825
16	N	-0.001330	-0.428989	-0.016448	-0.000018	0.000000	0.000001
17	C	0.005267	-0.246017	0.000241	0.000065	0.000001	0.000000
18	C	-0.007408	-0.613592	0.006533	-0.000002	0.000000	0.000000
19	N	-0.059640	0.322884	0.003505	0.000004	0.000001	0.000002
20	H	0.000058	-0.031268	-0.000491	0.000000	0.000000	0.000000
21	H	0.000042	0.072758	-0.000487	0.000000	0.000000	0.000000
22	H	-0.000447	0.031567	0.000075	0.000000	0.000000	0.000000
23	H	0.000994	0.013466	-0.000416	0.000000	0.000000	0.000000
24	O	0.002173	0.379177	-0.027147	-0.000171	0.000000	0.000000
25	O	-0.001372	-0.026565	0.003991	0.000001	0.000000	0.000000

		13	14	15	16	17	18
1	C	-0.228464	-0.157519	-2.935096	0.029795	0.024264	-0.091719
2	C	-0.035851	0.098949	-2.282224	-0.048498	0.000923	-0.030898
3	C	-0.049310	0.015265	-1.269897	-0.014762	0.006855	-0.013865
4	C	0.023552	0.000468	0.139698	-0.000130	-0.000101	0.001498
5	C	-0.062283	-0.003501	-0.186997	-0.001265	-0.000281	-0.001443
6	C	0.668683	-0.022030	0.020929	0.000503	0.000556	-0.000578
7	N	-0.004432	0.397550	0.048696	-0.001330	0.005267	-0.007408
8	C	0.037686	0.030513	-15.839845	-0.428989	-0.246017	-0.613592
9	N	-0.000394	0.010903	-0.132128	-0.016448	0.000241	0.006533
10	H	0.000010	0.000001	0.011636	-0.000018	0.000065	-0.000002
11	H	-0.000245	0.000000	0.001143	0.000000	0.000001	0.000000
12	H	-0.003699	-0.000011	0.000825	0.000001	0.000000	0.000000
13	H	0.539424	-0.000123	0.003488	0.000010	0.000001	-0.000010
14	H	-0.000123	0.449185	-0.041793	-0.001178	-0.001535	0.002105
15	C	0.003488	-0.041793	27.336217	0.307044	0.045347	0.510977
16	N	0.000010	-0.001178	0.307044	7.879101	0.010407	0.001872

17	C	0.000001	-0.001535	0.045347	0.010407	5.679202	-0.575951
18	C	-0.000010	0.002105	0.510977	0.001872	-0.575951	5.918084
19	N	0.000107	0.008914	-0.364884	-0.146423	-0.073632	0.031614
20	H	0.000000	-0.000003	0.053252	-0.062059	0.485957	-0.059449
21	H	0.000000	0.000004	-0.060552	-0.035943	0.443823	-0.038030
22	H	0.000000	0.000006	0.013075	0.006448	-0.080667	0.448225
23	H	0.000000	-0.000029	-0.052896	-0.012732	-0.020614	0.464351
24	O	0.000000	-0.000081	-0.563283	0.285040	-0.065484	-0.015612
25	O	-0.000078	-0.000109	-0.231723	-0.006814	0.006880	-0.063648

		19	20	21	22	23	24
1	C	-0.006822	-0.001007	0.002289	-0.000025	0.001245	0.045696
2	C	0.016533	-0.001357	0.000090	0.000555	0.002196	-0.010725
3	C	-0.001782	-0.000118	0.000122	0.000005	0.000254	0.012593
4	C	-0.000312	0.000005	-0.000009	-0.000001	-0.000005	-0.001486
5	C	0.000031	-0.000004	0.000008	0.000000	0.000013	0.000892
6	C	0.000148	0.000002	-0.000004	0.000000	0.000002	-0.000101
7	N	-0.059640	0.000058	0.000042	-0.000447	0.000994	0.002173
8	C	0.322884	-0.031268	0.072758	0.031567	0.013466	0.379177
9	N	0.003505	-0.000491	-0.000487	0.000075	-0.000416	-0.027147
10	H	0.000004	0.000000	0.000000	0.000000	0.000000	-0.000171
11	H	0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
12	H	0.000002	0.000000	0.000000	0.000000	0.000000	0.000000
13	H	0.000107	0.000000	0.000000	0.000000	0.000000	0.000000
14	H	0.008914	-0.000003	0.000004	0.000006	-0.000029	-0.000081
15	C	-0.364884	0.053252	-0.060552	0.013075	-0.052896	-0.563283
16	N	-0.146423	-0.062059	-0.035943	0.006448	-0.012732	0.285040
17	C	-0.073632	0.485957	0.443823	-0.080667	-0.020614	-0.065484
18	C	0.031614	-0.059449	-0.038030	0.448225	0.464351	-0.015612
19	N	7.592934	-0.009450	0.011411	-0.046666	-0.024951	-0.009699
20	H	-0.009450	0.538228	-0.027200	-0.006342	0.003789	-0.002944
21	H	0.011411	-0.027200	0.501616	0.003767	-0.014807	-0.008030
22	H	-0.046666	-0.006342	0.003767	0.520148	-0.028518	-0.002678
23	H	-0.024951	0.003789	-0.014807	-0.028518	0.521698	0.004000
24	O	-0.009699	-0.002944	-0.008030	-0.002678	0.004000	8.362842
25	O	0.406865	0.000835	-0.000559	-0.000234	-0.001546	-0.002442

		25
1	C	0.019652
2	C	0.039759
3	C	0.006480
4	C	0.000084
5	C	-0.000188
6	C	0.000142
7	N	-0.001372
8	C	-0.026565
9	N	0.003991
10	H	0.000001
11	H	0.000000
12	H	0.000000
13	H	-0.000078
14	H	-0.000109
15	C	-0.231723
16	N	-0.006814
17	C	0.006880
18	C	-0.063648
19	N	0.406865
20	H	0.000835
21	H	-0.000559
22	H	-0.000234
23	H	-0.001546
24	O	-0.002442
25	O	8.405578

Mulliken atomic charges:

		1
1	C	0.272954
2	C	0.450845

```
     3  C   -0.059928
     4  C   -0.253731
     5  C   -0.390184
     6  C    0.523218
     7  N   -1.071913
     8  C    0.847937
     9  N   -1.153624
    10  H    0.120936
    11  H    0.106068
    12  H    0.107374
    13  H    0.111931
    14  H    0.214050
    15  C    1.468992
    16  N   -0.743631
    17  C    0.354494
    18  C    0.126945
    19  N   -0.650690
    20  H    0.119567
    21  H    0.149692
    22  H    0.141706
    23  H    0.144509
    24  O   -0.382530
    25  O   -0.554988
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
              1
     1  C    0.272954
     2  C    0.450845
     3  C    0.061008
     4  C   -0.147662
     5  C   -0.282810
     6  C    0.635149
     7  N   -0.857863
     8  C    0.847937
     9  N   -1.153624
    10  H    0.000000
    11  H    0.000000
    12  H    0.000000
    13  H    0.000000
    14  H    0.000000
    15  C    1.468992
    16  N   -0.743631
    17  C    0.623753
    18  C    0.413160
    19  N   -0.650690
    20  H    0.000000
    21  H    0.000000
    22  H    0.000000
    23  H    0.000000
    24  O   -0.382530
    25  O   -0.554988
Sum of Mulliken charges=   0.00000
          Atomic-Atomic Spin Densities.
              1          2          3          4          5          6
     1  C    0.042585  -0.023270  -0.037417  -0.000006  -0.006278  -0.008049
     2  C   -0.023270   0.109115  -0.015533  -0.011562   0.000347  -0.016657
     3  C   -0.037417  -0.015533   0.069444   0.004778   0.001669  -0.007169
     4  C   -0.000006  -0.011562   0.004778   0.026641  -0.000891  -0.004927
     5  C   -0.006278   0.000347   0.001669  -0.000891  -0.030067   0.005260
     6  C   -0.008049  -0.016657  -0.007169  -0.004927   0.005260   0.046405
     7  N    0.004770  -0.007539   0.000230  -0.001275   0.001141   0.004420
     8  C   -0.023046   0.072536  -0.003862   0.000644  -0.001773   0.000033
     9  N   -0.000270   0.014580   0.003129   0.002369  -0.001612  -0.004225
    10  H    0.000152   0.000529  -0.000934  -0.000361   0.000006  -0.000006
    11  H   -0.000207  -0.000250  -0.000058  -0.000009   0.000578   0.000037
```

12	H	0.000322	0.000245	-0.000523	0.000409	-0.000710	-0.000286
13	H	-0.000935	-0.000179	-0.000200	-0.000063	0.000663	0.000878
14	H	0.000144	-0.000860	-0.000368	-0.000008	-0.000007	0.000055
15	C	0.032605	-0.107828	-0.040540	-0.002126	0.001440	0.003997
16	N	-0.000517	0.002573	0.000196	-0.000019	0.000033	0.000002
17	C	0.002975	-0.001016	-0.002092	-0.000372	0.000207	0.000188
18	C	-0.002691	-0.000036	0.001993	0.000410	-0.000272	-0.000447
19	N	0.002097	-0.000876	0.000307	0.000012	0.000078	-0.000224
20	H	-0.000039	0.000133	0.000017	0.000001	0.000000	0.000000
21	H	-0.000062	-0.000062	-0.000014	0.000000	0.000000	0.000000
22	H	-0.000024	-0.000020	-0.000002	0.000000	0.000000	0.000000
23	H	0.000253	0.000224	0.000032	-0.000001	0.000002	0.000000
24	O	0.002674	0.001687	-0.000395	-0.000037	0.000052	-0.000013
25	O	-0.005421	0.001973	-0.000009	0.000080	-0.000140	-0.000104

		7	8	9	10	11	12
1	C	0.004770	-0.023046	-0.000270	0.000152	-0.000207	0.000322
2	C	-0.007539	0.072536	0.014580	0.000529	-0.000250	0.000245
3	C	0.000230	-0.003862	0.003129	-0.000934	-0.000058	-0.000523
4	C	-0.001275	0.000644	0.002369	-0.000361	-0.000009	0.000409
5	C	0.001141	-0.001773	-0.001612	0.000006	0.000578	-0.000710
6	C	0.004420	0.000033	-0.004225	-0.000006	0.000037	-0.000286
7	N	0.000050	-0.012556	-0.006645	-0.000015	0.000003	0.000004
8	C	-0.012556	0.176204	0.007145	0.000365	-0.000006	0.000124
9	N	-0.006645	0.007145	-0.059616	0.000136	-0.000012	0.000002
10	H	-0.000015	0.000365	0.000136	0.000841	0.000003	0.000000
11	H	0.000003	-0.000006	-0.000012	0.000003	-0.000311	-0.000004
12	H	0.000004	0.000124	0.000002	0.000000	-0.000004	0.001388
13	H	0.000000	-0.000175	-0.000065	0.000000	0.000001	-0.000004
14	H	0.000131	-0.000581	-0.000197	0.000000	0.000000	0.000000
15	C	0.013661	-0.183317	-0.010173	-0.000079	0.000004	0.000001
16	N	0.001631	0.021357	0.000379	-0.000003	0.000000	0.000000
17	C	0.000864	-0.005811	-0.002603	0.000004	0.000000	0.000000
18	C	-0.000676	0.035688	0.003858	-0.000005	0.000000	0.000000
19	N	-0.001037	-0.037812	0.000010	-0.000001	0.000000	0.000000
20	H	-0.000031	0.002861	0.000081	0.000000	0.000000	0.000000
21	H	0.000009	-0.005058	-0.000016	0.000000	0.000000	0.000000
22	H	0.000019	-0.001295	-0.000031	0.000000	0.000000	0.000000
23	H	-0.000101	0.005577	0.000130	0.000000	0.000000	0.000000
24	O	0.000175	0.012594	0.003191	0.000010	0.000000	0.000000
25	O	0.000105	-0.008261	0.000076	0.000000	0.000000	0.000000

		13	14	15	16	17	18
1	C	-0.000935	0.000144	0.032605	-0.000517	0.002975	-0.002691
2	C	-0.000179	-0.000860	-0.107828	0.002573	-0.001016	-0.000036
3	C	-0.000200	-0.000368	-0.040540	0.000196	-0.002092	0.001993
4	C	-0.000063	-0.000008	-0.002126	-0.000019	-0.000372	0.000410
5	C	0.000663	-0.000007	0.001440	0.000033	0.000207	-0.000272
6	C	0.000878	0.000055	0.003997	0.000002	0.000188	-0.000447
7	N	0.000000	0.000131	0.013661	0.001631	0.000864	-0.000676
8	C	-0.000175	-0.000581	-0.183317	0.021357	-0.005811	0.035688
9	N	-0.000065	-0.000197	-0.010173	0.000379	-0.002603	0.003858
10	H	0.000000	0.000000	-0.000079	-0.000003	0.000004	-0.000005
11	H	0.000001	0.000000	0.000004	0.000000	0.000000	0.000000
12	H	-0.000004	0.000000	0.000001	0.000000	0.000000	0.000000
13	H	-0.000475	0.000000	0.000213	0.000001	0.000005	-0.000012
14	H	0.000000	0.000135	0.002123	0.000043	0.000076	-0.000224
15	C	0.000213	0.002123	0.088831	-0.059634	0.053776	-0.079441
16	N	0.000001	0.000043	-0.059634	0.439537	-0.005600	-0.002104
17	C	0.000005	0.000076	0.053776	-0.005600	-0.000026	-0.028235
18	C	-0.000012	-0.000224	-0.079441	-0.002104	-0.028235	0.071319
19	N	0.000000	-0.000444	0.031438	-0.010453	0.008704	-0.021340
20	H	0.000000	0.000000	-0.004402	-0.004722	-0.009791	0.010565
21	H	0.000000	0.000000	0.004583	-0.002911	0.008607	-0.006291
22	H	0.000000	0.000001	0.002429	0.000065	0.002938	-0.004353
23	H	0.000000	0.000000	-0.010253	-0.000668	-0.002178	0.010161
24	O	0.000000	0.000002	0.017172	-0.140054	0.004972	-0.006647

25	O	-0.000006	0.000019	0.022958	0.003490	0.002214	0.005728
		19	20	21	22	23	24
1	C	0.002097	-0.000039	-0.000062	-0.000024	0.000253	0.002674
2	C	-0.000876	0.000133	-0.000062	-0.000020	0.000224	0.001687
3	C	0.000307	0.000017	-0.000014	-0.000002	0.000032	-0.000395
4	C	0.000012	0.000001	0.000000	0.000000	-0.000001	-0.000037
5	C	0.000078	0.000000	0.000000	0.000000	0.000002	0.000052
6	C	-0.000224	0.000000	0.000000	0.000000	0.000000	-0.000013
7	N	-0.001037	-0.000031	0.000009	0.000019	-0.000101	0.000175
8	C	-0.037812	0.002861	-0.005058	-0.001295	0.005577	0.012594
9	N	0.000010	0.000081	-0.000016	-0.000031	0.000130	0.003191
10	H	-0.000001	0.000000	0.000000	0.000000	0.000000	0.000010
11	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
12	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
13	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
14	H	-0.000444	0.000000	0.000000	0.000001	0.000000	0.000002
15	C	0.031438	-0.004402	0.004583	0.002429	-0.010253	0.017172
16	N	-0.010453	-0.004722	-0.002911	0.000065	-0.000668	-0.140054
17	C	0.008704	-0.009791	0.008607	0.002938	-0.002178	0.004972
18	C	-0.021340	0.010565	-0.006291	-0.004353	0.010161	-0.006647
19	N	0.256203	0.003014	-0.001223	-0.000108	-0.003119	0.002199
20	H	0.003014	0.008902	-0.001120	-0.000030	-0.000087	-0.000977
21	H	-0.001223	-0.001120	0.002135	-0.000074	0.000063	0.004800
22	H	-0.000108	-0.000030	-0.000074	0.001123	-0.000996	0.000085
23	H	-0.003119	-0.000087	0.000063	-0.000996	0.009064	0.000214
24	O	0.002199	-0.000977	0.004800	0.000085	0.000214	0.729231
25	O	-0.075642	0.000012	-0.000083	0.000615	0.000226	-0.000429
		25					
1	C	-0.005421					
2	C	0.001973					
3	C	-0.000009					
4	C	0.000080					
5	C	-0.000140					
6	C	-0.000104					
7	N	0.000105					
8	C	-0.008261					
9	N	0.000076					
10	H	0.000000					
11	H	0.000000					
12	H	0.000000					
13	H	-0.000006					
14	H	0.000019					
15	C	0.022958					
16	N	0.003490					
17	C	0.002214					
18	C	0.005728					
19	N	-0.075642					
20	H	0.000012					
21	H	-0.000083					
22	H	0.000615					
23	H	0.000226					
24	O	-0.000429					
25	O	0.245480					

Mulliken atomic spin densities:

		1
1	C	-0.019652
2	C	0.018254
3	C	-0.027321
4	C	0.013689
5	C	-0.030274
6	C	0.019168
7	N	-0.002663
8	C	0.051574
9	N	-0.050378
10	H	0.000642

```
   11  H   -0.000229
   12  H    0.000968
   13  H   -0.000352
   14  H    0.000038
   15  C   -0.222561
   16  N    0.242619
   17  C    0.027805
   18  C   -0.013051
   19  N    0.151786
   20  H    0.004386
   21  H    0.003282
   22  H    0.000341
   23  H    0.008543
   24  O    0.630505
   25  O    0.192882
Sum of Mulliken spin densities=   1.00000
                     Isotropic Fermi Contact Couplings
    Atom                a.u.       MegaHertz       Gauss      10(-4) cm-1
  1  C(13)             -0.00101      -1.13326      -0.40437      -0.37801
  2  C(13)              0.00255       2.86722       1.02310       0.95640
  3  C(13)             -0.00118      -1.33200      -0.47529      -0.44431
  4  C(13)              0.00143       1.60705       0.57343       0.53605
  5  C(13)             -0.00161      -1.80441      -0.64386      -0.60189
  6  C(13)              0.00151       1.69650       0.60535       0.56589
  7  N(14)             -0.00059      -0.19006      -0.06782      -0.06340
  8  C(13)              0.01096      12.31590       4.39462       4.10814
  9  N(14)             -0.00442      -1.42905      -0.50992      -0.47668
 10  H                  0.00029       1.28335       0.45793       0.42808
 11  H                 -0.00010      -0.45015      -0.16062      -0.15015
 12  H                  0.00035       1.57107       0.56060       0.52405
 13  H                 -0.00016      -0.69634      -0.24847      -0.23227
 14  H                  0.00005       0.23412       0.08354       0.07809
 15  C(13)             -0.00745      -8.37029      -2.98673      -2.79203
 16  N(14)              0.16286      52.61988      18.77609      17.55210
 17  C(13)              0.00692       7.77725       2.77512       2.59421
 18  C(13)             -0.00497      -5.58404      -1.99252      -1.86264
 19  N(14)              0.02627       8.48637       3.02815       2.83075
 20  H                  0.00314      14.04331       5.01100       4.68435
 21  H                  0.00076       3.41911       1.22002       1.14049
 22  H                  0.00038       1.68676       0.60188       0.56264
 23  H                  0.00537      24.02394       8.57234       8.01352
 24  O(17)              0.04440     -26.91354      -9.60342      -8.97739
 25  O(17)              0.01711     -10.37287      -3.70130      -3.46002
Electronic spatial extent (au):  <R**2>=  4017.2159
Charge=     0.0000 electrons
Dipole moment (Debye):
   X=    -2.0175    Y=     1.8544    Z=     1.7462  Tot=     3.2494
Quadrupole moment (Debye-Ang):
  XX=   -63.5972   YY=  -101.4711   ZZ=   -93.0336
  XY=     3.4499   XZ=    -3.7790   YZ=     3.4457
Octapole moment (Debye-Ang**2):
 XXX=   -86.5670  YYY=     6.7669  ZZZ=     2.1481  XYY=    36.0087
 XXY=    -9.6784  XXZ=    14.4366  XZZ=   -26.9594  YZZ=    -0.9684
 YYZ=     5.5238  XYZ=    -3.0551
Hexadecapole moment (Debye-Ang**3):
XXXX= -3593.2946 YYYY=  -996.8842 ZZZZ=  -138.3409 XXXY=     9.7502
XXXZ=   -28.1891 YYYX=    25.0703 YYYZ=    14.8455 ZZZX=   -12.2516
ZZZY=    -4.1809 XXYY=  -875.9154 XXZZ=  -768.6352 YYZZ=  -187.2395
XXYZ=    23.8189 YYXZ=    -7.3953 ZZXY=     6.5174
N-N= 1.046645973509D+03 E-N=-3.856023948285D+03  KE= 7.520871466376D+02
Leave Link  601 at Wed Nov 20 12:12:46 2002, MaxMem=   13107200 cpu:      27.3
(Enter /export/local/gauss/g99/l9999.exe)

Test job not archived.
1\1\GINC-SLV25\SP\UTD-PBE1PBE-FC\6-311+G(3df,2p)\C10H9N4O2(2)\COURS\20
```

-Nov-2002\0\\#P PBE1PBE/6-311+G(3DF,2P) GEOM=CONNECTIVITY TD(NSTATE=2,
50-50) TEST\\Energies d'excitation de NITBzImH (PBE1PBE)\\0,2\C\C,1,1.
330934\C,2,1.350248,1,121.935991\C,3,1.408727,2,118.001611,1,-0.000006
,0\C,4,1.413281,3,119.535849,2,-0.000002,0\C,1,1.347269,2,123.80464,3,
0.000007,0\N,1,1.439962,2,106.494709,3,-179.999995,0\C,7,1.333695,1,10
5.190406,2,-0.000021,0\N,2,1.315146,1,110.593463,6,-179.999992,0\H,3,1
.07,2,120.999196,1,179.999995,0\H,4,1.07,3,120.232067,2,179.999999,0\H
,5,1.07,4,120.36888,3,-179.999991,0\H,6,1.07,1,121.270169,2,180.,0\H,7
,1.,1,127.4048,2,179.99998,0\C,8,1.54,7,125.109385,1,-179.999969,0\N,1
5,1.473173,8,124.804551,7,178.885544,0\C,16,1.477753,15,104.823744,8,1
60.718154,0\C,17,1.537652,16,103.830125,15,2.756818,0\N,15,1.310301,8,
124.976471,7,1.114501,0\H,17,1.07,16,105.173774,15,125.394242,0\H,17,1
.07,16,116.952153,15,-113.343008,0\H,18,1.07,17,111.887975,16,142.3678
2,0\H,18,1.07,17,109.480123,16,-96.728372,0\O,16,1.36,15,118.062246,8,
35.77404,0\O,19,1.36,15,126.322048,8,26.702506,0\\Version=x86-Linux-G9
9RevB.08+\State=2-A\HF=-755.1328514\S2=0.819606\S2-1=0.\S2A=0.750965\R
MSD=2.826e-09\PG=C01 [X(C10H9N4O2)]\\@

ONE BIG VICE IN A MAN IS APT TO KEEP OUT MANY SMALLER ONES.

-- BRET HARTE

Job cpu time: 9 days 19 hours 30 minutes 41.2 seconds.
File lengths (MBytes): RWF= 389 Int=   0 D2E=   0 Chk=   57 Scr=   1
Normal termination of Gaussian 99.