```
AM1 BONDS ESP VECTORS PRECISE +
 CHARGE=-1
 Phenolate anion

                                AM1    CALCULATION
                                       VERSION  6.00

          FINAL HEAT OF FORMATION =        -29.72681 KCAL

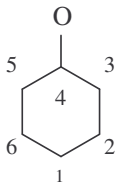
          TOTAL ENERGY            =      -1157.60678 EV
          ELECTRONIC ENERGY       =      -4252.89816 EV
          CORE-CORE REPULSION     =       3095.29138 EV

          IONIZATION POTENTIAL    =          2.83833
          NO. OF FILLED LEVELS    =         18
          MOLECULAR WEIGHT        =         93.105

          SCF CALCULATIONS        =          2
          COMPUTATION TIME        =         10.000 SECONDS
```

EIGENVECTORS

Orb		**13**	**14**	**15**	**16**	**17**	**18**	19	20	21	22	23	24
					π3	*lp*	*π4*	*π5*	*π6*				
Ei		*-7.38*	*-7.26*	*-6.34*	*-5.03*	*-4.26*	*-2.84*	*5.34*	*5.90*	*8.15*	*8.32*	*8.57*	*8.69*
S	C 1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.04	0.02	-0.42
PX	C 1	0.28	-0.17	0.00	0.00	0.03	0.00	0.00	0.00	0.00	-0.13	-0.15	0.16
PY	C 1	-0.21	-0.24	0.00	0.00	-0.01	0.00	0.00	0.00	0.00	-0.24	0.05	0.29
PZ	**C 1**	**0.00**	**0.00**	**-0.49**	**0.00**	**0.00**	**0.48**	**-0.01**	**0.57**	**0.26**	**0.00**	**0.00**	**0.00**
S	C 2	-0.01	0.01	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.28	-0.14	0.21
PX	C 2	-0.26	0.21	0.00	0.00	-0.01	0.00	0.00	0.00	0.00	0.06	-0.30	-0.03
PY	C 2	0.12	0.27	0.00	0.00	0.07	0.00	0.00	0.00	0.00	-0.32	0.27	0.06
PZ	**C 2**	**0.00**	**0.00**	**-0.31**	**-0.50**	**0.00**	**0.06**	**0.50**	**-0.41**	**-0.29**	**0.00**	**0.00**	**0.00**
S	C 3	0.03	-0.01	0.00	0.00	-0.10	0.00	0.00	0.00	0.00	-0.04	0.00	-0.23
PX	C 3	0.28	-0.19	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.03	-0.19	-0.01
PY	C 3	-0.15	-0.27	0.00	0.00	-0.19	0.00	0.00	0.00	0.00	-0.08	0.03	0.11
PZ	**C 3**	**0.00**	**0.00**	**0.04**	**-0.49**	**0.00**	**-0.44**	**-0.50**	**-0.03**	**0.40**	**0.00**	**0.00**	**0.00**
S	C 4	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.14	0.00	0.08
PX	C 4	-0.27	0.18	0.00	0.00	-0.10	0.00	0.00	0.00	0.00	-0.03	-0.17	-0.02
PY	C 4	0.17	0.26	0.00	0.00	0.04	0.00	0.00	0.00	0.00	-0.07	0.08	-0.03
PZ	**C 4**	**0.00**	**0.00**	**0.43**	**0.00**	**0.00**	**-0.16**	**0.00**	**0.49**	**-0.60**	**0.00**	**0.00**	**0.00**
S	C 5	-0.03	0.00	0.00	0.00	0.10	0.00	0.00	0.00	0.00	-0.04	0.02	-0.21
PX	C 5	0.25	-0.19	0.00	0.00	0.23	0.00	0.00	0.00	0.00	-0.08	-0.14	0.08
PY	C 5	-0.23	-0.26	0.00	0.00	0.01	0.00	0.00	0.00	0.00	-0.02	0.12	0.06
PZ	**C 5**	**0.00**	**0.00**	**0.05**	**0.49**	**0.00**	**-0.44**	**0.51**	**-0.02**	**0.40**	**0.00**	**0.00**	**0.00**
S	C 6	0.01	0.01	0.00	0.00	-0.03	0.00	0.00	0.00	0.00	0.27	0.13	0.22
PX	C 6	-0.21	0.17	0.00	0.00	-0.07	0.00	0.00	0.00	0.00	-0.28	-0.42	0.03
PY	C 6	0.23	0.28	0.00	0.00	-0.05	0.00	0.00	0.00	0.00	-0.12	0.10	0.01
PZ	**C 6**	**0.00**	**0.00**	**-0.30**	**0.51**	**0.00**	**0.04**	**-0.49**	**-0.42**	**-0.30**	**0.00**	**0.00**	**0.00**
S	H 7	0.04	0.31	0.00	0.00	-0.01	0.00	0.00	0.00	0.00	-0.23	-0.04	0.61
S	H 8	-0.26	-0.13	0.00	0.00	-0.08	0.00	0.00	0.00	0.00	-0.50	0.43	-0.10
S	H 9	0.28	-0.19	0.00	0.00	0.07	0.00	0.00	0.00	0.00	0.00	0.20	0.21
S	H 10	-0.32	-0.14	0.00	0.00	-0.06	0.00	0.00	0.00	0.00	0.02	-0.20	0.18
S	H 11	0.24	-0.17	0.00	0.00	0.09	0.00	0.00	0.00	0.00	-0.46	-0.46	-0.14
S	O 12	-0.01	-0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01
PX	O 12	-0.26	-0.13	0.00	0.00	0.82	0.00	0.00	0.00	0.00	0.02	0.04	0.03
PY	O 12	0.09	-0.38	0.00	0.00	-0.39	0.00	0.00	0.00	0.00	0.04	-0.03	0.05
PZ	**O 12**	**0.00**	**0.00**	**0.62**	**0.00**	**0.00**	**0.59**	**0.00**	**-0.30**	**0.27**	**0.00**	**0.00**	**0.00**

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AM1 BONDS ESP VECTORS PRECISE +
 CHARGE=0 UHF
 Phenoxyl radical

                                AM1    CALCULATION
                                       VERSION  6.00

          FINAL HEAT OF FORMATION =         16.64809 KCAL

          TOTAL ENERGY            =      -1155.59582 EV
          ELECTRONIC ENERGY       =      -4250.88720 EV
          CORE-CORE REPULSION     =       3095.29138 EV

          IONIZATION POTENTIAL    =         10.02345
          NO. OF ALPHA ELECTRONS  =         18
          NO. OF BETA  ELECTRONS  =         17
          MOLECULAR WEIGHT        =         93.105

          SCF CALCULATIONS        =          2
          COMPUTATION TIME        =         10.000 SECONDS
```

EIGENVECTORS

	Orb	**13**	**14**	**15**	**16**	**17**	**18**	19	20	21	22	23	24
					lp	*π3*	*π4*	*π5*	*π6*				
α	*Ei*	*-13.16*	*-13.03*	*-12.87*	*-11.48*	*-10.63*	*-10.02*	*0.20*	*0.39*	*2.39*	*3.32*	*3.56*	*3.56*
					π3	*lp*	*π4*	*π5*	*π6*				
β	*Ei*	*-12.87*	*-12.77*	*-11.31*	*-11.07*	*-10.43*	*-1.28*	*0.53*	*1.13*	*2.78*	*3.36*	*3.56*	*3.71*

```
AM1 BONDS ESP VECTORS PRECISE +
 CHARGE=1 UHF TRIPLET
 Phenoxyl cation triplet

                                AM1    CALCULATION
                                       VERSION  6.00

          FINAL HEAT OF FORMATION =        235.20349 KCAL

          TOTAL ENERGY            =      -1146.11854 EV
          ELECTRONIC ENERGY       =      -4241.40992 EV
          CORE-CORE REPULSION     =       3095.29138 EV

          IONIZATION POTENTIAL    =         15.77211
          NO. OF ALPHA ELECTRONS  =         18
          NO. OF BETA  ELECTRONS  =         16
          MOLECULAR WEIGHT        =         93.105

          SCF CALCULATIONS        =          2
          COMPUTATION TIME        =         10.000 SECONDS
```

EIGENVECTORS

Orb	**13**	**14**	**15**	**16**	**17**	**18**	19	20	21	22	23	24
				?	*π3*	*π4*	*π5*	*π6*				
Ei	*-20.07*	*-19.03*	*-18.27*	*-17.62*	*-15.89*	*-15.80*	*-6.15*	*-5.28*	*-3.44*	*-3.26*	*-2.32*	*-2.14*
				π3	*π4*	*lp*	*π5*	*π6*				
Ei	*-18.15*	*-17.78*	*-17.48*	*-15.77*	*-8.48*	*-7.46*	*-4.95*	*-4.78*	*-2.86*	*-2.82*	*-2.00*	*-1.82*

```
AM1 BONDS ESP VECTORS PRECISE +
 CHARGE=1
 Phenoxyl cation singlet

                                AM1    CALCULATION
                                       VERSION  6.00

          FINAL HEAT OF FORMATION =        238.48266 KCAL

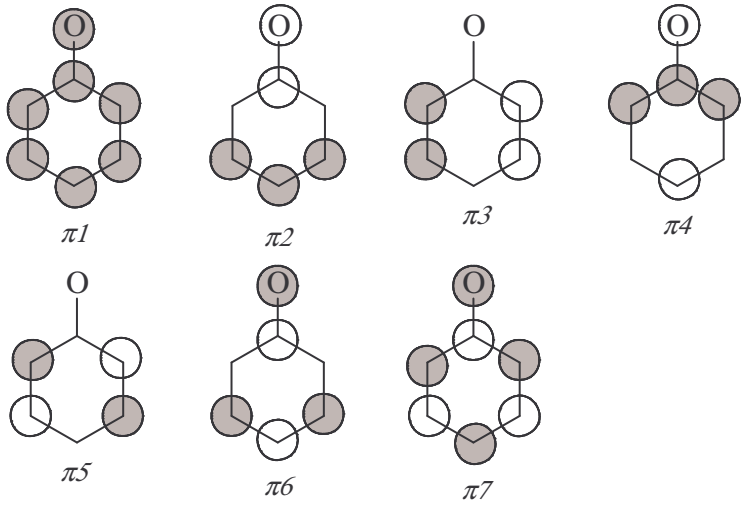
          TOTAL ENERGY            =      -1145.97635 EV
          ELECTRONIC ENERGY       =      -4241.26773 EV
          CORE-CORE REPULSION     =       3095.29138 EV

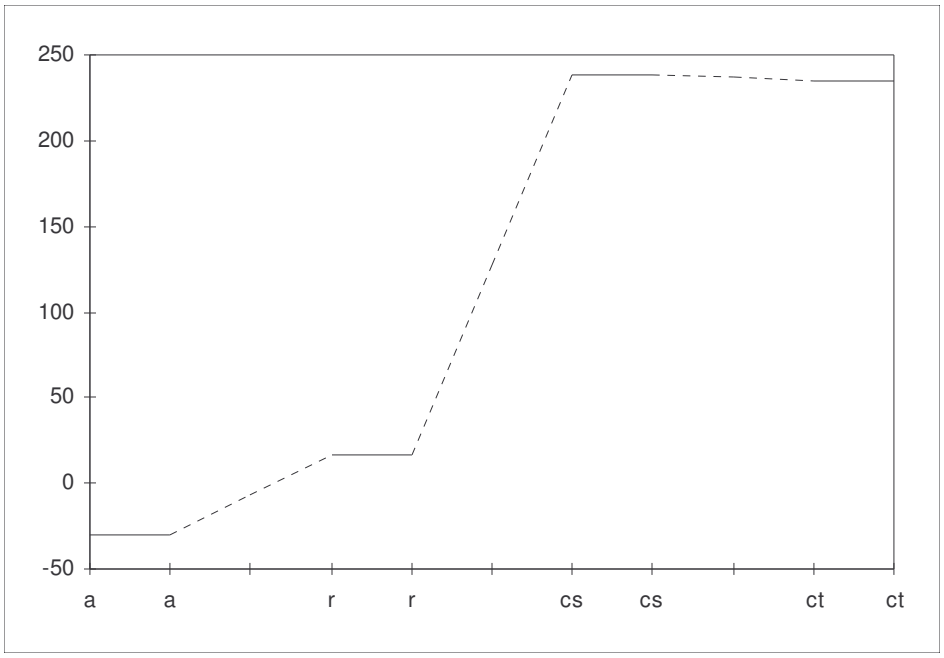
          IONIZATION POTENTIAL    =         15.95867
          NO. OF FILLED LEVELS    =         17
          MOLECULAR WEIGHT        =         93.105

          SCF CALCULATIONS        =          2
          COMPUTATION TIME        =         10.000 SECONDS

EIGENVECTORS
```

Orb	**13**	**14**	**15**	**16**	**17**	18	19	20	21	22	23	24
				lp	*π3*	*π4*	*π5*	*π6*				
Ei	*-18.58*	*-18.50*	*-17.38*	*-17.09*	*-15.96*	*-8.77*	*-5.39*	*-5.16*	*-3.30*	*-2.73*	*-2.11*	*-2.08*

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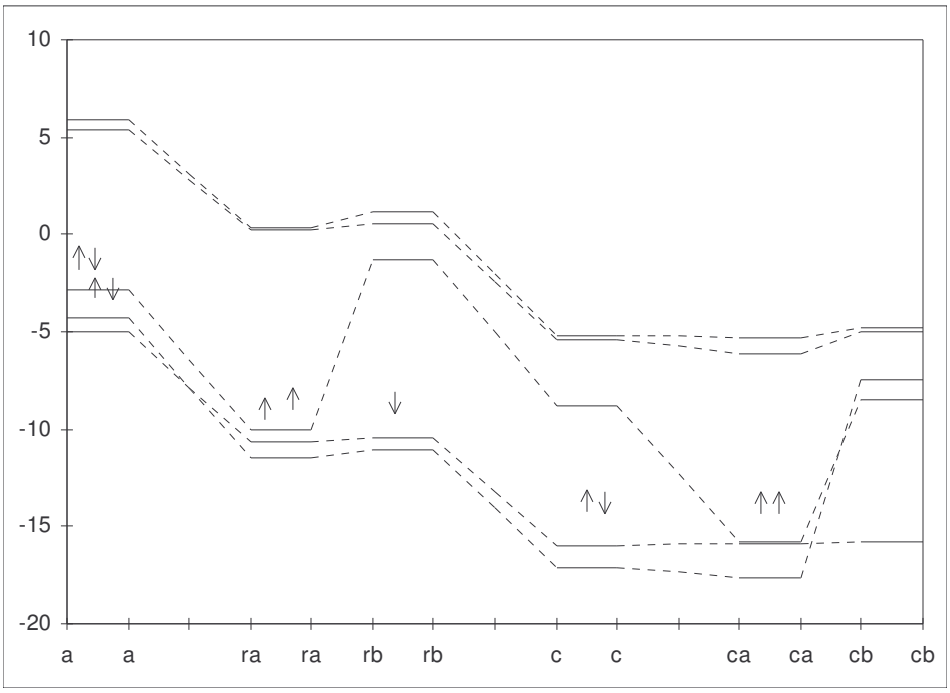
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*************************************************************************
** FRANK J. SEILER RES. LAB., U.S. AIR FORCE ACADEMY, COLO. SPGS., CO. 80840 **
*************************************************************************

                              AM1 CALCULATION RESULTS

*************************************************************************
*          MOPAC:  VERSION  6.00              CALC'D. Today
*  VECTORS  - FINAL EIGENVECTORS TO BE PRINTED
*  BONDS    - FINAL BOND-ORDER MATRIX TO BE PRINTED
*  ESP      - ELECTROSTATIC POTENTIAL CALCULATION
*   T=      - A TIME OF360000.0 SECONDS REQUESTED
*  DUMP=N   - RESTART FILE WRITTEN EVERY  3600.0 SECONDS
*  AM1      - THE AM1 HAMILTONIAN TO BE USED
*  PRECISE  - CRITERIA TO BE INCREASED BY 100 TIMES
*************************************************************************030BY030
AM1 BONDS ESP VECTORS PRECISE
Phenol molecule
```

ATOM NUMBER (I)	CHEMICAL SYMBOL	BOND LENGTH (ANGSTROMS) NA:I	BOND ANGLE (DEGREES) NB:NA:I	TWIST ANGLE (DEGREES) NC:NB:NA:I	NA	NB	NC
1	C						
2	C	1.39394			1		
3	C	1.39345	120.45278		2	1	
4	C	1.40203	119.02975	.02212	3	2	1
5	C	1.40493	121.02234	.00091	4	3	2
6	C	1.39125	118.86839	-.01402	5	4	3
7	H	1.09914	120.02371	179.95797	1	2	3
8	H	1.10022	119.55454	-179.99579	2	3	4
9	H	1.09845	120.37576	-179.99308	3	4	5
10	H	1.09855	119.61084	179.98820	5	4	3
11	H	1.10041	119.57230	-179.99430	6	5	4
12	O	1.37692	122.58831	179.99793	4	3	2
13	H	.96802	107.90180	-.03374	12	4	3

CARTESIAN COORDINATES

NO.	ATOM	X	Y	Z
1	C	.0000	.0000	.0000
2	C	1.3939	.0000	.0000
3	C	2.1002	1.2012	.0000
4	C	1.3882	2.4090	.0005
5	C	-.0166	2.4214	.0010
6	C	-.6991	1.2090	.0007
7	H	-.5500	-.9517	-.0007
8	H	1.9439	-.9529	-.0003
9	H	3.1986	1.2039	-.0003
10	H	-.5510	3.3812	.0015
11	H	-1.7995	1.2052	.0010
12	O	2.0111	3.6370	.0005
13	H	2.9672	3.4857	.0008

```
  H: (AM1): M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)
  C: (AM1): M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)
  O: (AM1): M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)

          RHF CALCULATION, NO. OF DOUBLY OCCUPIED LEVELS = 18
```

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AM1 BONDS ESP VECTORS PRECISE
Phenol molecule

    GRADIENTS WERE INITIALLY ACCEPTABLY SMALL
    SCF FIELD WAS ACHIEVED

                              AM1    CALCULATION
                                                    VERSION  6.00
                                                    Today

        FINAL HEAT OF FORMATION =        -22.24764 KCAL

        TOTAL ENERGY            =      -1170.93820 EV
        ELECTRONIC ENERGY       =      -4456.19061 EV
        CORE-CORE REPULSION     =       3285.25241 EV

        IONIZATION POTENTIAL    =          9.11483
        NO. OF FILLED LEVELS    =         18
        MOLECULAR WEIGHT        =     94.113

        SCF CALCULATIONS  =                2
        COMPUTATION TIME =  10.000 SECONDS
```

ATOM NUMBER (I)	CHEMICAL SYMBOL	BOND LENGTH (ANGSTROMS) NA:I	BOND ANGLE (DEGREES) NB:NA:I	TWIST ANGLE (DEGREES) NC:NB:NA:I	NA	NB	NC
1	C						
2	C	1.39394			1		
3	C	1.39345	120.45278		2	1	
4	C	1.40203	119.02975	.02212	3	2	1
5	C	1.40493	121.02234	.00091	4	3	2
6	C	1.39125	118.86839	-.01402	5	4	3
7	H	1.09914	120.02371	179.95797	1	2	3
8	H	1.10022	119.55454	-179.99579	2	3	4
9	H	1.09845	120.37576	-179.99308	3	4	5
10	H	1.09855	119.61084	179.98820	5	4	3
11	H	1.10041	119.57230	-179.99430	6	5	4
12	O	1.37692	122.58831	179.99793	4	3	2
13	H	.96802	107.90180	-.03374	12	4	3

EIGENVECTORS

ROOT NO.			1	2	3	4	5	6
			-40.14349	-37.37962	-31.62254	-30.25537	-23.68517	-23.00186
S	C	1	-.24850	.34712	-.01474	.48226	-.12416	.33101
PX	C	1	-.04385	.04435	-.17791	-.00652	-.23814	-.15858
PY	C	1	-.07386	.07826	.10200	.00384	.17568	-.01739
PZ	C	1	-.00003	.00003	.00006	.00001	.00009	-.00001
S	C	2	-.26465	.31093	-.43640	.17884	-.26295	-.30242
PX	C	2	.03385	-.06724	-.07710	-.17673	.15813	-.21229
PY	C	2	-.08375	.05516	-.06822	-.10721	.17093	-.00214
PZ	C	2	-.00001	.00000	.00002	-.00001	.00003	.00002
S	C	3	-.32941	.16674	-.43261	-.30600	.34826	-.02510
PX	C	3	.09053	-.07983	.02088	.03014	.10978	-.02997
PY	C	3	-.04602	-.08733	.10453	-.13645	.08891	.33069
PZ	C	3	-.00004	.00000	.00001	-.00005	.00000	.00006
S	C	4	-.47004	-.06535	.02368	-.40940	-.14273	.36156
PX	C	4	-.02392	-.13479	-.19345	.07127	.25831	.15196
PY	C	4	-.02560	-.21518	.11686	.12715	-.23076	.00140
PZ	C	4	-.00001	-.00002	.00008	.00000	-.00013	-.00006
S	C	5	-.31410	.18255	.44865	-.27724	-.20884	-.28992
PX	C	5	-.08251	-.03320	-.06530	-.14022	-.19859	.22338
PY	C	5	.05933	-.10915	-.06836	-.04919	-.19154	.01440
PZ	C	5	.00005	-.00003	-.00002	.00002	.00000	-.00007
S	C	6	-.25956	.31639	.42248	.21003	.37102	-.04927
PX	C	6	-.08861	.08235	.02116	-.00376	-.10106	.02329
PY	C	6	-.01065	-.02718	.11199	-.19897	-.03693	-.31730
PZ	C	6	.00002	-.00003	.00003	-.00008	.00001	-.00015
S	H	7	-.06129	.09589	-.00536	.18802	-.06881	.18949
S	H	8	-.06609	.08508	-.15967	.07205	-.14572	-.18286
S	H	9	-.09245	.02870	-.15939	-.10378	.20663	-.03017
S	H	10	-.08451	.03609	.16077	-.09497	-.12338	-.17279
S	H	11	-.06439	.08674	.15371	.08412	.20674	-.03237
S	O	12	-.50220	-.65009	.01658	.32977	.00756	-.18499
PX	O	12	.00286	-.04163	-.05640	.11097	.26115	-.15351
PY	O	12	.14008	.10633	.00715	.08153	.05132	-.23661
PZ	O	12	-.00001	-.00001	.00001	.00002	-.00002	-.00006
S	H	13	-.16603	-.20231	-.03042	.11339	.15991	-.10488

ROOT NO.			7	8	9	10	11	12
			-18.99673	-17.42490	-16.54528	-15.04607	-15.03445	-14.40737
S	C	1	-.08125	-.12476	-.18142	.00456	.10953	-.01777
PX	C	1	-.14059	.04262	.27352	.01283	.30370	.13660
PY	C	1	-.01223	.38047	.07968	.00404	.10584	-.27910
PZ	C	1	.00001	.00020	.00013	-.14155	.00600	-.00001
S	C	2	.09167	.03877	.19666	-.00313	-.07361	.00782
PX	C	2	.23427	.03743	-.10052	-.01490	-.35187	-.18933
PY	C	2	-.07782	.29867	-.18639	.00743	.18203	.13646
PZ	C	2	-.00005	.00009	.00005	-.17607	.00745	.00019
S	C	3	.07583	-.03887	-.21536	.00415	.09766	.07760
PX	C	3	.20101	-.27188	-.20425	.00702	.17276	-.33742
PY	C	3	-.16407	-.19085	.15762	.00328	.06825	.16899
PZ	C	3	-.00010	.00001	.00012	-.27640	.01154	.00036
S	C	4	-.00429	-.00004	.14677	-.00739	-.17744	.02156
PX	C	4	.14229	-.15605	.28379	.01173	.28105	.11003
PY	C	4	.36828	.00358	.03649	.00450	.11477	-.25404
PZ	C	4	-.00004	-.00006	-.00005	-.49903	.02084	.00032
S	C	5	-.09905	-.18208	-.12731	.00272	.06474	-.05649
PX	C	5	-.11798	.19928	-.12496	-.01537	-.36114	-.17514
PY	C	5	.10621	-.22433	-.23772	-.00137	-.02868	.12138
PZ	C	5	.00003	-.00019	-.00002	-.26779	.01137	.00037
S	C	6	.18781	.10248	.15487	-.00263	-.06198	-.02657
PX	C	6	-.25045	.16558	-.07556	.01196	.29044	-.39993
PY	C	6	-.04417	-.12476	.21321	.00859	.19368	.16284
PZ	C	6	.00003	-.00009	.00017	-.17406	.00737	.00036
S	H	7	.01307	-.29277	-.23447	-.00480	-.12065	.12423
S	H	8	.15826	-.14021	.17818	-.01213	-.29176	-.16264
S	H	9	.15213	-.20779	-.25328	.00748	.18093	-.22922
S	H	10	.04757	-.27487	-.16894	.00606	.14744	.11833
S	H	11	.24298	-.05923	.13117	-.01045	-.25221	.29601
S	O	12	.00922	.17903	-.16971	.00153	.03004	.15468
PX	O	12	-.51410	-.30215	.13298	-.00836	-.19532	-.19398
PY	O	12	-.23403	.17884	-.41263	-.00436	-.11668	.30899
PZ	O	12	-.00013	-.00010	-.00006	-.72095	.03013	.00059
S	H	13	-.33377	-.22344	.09589	-.00638	-.14553	-.18495

			ROOT NO. 13	14	15	16	17	18			ROOT NO. 19	20	21	22	23	24
			-14.27085	-12.64390	-12.50657	-11.94064	-9.85152	-9.11483			.39685	.50811	2.83915	3.02693	3.80103	3.83401
S	C	1	-.02506	-.00006	.02259	.00105	-.00001	-.00002	S	C	1	.00002	.00003	-.00008	-.00888	-.01070	-.12216
PX	C	1	.03834	.00090	-.27627	-.25549	-.00004	.00008	PX	C	1	.00004	-.00002	.00003	.00816	.12992	-.18032
PY	C	1	-.18496	.00128	-.33826	.21156	-.00001	.00036	PY	C	1	.00008	-.00034	.00037	.04169	-.14744	-.06978
PZ	C	1	.00006	.46337	.00163	-.00020	.04008	-.53194	PZ	C	1	-.13245	.53588	-.41945	.00006	-.00014	-.00008
S	C	2	-.04798	.00018	-.03992	.00571	-.00005	.00000	S	C	2	-.00005	-.00005	.00005	.09880	.15687	.13330
PX	C	2	-.01718	-.00085	.26494	.24355	.00001	-.00006	PX	C	2	.00000	-.00005	.00005	.07426	.24082	-.15208
PY	C	2	-.37984	-.00118	.23338	-.21648	.00006	.00001	PY	C	2	.00008	.00005	.00002	.06728	-.21670	-.06252
PZ	C	2	.00010	.41821	.00175	-.00028	-.46441	-.25418	PZ	C	2	-.42297	-.41340	.40492	.00000	-.00002	.00000
S	C	3	.01166	-.00012	.02646	-.00019	.00001	-.00006	S	C	3	-.00001	.00005	-.00005	-.12824	-.15899	-.30935
PX	C	3	.23168	.00098	-.24651	-.22279	-.00017	.00015	PX	C	3	.00014	-.00005	-.00008	.08651	.31636	-.28186
PY	C	3	.25619	.00106	-.24346	.23592	.00007	-.00003	PY	C	3	-.00009	-.00004	.00018	-.03581	-.27831	-.15499
PZ	C	3	.00024	.28968	.00135	-.00003	-.52852	.32636	PZ	C	3	.54281	-.12295	-.37941	-.00009	-.00017	.00003
S	C	4	.02724	.00014	-.03630	-.00668	.00001	.00000	S	C	4	.00003	-.00001	-.00003	.40446	.21896	.18687
PX	C	4	-.04386	-.00028	.10546	.28435	.00000	.00014	PX	C	4	-.00006	.00019	.00013	.07256	.28781	-.17953
PY	C	4	-.16549	-.00049	.07851	-.20460	.00000	-.00013	PY	C	4	.00006	-.00016	-.00007	.31355	-.23056	-.23017
PZ	C	4	.00036	.04969	.00033	-.00012	-.02182	.47650	PZ	C	4	-.17756	.57133	.40322	.00015	-.00015	.00002
S	C	5	-.01910	-.00012	.04586	.01342	.00001	.00000	S	C	5	-.00003	.00004	-.00002	-.22297	-.03910	-.16670
PX	C	5	.05562	.00057	-.14768	-.27782	.00017	.00019	PX	C	5	-.00015	-.00012	-.00007	-.20939	.13963	-.20771
PY	C	5	-.42661	.00128	-.28922	.18142	-.00020	-.00010	PY	C	5	.00017	.00013	.00023	.09826	-.14590	-.11785
PZ	C	5	.00006	.26928	.00114	.00000	.49183	.37357	PZ	C	5	-.39832	-.38689	-.40725	.00012	-.00013	-.00001
S	C	6	.04501	.00014	-.04416	-.00478	.00002	.00002	S	C	6	.00002	.00001	-.00001	.14298	.03440	.10694
PX	C	6	.14189	-.00051	.18901	.27130	.00016	-.00008	PX	C	6	.00016	-.00004	.00015	-.00331	.13670	-.18711
PY	C	6	.25364	-.00149	.27186	-.19352	-.00024	.00003	PY	C	6	-.00024	.00004	-.00010	.14971	-.13849	-.08537
PZ	C	6	.00024	.40477	.00173	-.00046	.51060	-.17807	PZ	C	6	.56173	-.14233	.42141	.00003	-.00005	.00005
S	H	7	.09567	-.00166	.40210	-.05149	.00000	-.00007	S	H	7	-.00001	-.00009	.00022	.06557	-.05383	-.04470
S	H	8	.22498	.00056	-.09039	.30011	.00005	.00004	S	H	8	.00003	-.00002	.00006	-.07980	-.45281	-.09628
S	H	9	.18396	.00075	-.20976	-.22534	-.00004	.00003	S	H	9	-.00002	-.00005	.00004	-.00748	-.16344	.54200
S	H	10	-.31107	.00077	-.13059	.28422	.00000	.00000	S	H	10	.00001	-.00003	-.00002	-.02255	.25430	.16668
S	H	11	-.08630	.00064	-.20103	-.26065	-.00002	.00007	S	H	11	-.00001	-.00005	.00006	-.15844	.10854	-.28870
S	O	12	.15127	.00014	-.01684	.06558	.00000	.00004	S	O	12	-.00002	.00004	.00002	-.22584	.03048	.05939
PX	O	12	-.21588	.00008	-.01148	-.09337	.00000	.00003	PX	O	12	-.00002	.00005	.00006	-.15188	.11690	.03357
PY	O	12	.30810	.00107	-.22821	.12597	-.00002	.00005	PY	O	12	.00003	.00000	.00001	.49152	.07077	-.11928
PZ	O	12	.00060	-.53632	-.00220	.00043	.01731	-.38420	PZ	O	12	.05644	-.17451	-.10065	-.00009	.00006	.00001
S	H	13	-.18202	-.00004	-.01344	-.11509	.00000	-.00008	S	H	13	.00005	-.00012	-.00010	.43343	-.18136	-.10001

NET ATOMIC CHARGES AND DIPOLE CONTRIBUTIONS

ATOM NO.	TYPE	CHARGE	ATOM ELECTRON DENSITY
1	C	-.1656	4.1656
2	C	-.0917	4.0917
3	C	-.2132	4.2132
4	C	.0778	3.9222
5	C	-.1566	4.1566
6	C	-.0970	4.0970
7	H	.1333	.8667
8	H	.1320	.8680
9	H	.1328	.8672
10	H	.1498	.8502
11	H	.1339	.8661
12	O	-.2528	6.2528
13	H	.2173	.7827

DIPOLE	X	Y	Z	TOTAL
POINT-CHG.	.115	-.731	.000	.740
HYBRID	.656	-.231	.000	.696
SUM	.771	-.963	.000	1.233

CARTESIAN COORDINATES

NO.	ATOM	X	Y	Z
1	C	.0000	.0000	.0000
2	C	1.3939	.0000	.0000
3	C	2.1002	1.2012	.0000
4	C	1.3882	2.4090	.0005
5	C	-.0166	2.4214	.0010
6	C	-.6991	1.2090	.0007
7	H	-.5500	-.9517	-.0007
8	H	1.9439	-.9529	-.0003
9	H	3.1986	1.2039	-.0003
10	H	-.5510	3.3812	.0015
11	H	-1.7995	1.2052	.0010
12	O	2.0111	3.6370	.0005
13	H	2.9672	3.4857	.0008

BOND ORDERS AND VALENCIES

		C 1	C 2	C 3	C 4	C 5	C 6
C	1	3.935587					
C	2	1.422314	3.935920				
C	3	.007413	1.415561	3.926596			
C	4	.105203	.005319	1.361968	3.920484		
C	5	.006690	.108180	.011031	1.349412	3.926955	
C	6	1.400852	.005623	.106937	.006684	1.435525	3.935780
H	7	.949504	.007222	.007797	.000076	.007665	.007165
H	8	.007193	.949067	.007322	.007820	.000020	.007767
H	9	.007594	.006104	.947311	.009439	.006522	.000078
H	10	.007709	.000071	.006617	.007637	.944950	.006874
H	11	.007208	.007662	.000025	.008135	.007127	.948595
O	12	.013892	.008781	.051433	1.056609	.038097	.008113
H	13	.000015	.000015	.003181	.002181	.011737	.001568

		H 7	H 8	H 9	H 10	H 11	O 12
H	7	.982223					
H	8	.000566	.982575				
H	9	.000724	.000662	.982352			
H	10	.000745	.000167	.000823	.977574		
H	11	.000553	.000879	.000165	.000590	.982071	
O	12	.000185	.001066	.001084	.001386	.000763	2.113218
H	13	.000022	.000046	.001846	.000005	.000369	.931808

		H 13
H	13	.952791

TOTAL CPU TIME: 25.00 SECONDS

== MOPAC DONE ==