Supporting Information

Diels-Alder reaction of acenes with singlet and triplet oxygen - theoretical study of two-state reactivity

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Computational details:

Density functional theory (DFT)[1] with B3LYP hybrid functional[2] and 6-31G* basis set have been used throughout the paper. The structures of all the critical points have been fully optimized using an analytical gradient procedure with the methods available in the Gaussian 03 package of programs.[3] In the cases where the direction of the negative eigenvector was not clear, IRC calculations were also performed. Spin-projected energies have been calculated with the approximate spin-correction procedure proposed by Yamaguchi et al.[4] To evaluate the effect of spin projection on the singlet energy, we have computed at the UB3LYP/6-31G* singlet (^1E(UB)), triplet (^3E(UB)), and singlet spin-corrected (^1E(SC)) energies.

$$\psi_{(UB)} = c_s\,{}^1\phi + c_T\,{}^3\phi$$

$$^1E_{(SC)} = {}^1E_{(UB)} + fsc[{}^1E_{(UB)} - {}^3E_{(UB)}]$$

$$f_{sc} = C_T^{\,2}/1 - C_s^{\,2} = {}^1\langle S^2\rangle/({}^3\langle S^2\rangle - {}^1\langle S^2\rangle)$$

It is assumed that singlet energy contamination arises only by the first higher multiplicity state.

The open-shell electronic structure of the O_2 molecule represents a particular challenge for *ab initio* calculations. Indeed even G3(MP2) theory is unable to reproduce $^3\Sigma_g$-$O_2 \rightarrow {}^1\Delta_g$-$O_2$ excitation energy.[5] However DFT after spin projection reproduce $^3\Sigma_g$-$O_2 \rightarrow {}^1\Delta_g$-$O_2$ excitation energy very nicely.

[1] (a) Parr, R. G.; Yang, W. *Density-functional theory of atoms and molecules*, Oxford University Press, New York, 1989. (b) Koch, W.; Holthausen, M. C. *A Chemist's guide to density functional theory*, Wiley-VCH, New York, 2000.

[2] (a) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785. (b) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.

[3] Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Jr., Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, 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.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; 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, A. 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.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

[4] Yamaguchi, K.; Jensen, F.; Dorigo, A.; Houk, K. N.; *Chem. Phys. Lett*. **1988**, *149*, 537; Yamanaka, S.; Kawakami, T.; Nagao, H.; Yamaguchi, K. *Chem. Phys. Lett*. **1994**, *231*, 25; Goldstein, E.; Beno, B.; Houk, K. N. *J. Am. Chem. Soc.* **1996**, *118*, 6036.

[5] S-H. Chien, M.-F. Cheng, K.-C. Lau and W.-K. Li, *J. Phys. Chem. A*, 2005, **109**, 7509.

Table S1:

	PG	B3LYP/6-31G(d)	ZPE	$E_{corrected}$	[a]CASSCF
$^1O_2$		-150.3033948	2.36		-149.6099858
$^3O_2$		-150.3200421	2.37		
1		-232.2486606	63.23		-230.7429973
1+$^1O_2$ (T_1)		-382.5012145	65.32	-382.504222	
1+$^1O_2$ (M_1)		-382.5014657	65.84	-382.5028516	-380.3209835
1+$^1O_2$ (T)		-382.4932402	66.46		-380.3041488
1+$^1O_2$ (P)		-382.5191687	67.93		
1+$^1O_2$ (T_{RO})		-382.4768656	65.02	-382.4661699	
1+$^1O_2$ (P_2)		-382.5019431	65.09	-382.5019849	
1+$^1O_2$ (T_E)		-382.4607604	59.82	-382.4447965	
Benzoquinone		-381.4516871	53.57		
2		-385.8927291	92.76		
2+$^1O_2$ (T_1)		-536.1565478	95.06	-536.1604076	
2+$^1O_2$ (M_1)		-536.1583375	95.77	-536.1586988	
2+$^1O_2$ (T)		-536.1477804	96.05		
2+$^1O_2$ (P)		-536.184637	97.92		
2+$^1O_2$ (T_{RO})		-536.1432136	95.21	-536.1330544	
2+$^1O_2$ (P_2)		-536.1616558	94.86	-536.1617572	
2+$^1O_2$ (T_E)		-536.1265587	89.84	-536.1093438	
Naphthoquinone					
3		-539.5305235	122.08		-536.0369129
3+$^1O_2$ (T_1)		-689.8090488	124.60	-689.8141892	
3+$^1O_2$ (M_1)		-689.8131902	125.53	-689.8138105	-685.6505846
3+$^1O_2$ (T_R)		-689.8086438	125.16	-689.8090241	
3+$^1O_2$ (M_2)		-689.810809	125.44	-689.8114898	
3+$^1O_2$ (T_2)		-689.8003893	125.63	-689.7824535	-685.6390144
3+$^1O_2$ (T_U)		-689.7970104	125.17	-689.7792987	-685.6267082
3+$^1O_2$ (P)		-689.8494462	127.81		
3+$^1O_2$ (T_{RO})		-689.8080172	124.65		
3+$^1O_2$ (P_2)		-689.8220437	124.71	-689.8221874	
3+$^1O_2$ (T_E)		-689.7925828	119.89	-689.7745591	
Anthraquinone		-688.7791278	113.46		
3+$^3O_2$ (T_1)		-689.8128047	124.67		
3+$^3O_2$ (M_1)		-689.8139199	125.43		
3+$^3O_2$ (T_R)		-689.8093465	124.81		
3+$^3O_2$ (T_s)		-689.8107699	124.61		
3+$^3O_2$ (M_2)		-689.8116827	125.36		
3+$^3O_2$ (T_2)		-689.7403966	124.79		
3+$^3O_2$ (P)		-689.8221834	124.69		
3+$^3O_2$ (T_E)		-689.7907595	119.95		
^{3}Anthraquinone		-688.6860769	111.02		
5		-846.7999431	180.47		
5+$^1O_2$ (T_1)		-997.094951	182.99	-997.1024181	
5+$^1O_2$ (M_1)		-997.1025755	184.26	-997.1029228	
5+$^1O_2$ (T_R)		-997.0979926	183.92	-997.0981332	
5+$^1O_2$ (M_2)		-997.099795	184.16	-997.1002503	
5+$^1O_2$ (T_2)		-997.088065	184.41	-997.0703305	
5+$^1O_2$ (P)		-997.1393842	186.59		
5+$^1O_2$ (T_{RO})		-997.0979446	183.57		
5+$^1O_2$ (P_2)		-997.1096491	183.40	-997.109748	

5+$^1O_2$ (T_E)		-997.0853841	178.83	-997.0661122	
Pentacenequinone		-996.0682771	172.25		
5+$^3O_2$ (T_1)		-997.0993111	183.21		
5+$^3O_2$ (M_1)		-997.1029352	184.23		
5+$^3O_2$ (T_R)		-997.0981427	183.86		
5+$^3O_2$ (T_s)		try			
5+$^3O_2$ (M_2)		-997.1002649	184.16		
5+$^3O_2$ (T_2)		-997.0298478	183.56		
5+$^3O_2$ (P)		-997.1097492	183.39		
5+$^3O_2$ (T_E)		-997.0785652	178.65		
^{3}Pentacenequinone		-995.9624885	171.26		

[a]Oxygen(8,6) Benzene(4,4) Anthracene(6,6)Benzene+$^1O_2$ (12,10) Anthracene+$^1O_2$ (14, 12).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	0.000000	0.000000	0.607609
2	8	0.000000	0.000000	-0.607609

$^3O_2$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	0.000000	0.000000	0.607296
2	8	0.000000	0.000000	-0.607296

H_2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	1	0.000000	0.000000	0.371394
2	1	0.000000	0.000000	-0.371394

1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.396490	0.000000
2	6	1.209396	0.698245	0.000000
3	6	1.209396	-0.698245	0.000000
4	6	0.000000	-1.396490	0.000000
5	6	-1.209396	-0.698245	0.000000
6	6	-1.209396	0.698245	0.000000
7	1	0.000000	2.483191	0.000000
8	1	2.150506	1.241595	0.000000
9	1	2.150506	-1.241595	0.000000
10	1	0.000000	-2.483191	0.000000
11	1	-2.150506	-1.241595	0.000000
12	1	-2.150506	1.241595	0.000000

T_1 ($1+^1O_2$)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.069360	1.169225	0.410940
2	6	-1.349357	1.322726	-0.060751
3	6	-2.156905	0.197285	-0.340597
4	6	-1.654707	-1.106875	-0.113499
5	1	-3.166907	0.332041	-0.715210
6	6	-0.380606	-1.300121	0.354775
7	6	0.530619	-0.164848	0.569111
8	1	1.196129	-0.265365	1.428911
9	8	2.819775	0.168353	-0.185242
10	8	1.673436	-0.275484	-0.601445
11	1	0.558276	2.028948	0.625881
12	1	-1.753726	2.320423	-0.210467
13	1	-2.298378	-1.963567	-0.295967
14	1	0.000817	-2.299790	0.540473

M_1 ($1+^1O_2$)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.038043	1.169418	0.330975
2	6	-1.341710	1.333364	-0.053610
3	6	-2.183840	0.216342	-0.272190
4	6	-1.678400	-1.095943	-0.089925
5	1	-3.214336	0.363342	-0.579780
6	6	-0.381240	-1.309265	0.288154
7	6	0.561045	-0.179853	0.500093
8	1	1.139506	-0.272255	1.426830
9	8	2.805510	0.203883	-0.135592
10	8	1.682595	-0.327758	-0.557951
11	1	0.618246	2.020011	0.489246
12	1	-1.740419	2.335247	-0.191161
13	1	-2.339276	-1.944899	-0.245650
14	1	0.004566	-2.314823	0.427877

T ($1+^1O_2$)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.342892	0.425393	-0.656287
2	6	0.370873	1.375447	-0.691155
3	6	-0.934648	0.925975	-0.310307
4	6	-1.343018	-0.425329	-0.656105
5	6	-0.371005	-1.375374	-0.691217
6	6	0.934571	-0.925934	-0.310516
7	1	2.398353	0.663872	-0.738470
8	1	0.590284	2.434147	-0.781430

9	1	-1.714299	1.662605	-0.140961
10	1	-2.398492	-0.663803	-0.738129
11	1	-0.590430	-2.434063	-0.781581
12	1	1.714258	-1.662585	-0.141427
13	8	-0.575880	0.320040	1.451053
14	8	0.576172	-0.320196	1.450887

P_1 ($1+^1O_2$)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.252271	-0.667251	-0.698890
2	6	1.252325	0.667025	-0.699057
3	6	-0.000072	1.228810	-0.056886
4	6	-1.252271	0.667251	-0.698890
5	6	-1.252325	-0.667025	-0.699057
6	6	0.000072	-1.228810	-0.056886
7	1	2.075585	-1.303018	-1.008118
8	1	2.075151	1.303169	-1.008617
9	1	0.000498	2.312743	0.067150
10	1	-2.075585	1.303018	-1.008118
11	1	-2.075151	-1.303169	-1.008617
12	1	-0.000498	-2.312743	0.067150
13	8	0.000072	0.732490	1.334823
14	8	-0.000072	-0.732490	1.334823

T_{RO} ($1+^1O_2$)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.716105	1.233657	-0.653331
2	6	0.614150	1.283092	-0.663531
3	6	1.310348	0.057272	-0.080438
4	6	0.716306	-1.233017	-0.654150
5	1	2.402991	0.086189	-0.213875
6	6	-0.613946	-1.282376	-0.664749
7	6	-1.310253	-0.057038	-0.080744
8	1	-2.402874	-0.085974	-0.214401
9	8	1.111384	0.018949	1.314295
10	8	-1.111842	-0.020396	1.314139
11	1	-1.187358	-2.150223	-0.977690
12	1	1.367341	-2.055720	-0.932695
13	1	1.187622	2.151226	-0.975568
14	1	-1.367052	2.056537	-0.931582

P_2 ($1+^1O_2$)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.666479	1.266224	0.124896
2	6	-0.666479	1.266224	0.124896
3	6	-1.487233	0.000000	0.249764

4	6	-0.666479	-1.266224	0.124897
5	1	-1.955679	0.000000	1.268958
6	6	0.666479	-1.266224	0.124897
7	6	1.487233	0.000000	0.249764
8	1	1.955679	0.000000	1.268958
9	8	-2.617384	0.000000	-0.537180
10	8	2.617384	0.000000	-0.537180
11	1	1.236922	2.185346	0.015567
12	1	-1.236922	2.185346	0.015567
13	1	-1.236922	-2.185346	0.015567
14	1	1.236922	-2.185346	0.015567

T_E ($1+{}^1O_2$)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.268584	0.666456	-0.405576
2	6	-1.268584	-0.666456	-0.405576
3	6	0.000000	-1.291970	0.160783
4	6	1.268584	-0.666456	-0.405576
5	1	0.000000	-0.617557	1.278103
6	6	1.268584	0.666456	-0.405576
7	6	0.000000	1.291970	0.160783
8	1	0.000000	0.617557	1.278103
9	8	0.000000	-2.544102	0.507347
10	8	0.000000	2.544102	0.507347
11	1	-2.079898	1.315628	-0.717335
12	1	-2.079898	-1.315628	-0.717335
13	1	2.079898	-1.315628	-0.717335
14	1	2.079898	1.315628	-0.717335

BENZOQUINONE

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.268942	0.671502
2	6	0.000000	1.268942	-0.671502
3	6	0.000000	0.000000	-1.445451
4	6	0.000000	-1.268942	-0.671502
5	6	0.000000	-1.268942	0.671502
6	6	0.000000	0.000000	1.445451
7	1	0.000000	2.182959	1.259075
8	1	0.000000	2.182959	-1.259075
9	1	0.000000	-2.182959	-1.259075
10	1	0.000000	-2.182959	1.259075
11	8	0.000000	0.000000	-2.670391
12	8	0.000000	0.000000	2.670391

NAPHTHALENE.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.433783	-0.708367	0.000000

2	6	1.244882	-1.402418	0.000000
3	6	0.000000	-0.717154	0.000000
4	6	0.000000	0.717154	0.000000
5	6	1.244882	1.402418	0.000000
6	6	2.433783	0.708367	0.000000
7	1	-1.242503	-2.490179	0.000000
8	1	3.378204	-1.246174	0.000000
9	1	1.242503	-2.490179	0.000000
10	6	-1.244882	-1.402418	0.000000
11	6	-1.244882	1.402418	0.000000
12	1	1.242503	2.490179	0.000000
13	1	3.378204	1.246174	0.000000
14	6	-2.433783	0.708367	0.000000
15	6	-2.433783	-0.708367	0.000000
16	1	-1.242503	2.490179	0.000000
17	1	-3.378204	1.246174	0.000000
18	1	-3.378204	-1.246174	0.000000

NAPHOXYANTITS_2.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.822333	1.101293	0.571647
2	6	1.117896	2.210664	0.131402
3	6	-0.229748	2.115218	-0.222625
4	6	-0.933114	0.874120	-0.106860
5	1	-0.770324	2.993376	-0.564941
6	6	-0.236303	-0.285367	0.337928
7	6	1.215622	-0.216784	0.575821
8	1	1.607292	-0.923542	1.305669
9	6	-0.932323	-1.490870	0.494984
10	6	-2.293751	-1.569386	0.217999
11	1	-0.392941	-2.373662	0.829426
12	1	-2.820452	-2.510834	0.344813
13	6	-2.984637	-0.431535	-0.228503
14	6	-2.315005	0.771579	-0.387263
15	1	-4.047003	-0.493852	-0.447705
16	1	-2.849494	1.655256	-0.727519
17	8	2.995978	-1.641451	-0.457112
18	8	1.929139	-1.005500	-0.789148
19	1	2.868913	1.181008	0.848548
20	1	1.617254	3.174261	0.074607

NAPHOXYANTIMINIMA_1.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.852160	1.123676	0.405259
2	6	1.101103	2.231384	0.085578
3	6	-0.277573	2.137419	-0.156888
4	6	-0.957214	0.877471	-0.066713
5	1	-0.850774	3.024525	-0.410295
6	6	-0.226916	-0.297071	0.257626

7	6	1.260351	-0.237036	0.458143
8	1	1.587117	-0.803911	1.336115
9	6	-0.894106	-1.518097	0.366551
10	6	-2.270763	-1.603089	0.155447
11	1	-0.326832	-2.413311	0.608955
12	1	-2.774941	-2.561314	0.241214
13	6	-2.998126	-0.450197	-0.166643
14	6	-2.350576	0.772883	-0.273750
15	1	-4.070408	-0.511889	-0.330893
16	1	-2.913649	1.670171	-0.518868
17	8	3.032276	-1.584647	-0.306533
18	8	1.894405	-1.043863	-0.682568
19	1	2.921747	1.196546	0.575870
20	1	1.584252	3.203196	0.023060

NAPHTHOXYGENPARATS_1.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.025504	-0.564291	-1.000434
2	6	1.979947	0.810229	-0.983135
3	6	0.903439	1.405824	-0.299793
4	6	-0.376325	0.722973	-0.210178
5	6	-0.354448	-0.689949	-0.287547
6	6	0.959421	-1.283331	-0.351336
7	1	2.901041	-1.102746	-1.347814
8	1	2.832718	1.406429	-1.291990
9	1	0.920379	2.473213	-0.097193
10	1	1.036700	-2.364522	-0.279825
11	8	1.302914	0.478300	1.560183
12	8	1.715763	-0.721575	1.275131
13	6	-1.549850	-1.416989	-0.166729
14	6	-2.755643	-0.746272	-0.017665
15	1	-1.523227	-2.503346	-0.201405
16	1	-3.683762	-1.306400	0.052806
17	6	-2.778983	0.657540	0.053628
18	6	-1.600956	1.387146	-0.026228
19	1	-3.726764	1.174375	0.177254
20	1	-1.619138	2.471914	0.042153

NAPHOXYPROD.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.162775	-1.843358	0.667946
2	6	-1.162775	-1.843358	-0.667946
3	6	-0.021202	-1.027876	-1.239146
4	6	-0.060523	0.384799	-0.701233
5	6	-0.060523	0.384799	0.701233
6	6	-0.021202	-1.027876	1.239146
7	1	-1.830262	-2.421446	1.298934
8	1	-1.830262	-2.421446	-1.298934
9	1	0.087876	-1.092154	-2.323850
10	1	0.087876	-1.092154	2.323850

11	8	1.219049	-1.633920	-0.736609
12	8	1.219049	-1.633920	0.736609
13	6	-0.037732	1.578716	1.408713
14	6	-0.042165	2.786978	0.697526
15	1	-0.021878	1.579755	2.496068
16	1	-0.041746	3.729654	1.238003
17	6	-0.042165	2.786978	-0.697526
18	6	-0.037732	1.578716	-1.408713
19	1	-0.041746	3.729654	-1.238003
20	1	-0.021878	1.579755	-2.496068

NAPHTHALENERINGOPENENI

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.905893	-0.687598	-1.078295
2	6	-1.892855	0.645118	-1.107262
3	6	-1.012644	1.316091	-0.055983
4	6	0.380839	0.695524	-0.067378
5	1	-0.960625	2.408830	-0.191673
6	6	0.382833	-0.707214	-0.054836
7	6	-1.002108	-1.329961	-0.019210
8	1	-0.977705	-2.424866	-0.136438
9	8	-1.597493	1.141447	1.210517
10	8	-1.628621	-1.072737	1.212638
11	1	-2.514869	1.238051	-1.771486
12	1	-2.556181	-1.310248	-1.684113
13	6	1.578667	1.398769	-0.060257
14	6	1.584145	-1.404824	-0.038281
15	6	2.794101	-0.697877	-0.039469
16	6	2.790984	0.695752	-0.050057
17	1	1.577135	2.486411	-0.067200
18	1	1.585898	-2.492653	-0.025540
19	1	3.736176	-1.239277	-0.031258
20	1	3.730673	1.241384	-0.051366

SBNAPHOXYPROD.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.251104	-0.666178	-0.067513
2	6	2.251104	0.666178	-0.067513
3	6	1.021992	1.483342	0.266029
4	6	-0.285804	0.700696	0.145476
5	1	1.125323	1.790725	1.341142
6	6	-0.285804	-0.700696	0.145476
7	6	1.021992	-1.483342	0.266029
8	1	1.125323	-1.790725	1.341142
9	6	-1.495609	-1.392968	0.029595
10	6	-2.697763	-0.698987	-0.079901
11	1	-1.476389	-2.478197	0.008732
12	1	-3.632348	-1.245825	-0.171162
13	6	-2.697763	0.698987	-0.079901
14	6	-1.495609	1.392968	0.029595

15	1	-3.632348	1.245825	-0.171162
16	1	-1.476389	2.478197	0.008732
17	8	1.009540	2.717509	-0.329716
18	8	1.009540	-2.717509	-0.329716
19	1	3.143574	1.240400	-0.303103
20	1	3.143574	-1.240400	-0.303103

H2ELIMINATIONS.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.049464	1.514864	1.410518
2	6	-0.055689	0.326322	0.699471
3	6	-0.055689	0.326322	-0.699471
4	6	0.049464	1.514864	-1.410518
5	6	0.175542	2.715337	-0.697880
6	6	0.175542	2.715337	0.697880
7	1	0.030677	1.501545	2.496153
8	1	0.030677	1.501545	-2.496153
9	1	0.263826	3.653729	-1.238338
10	1	0.263826	3.653729	1.238338
11	6	-0.214737	-1.060280	-1.310359
12	6	0.723352	-2.077687	-0.666552
13	1	-1.268452	-1.377297	-0.629687
14	6	0.723352	-2.077687	0.666552
15	6	-0.214737	-1.060280	1.310359
16	1	-1.268452	-1.377297	0.629687
17	8	-0.547487	-1.192981	-2.555358
18	8	-0.547487	-1.192981	2.555358
19	1	1.286250	-2.745470	-1.310326
20	1	1.286250	-2.745470	1.310326

NAPHTHAQUINONE
(anthra)SBMINIMA143.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.476594	0.790400	-0.588355
2	6	1.235428	0.230752	-0.284780
3	6	1.154774	-1.129516	0.130308
4	6	2.355785	-1.872619	0.246259
5	6	3.581591	-1.296679	-0.049136
6	6	3.647569	0.037971	-0.473766
7	1	2.526066	1.830209	-0.897123
8	1	2.300076	-2.910935	0.564136
9	1	4.491697	-1.883231	0.042877
10	1	4.606557	0.488656	-0.712181
11	6	-0.113112	-1.725905	0.374449
12	6	-1.331980	-1.030037	0.139840
13	1	-0.153340	-2.763967	0.694483
14	6	-1.303954	0.332884	-0.268696
15	6	-0.003112	1.075240	-0.326703
16	1	0.023973	1.799984	-1.143609
17	6	-2.498031	0.997481	-0.546210

18	6	-3.727122	0.346774	-0.424038
19	1	-2.466419	2.040836	-0.851083
20	1	-4.648051	0.878478	-0.644537
21	6	-3.766225	-0.992816	-0.011440
22	6	-2.589201	-1.671216	0.265025
23	1	-4.720783	-1.502311	0.088477
24	1	-2.616934	-2.712466	0.576676
25	8	0.752187	3.039324	0.737427
26	8	-0.009297	1.982983	0.910740

ANTHRACENE.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.660679	-0.713146	0.000016
2	6	2.479530	-1.407037	-0.000045
3	6	1.223922	-0.722624	-0.000027
4	6	1.223924	0.722625	-0.000020
5	6	2.479532	1.407036	0.000024
6	6	3.660681	0.713142	0.000058
7	6	0.000000	-1.403377	-0.000022
8	6	0.000001	1.403379	-0.000026
9	6	-1.223922	0.722626	-0.000023
10	6	-1.223923	-0.722623	-0.000006
11	6	-2.479531	-1.407037	0.000025
12	1	-2.476863	-2.494580	0.000063
13	6	-3.660680	-0.713145	0.000052
14	6	-3.660679	0.713143	0.000006
15	6	-2.479531	1.407037	-0.000028
16	1	-0.000006	-2.491747	-0.000044
17	1	4.607361	-1.246655	0.000042
18	1	2.476860	-2.494580	-0.000093
19	1	2.476864	2.494579	0.000026
20	1	4.607357	1.246660	0.000113
21	1	-0.000004	2.491749	-0.000045
22	1	-4.607358	-1.246660	0.000086
23	1	-4.607358	1.246658	0.000021
24	1	-2.476867	2.494580	-0.000070

TEMP12REOPTFREQ_1.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.436997	0.742827	-0.748435
2	6	1.184358	0.202177	-0.421858
3	6	1.104393	-1.125211	0.110052
4	6	2.307140	-1.854196	0.295878
5	6	3.531737	-1.296997	-0.029057
6	6	3.601897	0.004725	-0.556360
7	1	2.489570	1.748387	-1.153192
8	1	2.251713	-2.863658	0.696022
9	1	4.443214	-1.869742	0.119037
10	1	4.565352	0.435055	-0.813557

11	6	-0.162416	-1.683658	0.403895
12	6	-1.367640	-0.983562	0.148551
13	1	-0.214192	-2.694140	0.802321
14	6	-1.312519	0.347519	-0.371983
15	6	-0.021150	0.999672	-0.521991
16	1	0.015987	1.843274	-1.206913
17	6	-2.506811	1.026200	-0.658440
18	6	-3.740041	0.422346	-0.443937
19	1	-2.457188	2.040809	-1.046027
20	1	-4.655768	0.960045	-0.672043
21	6	-3.801910	-0.885546	0.073253
22	6	-2.639355	-1.575657	0.363605
23	1	-4.767404	-1.354326	0.242610
24	1	-2.685337	-2.587639	0.758450
25	8	1.139095	2.695327	1.086918
26	8	0.026651	2.091934	0.964863

ANTHOXYSINGBIRADANTITSCALCALL.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.440030	0.854504	-0.780226
2	6	1.215664	0.310474	-0.396090
3	6	1.163134	-1.014756	0.121743
4	6	2.373811	-1.738513	0.250285
5	6	3.582755	-1.177479	-0.131868
6	6	3.621884	0.121920	-0.657028
7	1	2.471681	1.869632	-1.168665
8	1	2.340034	-2.750981	0.645113
9	1	4.501124	-1.749163	-0.029136
10	1	4.567772	0.561010	-0.960207
11	6	-0.092636	-1.600896	0.444493
12	6	-1.323027	-0.945553	0.165098
13	1	-0.113566	-2.609352	0.849924
14	6	-1.314588	0.377658	-0.363444
15	6	-0.025952	1.127826	-0.452056
16	1	-0.019245	1.838691	-1.282410
17	6	-2.518048	0.993535	-0.706219
18	6	-3.736858	0.336291	-0.526309
19	1	-2.502717	2.003628	-1.108696
20	1	-4.665268	0.829784	-0.798502
21	6	-3.757186	-0.959280	0.010128
22	6	-2.570557	-1.591556	0.348249
23	1	-4.704239	-1.471874	0.155038
24	1	-2.583070	-2.601241	0.751425
25	8	0.888518	2.051466	1.613494
26	8	-0.093900	2.137885	0.759703

SBSYMMETRICMINIMA_1.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.486078	-0.972334	-0.715540
2	6	-1.269886	-0.379671	-0.378312

3	6	-1.244363	0.960276	0.099133
4	6	-2.474281	1.649169	0.240674
5	6	-3.674899	1.040704	-0.090912
6	6	-3.687047	-0.274041	-0.578458
7	1	-2.495519	-1.998065	-1.077048
8	1	-2.461748	2.672523	0.607751
9	1	-4.607769	1.586408	0.021875
10	1	-4.626134	-0.750147	-0.844922
11	6	0.000062	1.592845	0.374635
12	6	1.244475	0.960234	0.099176
13	1	0.000073	2.614941	0.744630
14	6	1.269967	-0.379705	-0.378301
15	6	0.000027	-1.172995	-0.443591
16	1	0.000024	-1.867723	-1.289350
17	6	2.486153	-0.972407	-0.715490
18	6	3.687141	-0.274160	-0.578346
19	1	2.495570	-1.998130	-1.077022
20	1	4.626221	-0.750293	-0.844788
21	6	3.675023	1.040574	-0.090766
22	6	2.474416	1.649076	0.240787
23	1	4.607909	1.586243	0.022066
24	1	2.461906	2.672422	0.607889
25	8	-0.000686	-1.624741	1.880382
26	8	0.000088	-2.196955	0.697217

TSSYMMETRICBIRAD_5.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.408680	-1.225343	-0.703570
2	6	-1.249669	-0.611866	-0.237829
3	6	-1.241475	0.774105	0.050016
4	6	-2.422705	1.515259	-0.111944
5	6	-3.574127	0.895544	-0.591562
6	6	-3.568635	-0.470085	-0.896334
7	1	-2.411384	-2.293476	-0.907495
8	1	-2.428059	2.576347	0.124433
9	1	-4.481742	1.476830	-0.729257
10	1	-4.470476	-0.947509	-1.268854
11	6	0.009693	1.353926	0.482731
12	6	1.247062	0.785352	0.056073
13	1	0.004989	2.365659	0.881176
14	6	1.246793	-0.594407	-0.283202
15	6	0.005173	-1.331495	0.101128
16	1	0.011669	-2.387579	-0.173225
17	6	2.413425	-1.203662	-0.745932
18	6	3.579876	-0.454333	-0.887409
19	1	2.409258	-2.263087	-0.990778
20	1	4.481249	-0.923645	-1.271506
21	6	3.600557	0.901797	-0.518644
22	6	2.454058	1.514249	-0.036918
23	1	4.520410	1.472173	-0.612887
24	1	2.466904	2.562791	0.249990
25	8	-0.290250	-0.244567	2.202885
26	8	0.208886	-1.347026	1.626963

ANTHRAOXYPRODSINGLET.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.408130	2.309400	-0.489355
2	6	-0.701834	1.237336	0.040995
3	6	0.702145	1.237222	0.040707
4	6	1.408278	2.309164	-0.490020
5	6	0.697887	3.381224	-1.045311
6	6	-0.697887	3.381385	-1.044954
7	1	-2.495469	2.316274	-0.477538
8	1	2.495627	2.315990	-0.478868
9	1	1.238259	4.219978	-1.475592
10	1	-1.238267	4.220268	-1.474963
11	6	1.248896	-0.000197	0.715337
12	6	0.701834	-1.237336	0.040995
13	1	2.334394	-0.000227	0.844173
14	6	-0.702145	-1.237222	0.040707
15	6	-1.248896	0.000197	0.715337
16	1	-2.334394	0.000227	0.844173
17	6	-1.408278	-2.309164	-0.490020
18	6	-0.697887	-3.381224	-1.045311
19	1	-2.495627	-2.315990	-0.478868
20	1	-1.238259	-4.219978	-1.475592
21	6	0.697887	-3.381385	-1.044954
22	6	1.408130	-2.309400	-0.489355
23	1	1.238267	-4.220268	-1.474963
24	1	2.495469	-2.316274	-0.477538
25	8	0.740167	0.000546	2.087299
26	8	-0.740167	-0.000546	2.087299

SBANTHRAOXYPROD.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.441856	-1.395364	-0.140098
2	6	1.274695	-0.700727	0.188238
3	6	1.274693	0.700735	0.188236
4	6	2.441851	1.395374	-0.140104
5	6	3.602847	0.698678	-0.470149
6	6	3.602850	-0.698666	-0.470145
7	1	2.422321	-2.480188	-0.142598
8	1	2.422312	2.480198	-0.142607
9	1	4.505409	1.245037	-0.730347
10	1	4.505413	-1.245024	-0.730340
11	6	-0.000003	1.458308	0.559947
12	6	-1.274696	0.700727	0.188234
13	1	-0.000011	1.547288	1.680274
14	6	-1.274694	-0.700732	0.188233
15	6	0.000005	-1.458307	0.559945
16	1	0.000009	-1.547307	1.680272
17	6	-2.441850	-1.395374	-0.140097
18	6	-3.602856	-0.698680	-0.470143

19	1	-2.422300	-2.480199	-0.142590
20	1	-4.505418	-1.245034	-0.730334
21	6	-3.602841	0.698660	-0.470148
22	6	-2.441858	1.395374	-0.140107
23	1	-4.505410	1.245018	-0.730347
24	1	-2.422324	2.480194	-0.142611
25	8	-0.000018	2.779122	0.221267
26	8	0.000021	-2.779123	0.221255

ANTHRACENE910OXYGENTS_2.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.467460	-1.416165	-0.401164
2	6	-1.241086	-0.723403	-0.253034
3	6	-1.244709	0.702995	-0.222156
4	6	-2.470910	1.394509	-0.359374
5	6	-3.647160	0.695578	-0.539228
6	6	-3.646785	-0.718919	-0.558776
7	1	-2.463126	-2.503268	-0.400841
8	1	-2.472853	2.481140	-0.330959
9	1	-4.583544	1.232933	-0.661601
10	1	-4.582256	-1.254562	-0.693412
11	6	0.005280	1.371171	-0.007193
12	6	1.241075	0.723448	-0.252993
13	1	-0.004732	2.452019	0.108881
14	6	1.244706	-0.702959	-0.222216
15	6	-0.005288	-1.371162	-0.007313
16	1	0.004715	-2.452023	0.108641
17	6	2.470911	-1.394457	-0.359478
18	6	3.647156	-0.695506	-0.539275
19	1	2.472864	-2.481090	-0.331138
20	1	4.583544	-1.232849	-0.661679
21	6	3.646776	0.718994	-0.558734
22	6	2.467451	1.416225	-0.401069
23	1	4.582245	1.254648	-0.693335
24	1	2.463111	2.503328	-0.400670
25	8	-0.231169	0.594892	2.003077
26	8	0.231204	-0.595189	2.002938

ANTHRACENEOXYSBRINGOPENING_1.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.254868	-0.695041	0.042637
2	6	-1.238110	0.707264	0.018295
3	6	0.003003	1.342228	0.626555
4	6	1.256993	0.694359	0.040026
5	1	0.026438	2.434277	0.469432
6	6	1.242530	-0.708662	0.027420
7	6	0.000362	-1.341388	0.633711
8	1	-0.029962	-2.433449	0.481596
9	8	0.015293	1.163869	2.016076
10	8	-0.036863	-1.135470	2.018551

11	6	2.360301	1.390320	-0.441868
12	6	2.330774	-1.410975	-0.479487
13	6	3.438811	-0.712526	-0.973405
14	6	3.453710	0.681915	-0.953634
15	1	2.370643	2.477614	-0.427985
16	1	2.320997	-2.498714	-0.489562
17	1	4.289197	-1.259497	-1.371278
18	1	4.314218	1.222208	-1.338590
19	6	-2.324906	1.405327	-0.498140
20	6	-2.359291	-1.396038	-0.430205
21	6	-3.432655	0.702899	-0.986253
22	6	-3.450238	-0.691620	-0.951365
23	1	-2.314343	2.492821	-0.518872
24	1	-4.281680	1.246690	-1.391325
25	1	-4.310820	-1.234554	-1.332311
26	1	-2.370617	-2.482956	-0.403848

H2ELIMINATIONSBTS_1.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.355053	1.409384	-0.326737
2	6	-1.260710	0.699618	0.152030
3	6	-1.260710	-0.699618	0.152030
4	6	-2.355053	-1.409384	-0.326737
5	6	-3.453409	-0.697905	-0.827415
6	6	-3.453409	0.697905	-0.827415
7	1	-2.347683	2.494940	-0.303788
8	1	-2.347683	-2.494940	-0.303788
9	1	-4.315493	-1.238829	-1.207829
10	1	-4.315493	1.238829	-1.207829
11	6	0.000000	-1.327844	0.737058
12	6	1.260710	-0.699618	0.152030
13	1	0.000000	-0.643647	1.826234
14	6	1.260710	0.699618	0.152030
15	6	0.000000	1.327844	0.737058
16	1	0.000000	0.643647	1.826234
17	6	2.355053	1.409384	-0.326737
18	6	3.453409	0.697905	-0.827415
19	1	2.347683	2.494940	-0.303788
20	1	4.315493	1.238829	-1.207829
21	6	3.453409	-0.697905	-0.827415
22	6	2.355053	-1.409384	-0.326737
23	1	4.315493	-1.238829	-1.207829
24	1	2.347683	-2.494940	-0.303788
25	8	0.000000	-2.568672	1.100014
26	8	0.000000	2.568672	1.100014

SBANTHRAQUINONE.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.490748	-1.398600	0.000322
2	6	1.275414	-0.704361	-0.000275

3	6	1.275539	0.704510	-0.000440
4	6	2.491025	1.398512	0.000150
5	6	3.695383	0.699765	0.000475
6	6	3.695228	-0.700119	0.000527
7	1	2.464168	-2.483325	0.000445
8	1	2.464676	2.483228	0.000191
9	1	4.636438	1.242863	0.000775
10	1	4.636153	-1.243435	0.000929
11	6	0.000110	1.478552	-0.000656
12	6	-1.275396	0.704511	-0.000575
13	6	-1.275398	-0.704319	-0.000210
14	6	-0.000021	-1.478311	-0.000579
15	6	-2.490853	-1.398528	0.000437
16	6	-3.695377	-0.700152	0.000614
17	1	-2.464063	-2.483278	0.000886
18	1	-4.636446	-1.243210	0.001010
19	6	-3.695517	0.699813	0.000239
20	6	-2.490993	1.398540	0.000196
21	1	-4.636449	1.243185	0.000501
22	1	-2.464698	2.483258	0.000698
23	8	0.000098	2.704919	-0.000191
24	8	0.000008	-2.704689	-0.000658

Triplet Path:
ANTHOXYTBANTI_3.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.449426	0.754711	-0.712123
2	6	1.202295	0.215549	-0.371947
3	6	1.122607	-1.120451	0.130573
4	6	2.324440	-1.857203	0.288357
5	6	3.547304	-1.300613	-0.044632
6	6	3.614818	0.008485	-0.551816
7	1	2.500450	1.769585	-1.093302
8	1	2.269310	-2.873863	0.669926
9	1	4.457964	-1.880182	0.080175
10	1	4.575531	0.439366	-0.818305
11	6	-0.144333	-1.688820	0.415439
12	6	-1.353490	-0.994036	0.155593
13	1	-0.192514	-2.706566	0.795028
14	6	-1.305945	0.344886	-0.338779
15	6	-0.012594	1.030566	-0.440123
16	1	0.022224	1.846750	-1.159850
17	6	-2.499398	1.013489	-0.639608
18	6	-3.731259	0.391133	-0.463313
19	1	-2.454516	2.035619	-1.007789
20	1	-4.648038	0.921595	-0.703593
21	6	-3.787124	-0.924305	0.031587
22	6	-2.621485	-1.604767	0.335379
23	1	-4.749638	-1.408332	0.172928
24	1	-2.662794	-2.623888	0.711915
25	8	1.004523	2.829457	0.979131
26	8	0.001783	2.029065	0.969037

ANTHRACENE910OXYGENTRIPLETBIRADANTIMIN.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.470067	0.781962	-0.625599
2	6	1.229620	0.232093	-0.299506
3	6	1.148473	-1.121310	0.139107
4	6	2.348195	-1.866140	0.258305
5	6	3.572766	-1.299144	-0.057800
6	6	3.639077	0.027502	-0.507762
7	1	2.520418	1.815378	-0.954251
8	1	2.292138	-2.898744	0.594213
9	1	4.481991	-1.886682	0.036665
10	1	4.597490	0.470213	-0.762857
11	6	-0.119801	-1.709688	0.398474
12	6	-1.336712	-1.016787	0.150781
13	1	-0.161595	-2.742254	0.735812
14	6	-1.304619	0.339281	-0.281895
15	6	-0.004829	1.075282	-0.336298
16	1	0.024303	1.816242	-1.137785
17	6	-2.497183	1.000901	-0.576577
18	6	-3.726850	0.353838	-0.449043
19	1	-2.462579	2.038698	-0.899554
20	1	-4.646220	0.882116	-0.683860
21	6	-3.769913	-0.978545	-0.011553
22	6	-2.596006	-1.653613	0.282874
23	1	-4.725947	-1.484298	0.093156
24	1	-2.626933	-2.688850	0.613640
25	8	0.816511	2.982041	0.807402
26	8	-0.017358	1.978509	0.925570

TRBANTITSROTATION.LO

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.440417	0.860869	-0.777984
2	6	1.212129	0.306238	-0.414041
3	6	1.163648	-1.019235	0.106621
4	6	2.378671	-1.734818	0.249517
5	6	3.587174	-1.164872	-0.116028
6	6	3.624028	0.137435	-0.638296
7	1	2.469722	1.876573	-1.165194
8	1	2.347224	-2.747002	0.645266
9	1	4.508628	-1.729344	-0.001792
10	1	4.571251	0.583273	-0.927210
11	6	-0.089704	-1.609654	0.422970
12	6	-1.319594	-0.951788	0.152377
13	1	-0.109564	-2.619089	0.826094
14	6	-1.310992	0.373051	-0.374526
15	6	-0.026623	1.111290	-0.483678
16	1	-0.023458	1.836633	-1.299943
17	6	-2.518277	0.993999	-0.702461
18	6	-3.735696	0.340854	-0.510453
19	1	-2.503745	2.004754	-1.103230

20	1	-4.665661	0.838044	-0.770450
21	6	-3.755005	-0.957469	0.022428
22	6	-2.567919	-1.594419	0.346143
23	1	-4.702494	-1.466793	0.175702
24	1	-2.579494	-2.604976	0.747180
25	8	0.844981	2.011732	1.650454
26	8	-0.070726	2.173148	0.746803

MINIMAOFSYMTS.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.482062	-0.975247	-0.735704
2	6	-1.266994	-0.386139	-0.384635
3	6	-1.243639	0.950903	0.102673
4	6	-2.474209	1.639953	0.241100
5	6	-3.672203	1.035432	-0.104907
6	6	-3.682128	-0.276024	-0.603510
7	1	-2.489830	-1.998385	-1.104539
8	1	-2.463574	2.660370	0.616312
9	1	-4.605515	1.581017	0.004738
10	1	-4.619931	-0.748198	-0.881293
11	6	0.000024	1.579997	0.386704
12	6	1.243686	0.950889	0.102681
13	1	0.000030	2.599316	0.764415
14	6	1.267024	-0.386155	-0.384616
15	6	0.000011	-1.176625	-0.435467
16	1	0.000014	-1.903680	-1.252574
17	6	2.482088	-0.975280	-0.735670
18	6	3.682166	-0.276075	-0.603469
19	1	2.489844	-1.998422	-1.104498
20	1	4.619965	-0.748261	-0.881238
21	6	3.672239	1.035380	-0.104876
22	6	2.474260	1.639930	0.241120
23	1	4.605558	1.580955	0.004775
24	1	2.463637	2.660345	0.616330
25	8	-0.000176	-1.571102	1.914289
26	8	-0.000044	-2.175233	0.751841

ANTHRAOXYTSTRIPLETI_2FREQ.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.363651	-1.225889	-0.735614
2	6	-1.241203	-0.631915	-0.168502
3	6	-1.239807	0.752016	0.125367
4	6	-2.388542	1.511574	-0.129150
5	6	-3.508585	0.909318	-0.701943
6	6	-3.497120	-0.453984	-1.011119
7	1	-2.362661	-2.291638	-0.951969
8	1	-2.394837	2.573822	0.102602
9	1	-4.393152	1.504998	-0.910213
10	1	-4.374014	-0.919058	-1.452636
11	6	0.000000	1.285718	0.694929

12	6	1.239807	0.752016	0.125367
13	1	0.000000	2.310583	1.059601
14	6	1.241203	-0.631915	-0.168501
15	6	0.000000	-1.382828	0.256700
16	1	0.000000	-2.418354	-0.097335
17	6	2.363651	-1.225889	-0.735614
18	6	3.497120	-0.453984	-1.011119
19	1	2.362661	-2.291639	-0.951969
20	1	4.374014	-0.919059	-1.452636
21	6	3.508585	0.909318	-0.701943
22	6	2.388542	1.511574	-0.129151
23	1	4.393151	1.504998	-0.910214
24	1	2.394837	2.573822	0.102601
25	8	0.000000	0.053432	2.172507
26	8	0.000000	-1.475838	1.727984

IRCREVERSETRIPLETTS-IITOOPT(TRIPLETPROD)_1.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.441008	1.395503	-0.142114
2	6	-1.274581	0.700722	0.188355
3	6	-1.274548	-0.700681	0.188393
4	6	-2.440931	-1.395587	-0.141946
5	6	-3.601268	-0.698818	-0.474141
6	6	-3.601303	0.698616	-0.474223
7	1	-2.421415	2.480326	-0.144490
8	1	-2.421251	-2.480412	-0.144208
9	1	-4.503369	-1.245112	-0.736072
10	1	-4.503437	1.244828	-0.736214
11	6	0.000027	-1.457294	0.562271
12	6	1.274598	-0.700686	0.188440
13	1	-0.000082	-1.540631	1.683321
14	6	1.274572	0.700718	0.188416
15	6	-0.000010	1.457475	0.562287
16	1	-0.000063	1.540516	1.683333
17	6	2.440988	1.395535	-0.142032
18	6	3.601288	0.698685	-0.474207
19	1	2.421390	2.480355	-0.144339
20	1	4.503399	1.244930	-0.736208
21	6	3.601283	-0.698747	-0.474193
22	6	2.440976	-1.395558	-0.141989
23	1	4.503385	-1.245011	-0.736183
24	1	2.421324	-2.480380	-0.144322
25	8	0.000053	-2.779017	0.229688
26	8	-0.000100	2.779179	0.229747

H2ELIMINATION.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.469747	-1.403206	-0.131835
2	6	1.277816	-0.704922	0.102764
3	6	1.282927	0.699507	0.131318

4	6	2.477794	1.390338	-0.079770
5	6	3.658577	0.689165	-0.319939
6	6	3.656482	-0.710158	-0.342519
7	1	2.431981	-2.487475	-0.150968
8	1	2.467710	2.475170	-0.063380
9	6	0.000000	1.462022	0.450592
10	6	-1.282927	0.699507	0.131318
11	1	0.000000	1.586920	1.568383
12	6	-1.277816	-0.704922	0.102764
13	6	0.000000	-1.483129	0.266680
14	1	0.000000	-1.267842	1.973123
15	6	-2.469747	-1.403206	-0.131835
16	6	-3.656482	-0.710158	-0.342519
17	1	-2.431981	-2.487475	-0.150968
18	6	-3.658577	0.689165	-0.319939
19	6	-2.477794	1.390338	-0.079770
20	1	-2.467710	2.475170	-0.063380
21	8	0.000000	2.769296	0.062969
22	8	0.000000	-2.726489	0.224928
23	1	-4.578434	-1.254025	-0.528450
24	1	-4.582723	1.234541	-0.491472
25	1	4.578434	-1.254025	-0.528450
26	1	4.582723	1.234541	-0.491472

TRIPLETANTHRAQUINONE.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.490058	1.409348	0.000000
2	6	1.257245	0.710287	0.000000
3	6	1.255034	-0.708024	0.000000
4	6	2.482288	-1.391214	0.000000
5	6	3.683481	-0.699024	0.000000
6	6	3.682164	0.709524	0.000000
7	1	2.485439	2.495365	0.000000
8	1	2.446763	-2.476174	0.000000
9	1	4.624875	-1.240761	0.000000
10	1	4.623198	1.252716	0.000000
11	6	0.000040	-1.486432	0.000000
12	6	-1.254954	-0.708047	0.000000
13	6	-1.257135	0.710139	0.000000
14	6	0.000000	1.416225	0.000000
15	6	-2.490237	1.409226	0.000000
16	6	-3.682282	0.709244	0.000000
17	1	-2.485572	2.495219	0.000000
18	1	-4.623314	1.252452	0.000000
19	6	-3.683286	-0.699215	0.000000
20	6	-2.482072	-1.391384	0.000000
21	1	-4.624471	-1.241320	0.000000
22	1	-2.446647	-2.476341	0.000000
23	8	-0.000087	-2.724126	0.000000
24	8	-0.000204	2.723492	0.000000

TETRACENE.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.235379	1.406343
2	6	0.000000	0.000000	0.726336
3	6	0.000000	0.000000	-0.726336
4	6	0.000000	1.235379	-1.406343
5	6	0.000000	2.450534	-0.726024
6	6	0.000000	2.450534	0.726024
7	1	0.000000	1.235250	2.494599
8	1	0.000000	1.235250	-2.494599
9	6	0.000000	-1.235379	-1.406343
10	6	0.000000	-2.450534	-0.726024
11	1	0.000000	-1.235250	-2.494599
12	6	0.000000	-2.450534	0.726024
13	6	0.000000	-1.235379	1.406343
14	1	0.000000	-1.235250	2.494599
15	6	0.000000	-3.711088	-1.409290
16	6	0.000000	-4.888894	-0.715348
17	1	0.000000	-3.708839	-2.496800
18	1	0.000000	-5.836288	-1.247457
19	6	0.000000	-4.888894	0.715348
20	6	0.000000	-3.711088	1.409290
21	1	0.000000	-5.836288	1.247457
22	1	0.000000	-3.708839	2.496800
23	6	0.000000	3.711088	-1.409290
24	6	0.000000	4.888894	-0.715348
25	1	0.000000	3.708839	-2.496800
26	1	0.000000	5.836288	-1.247457
27	6	0.000000	4.888894	0.715348
28	6	0.000000	3.711088	1.409290
29	1	0.000000	5.836288	1.247457
30	1	0.000000	3.708839	2.496800

TETRACENE9,10OXYTS_2.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.525467	1.433345	-0.488598
2	6	2.294080	0.739679	-0.314422
3	6	2.300620	-0.696854	-0.309273
4	6	3.533267	-1.381518	-0.493434
5	6	4.699011	-0.679981	-0.685876
6	6	4.696070	0.741672	-0.681564
7	1	3.519710	2.520324	-0.474813
8	1	3.535811	-2.468491	-0.486393
9	1	5.634312	-1.211441	-0.838219
10	1	5.628895	1.278689	-0.828684
11	6	1.076972	-1.378708	-0.095429
12	6	-0.174272	-0.717147	-0.158155
13	1	1.090483	-2.464128	-0.036474
14	6	-0.175702	0.725436	-0.113394
15	6	1.081131	1.399009	-0.062209
16	1	1.081003	2.482381	0.030617

17	6	-1.396770	1.409229	-0.113858
18	6	-2.617369	0.725080	-0.166466
19	1	-1.398164	2.496361	-0.077096
20	6	-2.616802	-0.721464	-0.203397
21	6	-1.394992	-1.403564	-0.187392
22	1	-1.392532	-2.491269	-0.204526
23	8	1.480833	-0.670557	2.072283
24	8	1.037059	0.505419	2.170461
25	6	-3.870931	-1.406551	-0.253461
26	6	-5.051914	-0.712893	-0.266129
27	6	-5.052538	0.713108	-0.231105
28	6	-3.873024	1.408288	-0.183741
29	1	-3.866986	-2.493575	-0.279495
30	1	-5.997913	-1.246012	-0.302590
31	1	-5.999358	1.246045	-0.241232
32	1	-3.872226	2.495234	-0.155637

TETRAOXYGENPRODUCT.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.162788	1.408654	-0.866930
2	6	2.252385	0.702270	-0.090358
3	6	2.252654	-0.701981	-0.090430
4	6	3.163443	-1.407997	-0.866912
5	6	4.068538	-0.697579	-1.665058
6	6	4.068214	0.698598	-1.665039
7	1	3.171036	2.495982	-0.858842
8	1	3.171992	-2.495322	-0.858823
9	1	4.778547	-1.237582	-2.285481
10	1	4.777881	1.238965	-2.285542
11	6	1.212617	-1.251457	0.858304
12	6	-0.148607	-0.712703	0.483932
13	1	1.245927	-2.336868	0.983081
14	6	-0.148693	0.712321	0.484565
15	6	1.212381	1.251005	0.858978
16	1	1.245637	2.336329	0.984505
17	6	-1.290907	1.414098	0.203816
18	6	-2.493452	0.717615	-0.115117
19	1	-1.297035	2.502154	0.215588
20	6	-2.493387	-0.717583	-0.115730
21	6	-1.290783	-1.414273	0.202565
22	1	-1.296875	-2.502344	0.213268
23	8	1.527791	-0.742023	2.190765
24	8	1.528822	0.740606	2.190877
25	6	-3.695657	-1.401373	-0.433579
26	6	-4.846525	-0.707230	-0.737455
27	6	-4.846581	0.707595	-0.736879
28	6	-3.695764	1.401576	-0.432437
29	1	-3.693486	-2.488914	-0.432660
30	1	-5.759371	-1.245290	-0.978021
31	1	-5.759462	1.245784	-0.977022
32	1	-3.693677	2.489117	-0.430618

Pentacene

PENTACENE.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.408475	-0.000072
2	6	0.000000	0.728523	1.226580
3	6	0.000000	-0.728523	1.226580
4	6	0.000000	-1.408475	-0.000072
5	6	0.000000	-0.728630	-1.226502
6	6	0.000000	0.728630	-1.226502
7	1	0.000000	2.496604	0.000028
8	1	0.000000	-2.496604	0.000028
9	6	0.000000	-1.407868	2.467530
10	6	0.000000	-0.727797	3.678967
11	1	0.000000	-2.496125	2.467947
12	6	0.000000	0.727797	3.678967
13	6	0.000000	1.407868	2.467530
14	1	0.000000	2.496125	2.467947
15	6	0.000000	-1.410440	4.942089
16	6	0.000000	-0.716533	6.118242
17	1	0.000000	-1.247766	7.066226
18	6	0.000000	0.716533	6.118242
19	6	0.000000	1.410440	4.942089
20	1	0.000000	1.247766	7.066226
21	6	0.000000	-1.407830	-2.467762
22	6	0.000000	-0.727601	-3.678779
23	1	0.000000	-2.496077	-2.467937
24	6	0.000000	0.727601	-3.678779
25	6	0.000000	1.407830	-2.467762
26	1	0.000000	2.496077	-2.467937
27	6	0.000000	-1.410363	-4.942044
28	6	0.000000	-0.716474	-6.118252
29	1	0.000000	-2.497899	-4.940167
30	1	0.000000	-1.248000	-7.066070
31	6	0.000000	0.716474	-6.118252
32	6	0.000000	1.410363	-4.942044
33	1	0.000000	2.497899	-4.940167
34	1	0.000000	1.248000	-7.066070
35	1	0.000000	2.498030	4.939985
36	1	0.000000	-2.498030	4.939985

PENTACENEOXYGENANTITS_1.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.396596	1.055049	-0.569387
2	6	1.177932	0.415564	-0.376705
3	6	1.154726	-0.971570	0.050045
4	6	2.375004	-1.642640	0.219638
5	6	3.612890	-1.003334	0.008014
6	6	3.629413	0.378954	-0.393537
7	1	2.409734	2.092191	-0.891067

8	1	2.366476	-2.685791	0.528484
9	6	-0.089606	-1.601198	0.274584
10	6	-1.321042	-0.926670	0.095085
11	1	-0.103045	-2.643671	0.584065
12	6	-1.312286	0.464411	-0.312876
13	6	-0.048885	1.140051	-0.454379
14	1	-0.045277	2.095582	-0.968838
15	6	-2.516009	1.124200	-0.518162
16	6	-3.761061	0.482699	-0.335308
17	1	-2.504353	2.169255	-0.820636
18	6	-3.777688	-0.897991	0.077521
19	6	-2.556484	-1.565519	0.280204
20	1	-2.570173	-2.609280	0.586990
21	8	1.274270	2.493792	1.574249
22	8	0.083606	2.198148	1.307382
23	6	4.877383	1.019263	-0.604107
24	6	6.061590	0.335731	-0.429526
25	6	4.854944	-1.678363	0.177982
26	6	6.047985	-1.025891	-0.035169
27	6	-5.036871	-1.539969	0.262298
28	6	-6.212843	-0.859591	0.052583
29	6	-6.194388	0.500889	-0.353653
30	6	-4.997203	1.152975	-0.542371
31	1	-4.979935	2.195298	-0.851770
32	1	-7.132123	1.025418	-0.514273
33	1	-7.165341	-1.361836	0.197964
34	1	-5.049750	-2.581663	0.573864
35	1	4.883593	2.064579	-0.903235
36	1	7.010587	0.838668	-0.592692
37	1	6.987894	-1.554206	0.099638
38	1	4.844116	-2.722370	0.481792

PENTACENEOXYGENANTIMINIMA_1.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.436055	1.072394	-0.436391
2	6	1.240371	0.475195	-0.123437
3	6	1.203870	-0.916471	0.258545
4	6	2.412443	-1.619587	0.338125
5	6	3.651567	-1.013697	0.035863
6	6	3.669610	0.362435	-0.371234
7	1	2.453897	2.121860	-0.717105
8	1	2.395617	-2.668525	0.626470
9	6	-0.045462	-1.550921	0.489891
10	6	-1.286500	-0.898752	0.260716
11	1	-0.052825	-2.598603	0.780098
12	6	-1.301100	0.493960	-0.114364
13	6	-0.024033	1.279559	-0.089124
14	1	-0.017807	2.080854	-0.830430
15	6	-2.488895	1.115733	-0.407659
16	6	-3.734715	0.429505	-0.342990
17	1	-2.491183	2.168499	-0.683672
18	6	-3.736860	-0.950903	0.051075
19	6	-2.507111	-1.580596	0.342024

20	1	-2.507834	-2.630982	0.625338
21	8	0.756624	3.066656	1.232458
22	8	-0.074528	2.050848	1.236522
23	6	4.907391	0.971448	-0.687390
24	6	6.086803	0.258516	-0.607075
25	6	4.883883	-1.720655	0.107908
26	6	6.072444	-1.098836	-0.205962
27	6	-4.981189	-1.636761	0.124825
28	6	-6.160606	-0.991456	-0.174920
29	6	-6.154642	0.370037	-0.562900
30	6	-4.963991	1.063279	-0.644361
31	1	-4.955890	2.109825	-0.939804
32	1	-7.091889	0.867538	-0.795727
33	1	-7.103753	-1.527629	-0.113915
34	1	-4.984940	-2.682455	0.422865
35	1	4.914908	2.015280	-0.991986
36	1	7.030780	0.737829	-0.850809
37	1	7.006635	-1.650636	-0.146104
38	1	4.871510	-2.763438	0.415955

PENTACENEOXYGENROTTS_1.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.421761	1.136624	-0.487644
2	6	1.233646	0.544112	-0.142734
3	6	1.206185	-0.840629	0.260689
4	6	2.416073	-1.541725	0.325471
5	6	3.647451	-0.940199	-0.015135
6	6	3.656514	0.429409	-0.444707
7	1	2.435154	2.183247	-0.785768
8	1	2.407091	-2.585833	0.630961
9	6	-0.040562	-1.470965	0.519727
10	6	-1.283159	-0.829787	0.271381
11	1	-0.043818	-2.511446	0.834903
12	6	-1.298497	0.552628	-0.144724
13	6	-0.026150	1.337533	-0.095051
14	1	-0.024645	2.159645	-0.814652
15	6	-2.483945	1.157870	-0.480036
16	6	-3.727490	0.467100	-0.411383
17	1	-2.487226	2.200230	-0.792964
18	6	-3.730223	-0.898599	0.031396
19	6	-2.502049	-1.513526	0.359453
20	1	-2.502359	-2.555028	0.673977
21	8	0.825341	1.918671	2.106492
22	8	-0.131617	2.141094	1.246002
23	6	4.886584	1.033234	-0.799067
24	6	6.067405	0.321369	-0.735448
25	6	4.881364	-1.645879	0.038957
26	6	6.062124	-1.029539	-0.312628
27	6	-4.972407	-1.587373	0.110830
28	6	-6.150262	-0.959273	-0.229377
29	6	-6.143834	0.387263	-0.665906
30	6	-4.954919	1.083001	-0.754137
31	1	-4.947253	2.118453	-1.086524

32	1	-7.079423	0.871831	-0.930668
33	1	-7.091855	-1.497568	-0.163457
34	1	-4.975902	-2.621909	0.445630
35	1	4.887466	2.072226	-1.120222
36	1	7.005438	0.796332	-1.008756
37	1	6.997448	-1.580657	-0.265827
38	1	4.876439	-2.683543	0.363858

PENTACENEOXYGENSYNMINIMA.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.461495	-1.177505	-0.446082
2	6	-1.271413	-0.566289	-0.141044
3	6	-1.245268	0.831265	0.213149
4	6	-2.459478	1.526075	0.275125
5	6	-3.692836	0.906026	-0.020593
6	6	-3.700632	-0.477739	-0.402396
7	1	-2.472550	-2.232875	-0.712335
8	1	-2.451879	2.579809	0.545636
9	6	-0.000003	1.478541	0.432834
10	6	1.245265	0.831269	0.213147
11	1	-0.000004	2.531342	0.703639
12	6	1.271415	-0.566287	-0.141034
13	6	0.000001	-1.363325	-0.092332
14	1	0.000005	-2.164264	-0.837067
15	6	2.461497	-1.177502	-0.446067
16	6	3.700633	-0.477730	-0.402391
17	1	2.472558	-2.232877	-0.712303
18	6	3.692832	0.906036	-0.020602
19	6	2.459472	1.526084	0.275112
20	1	2.451871	2.579820	0.545614
21	8	0.000054	-1.475728	2.266749
22	8	-0.000024	-2.209655	1.175043
23	6	-4.933180	-1.100924	-0.712878
24	6	-6.117282	-0.394706	-0.650905
25	6	-4.930708	1.605377	0.033263
26	6	-6.113454	0.970050	-0.274278
27	6	4.930702	1.605395	0.033245
28	6	6.113447	0.970048	-0.274295
29	6	6.117275	-0.394711	-0.650907
30	6	4.933175	-1.100938	-0.712859
31	1	4.932868	-2.150072	-0.999291
32	1	7.057008	-0.884455	-0.890233
33	1	7.051568	1.516464	-0.228343
34	1	4.926658	2.653581	0.322467
35	1	-4.932877	-2.150051	-0.999337
36	1	-7.057014	-0.884452	-0.890231
37	1	-7.051573	1.516470	-0.228313
38	1	-4.926659	2.653560	0.322498

PENATCENEOXYSBTS-II.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.383961	-1.347939	-0.195217
2	6	-1.252065	-0.721903	0.258363
3	6	-1.239395	0.697671	0.471447
4	6	-2.394841	1.429702	0.253854
5	6	-3.575101	0.806766	-0.224570
6	6	-3.570158	-0.608388	-0.466956
7	1	-2.394107	-2.426610	-0.338259
8	1	-2.399797	2.502737	0.432501
9	6	0.011652	1.282893	0.894927
10	6	1.247729	0.697263	0.477534
11	1	0.012235	2.310415	1.250379
12	6	1.239672	-0.711594	0.189952
13	6	0.004522	-1.425259	0.652833
14	1	0.006276	-2.492612	0.423336
15	6	2.368893	-1.333027	-0.284286
16	6	3.566468	-0.601040	-0.506308
17	1	2.362832	-2.403181	-0.481252
18	6	3.600307	0.798290	-0.172473
19	6	2.433979	1.414956	0.329672
20	1	2.457563	2.474470	0.575231
21	8	-0.309862	-0.217069	2.659009
22	8	0.199007	-1.362712	2.150341
23	6	-4.751215	-1.226361	-0.950049
24	6	-4.766061	1.539512	-0.479498
25	6	4.738625	-1.209467	-1.025422
26	6	4.811810	1.520005	-0.371857
27	6	5.929811	0.897441	-0.875615
28	6	5.893577	-0.481095	-1.205798
29	6	-5.896576	0.908991	-0.949577
30	6	-5.890072	-0.486789	-1.187077
31	1	4.835982	2.577261	-0.118649
32	1	6.847349	1.460584	-1.022498
33	1	6.784043	-0.962056	-1.601120
34	1	4.710885	-2.267393	-1.275709
35	1	-4.744677	-2.298980	-1.129480
36	1	-6.788255	-0.973593	-1.556999
37	1	-6.799992	1.482081	-1.139563
38	1	-4.769101	2.611356	-0.295993

PENTACENOXYGENEPRODUCT.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-5.519844	-1.578956	0.707622
2	6	-5.519811	-1.579098	-0.707451
3	6	-4.470166	-1.018150	1.401643
4	6	-4.470099	-1.018434	-1.401536
5	6	-3.373199	-0.431955	-0.717687
6	6	-3.373237	-0.431807	0.717724
7	6	-2.278127	0.157395	1.414019
8	1	-2.286295	0.166518	2.502077
9	6	-1.233321	0.699136	0.712438
10	6	-1.233303	0.699025	-0.712500
11	6	-2.278062	0.157136	-1.414039

12	1	-4.468623	-1.016058	2.489171
13	1	-4.468504	-1.016555	-2.489065
14	1	-2.286169	0.166055	-2.502098
15	6	1.233291	0.699002	-0.712504
16	6	1.233262	0.699027	0.712449
17	6	2.278081	0.157172	-1.414033
18	6	2.278062	0.157287	1.414026
19	6	3.373206	-0.431950	-0.717680
20	1	2.286197	0.166104	-2.502093
21	6	3.373209	-0.431862	0.717727
22	1	2.286226	0.166367	2.502085
23	6	4.470128	-1.018379	-1.401529
24	6	4.470130	-1.018208	1.401650
25	6	5.519838	-1.579049	-0.707441
26	1	4.468561	-1.016458	-2.489057
27	6	5.519838	-1.578966	0.707630
28	1	4.468559	-1.016164	2.489177
29	6	-0.000006	1.383944	1.253123
30	6	0.000001	1.383841	-1.253273
31	8	-0.000027	2.750384	-0.742295
32	8	0.000126	2.750498	0.741948
33	1	0.000022	1.514131	-2.338572
34	1	-0.000015	1.514375	2.338409
35	1	-6.352834	-2.023203	-1.245502
36	1	-6.352883	-2.022969	1.245724
37	1	6.352883	-2.023112	-1.245492
38	1	6.352871	-2.022988	1.245733

PENTACENERINGOPENING_5.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.252286	-0.687579	0.663549
2	6	-1.234845	0.734817	0.598547
3	6	0.001581	1.381490	1.200606
4	6	1.253232	0.725088	0.624300
5	1	0.021929	2.469613	1.017345
6	6	1.240415	-0.699999	0.643659
7	6	0.003708	-1.317438	1.271401
8	1	-0.030630	-2.411812	1.142268
9	8	0.000448	1.241752	2.593473
10	8	-0.039672	-1.062522	2.645943
11	6	2.330864	1.404170	0.115226
12	6	2.304838	-1.407888	0.146141
13	6	3.438556	-0.735098	-0.392691
14	6	3.451881	0.698165	-0.407136
15	1	2.341198	2.492200	0.098294
16	1	2.296946	-2.496385	0.159243
17	6	-2.297048	1.411284	0.054271
18	6	-2.333322	-1.397758	0.204648
19	6	-3.431267	0.708067	-0.442293
20	6	-3.450101	-0.723527	-0.364008
21	1	-2.287650	2.498309	-0.000657
22	1	-2.345812	-2.484231	0.259713
23	6	4.581399	1.368124	-0.945574

24	6	5.651409	0.658668	-1.445475
25	6	4.556112	-1.436068	-0.915841
26	6	-4.581078	-1.423797	-0.860203
27	6	-4.546020	1.377058	-1.011458
28	6	-5.629804	0.668777	-1.482576
29	6	-5.647813	-0.744626	-1.406131
30	6	5.638578	-0.756464	-1.430499
31	1	4.544392	-2.523438	-0.902812
32	1	4.589190	2.455556	-0.954977
33	1	6.510475	1.184372	-1.853215
34	1	6.487810	-1.306054	-1.827244
35	1	-4.592136	-2.509494	-0.799492
36	1	-4.530932	2.462885	-1.068892
37	1	-6.476646	1.194273	-1.915391
38	1	-6.508291	-1.292427	-1.780298

SBPENTACENEOXYGENPRODUCT.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.402291	1.401304	0.211107
2	6	-1.270786	0.711740	0.583289
3	6	-1.270796	-0.711705	0.583286
4	6	-2.402306	-1.401269	0.211102
5	6	-3.580980	-0.716577	-0.182363
6	6	-3.580980	0.716604	-0.182364
7	1	-2.386386	2.487103	0.211767
8	1	-2.386339	-2.487069	0.211784
9	6	-0.000006	-1.449222	1.007058
10	6	1.270780	-0.711697	0.583286
11	1	-0.000005	-1.458576	2.131354
12	6	1.270787	0.711690	0.583285
13	6	0.000019	1.449230	1.007061
14	1	0.000029	1.458577	2.131356
15	6	2.402334	1.401268	0.211087
16	6	3.580944	0.716548	-0.182356
17	1	2.386362	2.487066	0.211769
18	6	3.580941	-0.716589	-0.182350
19	6	2.402321	-1.401288	0.211097
20	1	2.386341	-2.487086	0.211786
21	8	-0.000003	-2.788366	0.760464
22	8	0.000049	2.788377	0.760469
23	6	-4.760290	1.404131	-0.577389
24	6	-5.887212	0.708718	-0.952994
25	6	-4.760281	-1.404178	-0.577369
26	6	-5.887211	-0.708709	-0.952988
27	6	4.760304	-1.404193	-0.577382
28	6	5.887183	-0.708757	-0.952988
29	6	4.760297	1.404180	-0.577393
30	6	5.887187	0.708761	-0.952996
31	1	-4.756417	-2.491497	-0.577701
32	1	-6.783425	-1.245100	-1.252675
33	1	-6.783431	1.245066	-1.252719
34	1	-4.756424	2.491461	-0.577711
35	1	4.756292	2.491502	-0.577696

36	1	6.783458	1.245022	-1.252723
37	1	6.783471	-1.244994	-1.252715
38	1	4.756354	-2.491515	-0.577694

H2ELIMINATIONSBTS_3.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.333517	1.413706	0.215754
2	6	-1.256176	0.710098	0.689619
3	6	-1.256176	-0.710098	0.689619
4	6	-2.333517	-1.413706	0.215754
5	6	-3.460476	-0.717653	-0.310757
6	6	-3.460476	0.717653	-0.310757
7	1	-2.327180	2.500056	0.242593
8	1	-2.327180	-2.500056	0.242593
9	6	0.000000	-1.342306	1.277684
10	6	1.256176	-0.710098	0.689619
11	1	0.000000	-0.661516	2.352918
12	6	1.256176	0.710098	0.689619
13	6	0.000000	1.342306	1.277684
14	1	0.000000	0.661516	2.352918
15	6	2.333517	1.413706	0.215754
16	6	3.460476	0.717653	-0.310757
17	1	2.327180	2.500056	0.242593
18	6	3.460476	-0.717653	-0.310757
19	6	2.333517	-1.413706	0.215754
20	1	2.327180	-2.500056	0.242593
21	8	0.000000	-2.585080	1.630729
22	8	0.000000	2.585080	1.630729
23	6	4.591672	-1.402414	-0.822345
24	6	4.591672	1.402414	-0.822345
25	6	-4.591672	-1.402414	-0.822345
26	6	-4.591672	1.402414	-0.822345
27	6	5.676986	0.706690	-1.313827
28	6	5.676986	-0.706690	-1.313827
29	6	-5.676986	0.706690	-1.313827
30	6	-5.676986	-0.706690	-1.313827
31	1	-4.589532	-2.489650	-0.821284
32	1	-6.536169	-1.244888	-1.704397
33	1	-6.536169	1.244888	-1.704397
34	1	-4.589532	2.489650	-0.821284
35	1	4.589532	-2.489650	-0.821284
36	1	6.536169	-1.244888	-1.704397
37	1	6.536169	1.244888	-1.704397
38	1	4.589532	2.489650	-0.821284

PENTACENEQUINONE_1.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.471594	1.400758	0.000000
2	6	1.272647	0.714909	0.000000
3	6	1.272646	-0.714908	0.000000

4	6	2.471594	-1.400759	0.000000
5	6	3.711549	-0.717981	0.000000
6	6	3.711548	0.717981	0.000000
7	1	2.445197	2.486662	0.000000
8	1	2.445197	-2.486661	0.000000
9	6	0.000000	-1.491158	0.000000
10	6	-1.272647	-0.714908	0.000000
11	6	-1.272647	0.714908	0.000000
12	6	0.000000	1.491158	0.000000
13	6	-2.471594	1.400759	0.000000
14	6	-3.711548	0.717980	0.000000
15	1	-2.445197	2.486663	0.000000
16	6	-3.711549	-0.717980	0.000000
17	6	-2.471594	-1.400759	0.000000
18	1	-2.445197	-2.486663	0.000000
19	6	4.954883	1.406112	0.000000
20	6	6.141774	0.708947	0.000000
21	6	4.954884	-1.406112	0.000000
22	6	6.141773	-0.708946	0.000000
23	6	-4.954884	-1.406113	0.000000
24	6	-6.141773	-0.708945	0.000000
25	6	-6.141773	0.708945	0.000000
26	6	-4.954882	1.406112	0.000000
27	1	-4.950748	2.493110	0.000000
28	1	-7.087330	1.244036	0.000000
29	1	-7.087329	-1.244035	0.000000
30	1	-4.950748	-2.493111	0.000000
31	1	4.950747	2.493110	0.000000
32	1	7.087330	1.244037	0.000000
33	1	7.087329	-1.244036	0.000000
34	1	4.950747	-2.493111	0.000000
35	8	0.000000	2.718772	0.000000
36	8	0.000000	-2.718772	0.000000

Triplet path
PENTOXYANTITS.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.413031	1.062603	-0.533318
2	6	1.203201	0.440187	-0.286258
3	6	1.177080	-0.946860	0.130329
4	6	2.394639	-1.627706	0.269393
5	6	3.632614	-1.000474	0.019890
6	6	3.647980	0.376774	-0.393855
7	1	2.426088	2.102141	-0.847690
8	1	2.385001	-2.671503	0.576067
9	6	-0.069041	-1.579026	0.357448
10	6	-1.304353	-0.914138	0.154981
11	1	-0.079924	-2.622276	0.663836
12	6	-1.303578	0.475648	-0.248253
13	6	-0.035571	1.190234	-0.318226
14	1	-0.031534	2.098094	-0.916217
15	6	-2.501989	1.121090	-0.487791
16	6	-3.749053	0.463707	-0.346160

17	1	-2.494709	2.167810	-0.784923
18	6	-3.760753	-0.915338	0.064855
19	6	-2.535764	-1.568237	0.303424
20	1	-2.545559	-2.613086	0.606526
21	8	1.082332	2.664924	1.523802
22	8	-0.038529	2.125870	1.273497
23	6	4.892730	1.005056	-0.649119
24	6	6.076806	0.313281	-0.504771
25	6	4.873296	-1.684876	0.157568
26	6	6.064612	-1.044116	-0.097940
27	6	-5.015954	-1.572928	0.210628
28	6	-6.193989	-0.906239	-0.034906
29	6	-6.179622	0.453170	-0.439347
30	6	-4.983385	1.119669	-0.590886
31	1	-4.969021	2.162473	-0.898939
32	1	-7.117814	0.967177	-0.628620
33	1	-7.144121	-1.420520	0.081069
34	1	-5.025923	-2.614984	0.521061
35	1	4.898089	2.047643	-0.957813
36	1	7.024189	0.807151	-0.701660
37	1	7.003943	-1.579102	0.012506
38	1	4.863247	-2.726270	0.470290

ANTIMINIMA.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.434015	1.072857	-0.442780
2	6	1.238423	0.476503	-0.126185
3	6	1.202430	-0.914025	0.260070
4	6	2.411230	-1.616960	0.340649
5	6	3.649693	-1.011907	0.035219
6	6	3.667261	0.363050	-0.376481
7	1	2.451574	2.121029	-0.727927
8	1	2.394751	-2.664958	0.632416
9	6	-0.046780	-1.547715	0.493719
10	6	-1.287481	-0.895997	0.262484
11	1	-0.054228	-2.594556	0.786982
12	6	-1.301235	0.495488	-0.117123
13	6	-0.024969	1.279378	-0.090529
14	1	-0.018393	2.085660	-0.826324
15	6	-2.488985	1.117169	-0.412889
16	6	-3.734646	0.431580	-0.346984
17	1	-2.490569	2.169093	-0.692048
18	6	-3.737626	-0.947722	0.051815
19	6	-2.508713	-1.577040	0.345681
20	1	-2.510136	-2.626385	0.632828
21	8	0.783486	3.035734	1.262735
22	8	-0.078964	2.048181	1.243001
23	6	4.904950	0.970894	-0.696078
24	6	6.084263	0.258229	-0.614709
25	6	4.882273	-1.718662	0.108197
26	6	6.070349	-1.097965	-0.209021
27	6	-4.982513	-1.632792	0.127071
28	6	-6.161314	-0.988083	-0.175639

29	6	-6.154541	0.372281	-0.568331
30	6	-4.963756	1.064749	-0.651380
31	1	-4.955075	2.110290	-0.950362
32	1	-7.091483	0.869289	-0.803444
33	1	-7.104756	-1.523599	-0.113448
34	1	-4.986870	-2.677468	0.428656
35	1	4.912190	2.013733	-1.004069
36	1	7.028015	0.736656	-0.861056
37	1	7.004633	-1.649523	-0.148399
38	1	4.870186	-2.760434	0.419661

PENTOXYROTTS.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.423960	1.135616	-0.487059
2	6	1.233526	0.539536	-0.153791
3	6	1.206010	-0.846474	0.245258
4	6	2.417068	-1.546047	0.314550
5	6	3.649278	-0.941254	-0.014783
6	6	3.659084	0.430728	-0.437666
7	1	2.437543	2.183341	-0.781338
8	1	2.407691	-2.591246	0.616282
9	6	-0.040132	-1.479178	0.498546
10	6	-1.282836	-0.835587	0.256822
11	1	-0.043281	-2.521119	0.808799
12	6	-1.298474	0.548713	-0.152760
13	6	-0.025879	1.331857	-0.113735
14	1	-0.026197	2.147988	-0.839908
15	6	-2.485771	1.157049	-0.477357
16	6	-3.729600	0.467902	-0.404005
17	1	-2.489634	2.200831	-0.785505
18	6	-3.731331	-0.900487	0.030484
19	6	-2.501974	-1.518573	0.347387
20	1	-2.501537	-2.561884	0.655872
21	8	0.807159	1.908498	2.101086
22	8	-0.119902	2.163628	1.219079
23	6	4.891002	1.038237	-0.780415
24	6	6.072229	0.328026	-0.711657
25	6	4.884254	-1.645226	0.044672
26	6	6.066204	-1.025245	-0.295363
27	6	-4.958558	1.087595	-0.734856
28	6	-6.147695	0.392918	-0.643060
29	6	-6.153067	-0.956404	-0.214841
30	6	-4.973939	-1.588171	0.113698
31	1	-4.976645	-2.624731	0.442193
32	1	-7.094964	-1.493814	-0.146063
33	1	-7.084381	0.880281	-0.898660
34	1	-4.951615	2.125038	-1.060983
35	1	4.892430	2.078735	-1.096634
36	1	7.011493	0.805743	-0.975790
37	1	7.002177	-1.574899	-0.244528
38	1	4.878709	-2.684453	0.364523

PENOXYSYMMINIMA.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.458743	-1.181843	-0.446006
2	6	-1.269984	-0.570916	-0.133701
3	6	-1.245001	0.826435	0.221424
4	6	-2.459554	1.521416	0.278898
5	6	-3.691143	0.901974	-0.024603
6	6	-3.697301	-0.481280	-0.409189
7	1	-2.468686	-2.237104	-0.712705
8	1	-2.453251	2.574769	0.550894
9	6	0.000017	1.473014	0.444335
10	6	1.245052	0.826482	0.221296
11	1	-0.000009	2.525436	0.716660
12	6	1.269977	-0.570908	-0.133674
13	6	0.000023	-1.366189	-0.072391
14	1	-0.000051	-2.184290	-0.797835
15	6	2.458819	-1.181853	-0.445794
16	6	3.697356	-0.481326	-0.408997
17	1	2.468725	-2.237159	-0.712334
18	6	3.691177	0.902020	-0.024717
19	6	2.459586	1.521480	0.278656
20	1	2.453263	2.574868	0.550522
21	8	-0.000499	-1.429356	2.292313
22	8	0.000109	-2.186443	1.218110
23	6	-4.928541	-1.103289	-0.728041
24	6	-6.112537	-0.396739	-0.671479
25	6	-4.929254	1.601614	0.023592
26	6	-6.110341	0.967405	-0.291982
27	6	4.928625	-1.103407	-0.727667
28	6	6.112597	-0.396831	-0.671253
29	6	6.110371	0.967421	-0.292093
30	6	4.929285	1.601693	0.023317
31	1	4.926478	2.649373	0.314383
32	1	7.048555	1.514086	-0.250539
33	1	7.051183	-0.885667	-0.916867
34	1	4.927118	-2.152040	-1.015945
35	1	-4.927040	-2.151850	-1.016585
36	1	-7.051100	-0.885546	-0.917240
37	1	-7.048529	1.514050	-0.250285
38	1	-4.926454	2.649224	0.314913

PENOXYTS-II_2.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.345534	-1.332563	-0.305763
2	6	-1.242035	-0.773751	0.285052
3	6	-1.240963	0.611831	0.661182
4	6	-2.373644	1.376544	0.452989
5	6	-3.527059	0.822362	-0.160107
6	6	-3.513472	-0.556819	-0.556247
7	1	-2.348157	-2.386394	-0.577136
8	1	-2.381871	2.426112	0.739276

9	6	-0.000001	1.110425	1.254590
10	6	1.240955	0.611835	0.661169
11	1	-0.000001	2.112834	1.677013
12	6	1.242027	-0.773746	0.285036
13	6	0.000000	-1.545483	0.671776
14	1	0.000000	-2.557799	0.255309
15	6	2.345520	-1.332555	-0.305794
16	6	3.513455	-0.556811	-0.556280
17	1	2.348133	-2.386381	-0.577187
18	6	3.527048	0.822369	-0.160124
19	6	2.373637	1.376549	0.452976
20	1	2.381860	2.426120	0.739256
21	8	0.000011	-0.220916	2.658096
22	8	0.000010	-1.725032	2.125784
23	6	-4.698143	1.590658	-0.400545
24	6	-5.803324	1.026339	-0.998020
25	6	-5.789470	-0.335244	-1.385388
26	6	-4.668407	-1.107220	-1.167686
27	6	4.668400	-1.107215	-1.167710
28	6	5.789484	-0.335249	-1.385384
29	6	4.698151	1.590654	-0.400521
30	6	5.803339	1.026327	-0.997996
31	1	-4.655378	-2.153760	-1.463269
32	1	-6.667046	-0.769756	-1.856075
33	1	-6.692126	1.626089	-1.174216
34	1	-4.707307	2.636286	-0.101922
35	1	4.655384	-2.153773	-1.463226
36	1	6.667045	-0.769752	-1.856111
37	1	6.692155	1.626069	-1.174150
38	1	4.707342	2.636265	-0.101835

PENOXYTRIPLETPRODUCT.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.402503	1.401336	0.211072
2	6	-1.270859	0.711668	0.583003
3	6	-1.270858	-0.711667	0.583003
4	6	-2.402502	-1.401335	0.211072
5	6	-3.581095	-0.716652	-0.182101
6	6	-3.581096	0.716654	-0.182101
7	1	-2.386447	2.487121	0.211981
8	1	-2.386446	-2.487120	0.211980
9	6	0.000001	-1.449308	1.006301
10	6	1.270860	-0.711668	0.583004
11	1	0.000001	-1.457863	2.130721
12	6	1.270860	0.711668	0.583004
13	6	0.000001	1.449308	1.006301
14	1	0.000001	1.457862	2.130722
15	6	2.402503	1.401337	0.211072
16	6	3.581095	0.716653	-0.182102
17	1	2.386447	2.487122	0.211980
18	6	3.581095	-0.716653	-0.182101
19	6	2.402503	-1.401337	0.211073
20	1	2.386447	-2.487122	0.211981

21	8	0.000002	-2.788078	0.759787
22	8	0.000001	2.788079	0.759787
23	6	4.760557	-1.404209	-0.577071
24	6	4.760556	1.404209	-0.577072
25	6	-4.760562	1.404210	-0.577072
26	6	-4.760554	-1.404209	-0.577070
27	6	-5.887419	-0.708782	-0.952546
28	6	-5.887418	0.708775	-0.952546
29	6	5.887416	0.708780	-0.952547
30	6	5.887416	-0.708779	-0.952547
31	1	-4.756648	-2.491534	-0.577398
32	1	-6.783710	-1.245096	-1.252131
33	1	-6.783729	1.245097	-1.252137
34	1	-4.756666	2.491533	-0.577403
35	1	4.756657	-2.491533	-0.577401
36	1	6.783708	-1.245094	-1.252132
37	1	6.783708	1.245094	-1.252133
38	1	4.756656	2.491533	-0.577402

PENTACENERINGOPENING_5.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.252286	-0.687579	0.663549
2	6	-1.234845	0.734817	0.598547
3	6	0.001581	1.381490	1.200606
4	6	1.253232	0.725088	0.624300
5	1	0.021929	2.469613	1.017345
6	6	1.240415	-0.699999	0.643659
7	6	0.003708	-1.317438	1.271401
8	1	-0.030630	-2.411812	1.142268
9	8	0.000448	1.241752	2.593473
10	8	-0.039672	-1.062522	2.645943
11	6	2.330864	1.404170	0.115226
12	6	2.304838	-1.407888	0.146141
13	6	3.438556	-0.735098	-0.392691
14	6	3.451881	0.698165	-0.407136
15	1	2.341198	2.492200	0.098294
16	1	2.296946	-2.496385	0.159243
17	6	-2.297048	1.411284	0.054271
18	6	-2.333322	-1.397758	0.204648
19	6	-3.431267	0.708067	-0.442293
20	6	-3.450101	-0.723527	-0.364008
21	1	-2.287650	2.498309	-0.000657
22	1	-2.345812	-2.484231	0.259713
23	6	4.581399	1.368124	-0.945574
24	6	5.651409	0.658668	-1.445475
25	6	4.556112	-1.436068	-0.915841
26	6	-4.581078	-1.423797	-0.860203
27	6	-4.546020	1.377058	-1.011458
28	6	-5.629804	0.668777	-1.482576
29	6	-5.647813	-0.744626	-1.406131
30	6	5.638578	-0.756464	-1.430499
31	1	4.544392	-2.523438	-0.902812
32	1	4.589190	2.455556	-0.954977

33	1	6.510475	1.184372	-1.853215
34	1	6.487810	-1.306054	-1.827244
35	1	-4.592136	-2.509494	-0.799492
36	1	-4.530932	2.462885	-1.068892
37	1	-6.476646	1.194273	-1.915391
38	1	-6.508291	-1.292427	-1.780298

PENTACENEH2ELIMINATION_1.LOG

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.431190	-1.405427	0.142672
2	6	1.272080	-0.712395	0.431703
3	6	1.277219	0.714473	0.446373
4	6	2.434103	1.399794	0.162234
5	6	3.634474	0.710700	-0.156060
6	6	3.633763	-0.724518	-0.160281
7	1	2.399629	-2.491124	0.143586
8	1	2.427577	2.485450	0.181842
9	6	-0.000505	1.446024	0.848311
10	6	-1.275781	0.713815	0.442865
11	1	0.018635	1.409383	1.970181
12	6	-1.275407	-0.712837	0.441085
13	6	-0.000711	-1.481652	0.671351
14	1	-0.027912	-1.034979	2.336740
15	6	-2.437167	-1.405213	0.159357
16	6	-3.637057	-0.723000	-0.150964
17	1	-2.407667	-2.490986	0.165803
18	6	-3.631951	0.712300	-0.165021
19	6	-2.429389	1.400342	0.147730
20	1	-2.417531	2.486181	0.155001
21	8	0.005608	2.789185	0.641263
22	8	-0.000226	-2.719549	0.745114
23	6	-4.833454	1.397892	-0.485291
24	6	-4.842868	-1.412171	-0.456418
25	6	4.837088	-1.414769	-0.473559
26	6	4.839066	1.395476	-0.467375
27	6	5.987681	0.697151	-0.765509
28	6	5.987659	-0.720747	-0.768707
29	6	-5.990789	-0.717098	-0.760380
30	6	-5.985152	0.700462	-0.774891
31	1	4.838867	2.482658	-0.465121
32	1	6.903328	1.232866	-1.000810
33	1	6.902371	-1.256640	-1.006398
34	1	4.829889	-2.501877	-0.475604
35	1	-4.828863	2.484986	-0.496798
36	1	-6.898418	1.236935	-1.017479
37	1	-6.907479	-1.252311	-0.991815
38	1	-4.840029	-2.499224	-0.445487