Supporting Information

Computational study on the photophysics of protonated benzene

by

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Complete Reference 67

(67) MOLPRO is a package of ab initio programs written by Werner, H.-J. and Knowles, P. J. with contributions from Lindh, R.; Manby, F. R.; Schütz, M.; Celani, P.; Korona, T.; Mitrushenkov, A.; Rauhut, G.; Adler, T. B.; Amos, R. D.; Bernhardsson, A.; Berning, A.; Cooper, D. L.; Deegan, M. J. O.; Dobbyn, A. J.; Eckert, F.; Goll, E.; Hampel, C.; Hetzer, G.; Hrenar, T.; Knizia, G.; Köppl, C.; Liu, Y.; Lloyd, A. W.; Mata, R. A.; May, A. J.; McNicholas, S. J.; Meyer, W.; Mura, M. E.; Nicklaß, A.; Palmieri, P.; Pflüger, K.; Pitzer, R.; Reiher, M.; Schumann, U.; Stoll, H.; Stone, A. J.; Tarroni, R.; Thorsteinsson, T.; Wang, M.; Wolf, A., version 2008.1.

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(72) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Menucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratman, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B. G.; Chen, W.; Wong, M. W.; Gonzales, C.; Pople, J. A. *Gaussian 03, Revision C.02., Gaussian, Inc, Pittsburgh PA* **2004**.

Figure S1. Potential energy (PE) profiles calculated at the CC2/cc-pVDZ level along the minimum energy path for an elongation of the C2-C3 distance in C_s symmetry. The full line (blue) represents the PE profile of the reaction path determined for the S_1(1A",$\pi\pi^*$) state, the dashed line represents the PE profile of the ground electronic state S_0 at the geometry of the S_1 state. The structures correspond to the geometry for vertical excitation from the S_0 state (filled square) and the geometry at the conical intersectiopn point, respectively.

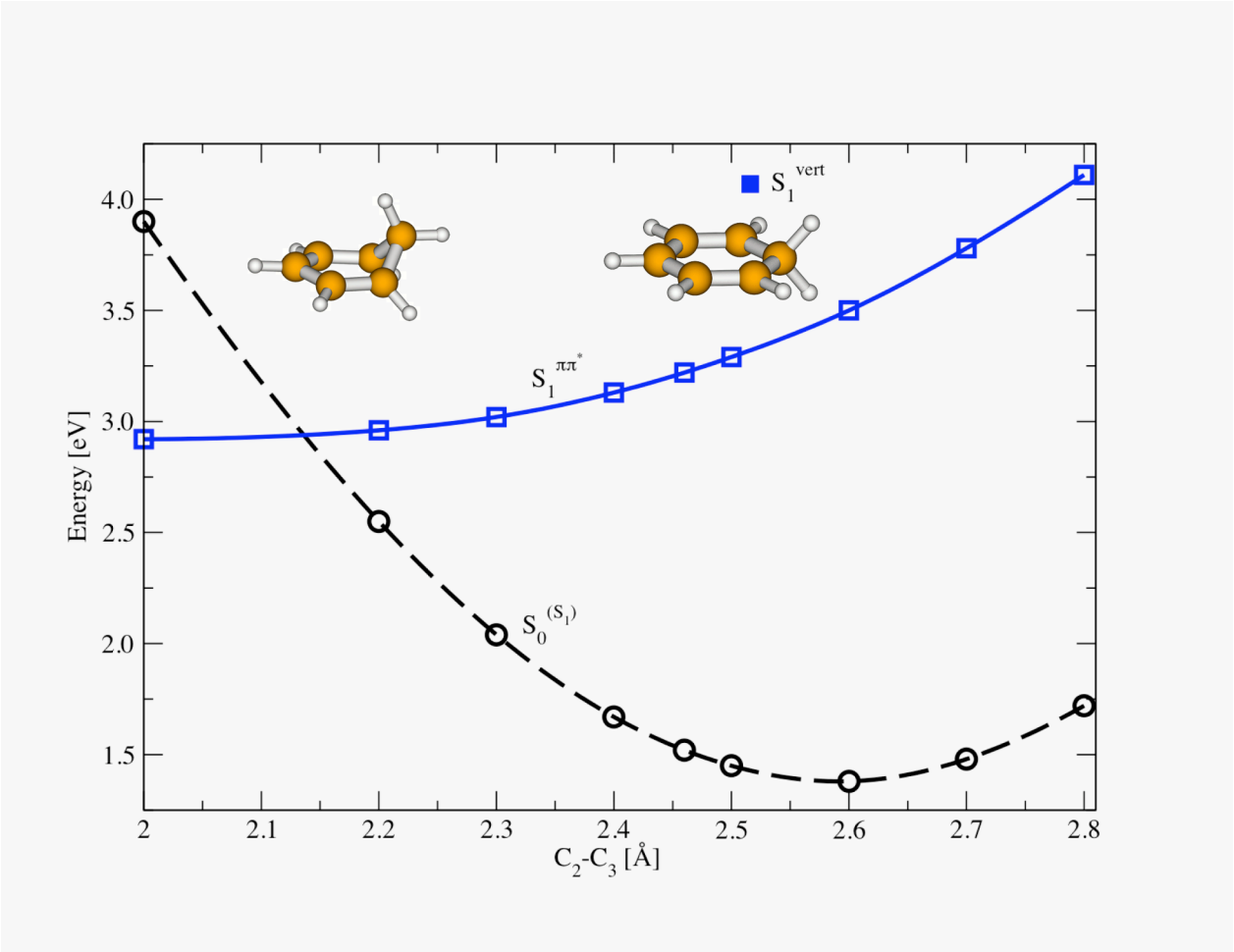

Table S1. Vertical excitation energies (ΔE) of the lowest excited singlet states of $C_6H_7^+$ calculated at different correlation levels of theory employing the cc-pVTZ basis set for the ground-state equilibrium geometry obtained at the MP2/cc-pVTZ level (*C_{2v} structure*). Oscillator strengths are given in parentheses.

state	ΔE/eV	ΔE/eV[a]	ΔE/eV
	CC2	CASPT2	TD-DFT
S_0, $1A_1$	0.0	0.0	0.0
S_1, $1B_2(\pi\pi^*)$	4.094 (0.14313)	3.37 (0.2756)	4.16 (0.1136)
S_2, $1A_2(\sigma\pi^*)$	5.514 (0.00000)	4.87 (0.0000)	5.12 (0.0000)
S_3, $2A_1(\pi\pi^*)$	5.709 (0.0956)	4.90 (0.0843)	5.65 (0.0561)
S_4, $1B_1(\sigma\pi^*)$	5.716 (0.00498)	5.08 (0.0099)	5.38 (0.0042)

[a] The oscillator strength f(CASPT2) was obtained by the use of the formula $f=A\bullet\mu\bullet\Delta E(CASPT2)$, where the transition moment μ was obtained at the CASSCF level.

Table S2. Vertical (ΔE_v) and adiabtic (ΔE_a) excitation energies of the lowest excited singlet states of $C_6H_7^+$ calculated at different correlation levels of theory obtained with the cc-pVDZ basis set for C_{2v} symmetric structures.

state	ΔE_v/eV	ΔE_a/eV	ΔE_v/eV	ΔE_a/eV	ΔE_v/eV	ΔE_a/eV
	CC2	CC2	CASPT2	CASPT2	TD-DFT	TD-DFT
S_0, $1A_1$	0.0		0.0		0.0	
S_1, $1B_2(\pi\pi^*)$	4.07	3.82	3.66	3.50	4.16	3.93
S_2, $1A_2(\sigma\pi^*)$	5.52	4.64	5.03	4.36	5.03	4.32
S_3, $2A_1(\pi\pi^*)$	5.67	5.46	4.83		5.63	5.46
S_4, $1B_1(\sigma\pi^*)$	5.71	5.23	5.25		5.37	5.01

Table S3. Comparison of calculated excited-state energies (in eV) for selected points on the PE profiles in Fig. 5 at different correlated levels of theory (CC2 and CASPT2) obtained with the cc-pVDZ basis set.

State (geometry)	ΔE_a(CC2)	ΔE_a(CASPT2)	ΔE_a(CC2)-ΔE_a(CASPT2)
B_2 (global minimum)	3.82	3.50	0.32
A_2 (global minimum)	4.64	4.36	0.28
B_2 (A_2)	4.54	4.25	0.29
A_2 (opt. at R_{CC}=2.30 Å)	4.70	4.41	0.29
B_2 (A_2(opt. at R_{CC}=2.30 Å))	4.73	4.45	0.28
A_2 (opt. at R_{CC}=2.75Å)	5.03	4.78	0.25
B_2 (A_2(opt. at R_{CC}=2.7Å))	4.99	4.69	0.30
B_1 (opt. at R_{CC}=2.80Å)	5.26	4.89	0.37
B_2 (B_1(opt. at R_{CC}=2.80Å))	5.31	4.93	0.38

Table S4. Various structures of $C_6H_7^+$ optimized at the MP2, CASSCF, or CC2 level

(1) Equilibrium geometry of the ground electronic state S_0 of $C_6H_7^+$ optimized at the MP2/cc-pVDZ level denoted as $1A_1$ (in C_{2v}) or 1A' (in C_s)

C -1.088157 -0.834530 0.000000
C -1.142108 0.634872 0.000000
C 0.134647 1.364138 0.000000
C 1.339441 0.680176 0.000000
C 1.324897 -0.736972 0.000000
C 0.128570 -1.496787 0.000000
H 2.283707 -1.270637 0.000000
H 0.175393 -2.588907 0.000000
H -2.030396 -1.394554 0.000000
H 0.112168 2.460024 0.000000
H 2.292203 1.216206 0.000000
H -1.766974 0.983023 0.857752
H -1.766974 0.983023 -0.857752

(2) local minimum of the $S_1(1B_2)$ excited state optimized at the CC2/cc-pVDZ level in C_{2v}

C 0.000000 -1.230995 -0.554003
C 0.000000 0.000000 -1.403313
C 0.000000 1.230995 -0.554003
C 0.000000 1.229018 0.861567
C 0.000000 0.000000 1.626762
C 0.000000 -1.229018 0.861567
H 0.000000 0.000000 2.719150
H 0.000000 -2.191825 1.383296
H 0.000000 -2.203967 -1.064189
H 0.000000 2.203967 -1.064189
H 0.000000 2.191825 1.383296
H -0.870791 0.000000 -2.102824
H 0.870791 0.000000 -2.102824

(3) local minimum of the $S_2(1A_2)$ excited state optimized at the CC2/cc-pVDZ level in C_{2v}

C 0.000000 -1.211054 -0.497953
C 0.000000 0.000000 -1.478167
C 0.000000 1.211054 -0.497953
C 0.000000 1.203323 0.846440
C 0.000000 0.000000 1.638641
C 0.000000 -1.203323 0.846440
H 0.000000 0.000000 2.729809
H 0.000000 -2.168627 1.388529
H 0.000000 -2.106520 -1.167243
H 0.000000 2.106520 -1.167243
H 0.000000 2.168627 1.388529
H -0.901962 0.000000 -2.118822
H 0.901962 0.000000 -2.118822

(4) local minimum of the $S_3(2A_1)$ excited state optimized at the CC2/cc-pVDZ level in C_{2v}

C 0.000000 -1.276071 -0.558490
C 0.000000 0.000000 -1.318131

C 0.000000 1.276071 -0.558490
C 0.000000 1.259915 0.877216
C 0.000000 0.000000 1.605232
C 0.000000 -1.259915 0.877216
H 0.000000 0.000000 2.700653
H 0.000000 -2.198269 1.442960
H 0.000000 -2.228932 -1.098209
H 0.000000 2.228932 -1.098209
H 0.000000 2.198269 1.442960
H -0.848161 0.000000 -2.059197
H 0.848161 0.000000 -2.059197

(5) local minimum of the $S_4(2B_1)$ excited state optimized at the CC2/cc-pVDZ level in C_{2v}

C 0.000000 -1.358683 -0.567447
C 0.000000 0.000000 -1.278102
C 0.000000 1.358683 -0.567447
C 0.000000 1.231133 0.820009
C 0.000000 0.000000 1.524095
C 0.000000 -1.231133 0.820009
H 0.000000 0.000000 2.622492
H 0.000000 -2.213830 1.328032
H 0.000000 -2.304132 -1.113731
H 0.000000 2.304132 -1.113731
H 0.000000 2.213830 1.328032
H -0.986664 0.000000 -1.808371
H 0.986664 0.000000 -1.808371

(6) chair(1) local minimum of the S_1(1A") excited state optimized at the CC2/cc-pVDZ level in C_s

C 0.712144 0.396934 -1.206085
C -0.659341 0.026190 -1.049678
C -0.659341 0.026190 1.049678
C 0.712144 0.396934 1.206085
C 1.477008 0.484774 0.000000
H 2.541806 0.733699 0.000000
H 1.111621 0.681803 -2.186310
H -1.468711 0.478074 -1.641888
H -1.468711 0.478074 1.641888
H 1.111621 0.681803 2.186310
C -1.016229 -0.991197 0.000000
H -2.073962 -1.276824 0.000000
H -0.316576 -1.842235 0.000000

(7) chair(2) S_1/S_0 conical Intersection point optimized at the CASSCF(6,6)/cc-pVDZ level in C_1

C 0.060519 -1.388476 0.024947
C -1.032990 -0.550263 -0.357107
C -0.069071 1.167890 -0.357215
C 1.216730 0.673120 0.025930
C 1.259272 -0.705709 0.348474
H 2.154302 -1.207640 0.680267
H -0.022246 -2.464346 -0.032681
H -1.688550 -0.793453 -1.184727
H -0.203093 1.851673 -1.186868
H 2.091665 1.304531 -0.033066

H -1.110556 0.622843 1.468589
H -2.187660 1.227189 0.130724
C -1.273747 0.714998 0.401308

(8) boat local minimum of the $S_3(2A')$ excited state optimized at the CC2/cc-pVDZ level in C_s

C 0.165488 0.461186 -1.286082
C -0.173853 1.158949 0.000000
C 0.165488 0.461186 1.286082
C 0.201666 -0.935933 1.282923
C -0.286905 -1.456010 0.000000
C 0.201666 -0.935933 -1.282923
H -1.367313 -1.140867 0.000000
H 0.609269 -1.526282 -2.112418
H 0.525792 1.035855 -2.149634
H 0.525792 1.035855 2.149634
H 0.609269 -1.526282 2.112418
H -1.310966 1.156457 0.000000
H 0.120077 2.218704 0.000000

Table S5. Various structures of $C_6H_7^+$ optimized at the DFT or TD-DFT level

(1) Equilibrium geometry of the ground electronic state S_0 of $C_6H_7^+$ optimized at the DFT level (B3-LYP/cc-pVDZ) described as $1A_1$ (in C_{2v}) or 1A' (in C_s)

C -1.081295 -0.835598 0.000000
C -1.140208 0.634112 0.000000
C 0.139250 1.359701 0.000000
C 1.334134 0.680576 0.000000
C 1.319824 -0.733882 0.000000
C 0.125960 -1.492462 0.000000
H 2.276564 -1.265972 0.000000
H 0.175653 -2.582645 0.000000
H -2.023376 -1.391317 0.000000
H 0.112857 2.453118 0.000000
H 2.286504 1.213488 0.000000
H -1.768875 0.983586 0.853061
H -1.768875 0.983586 -0.853061

(2) local minimum of the $S_1(1B_2)$ excited state optimized at the TD-DFT level (B3-LYP/cc-pVDZ) in C_{2v}

C 0.000000 -1.222453 -0.546382
C 0.000000 0.000000 -1.390626
C 0.000000 1.222453 -0.546382
C 0.000000 1.212379 0.868315
C 0.000000 0.000000 1.608728
C 0.000000 -1.212379 0.868315
H 0.000000 0.000000 2.698240
H 0.000000 -2.171270 1.392625
H 0.000000 -2.194280 -1.053095
H 0.000000 2.194280 -1.053095
H 0.000000 2.171270 1.392625
H -0.859514 0.000000 -2.115728
H 0.859514 0.000000 -2.115728

(3) local minimum of the $S_2(1A_2)$ excited state optimized at the TD-DFT level (B3-LYP/cc-pVDZ) in C_{2v}

C 0.000000 -1.217581 -0.489892
C 0.000000 0.000000 -1.436163
C 0.000000 1.217581 -0.489892
C 0.000000 1.195930 0.839779
C 0.000000 0.000000 1.630104
C 0.000000 -1.195930 0.839779
H 0.000000 0.000000 2.716424
H 0.000000 -2.149090 1.411282
H 0.000000 -2.137342 -1.121140
H 0.000000 2.137342 -1.121140
H 0.000000 2.149090 1.411282
H -0.890696 0.000000 -2.092103
H 0.890696 0.000000 -2.092103

(4) local minimum of the $S_3(2A_1)$ excited state optimized at the TD-DFT level (B3-LYP/cc-pVDZ) in C_{2v}

C 0.000000 -1.264069 -0.562044
C 0.000000 0.000000 -1.329106

C 0.000000 1.264069 -0.562044
C 0.000000 1.259016 0.852827
C 0.000000 0.000000 1.576092
C 0.000000 -1.259016 0.852827
H 0.000000 0.000000 2.669655
H 0.000000 -2.192477 1.418196
H 0.000000 -2.212237 -1.102315
H 0.000000 2.212237 -1.102315
H 0.000000 2.192477 1.418196
H -0.842303 0.000000 -2.078050
H 0.842303 0.000000 -2.078050

(5) local minimum of the $S_4(1B_1)$ excited state optimized at the TD-DFT level (B3-LYP/cc-pVDZ) in C_{2v}

C 0.000000 -1.343661 -0.570905
C 0.000000 0.000000 -1.303197
C 0.000000 1.343661 -0.570905
C 0.000000 1.224673 0.803908
C 0.000000 0.000000 1.492362
C 0.000000 -1.224673 0.803908
H 0.000000 0.000000 2.590661
H 0.000000 -2.206797 1.315858
H 0.000000 -2.291423 -1.105943
H 0.000000 2.291423 -1.105943
H 0.000000 2.206797 1.315858
H -0.972156 0.000000 -1.852666
H 0.972156 0.000000 -1.852666

Table S6. Part of the Gaussian 03 output file with the optimization of the conical intersection point (S_1/S_0) including g-h vectors in cartesian coordinates along with the optimized structure.

```
---------------------------------------------------------------------
 #P CAS(6,6)/cc-pVDZ geo=check guess=read Pop=(Full,NO) Opt(Conical) gf
 input iop(6/7=3) scf(Direct,Conver=5,maxcycle=99)
 ---------------------------------------------------------------------
 1/9=11,11=1,18=20,19=9,29=2,38=1/1,3;
 2/9=110,40=1/2;
 3/5=16,16=1,24=10,25=1,32=1/1,2,3;
 4/5=1,7=6,17=6,18=6/1,5;
 5/5=2,6=5,7=99,17=31000200,28=2,38=6/10;
 8/6=4,10=90,11=11,27=4294967296/1;
 11/42=1,45=1/1;
 10/6=1,10=600005,28=2/3;
 6/7=3,28=1,31=1/1;
 7//16;
 1/9=11,11=1,18=20,19=9/3(2);
 2/9=110/2;
 99//99;
 2/9=110/2;
 3/5=16,16=1,25=1,32=1/1,2,3;
 4/5=5,7=6,16=3,17=6,18=6/1,5;
 5/5=2,6=5,7=99,17=31000200,23=1,28=2,38=5/10;
 8/6=4,10=90,11=11,27=4294967296/1;
 11/42=1,45=1/1;
 10/6=1,10=600005,28=2/3;
 7//16;
 1/9=11,11=1,18=20,19=9/3(-8);
 2/9=110/2;
 6/7=3,19=2,28=1,31=1/1;
 99/9=1/99;
 Leave Link    1 at 18:00:27   on 02/11/08  , MaxMem=  134217728 cpu:      15.9
 (Enter /opt/gaussian/g03/l101.exe)
 ---------------------------
 Conical intersection search
 ---------------------------
 Redundant internal coordinates taken from checkpoint file:
 3-21G.chk
 Charge =  1 Multiplicity = 1
 C,0,0.0563556135,-1.387921942,0.0201025468
 C,0,-1.0349545657,-0.5591398899,-0.3832278941
 C,0,-0.0628953797,1.1742858328,-0.3837884454
 C,0,1.213584623,0.6758125091,0.0191846095
 C,0,1.254631445,-0.7035615637,0.3344121476
 H,0,2.1346482743,-1.1969150372,0.6833191378
 H,0,-0.0243610277,-2.4553247058,0.0003821533
 H,0,-1.6962508152,-0.7994109907,-1.1917545146
 H,0,-0.2028609278,1.8646380461,-1.191630013
 H,0,2.0824000918,1.3010641709,-0.0016470203
 H,0,-1.0841304039,0.6085189897,1.4617347085
 H,0,-2.1759553185,1.2202558605,0.1538860312
 C,0,-1.2656367149,0.7100539981,0.407601955
 Recover connectivity data from disk.
                    Isotopes and Nuclear Properties:

                    EIGENVALUES AND  EIGENVECTORS OF CI MATRIX
```

```
( 1)     EIGENVALUE    -230.9706578171
 (  102) 0.9416199 (   66)-0.2253594 (  158) 0.1084347 (   74)-0.1044664 (   39)
0.1013479 (  119)-0.0968649 (  122) 0.0654259
 (   19) 0.0422086 (  117) 0.0374973 (  163) 0.0349722 (  161)-0.0329320 (    6)-
0.0300522 (   97)-0.0281889 (  138)-0.0281416
 (   42)-0.0242372 (   85) 0.0216824 (  126)-0.0214490 (    8) 0.0214362 (   62)
0.0213526 (  124) 0.0205985 (  135)-0.0192260
 (  148)-0.0187466 (   61)-0.0174048 (   88)-0.0171583 (  133)-0.0168850 (   41)
0.0165253 (   83)-0.0152856 (   33) 0.0145777
 (   55)-0.0131429 (  160) 0.0118017 (  134)-0.0115000 (   92) 0.0112072 (  129)-
0.0111213 (   86)-0.0109563 (  118)-0.0106287
 (   32) 0.0103434 (   36)-0.0102793 (  123) 0.0099897 (  167) 0.0099509 (   57)
0.0099058 (   93) 0.0096748 (   11)-0.0095063
 (   81)-0.0093714 (   35) 0.0091711 (  108) 0.0082837 (   50) 0.0080708 (   18)
0.0079785 (   17)-0.0077991 (  147)-0.0070356
 (  165) 0.0068176 (


   ( 2)     EIGENVALUE    -230.9705338952
 (  158) 0.9390113 (  135)-0.1667081 (  133)-0.1463330 (  102)-0.1087633 (  134)-
0.0977419 (  167) 0.0863881 (   11)-0.0823424
 (   81)-0.0812279 (   50) 0.0699158 (  140) 0.0543035 (  110)-0.0489421 (  107)
0.0439707 (   58) 0.0433578 (   87)-0.0427733
 (  101)-0.0393899 (  175)-0.0311084 (   98) 0.0307372 (   12) 0.0278233 (   66)
0.0261427 (  141) 0.0247233 (  109) 0.0199127
 (  137)-0.0181529 (  100) 0.0174508 (  157) 0.0167885 (   99) 0.0162637 (   67)
0.0160677 (   54)-0.0142228 (    3) 0.0140720
 (  105) 0.0140693 (  106)-0.0128490 (  152) 0.0128437 (  171)-0.0125419 (   74)
0.0121380 (  155) 0.0120990 (   39)-0.0117257
 (  119) 0.0110912 (   76)-0.0107360 (  153)-0.0107270 (   44) 0.0103060 (   53)-
0.0102296 (   63)-0.0101154 (  169)-0.0099707
 (   68)-0.0093697 (    4)-0.0093124 (   27) 0.0089203 (   23)-0.0081057 (  103)-
0.0078420 (  166)-0.0076448 (   28)-0.0075737
 (  116)-0.0075220 (
 Final one electron symbolic density matrix:
               1             2             3             4             5
     1  0.403439E-01
     2  0.175387E-01  0.102533E+00
     3  0.508865E-01 -0.636050E-02  0.190208E+01
     4 -0.200855E-01  0.601725E-01 -0.295960E-02  0.198886E+01
     5 -0.614815E-02  0.503970E-01 -0.420770E-02 -0.240893E-01  0.857653E-01
     6 -0.942452E-01 -0.293484E+00 -0.305819E-01  0.344082E-02  0.221317E-01
               6
     6  0.188042E+01
 Density Matrix for State     1
               1             2             3             4             5
     1  0.930948E-01
     2 -0.175645E-01  0.988798E+00
     3 -0.508890E-01  0.635418E-02  0.190444E+01
     4  0.199049E-01 -0.600902E-01  0.297497E-02  0.197761E+01
     5  0.617329E-02 -0.504033E-01  0.416078E-02  0.239864E-01  0.273237E-01
     6  0.942269E-01  0.293264E+00  0.305970E-01 -0.319395E-02 -0.222611E-01
               6
     6  0.100874E+01
  Final State Averaged  Density Matrix
               1             2             3             4             5
     1  0.667193E-01
     2 -0.128753E-04  0.545665E+00
```

```
     3 -0.124120E-05 -0.315706E-05  0.190326E+01
     4 -0.902711E-04  0.411944E-04  0.768425E-05  0.198323E+01
     5  0.125658E-04 -0.313892E-05 -0.234601E-04 -0.514388E-04  0.565445E-01
     6 -0.915393E-05 -0.109584E-03  0.759814E-05  0.123436E-03 -0.646622E-04
               6
     6  0.144458E+01
 Ecx terms are ignored for the Tr den 1
 Ecx terms are ignored for the Tr den 2
 In PrCiAS Ecx terms are ignored for the Tr den 1
 In PrCiAS Ecx terms are ignored for the Tr den 2
 Ecx terms are ignored for the Tr den 1
 Ecx terms are ignored for the Tr den 2
MCSCF converged.
Leave Link  510 at 05:44:50   on 02/12/08  , MaxMem=  134217728 cpu:   11461.3
(Enter /opt/gaussian/g03/l801.exe)
Range of M.O.s used for correlation:     1   119
NBasis=   119 NAE=    21 NBE=    21 NFC=     0 NFV=     0
NROrb=    119 NOA=    21 NOB=    21 NVA=    98 NVB=    98
Leave Link  801 at 05:44:52   on 02/12/08  , MaxMem=  134217728 cpu:       0.2
(Enter /opt/gaussian/g03/l1101.exe)
Not using compressed storage, NAtomX=    13.
Will process  13 centers per pass.
Leave Link 1101 at 05:44:57   on 02/12/08  , MaxMem=  134217728 cpu:       8.5
(Enter /opt/gaussian/g03/l1003.exe)
Gradient Difference/Derivative Coupling Calculation
NO. OF ORBITALS         =119      NO. OF CORE-ORBITALS    = 18
NO. OF VALENCE-ORBITALS =  6      NO. OF VIRTUAL-ORBITALS = 95
One call to fofdir will do it.
Symmetry not used in FoFDir.
MinBra= 0 MaxBra= 2 Meth= 1.
IRaf=       1 NMat=   7 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 JSym2E=0.
JobTyp= 0 Pass  1:  I=   1 to   6  IAt=   2 to  13.
    State    2   State    1
    Energy difference=     -0.0001239
Derivative Coupling
       -0.0726759414       -0.0288626845       -0.0206873858
        0.0608622154       -0.0357022202       -0.0146087188
       -0.0556993950       -0.0276654418        0.0196831087
        0.0693225103       -0.0204864498        0.0209281538
       -0.0006128984        0.0732306960        0.0009873609
        0.0000424857        0.0000927235       -0.0004339083
        0.0009804140        0.0007370896       -0.0076724133
       -0.0041006403       -0.0098271501        0.0104209855
        0.0032239200       -0.0090578305       -0.0099396910
       -0.0017328851        0.0001339051        0.0057263792
        0.0009132507       -0.0069395146       -0.0005465719
       -0.0000022766       -0.0040414479       -0.0002960835
       -0.0005207594        0.0683883252       -0.0035612155
Unscaled Gradient Difference
        0.0190370624       -0.0241302112        0.0106840284
       -0.0054293314       -0.0196223887        0.0298684120
        0.0489557655        0.0491372694        0.0139716327
       -0.0474060390        0.0472088355       -0.0087600680
       -0.0051895255       -0.0342633147        0.0085087515
        0.0003640654       -0.0000409043       -0.0036834295
       -0.0038485812        0.0023833200       -0.0051771565
       -0.0020134140        0.0011003303       -0.0027605768
       -0.0054335773        0.0077282054        0.0067570144
       -0.0025778568       -0.0027954079       -0.0114704260
```

```
         0.0078233198        0.0032207905       -0.0046087932
        -0.0000308453        0.0018821296       -0.0025273446
        -0.0042510427       -0.0318086540       -0.0308020443
 Gradient of iOther State
        -0.0152728243       -0.0024811118       -0.0049488371
         0.0116031249       -0.0042064671       -0.0060347524
        -0.0156171473       -0.0105619211        0.0019694373
         0.0179204095       -0.0090394869        0.0047608618
         0.0004832823        0.0171090179       -0.0007855567
        -0.0000441588        0.0000182072        0.0003321596
         0.0006014361       -0.0001293290       -0.0007977153
        -0.0005013678       -0.0018977167        0.0021992478
         0.0012062294       -0.0025226114       -0.0025654168
        -0.0000323614        0.0003292173        0.0023440478
        -0.0007275355       -0.0016119064        0.0004225706
         0.0000171067       -0.0009450527        0.0002333312
         0.0003638061        0.0159391608        0.0028706221
 Gradient of iVec State.
         0.0037642381       -0.0266113230        0.0057351914
         0.0061737935       -0.0238288558        0.0238336596
         0.0333386182        0.0385753483        0.0159410701
        -0.0294856295        0.0381693486       -0.0039992062
        -0.0047062432       -0.0171542968        0.0077231948
         0.0003199066       -0.0000226971       -0.0033512700
        -0.0032471451        0.0022539911       -0.0059748718
        -0.0025147818       -0.0007973865       -0.0005613290
        -0.0042273479        0.0052055941        0.0041915976
        -0.0026102182       -0.0024661906       -0.0091263782
         0.0070957843        0.0016088841       -0.0041862226
        -0.0000137386        0.0009370770       -0.0022940134
        -0.0038872365       -0.0158694932       -0.0279314222
 The angle between DerCp and UGrDif has cos=-0.624
 and it is: 2.244 rad or :128.58 degrees.
 The length**2 of DerCp is:0.0323 and GrDif is:0.0156
 But the length of DerCp is:0.1797 and GrDif is:0.1250
------------------ Projection to constraints complement-------------
Angle of DerCp (L=0.1797) and UGrDif(L=0.1250) is 128.58 degs
Angle of Force (L=0.0941) and UGrDif(L=0.1250) is  15.63 degs
Angle of Force (L=0.0941) and DerCp (L=0.1797) is 112.95 degs
Angle of UGrDif(L=0.1250) and DerCp (L=0.1797) is 128.58 degs
Angle of UGrDif(L=0.1250) and Force (L=0.0001) is  90.00 degs
Angle of Dercpl(L=0.1797) and Force (L=0.0001) is  90.00 degs
 Projected Gradient of iVec State.
         0.0000064923       -0.0000111018       -0.0000017616
         0.0000011477        0.0000098736       -0.0000067356
        -0.0000052021        0.0000105403        0.0000029564
         0.0000254611        0.0000182279       -0.0000112317
         0.0000047078        0.0000008295        0.0000022820
        -0.0000104926       -0.0000031734       -0.0000077252
        -0.0000124828        0.0000082218       -0.0000006525
         0.0000101958        0.0000009986        0.0000048469
         0.0000074054       -0.0000102497       -0.0000041463
        -0.0000122594       -0.0000123339        0.0000081290
        -0.0000041417        0.0000063448       -0.0000020413
         0.0000140156       -0.0000018858       -0.0000001726
        -0.0000248471       -0.0000162919        0.0000162525
 Projected Ivec Gradient: RMS= 0.00001 MAX= 0.00003
 SCoeff= 1.9821761149155701 1E-3
 Scaled Projected Gradient of iVec State.
```

```
        0.0000442271       -0.0000589321        0.0000194160
       -0.0000096142       -0.0000290215        0.0000524689
        0.0000918368        0.0001079391        0.0000306506
       -0.0000685060        0.0001118041       -0.0000285957
       -0.0000055788       -0.0000670864        0.0000191479
       -0.0000097710       -0.0000032545       -0.0000150264
       -0.0000201113        0.0000129459       -0.0000109145
        0.0000062049        0.0000031797       -0.0000006250
       -0.0000033649        0.0000050689        0.0000092473
       -0.0000173692       -0.0000178749       -0.0000146074
        0.0000113655        0.0000127290       -0.0000111768
        0.0000139544        0.0000018449       -0.0000051823
       -0.0000332734       -0.0000793423       -0.0000448025
Leave Link 1003 at 05:55:35   on 02/12/08  , MaxMem=  134217728 cpu:    2446.3
(Enter /opt/gaussian/g03/l716.exe)
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6          -0.000008011    0.000072058   -0.000023442
   2          6           0.000026779    0.000018241   -0.000051360
   3          6          -0.000130087   -0.000050802   -0.000038998
   4          6           0.000002490   -0.000129579    0.000034843
   5          6           0.000039209    0.000054921   -0.000018565
   6          1           0.000008866   -0.000001237    0.000015866
   7          1           0.000010252   -0.000020590    0.000012733
   8          1          -0.000006994    0.000000278    0.000000048
   9          1           0.000001188   -0.000006481   -0.000008895
  10          1           0.000022650    0.000007794    0.000016149
  11          1          -0.000016999   -0.000005057    0.000010079
  12          1          -0.000013439    0.000005424    0.000003868
  13          6           0.000064098    0.000055031    0.000047673
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000130087 RMS     0.000040984
Leave Link  716 at 05:55:38   on 02/12/08  , MaxMem=  134217728 cpu:       0.3
(Enter /opt/gaussian/g03/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.000106916 RMS     0.000026106
Search for a local minimum.
Step number   6 out of a maximum of  72
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Swaping is turned off.
Update second derivatives using D2CorrX and points  1  2  3  4  5
                                                             6
    Eigenvalues ---    0.01255   0.01370   0.01747   0.01801   0.01909
    Eigenvalues ---    0.01940   0.02250   0.02623   0.05512   0.06469
    Eigenvalues ---    0.07667   0.10223   0.13663   0.15756   0.15800
    Eigenvalues ---    0.15962   0.16043   0.16792   0.18597   0.23752
    Eigenvalues ---    0.28199   0.29110   0.36500   0.36758   0.36992
    Eigenvalues ---    0.37008   0.37152   0.37428   0.38042   0.39759
    Eigenvalues ---    0.41728   0.44991   0.515161000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
    Eigenvalues --- 1000.000001000.000001000.000001000.000001000.00000
```

```
    Eigenvalues --- 1000.000001000.00000
Angle between quadratic step and forces=  62.03 degrees.
Linear search not attempted -- option 19 set.
Iteration  1 RMS(Cart)=  0.00033858 RMS(Int)=  0.00000011
Iteration  2 RMS(Cart)=  0.00000013 RMS(Int)=  0.00000004
```

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.70191	0.00001	0.00000	0.00003	0.00003	2.70194
R2	2.67751	-0.00002	0.00000	-0.00000	-0.00000	2.67751
R3	2.04203	0.00002	0.00000	0.00009	0.00009	2.04212
R4	2.04728	0.00000	0.00000	0.00002	0.00002	2.04731
R5	2.82406	0.00001	0.00000	0.00005	0.00005	2.82412
R6	2.70194	0.00008	0.00000	0.00016	0.00016	2.70210
R7	2.04730	0.00000	0.00000	0.00002	0.00002	2.04732
R8	2.82367	-0.00006	0.00000	-0.00016	-0.00016	2.82351
R9	2.67757	-0.00011	0.00000	-0.00021	-0.00021	2.67736
R10	2.04202	0.00002	0.00000	0.00010	0.00010	2.04212
R11	2.03786	0.00001	0.00000	0.00006	0.00006	2.03792
R12	2.04754	0.00001	0.00000	-0.00001	-0.00001	2.04754
R13	2.04483	0.00001	0.00000	0.00008	0.00008	2.04491
A1	2.01025	0.00003	0.00000	0.00007	0.00007	2.01031
A2	2.10675	0.00000	0.00000	0.00009	0.00009	2.10684
A3	2.16135	-0.00003	0.00000	-0.00011	-0.00011	2.16124
A4	2.13531	0.00001	0.00000	0.00015	0.00014	2.13545
A5	2.07538	-0.00001	0.00000	-0.00021	-0.00021	2.07517
A6	2.07243	-0.00000	0.00000	0.00007	0.00007	2.07250
A7	2.13515	-0.00000	0.00000	0.00017	0.00017	2.13533
A8	2.07550	-0.00000	0.00000	-0.00027	-0.00027	2.07522
A9	2.07246	0.00000	0.00000	0.00011	0.00011	2.07256
A10	2.01028	0.00003	0.00000	-0.00001	-0.00001	2.01028
A11	2.10675	-0.00000	0.00000	0.00009	0.00009	2.10685
A12	2.16129	-0.00003	0.00000	-0.00006	-0.00006	2.16123
A13	1.97290	-0.00005	0.00000	-0.00026	-0.00026	1.97264
A14	2.15087	0.00003	0.00000	0.00017	0.00017	2.15104
A15	2.15087	0.00002	0.00000	0.00015	0.00015	2.15102
A16	1.44005	-0.00006	0.00000	-0.00050	-0.00050	1.43954
A17	1.98682	0.00002	0.00000	0.00005	0.00005	1.98687
A18	1.99333	0.00001	0.00000	0.00004	0.00004	1.99336
A19	1.98699	0.00003	0.00000	0.00018	0.00018	1.98717
A20	1.99348	0.00001	0.00000	0.00006	0.00006	1.99355
A21	1.99688	-0.00002	0.00000	0.00004	0.00004	1.99693
D1	2.40367	0.00000	0.00000	0.00075	0.00075	2.40441
D2	-0.72484	-0.00001	0.00000	-0.00016	-0.00016	-0.72500
D3	-0.63632	-0.00000	0.00000	0.00027	0.00027	-0.63605
D4	2.51836	-0.00002	0.00000	-0.00064	-0.00064	2.51771
D5	-0.16741	-0.00001	0.00000	-0.00007	-0.00007	-0.16748
D6	3.11035	-0.00001	0.00000	-0.00053	-0.00053	3.10982
D7	2.86900	-0.00001	0.00000	0.00044	0.00044	2.86945
D8	-0.13642	0.00000	0.00000	-0.00003	-0.00003	-0.13645
D9	1.29155	0.00002	0.00000	0.00048	0.00048	1.29203
D10	-0.67737	0.00001	0.00000	0.00049	0.00049	-0.67688
D11	-3.01529	0.00000	0.00000	0.00033	0.00033	-3.01496
D12	-1.83743	0.00000	0.00000	-0.00040	-0.00040	-1.83783
D13	2.47683	-0.00000	0.00000	-0.00039	-0.00039	2.47645
D14	0.13891	-0.00001	0.00000	-0.00054	-0.00054	0.13836
D15	-2.40344	0.00001	0.00000	0.00003	0.00003	-2.40341
D16	0.63641	0.00001	0.00000	0.00026	0.00026	0.63667
D17	0.72458	0.00003	0.00000	0.00072	0.00072	0.72530
D18	-2.51876	0.00003	0.00000	0.00095	0.00095	-2.51781

```
  D19       -1.29140  -0.00002   0.00000  -0.00078  -0.00078  -1.29218
  D20        0.67735  -0.00002   0.00000  -0.00093  -0.00093   0.67642
  D21        3.01561  -0.00001   0.00000  -0.00060  -0.00060   3.01501
  D22        1.83711  -0.00000   0.00000  -0.00011  -0.00011   1.83700
  D23       -2.47733  -0.00000   0.00000  -0.00026  -0.00026  -2.47759
  D24       -0.13907   0.00001   0.00000   0.00007   0.00007  -0.13900
  D25        0.16760   0.00002   0.00000  -0.00014  -0.00014   0.16746
  D26       -3.11016   0.00001   0.00000   0.00033   0.00033  -3.10984
  D27       -2.86867   0.00001   0.00000  -0.00039  -0.00039  -2.86906
  D28        0.13676   0.00001   0.00000   0.00008   0.00008   0.13683
         Item               Value     Threshold  Converged?
Maximum Force            0.000107     0.000450     YES
RMS     Force            0.000026     0.000300     YES
Maximum Displacement     0.000957     0.001800     YES
RMS     Displacement     0.000339     0.001200     YES
Predicted change in Energy=-1.291833E-07
Optimization completed.
   -- Stationary point found.
                          ----------------------------
                          !   Optimized Parameters   !
                          ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.4298         -DE/DX =    0.0                 !
! R2    R(1,5)                  1.4169         -DE/DX =    0.0                 !
! R3    R(1,7)                  1.0806         -DE/DX =    0.0                 !
! R4    R(2,8)                  1.0834         -DE/DX =    0.0                 !
! R5    R(2,13)                 1.4944         -DE/DX =    0.0                 !
! R6    R(3,4)                  1.4298         -DE/DX =    0.0001              !
! R7    R(3,9)                  1.0834         -DE/DX =    0.0                 !
! R8    R(3,13)                 1.4942         -DE/DX =   -0.0001              !
! R9    R(4,5)                  1.4169         -DE/DX =   -0.0001              !
! R10   R(4,10)                 1.0806         -DE/DX =    0.0                 !
! R11   R(5,6)                  1.0784         -DE/DX =    0.0                 !
! R12   R(11,13)                1.0835         -DE/DX =    0.0                 !
! R13   R(12,13)                1.0821         -DE/DX =    0.0                 !
! A1    A(2,1,5)              115.1787         -DE/DX =    0.0                 !
! A2    A(2,1,7)              120.708          -DE/DX =    0.0                 !
! A3    A(5,1,7)              123.8361         -DE/DX =    0.0                 !
! A4    A(1,2,8)              122.3441         -DE/DX =    0.0                 !
! A5    A(1,2,13)             118.9104         -DE/DX =    0.0                 !
! A6    A(8,2,13)             118.7413         -DE/DX =    0.0                 !
! A7    A(4,3,9)              122.3352         -DE/DX =    0.0                 !
! A8    A(4,3,13)             118.9173         -DE/DX =    0.0                 !
! A9    A(9,3,13)             118.743          -DE/DX =    0.0                 !
! A10   A(3,4,5)              115.1808         -DE/DX =    0.0                 !
! A11   A(3,4,10)             120.7081         -DE/DX =    0.0                 !
! A12   A(5,4,10)             123.833          -DE/DX =    0.0                 !
! A13   A(1,5,4)              113.0388         -DE/DX =   -0.0001              !
! A14   A(1,5,6)              123.2358         -DE/DX =    0.0                 !
! A15   A(4,5,6)              123.236          -DE/DX =    0.0                 !
! A16   A(2,13,3)              82.5086         -DE/DX =   -0.0001              !
! A17   A(2,13,11)            113.8367         -DE/DX =    0.0                 !
! A18   A(2,13,12)            114.2092         -DE/DX =    0.0                 !
! A19   A(3,13,11)            113.8463         -DE/DX =    0.0                 !
! A20   A(3,13,12)            114.2181         -DE/DX =    0.0                 !
! A21   A(11,13,12)           114.4131         -DE/DX =    0.0                 !
! D1    D(5,1,2,8)            137.7201         -DE/DX =    0.0                 !
```

```
! D2    D(5,1,2,13)           -41.5301         -DE/DX =    0.0                 !
! D3    D(7,1,2,8)            -36.4586         -DE/DX =    0.0                 !
! D4    D(7,1,2,13)           144.2912         -DE/DX =    0.0                 !
! D5    D(2,1,5,4)             -9.5919         -DE/DX =    0.0                 !
! D6    D(2,1,5,6)            178.2101         -DE/DX =    0.0                 !
! D7    D(7,1,5,4)            164.3818         -DE/DX =    0.0                 !
! D8    D(7,1,5,6)             -7.8162         -DE/DX =    0.0                 !
! D9    D(1,2,13,3)            74.0006         -DE/DX =    0.0                 !
! D10   D(1,2,13,11)          -38.8104         -DE/DX =    0.0                 !
! D11   D(1,2,13,12)         -172.7636         -DE/DX =    0.0                 !
! D12   D(8,2,13,3)          -105.2769         -DE/DX =    0.0                 !
! D13   D(8,2,13,11)          141.9121         -DE/DX =    0.0                 !
! D14   D(8,2,13,12)            7.9588         -DE/DX =    0.0                 !
! D15   D(9,3,4,5)           -137.7067         -DE/DX =    0.0                 !
! D16   D(9,3,4,10)            36.4635         -DE/DX =    0.0                 !
! D17   D(13,3,4,5)            41.5153         -DE/DX =    0.0                 !
! D18   D(13,3,4,10)         -144.3145         -DE/DX =    0.0                 !
! D19   D(4,3,13,2)           -73.9917         -DE/DX =    0.0                 !
! D20   D(4,3,13,11)           38.8091         -DE/DX =    0.0                 !
! D21   D(4,3,13,12)          172.7819         -DE/DX =    0.0                 !
! D22   D(9,3,13,2)           105.2586         -DE/DX =    0.0                 !
! D23   D(9,3,13,11)         -141.9406         -DE/DX =    0.0                 !
! D24   D(9,3,13,12)           -7.9678         -DE/DX =    0.0                 !
! D25   D(3,4,5,1)              9.6026         -DE/DX =    0.0                 !
! D26   D(3,4,5,6)           -178.1993         -DE/DX =    0.0                 !
! D27   D(10,4,5,1)          -164.3626         -DE/DX =    0.0                 !
! D28   D(10,4,5,6)             7.8355         -DE/DX =    0.0                 !
--------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Largest change from initial coordinates is atom   12       0.021 Angstoms.
Leave Link  103 at 05:55:43   on 02/12/08  , MaxMem=  134217728 cpu:       6.1
(Enter /opt/gaussian/g03/l202.exe)
                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0        0.060218   -1.388643    0.025882
   2          6             0       -1.032986   -0.550431   -0.356998
   3          6             0       -0.069123    1.168500   -0.357303
   4          6             0        1.216325    0.672899    0.025254
   5          6             0        1.258968   -0.705880    0.348961
   6          1             0        2.153958   -1.207697    0.680774
   7          1             0       -0.022375   -2.464472   -0.032883
   8          1             0       -1.687073   -0.793386   -1.185759
   9          1             0       -0.203081    1.852774   -1.186485
  10          1             0        2.091260    1.304259   -0.034305
  11          1             0       -1.110266    0.623013    1.468692
  12          1             0       -2.187612    1.226893    0.131264
  13          6             0       -1.273638    0.714525    0.401482
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  C    1.429787   0.000000
    3  C    2.588927   1.970724   0.000000
    4  C    2.363586   2.588832   1.429807   0.000000
    5  C    1.416880   2.403247   2.403317   1.416910   0.000000
```

```
     6  H    2.201221   3.415491   3.415553   2.201250   1.078391
     7  H    1.080593   2.188593   3.647728   3.373552   2.209138
     8  H    2.208037   1.083375   2.674528   3.470773   3.322977
     9  H    3.470727   2.674356   1.083383   2.207970   3.322934
    10  H    3.373497   3.647591   2.188610   1.080590   2.209131
    11  H    2.738337   2.171655   2.171587   2.738435   2.938200
    12  H    3.450344   2.174958   2.174880   3.450353   3.957514
    13  C    2.518643   1.494429   1.494224   2.518571   2.904204
                   6          7          8          9         10
     6  H    0.000000
     7  H    2.612511   0.000000
     8  H    4.290584   2.625428   0.000000
     9  H    4.290544   4.472366   3.033874   0.000000
    10  H    2.612507   4.320971   4.472333   2.625336   0.000000
    11  H    3.824587   3.601499   3.063494   3.063537   3.601786
    12  H    5.007836   4.282683   2.463050   2.463038   4.282773
    13  C    3.939715   3.443887   2.228017   2.227856   3.443869
                  11         12         13
    11  H    0.000000
    12  H    1.820456   0.000000
    13  C    1.083513   1.082075   0.000000
Stoichiometry    C6H7(1+)
Framework group  C1[X(C6H7)]
Deg. of freedom    33
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        0.730522   -1.181738   -0.050753
   2          6             0       -0.662590   -0.985404   -0.305671
   3          6             0       -0.662859    0.985321   -0.305486
   4          6             0        0.730289    1.181849   -0.050803
   5          6             0        1.468895    0.000116    0.205327
   6          1             0        2.521288    0.000216    0.440693
   7          1             0        1.177387   -2.160426   -0.151565
   8          1             0       -1.189021   -1.517096   -1.089173
   9          1             0       -1.189286    1.516779   -1.089160
  10          1             0        1.177056    2.160544   -0.151940
  11          1             0       -1.132210   -0.000207    1.571808
  12          1             0       -2.485806   -0.000267    0.354502
  13          6             0       -1.417492   -0.000067    0.526526
---------------------------------------------------------------------
```