Efficiency of the $NICS_{zz}$-scan Curves to Probe the Antiaromaticity of Organic and Inorganic Rings/Cages

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Table S1.

Cartesian Coordinates, NICS-scan values and energies of selected antiaromatic organic and inorganic ring/cages computed at the B3LYP/GIAO/6-311+G(d,p)∪SDD(fourth and fifth row elements) level.

$[c\text{-}C_3H_3]^-$ (C_s), 1

```
Charge = -1 Multiplicity = 1
C,0,-0.9180347243,-0.5278646731,0.0140979881
C,0,0.6252229533,-0.364511879,-0.1715404683
C,0,-0.0250980219,0.7590459805,-0.2114140349
H,0,1.6022403287,-0.8052266143,0.0008484198
H,0,0.068141807,1.8297946556,-0.0678960719
H,0,-1.3524723427,-0.8123554698,-0.9740958327
```

Sum of electronic and zero-point Energies= -115.931848
Sum of electronic and thermal Energies= -115.927904
Sum of electronic and thermal Enthalpies= -115.926960
Sum of electronic and thermal Free Energies= -115.956210

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.0666	0.2554	-0.4553	0.2104	0.045
-4.9	-0.0686	0.2667	-0.4726	0.2208	0.0459
-4.8	-0.0705	0.2789	-0.4903	0.2318	0.0471
-4.7	-0.0721	0.292	-0.5084	0.2434	0.0486
-4.6	-0.0735	0.3064	-0.5269	0.2558	0.0506
-4.5	-0.0745	0.3223	-0.5457	0.269	0.0533
-4.4	-0.0749	0.3398	-0.5646	0.283	0.0568
-4.3	-0.0747	0.3595	-0.5837	0.298	0.0615
-4.2	-0.0737	0.3817	-0.6027	0.314	0.0677
-4.1	-0.0716	0.4068	-0.6215	0.3312	0.0756
-4	-0.0681	0.4355	-0.6399	0.3496	0.0859
-3.9	-0.063	0.4686	-0.6577	0.3696	0.099
-3.8	-0.0559	0.5069	-0.6747	0.3912	0.1157
-3.7	-0.0463	0.5513	-0.6903	0.4146	0.1367
-3.6	-0.0337	0.6031	-0.7043	0.4401	0.163
-3.5	-0.0174	0.6638	-0.7161	0.468	0.1958
-3.4	0.0033	0.7349	-0.725	0.4985	0.2364
-3.3	0.0293	0.8183	-0.7304	0.5318	0.2865
-3.2	0.0617	0.9162	-0.7312	0.5682	0.348
-3.1	0.1016	1.0311	-0.7264	0.608	0.4231
-3	0.1503	1.1657	-0.7147	0.6511	0.5146
-2.9	0.2095	1.323	-0.6944	0.6975	0.6255
-2.8	0.2807	1.506	-0.6639	0.7467	0.7593
-2.7	0.3658	1.7182	-0.621	0.798	0.9202
-2.6	0.4666	1.9629	-0.5631	0.8501	1.1128
-2.5	0.5852	2.2431	-0.4875	0.901	1.3421
-2.4	0.7237	2.5617	-0.3907	0.9478	1.6139

-2.3	0.8842	2.9214	-0.2687	0.9868	1.9346
-2.2	1.0693	3.3245	-0.1166	1.0134	2.3111
-2.1	1.2815	3.7732	0.0714	1.0218	2.7514
-2	1.524	4.2693	0.3027	1.0054	3.2639
-1.9	1.8003	4.8142	0.5866	0.9561	3.8581
-1.8	2.1142	5.408	0.9346	0.8643	4.5437
-1.7	2.4696	6.0478	1.361	0.7178	5.33
-1.6	2.8685	6.7233	1.8824	0.4996	6.2237
-1.5	3.3094	7.4113	2.517	0.1862	7.2251
-1.4	3.7827	8.0658	3.2823	-0.2567	8.3225
-1.3	4.2654	8.6053	4.191	-0.8765	9.4818
-1.2	4.714	8.8981	5.2438	-1.7363	10.6344
-1.1	5.0577	8.7514	6.4217	-2.911	11.6624
-1	5.195	7.9095	7.6756	-4.4767	12.3862
-0.9	4.9974	6.0739	8.9181	-6.4878	12.5617
-0.8	4.3245	2.9537	10.0198	-8.9426	11.8963
-0.7	3.0542	-1.6515	10.8143	-11.7448	10.0933
-0.6	1.1274	-7.7394	11.1216	-14.6739	6.9345
-0.5	-1.3968	-14.9944	10.8041	-17.3928	2.3984
-0.4	-4.2892	-22.7318	9.8641	-19.5221	-3.2097
-0.3	-7.1373	-29.9757	8.5638	-20.7926	-9.1831
-0.2	-9.4079	-35.7042	7.4804	-21.2179	-14.4863
-0.1	-10.5983	-39.1676	7.3727	-21.1449	-18.0227
0	-10.4146	-40.0711	8.8272	-21.0602	-19.0109
0.1	-8.8783	-38.5006	11.8658	-21.2328	-17.2678
0.2	-6.2981	-34.7269	15.8326	-21.4902	-13.2367
0.3	-3.1432	-29.1218	19.6922	-21.3484	-7.7734
0.4	0.1019	-22.2175	22.5232	-20.3718	-1.8457
0.5	3.0415	-14.7319	23.8562	-18.4441	3.7122
0.6	5.4179	-7.4506	23.7043	-15.7812	8.3306
0.7	7.1157	-1.0391	22.3862	-12.7679	11.7288
0.8	8.1367	4.0907	20.3193	-9.7802	13.8709
0.9	8.5633	7.8054	17.8846	-7.0847	14.8901
1	8.5212	10.1931	15.3705	-4.8168	15.0099
1.1	8.1471	11.4735	12.9677	-3.0056	14.4791
1.2	7.5662	11.9138	10.7849	-1.6132	13.527
1.3	6.8793	11.7685	8.8695	-0.5715	12.34
1.4	6.1587	11.248	7.228	0.1925	11.0555
1.5	5.4507	10.5092	5.8429	0.7429	9.7663
1.6	4.7819	9.6606	4.6852	1.1308	8.5298
1.7	4.165	8.7725	3.7225	1.3941	7.3784
1.8	3.6044	7.8892	2.924	1.5612	6.328
1.9	3.0998	7.0372	2.2622	1.6533	5.3839
2	2.6489	6.2325	1.7141	1.6872	4.5453
2.1	2.2483	5.4841	1.2607	1.6764	3.8077
2.2	1.8947	4.7976	0.8864	1.6328	3.1648
2.3	1.5845	4.1751	0.5783	1.566	2.6091
2.4	1.3143	3.617	0.3258	1.4843	2.1327
2.5	1.0806	3.1219	0.1199	1.3943	1.7276

2.6	0.88	2.6869	-0.0469	1.3013	1.3856
2.7	0.7091	2.3082	-0.1809	1.209	1.0992
2.8	0.5645	1.9813	-0.2878	1.1201	0.8612
2.9	0.443	1.7009	-0.3719	1.0361	0.6648
3	0.3416	1.4622	-0.4374	0.9581	0.5041
3.1	0.2575	1.2599	-0.4873	0.8863	0.3736
3.2	0.1883	1.0893	-0.5245	0.8208	0.2685
3.3	0.1316	0.946	-0.5512	0.7613	0.1847
3.4	0.0856	0.826	-0.5693	0.7074	0.1186
3.5	0.0484	0.7257	-0.5805	0.6587	0.067
3.6	0.0187	0.642	-0.5859	0.6146	0.0274
3.7	-0.0049	0.572	-0.5867	0.5746	-0.0026
3.8	-0.0234	0.5137	-0.5837	0.5384	-0.0247
3.9	-0.0377	0.4648	-0.5778	0.5054	-0.0406
4	-0.0486	0.4237	-0.5694	0.4753	-0.0516
4.1	-0.0567	0.3891	-0.5591	0.4478	-0.0587
4.2	-0.0625	0.3596	-0.5473	0.4225	-0.0629
4.3	-0.0666	0.3346	-0.5343	0.3993	-0.0647
4.4	-0.0692	0.3129	-0.5206	0.3778	-0.0649
4.5	-0.0707	0.294	-0.5062	0.3579	-0.0639
4.6	-0.0713	0.2774	-0.4914	0.3394	-0.062
4.7	-0.0712	0.2626	-0.4764	0.3221	-0.0595
4.8	-0.0706	0.2494	-0.4613	0.3061	-0.0567
4.9	-0.0696	0.2374	-0.4462	0.291	-0.0536
5	-0.0683	0.2264	-0.4312	0.2769	-0.0505

[*c*-C_4H_4] (D_{2h}), 2

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Charge =  0 Multiplicity = 1
 C,0,0.,0.78837095,-0.6668201
 C,0,0.,0.78837095,0.6668201
 C,0,0.,-0.78837095,0.6668201
 C,0,0.,-0.78837095,-0.6668201
 H,0,0.,-1.55266146,-1.43165058
 H,0,0.,1.55266146,-1.43165058
 H,0,0.,1.55266146,1.43165058
 H,0,0.,-1.55266146,1.43165058
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Sum of electronic and zero-point Energies= -154.660268
Sum of electronic and thermal Energies= -154.656487
Sum of electronic and thermal Enthalpies= -154.655543
Sum of electronic and thermal Free Energies= -154.684259

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.2061	0.4542	0.164	0.2633	0.1909
-4.9	0.2202	0.4779	0.1828	0.277	0.2009
-4.8	0.2358	0.5034	0.204	0.2917	0.2117
-4.7	0.2528	0.5305	0.228	0.3072	0.2233
-4.6	0.2716	0.5597	0.2551	0.3238	0.2359
-4.5	0.2923	0.5908	0.286	0.3414	0.2494
-4.4	0.3151	0.6244	0.3211	0.3603	0.2641
-4.3	0.3405	0.6603	0.3612	0.3803	0.28

-4.2	0.3686	0.6989	0.407	0.4016	0.2973
-4.1	0.4	0.7407	0.4595	0.4244	0.3163
-4	0.4351	0.7855	0.5197	0.4485	0.337
-3.9	0.4743	0.8339	0.5891	0.4742	0.3597
-3.8	0.5185	0.8863	0.6692	0.5015	0.3848
-3.7	0.5682	0.9428	0.7619	0.5304	0.4124
-3.6	0.6245	1.0039	0.8696	0.5608	0.4431
-3.5	0.6883	1.0701	0.9948	0.5928	0.4773
-3.4	0.761	1.1418	1.1411	0.6263	0.5155
-3.3	0.8439	1.2194	1.3123	0.6609	0.5585
-3.2	0.9389	1.3033	1.5133	0.6963	0.607
-3.1	1.0479	1.3939	1.7499	0.7318	0.6621
-3	1.1736	1.4914	2.0293	0.7664	0.725
-2.9	1.3186	1.5959	2.3598	0.7987	0.7972
-2.8	1.4862	1.707	2.7518	0.8264	0.8806
-2.7	1.6805	1.8237	3.2176	0.8465	0.9772
-2.6	1.9056	1.9447	3.7721	0.8549	1.0898
-2.5	2.1667	2.0671	4.4329	0.8457	1.2214
-2.4	2.4696	2.1874	5.2214	0.8116	1.3758
-2.3	2.821	2.3003	6.1627	0.7432	1.5571
-2.2	3.2287	2.3992	7.287	0.6289	1.7703
-2.1	3.7021	2.4761	8.6302	0.4548	2.0213
-2	4.2521	2.521	10.2354	0.2047	2.3163
-1.9	4.8923	2.523	12.154	-0.1397	2.6627
-1.8	5.6387	2.4692	14.447	-0.5987	3.0679
-1.7	6.5105	2.3444	17.187	-1.1946	3.539
-1.6	7.5292	2.13	20.4576	-1.9511	4.0811
-1.5	8.718	1.8014	24.3527	-2.8932	4.6946
-1.4	10.0986	1.3252	28.9707	-4.0451	5.3703
-1.3	11.6866	0.6549	34.4048	-5.4269	6.0818
-1.2	13.4841	-0.2723	40.7245	-7.0477	6.7754
-1.1	15.4713	-1.5359	47.9499	-8.8934	7.3575
-1	17.5972	-3.2263	56.018	-10.9095	7.6832
-0.9	19.7736	-5.428	64.7487	-12.9806	7.5526
-0.8	21.8766	-8.1912	73.8211	-14.9153	6.7241
-0.7	23.7599	-11.4952	82.7749	-16.4491	4.9539
-0.6	25.2792	-15.2176	91.0551	-17.2845	2.0669
-0.5	26.3279	-19.1241	98.1079	-17.1771	-1.947
-0.4	26.8742	-22.8971	103.5197	-16.0588	-6.8383
-0.3	26.9859	-26.1966	107.1544	-14.149	-12.0476
-0.2	26.8262	-28.7341	109.2127	-11.9779	-16.7562
-0.1	26.6073	-30.318	110.14	-10.2548	-20.0632
0	26.5105	-30.8545	110.3861	-9.5983	-21.2562
0.1	26.6073	-30.318	110.14	-10.2548	-20.0632
0.2	26.8262	-28.7341	109.2127	-11.9779	-16.7562
0.3	26.9859	-26.1966	107.1544	-14.149	-12.0476
0.4	26.8742	-22.8971	103.5197	-16.0588	-6.8383
0.5	26.3279	-19.1241	98.1079	-17.1771	-1.947
0.6	25.2792	-15.2176	91.0551	-17.2845	2.0669

0.7	23.7599	-11.4952	82.7749	-16.4491	4.9539
0.8	21.8766	-8.1912	73.8211	-14.9153	6.7241
0.9	19.7736	-5.428	64.7487	-12.9806	7.5526
1	17.5972	-3.2263	56.018	-10.9095	7.6832
1.1	15.4713	-1.5359	47.9499	-8.8934	7.3575
1.2	13.4841	-0.2723	40.7245	-7.0477	6.7754
1.3	11.6866	0.6549	34.4048	-5.4269	6.0818
1.4	10.0986	1.3252	28.9707	-4.0451	5.3703
1.5	8.718	1.8014	24.3527	-2.8932	4.6946
1.6	7.5292	2.13	20.4576	-1.9511	4.0811
1.7	6.5105	2.3444	17.187	-1.1946	3.539
1.8	5.6387	2.4692	14.447	-0.5987	3.0679
1.9	4.8923	2.523	12.154	-0.1397	2.6627
2	4.2521	2.521	10.2354	0.2047	2.3163
2.1	3.7021	2.4761	8.6302	0.4548	2.0213
2.2	3.2287	2.3992	7.287	0.6289	1.7703
2.3	2.821	2.3003	6.1627	0.7432	1.5571
2.4	2.4696	2.1874	5.2214	0.8116	1.3758
2.5	2.1667	2.0671	4.4329	0.8457	1.2214
2.6	1.9056	1.9447	3.7721	0.8549	1.0898
2.7	1.6805	1.8237	3.2176	0.8465	0.9772
2.8	1.4862	1.707	2.7518	0.8264	0.8806
2.9	1.3186	1.5959	2.3598	0.7987	0.7972
3	1.1736	1.4914	2.0293	0.7664	0.725
3.1	1.0479	1.3939	1.7499	0.7318	0.6621
3.2	0.9389	1.3033	1.5133	0.6963	0.607
3.3	0.8439	1.2194	1.3123	0.6609	0.5585
3.4	0.761	1.1418	1.1411	0.6263	0.5155
3.5	0.6883	1.0701	0.9948	0.5928	0.4773
3.6	0.6245	1.0039	0.8696	0.5608	0.4431
3.7	0.5682	0.9428	0.7619	0.5304	0.4124
3.8	0.5185	0.8863	0.6692	0.5015	0.3848
3.9	0.4743	0.8339	0.5891	0.4742	0.3597
4	0.4351	0.7855	0.5197	0.4485	0.337
4.1	0.4	0.7407	0.4595	0.4244	0.3163
4.2	0.3686	0.6989	0.407	0.4016	0.2973
4.3	0.3405	0.6603	0.3612	0.3803	0.28
4.4	0.3151	0.6244	0.3211	0.3603	0.2641
4.5	0.2923	0.5908	0.286	0.3414	0.2494
4.6	0.2716	0.5597	0.2551	0.3238	0.2359
4.7	0.2528	0.5305	0.228	0.3072	0.2233
4.8	0.2358	0.5034	0.204	0.2917	0.2117
4.9	0.2202	0.4779	0.1828	0.277	0.2009
5	0.2061	0.4542	0.164	0.2633	0.1909

cyclobutadienobenzene (C_{2v}), 3

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Charge =  0 Multiplicity = 1
C,0,0.,1.4431973825,-0.6215005236
C,0,0.,0.6885586071,-1.8417838617
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C,0,0.,-0.6885586071,-1.8417838617
C,0,0.,-1.4431973825,-0.6215005236
C,0,0.,-0.7108529147,0.5242911763
C,0,0.,0.7108529147,0.5242911763
C,0,0.,0.6749908281,2.0493492728
C,0,0.,-0.6749908281,2.0493492728
H,0,0.,2.5269127,-0.6420911655
H,0,0.,1.2199097141,-2.7868378435
H,0,0.,-1.2199097141,-2.7868378435
H,0,0.,-2.5269127,-0.6420911655
H,0,0.,1.4253716313,2.8277717652
H,0,0.,-1.4253716313,2.8277717652
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Sum of electronic and zero-point Energies= -308.328259
Sum of electronic and thermal Energies= -308.322519
Sum of electronic and thermal Enthalpies= -308.321575
Sum of electronic and thermal Free Energies= -308.357062

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.0294	0.6311	-0.5428	0.279	0.3521
-4.9	0.0347	0.6564	-0.5522	0.2889	0.3675
-4.8	0.0408	0.6831	-0.5607	0.2993	0.3838
-4.7	0.0478	0.7111	-0.5677	0.31	0.4011
-4.6	0.0557	0.7402	-0.5732	0.321	0.4192
-4.5	0.0648	0.7709	-0.5765	0.3324	0.4385
-4.4	0.0753	0.8031	-0.5773	0.3442	0.4589
-4.3	0.0873	0.8369	-0.575	0.3564	0.4805
-4.2	0.1011	0.8722	-0.569	0.3688	0.5034
-4.1	0.117	0.9094	-0.5583	0.3816	0.5278
-4	0.1354	0.9484	-0.5421	0.3947	0.5537
-3.9	0.1568	0.9895	-0.5192	0.4081	0.5814
-3.8	0.1815	1.0326	-0.4882	0.4216	0.611
-3.7	0.2103	1.0782	-0.4474	0.4354	0.6428
-3.6	0.2438	1.126	-0.3947	0.4491	0.6769
-3.5	0.283	1.1767	-0.3278	0.4629	0.7138
-3.4	0.3288	1.2301	-0.2436	0.4764	0.7537
-3.3	0.3827	1.2866	-0.1385	0.4895	0.7971
-3.2	0.446	1.3463	-0.0083	0.5018	0.8445
-3.1	0.5207	1.4096	0.1525	0.513	0.8966
-3	0.6088	1.4763	0.3501	0.5224	0.9539
-2.9	0.7129	1.5464	0.5924	0.529	1.0174
-2.8	0.836	1.6192	0.8887	0.5314	1.0878
-2.7	0.9814	1.6938	1.2503	0.5278	1.166
-2.6	1.1531	1.7685	1.6907	0.5154	1.2531
-2.5	1.3555	1.8401	2.2263	0.4903	1.3498
-2.4	1.5937	1.9046	2.8764	0.4477	1.4569
-2.3	1.8734	1.9559	3.6643	0.381	1.5749
-2.2	2.2012	1.9862	4.6176	0.282	1.7042
-2.1	2.5848	1.9852	5.7694	0.1407	1.8445
-2	3.0331	1.9403	7.1591	-0.0548	1.9951
-1.9	3.5568	1.8364	8.834	-0.3182	2.1546
-1.8	4.1684	1.655	10.8503	-0.6653	2.3203
-1.7	4.8826	1.3734	13.2745	-1.114	2.4874
-1.6	5.7159	0.9642	16.1835	-1.6841	2.6483
-1.5	6.6852	0.3918	19.6639	-2.398	2.7898
-1.4	7.8062	-0.3883	23.8069	-3.2795	2.8912
-1.3	9.0893	-1.432	28.6998	-4.3524	2.9204
-1.2	10.5346	-2.8055	34.4094	-5.6356	2.8301
-1.1	12.1265	-4.5795	40.959	-7.1342	2.5547

-1	13.8282	-6.8138	48.2983	-8.8254	2.0116
-0.9	15.5801	-9.5324	56.2726	-10.6398	1.1074
-0.8	17.3035	-12.6898	64.6005	-12.4451	-0.2447
-0.7	18.9108	-16.142	72.8744	-14.0424	-2.0996
-0.6	20.3197	-19.6386	80.5976	-15.1907	-4.4479
-0.5	21.469	-22.8596	87.2667	-15.6711	-7.1885
-0.4	22.3309	-25.499	92.4916	-15.3835	-10.1155
-0.3	22.9153	-27.3707	96.1167	-14.4392	-12.9315
-0.2	23.2654	-28.4801	98.2762	-13.1897	-15.2904
-0.1	23.4405	-28.9997	99.3213	-12.1355	-16.8642
0	23.4921	-29.1416	99.618	-11.7241	-17.4175
0.1	23.4405	-28.9997	99.3213	-12.1355	-16.8642
0.2	23.2654	-28.4801	98.2762	-13.1897	-15.2904
0.3	22.9153	-27.3707	96.1167	-14.4392	-12.9315
0.4	22.3309	-25.499	92.4916	-15.3835	-10.1155
0.5	21.469	-22.8596	87.2667	-15.6711	-7.1885
0.6	20.3197	-19.6386	80.5976	-15.1907	-4.4479
0.7	18.9108	-16.142	72.8744	-14.0424	-2.0996
0.8	17.3035	-12.6898	64.6005	-12.4451	-0.2447
0.9	15.5801	-9.5324	56.2726	-10.6398	1.1074
1	13.8282	-6.8138	48.2983	-8.8254	2.0116
1.1	12.1265	-4.5795	40.959	-7.1342	2.5547
1.2	10.5346	-2.8055	34.4094	-5.6356	2.8301
1.3	9.0893	-1.432	28.6998	-4.3524	2.9204
1.4	7.8062	-0.3883	23.8069	-3.2795	2.8912
1.5	6.6852	0.3918	19.6639	-2.398	2.7898
1.6	5.7159	0.9642	16.1835	-1.6841	2.6483
1.7	4.8826	1.3734	13.2745	-1.114	2.4874
1.8	4.1684	1.655	10.8503	-0.6653	2.3203
1.9	3.5568	1.8364	8.834	-0.3182	2.1546
2	3.0331	1.9403	7.1591	-0.0548	1.9951
2.1	2.5848	1.9852	5.7694	0.1407	1.8445
2.2	2.2012	1.9862	4.6176	0.282	1.7042
2.3	1.8734	1.9559	3.6643	0.381	1.5749
2.4	1.5937	1.9046	2.8764	0.4477	1.4569
2.5	1.3555	1.8401	2.2263	0.4903	1.3498
2.6	1.1531	1.7685	1.6907	0.5154	1.2531
2.7	0.9814	1.6938	1.2503	0.5278	1.166
2.8	0.836	1.6192	0.8887	0.5314	1.0878
2.9	0.7129	1.5464	0.5924	0.529	1.0174
3	0.6088	1.4763	0.3501	0.5224	0.9539
3.1	0.5207	1.4096	0.1525	0.513	0.8966
3.2	0.446	1.3463	-0.0083	0.5018	0.8445
3.3	0.3827	1.2866	-0.1385	0.4895	0.7971
3.4	0.3288	1.2301	-0.2436	0.4764	0.7537
3.5	0.283	1.1767	-0.3278	0.4629	0.7138
3.6	0.2438	1.126	-0.3947	0.4491	0.6769
3.7	0.2103	1.0782	-0.4474	0.4354	0.6428
3.8	0.1815	1.0326	-0.4882	0.4216	0.611
3.9	0.1568	0.9895	-0.5192	0.4081	0.5814
4	0.1354	0.9484	-0.5421	0.3947	0.5537
4.1	0.117	0.9094	-0.5583	0.3816	0.5278
4.2	0.1011	0.8722	-0.569	0.3688	0.5034
4.3	0.0873	0.8369	-0.575	0.3564	0.4805
4.4	0.0753	0.8031	-0.5773	0.3442	0.4589
4.5	0.0648	0.7709	-0.5765	0.3324	0.4385
4.6	0.0557	0.7402	-0.5732	0.321	0.4192
4.7	0.0478	0.7111	-0.5677	0.31	0.4011

4.8	0.0408	0.6831	-0.5607	0.2993	0.3838
4.9	0.0347	0.6564	-0.5522	0.2889	0.3675
5	0.0294	0.6311	-0.5428	0.279	0.3521

1,2,3,4,5,6-tricyclobutadieno[*a*,*c*,*e*]benzene (D_{3h}), 4

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Charge =  0 Multiplicity = 1
 C,0,0.,1.4248380752,0.025874802
 C,0,0.,0.6675433655,-1.2863346303
 C,0,0.,-0.6675433655,-1.2863346303
 C,0,0.,-1.4248380752,0.025874802
 C,0,0.,-0.7566159128,1.1817149071
 C,0,0.,0.7566159128,1.1817149071
 C,0,0.,0.6867597029,2.6523919039
 C,0,0.,-0.6867597029,2.6523919039
 C,0,0.,2.6629836538,-0.770394026
 C,0,0.,1.9765295805,-1.95993177
 H,0,0.,3.715404088,-0.5212096809
 H,0,0.,2.28820676,-2.9956018254
 H,0,0.,1.4286745695,3.4392593497
 H,0,0.,-1.4286745695,3.4392593497
 C,0,0.,-2.6629836538,-0.770394026
 C,0,0.,-1.9765295805,-1.95993177
 H,0,0.,-3.715404088,-0.5212096809
 H,0,0.,-2.28820676,-2.9956018254
```

Sum of electronic and zero-point Energies= -460.607798
Sum of electronic and thermal Energies= -460.599471
Sum of electronic and thermal Enthalpies= -460.598527
Sum of electronic and thermal Free Energies= -460.640173

NICS-scan (cyclobutadiene ring)

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.2223	0.6602	-1.327	0.3848	0.2754
-4.9	-0.2321	0.6854	-1.3817	0.4008	0.2846
-4.8	-0.2426	0.7117	-1.4394	0.4175	0.2942
-4.7	-0.2536	0.7394	-1.5003	0.4352	0.3042
-4.6	-0.2653	0.7686	-1.5646	0.4539	0.3147
-4.5	-0.2778	0.7991	-1.6325	0.4736	0.3255
-4.4	-0.291	0.8313	-1.7042	0.4945	0.3368
-4.3	-0.3051	0.865	-1.7802	0.5165	0.3485
-4.2	-0.32	0.9005	-1.8605	0.5398	0.3607
-4.1	-0.3359	0.9379	-1.9457	0.5645	0.3734
-4	-0.3528	0.9773	-2.0359	0.5907	0.3866
-3.9	-0.3709	1.019	-2.1317	0.6186	0.4004
-3.8	-0.3902	1.0627	-2.2333	0.6481	0.4146
-3.7	-0.4107	1.109	-2.3412	0.6796	0.4294
-3.6	-0.4327	1.1579	-2.4559	0.7131	0.4448
-3.5	-0.4562	1.2093	-2.5778	0.7487	0.4606
-3.4	-0.4812	1.2637	-2.7074	0.7868	0.4769
-3.3	-0.508	1.321	-2.845	0.8275	0.4935
-3.2	-0.5366	1.3814	-2.9912	0.8709	0.5105
-3.1	-0.5672	1.4449	-3.1464	0.9174	0.5275
-3	-0.5999	1.5112	-3.3107	0.9669	0.5443
-2.9	-0.6349	1.5799	-3.4845	1.0197	0.5602
-2.8	-0.6725	1.6502	-3.6676	1.0756	0.5746
-2.7	-0.713	1.7206	-3.8597	1.1345	0.5861
-2.6	-0.757	1.789	-4.0601	1.1958	0.5932
-2.5	-0.8052	1.8521	-4.2675	1.2588	0.5933
-2.4	-0.8582	1.9051	-4.4798	1.3219	0.5832
-2.3	-0.9173	1.9418	-4.6937	1.3832	0.5586

-2.2	-0.9834	1.9546	-4.9046	1.4403	0.5143
-2.1	-1.0575	1.9334	-5.1058	1.4898	0.4436
-2	-1.1404	1.8664	-5.2876	1.5276	0.3388
-1.9	-1.2322	1.7401	-5.4366	1.549	0.1911
-1.8	-1.332	1.5378	-5.5338	1.5478	-0.01
-1.7	-1.4377	1.2404	-5.5535	1.5168	-0.2764
-1.6	-1.5453	0.8242	-5.4601	1.4463	-0.6221
-1.5	-1.6491	0.2588	-5.2062	1.3232	-1.0644
-1.4	-1.7415	-0.4949	-4.7297	1.1291	-1.624
-1.3	-1.813	-1.4878	-3.9514	0.8385	-2.3263
-1.2	-1.8524	-2.7829	-2.7742	0.4169	-3.1998
-1.1	-1.846	-4.4523	-1.0857	-0.1791	-4.2732
-1	-1.7769	-6.5652	1.2345	-0.9986	-5.5666
-0.9	-1.6213	-9.1647	4.3008	-2.087	-7.0777
-0.8	-1.3462	-12.2364	8.1977	-3.471	-8.7654
-0.7	-0.9086	-15.674	12.9483	-5.1392	-10.5348
-0.6	-0.2634	-19.2646	18.4745	-7.0269	-12.2377
-0.5	0.6159	-22.7096	24.5574	-9.0116	-13.698
-0.4	1.7058	-25.6939	30.8114	-10.9288	-14.7651
-0.3	2.9032	-27.9827	36.6924	-12.6044	-15.3783
-0.2	4.0203	-29.4974	41.5583	-13.8917	-15.6057
-0.1	4.8243	-30.3135	44.7863	-14.6946	-15.6189
0	5.1182	-30.5642	45.9186	-14.9665	-15.5977
0.1	4.8243	-30.3135	44.7863	-14.6946	-15.6189
0.2	4.0203	-29.4974	41.5583	-13.8917	-15.6057
0.3	2.9032	-27.9827	36.6924	-12.6044	-15.3783
0.4	1.7058	-25.6939	30.8114	-10.9288	-14.7651
0.5	0.6159	-22.7096	24.5574	-9.0116	-13.698
0.6	-0.2634	-19.2646	18.4745	-7.0269	-12.2377
0.7	-0.9086	-15.674	12.9483	-5.1392	-10.5348
0.8	-1.3462	-12.2364	8.1977	-3.471	-8.7654
0.9	-1.6213	-9.1647	4.3008	-2.087	-7.0777
1	-1.7769	-6.5652	1.2345	-0.9986	-5.5666
1.1	-1.846	-4.4523	-1.0857	-0.1791	-4.2732
1.2	-1.8524	-2.7829	-2.7742	0.4169	-3.1998
1.3	-1.813	-1.4878	-3.9514	0.8385	-2.3263
1.4	-1.7415	-0.4949	-4.7297	1.1291	-1.624
1.5	-1.6491	0.2588	-5.2062	1.3232	-1.0644
1.6	-1.5453	0.8242	-5.4601	1.4463	-0.6221
1.7	-1.4377	1.2404	-5.5535	1.5168	-0.2764
1.8	-1.332	1.5378	-5.5338	1.5478	-0.01
1.9	-1.2322	1.7401	-5.4366	1.549	0.1911
2	-1.1404	1.8664	-5.2876	1.5276	0.3388
2.1	-1.0575	1.9334	-5.1058	1.4898	0.4436
2.2	-0.9834	1.9546	-4.9046	1.4403	0.5143
2.3	-0.9173	1.9418	-4.6937	1.3832	0.5586
2.4	-0.8582	1.9051	-4.4798	1.3219	0.5832
2.5	-0.8052	1.8521	-4.2675	1.2588	0.5933
2.6	-0.757	1.789	-4.0601	1.1958	0.5932
2.7	-0.713	1.7206	-3.8597	1.1345	0.5861
2.8	-0.6725	1.6502	-3.6676	1.0756	0.5746
2.9	-0.6349	1.5799	-3.4845	1.0197	0.5602
3	-0.5999	1.5112	-3.3107	0.9669	0.5443
3.1	-0.5672	1.4449	-3.1464	0.9174	0.5275
3.2	-0.5366	1.3814	-2.9912	0.8709	0.5105
3.3	-0.508	1.321	-2.845	0.8275	0.4935
3.4	-0.4812	1.2637	-2.7074	0.7868	0.4769
3.5	-0.4562	1.2093	-2.5778	0.7487	0.4606

3.6	-0.4327	1.1579	-2.4559	0.7131	0.4448
3.7	-0.4107	1.109	-2.3412	0.6796	0.4294
3.8	-0.3902	1.0627	-2.2333	0.6481	0.4146
3.9	-0.3709	1.019	-2.1317	0.6186	0.4004
4	-0.3528	0.9773	-2.0359	0.5907	0.3866
4.1	-0.3359	0.9379	-1.9457	0.5645	0.3734
4.2	-0.32	0.9005	-1.8605	0.5398	0.3607
4.3	-0.3051	0.865	-1.7802	0.5165	0.3485
4.4	-0.291	0.8313	-1.7042	0.4945	0.3368
4.5	-0.2778	0.7991	-1.6325	0.4736	0.3255
4.6	-0.2653	0.7686	-1.5646	0.4539	0.3147
4.7	-0.2536	0.7394	-1.5003	0.4352	0.3042
4.8	-0.2426	0.7117	-1.4394	0.4175	0.2942
4.9	-0.2321	0.6854	-1.3817	0.4008	0.2846
5	-0.2223	0.6602	-1.327	0.3848	0.2754

butalene (D_{2h}), 5

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Charge =  0 Multiplicity = 1
 C,0,1.39089903,-0.72594362,0.
 C,0,1.39089903,0.72594362,0.
 C,0,0.,0.78453918,0.
 C,0,0.,-0.78453918,0.
 C,0,-1.39089903,0.72594362,0.
 C,0,-1.39089903,-0.72594362,0.
 H,0,-2.18018729,1.47265685,0.
 H,0,-2.18018729,-1.47265685,0.
 H,0,2.18018729,-1.47265685,0.
 H,0,2.18018729,1.47265685,0.
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Sum of electronic and zero-point Energies= -230.804027
Sum of electronic and thermal Energies= -230.799279
Sum of electronic and thermal Enthalpies= -230.798335
Sum of electronic and thermal Free Energies= -230.830342

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.3279	0.5111	-1.4947	0.3676	0.1435
-4.9	-0.347	0.5357	-1.5768	0.3868	0.1489
-4.8	-0.3676	0.5618	-1.6647	0.4072	0.1546
-4.7	-0.3899	0.5895	-1.7592	0.429	0.1605
-4.6	-0.4139	0.619	-1.8606	0.4523	0.1667
-4.5	-0.4398	0.6503	-1.9698	0.4772	0.1731
-4.4	-0.468	0.6836	-2.0875	0.5038	0.1798
-4.3	-0.4984	0.719	-2.2143	0.5322	0.1868
-4.2	-0.5316	0.7566	-2.3513	0.5625	0.1941
-4.1	-0.5676	0.7966	-2.4994	0.5949	0.2017
-4	-0.6068	0.8393	-2.6596	0.6296	0.2097
-3.9	-0.6495	0.8847	-2.8334	0.6667	0.218
-3.8	-0.6963	0.9331	-3.0219	0.7063	0.2268
-3.7	-0.7474	0.9847	-3.2268	0.7486	0.2361
-3.6	-0.8034	1.0395	-3.4497	0.7936	0.2459
-3.5	-0.8649	1.0979	-3.6926	0.8415	0.2564
-3.4	-0.9325	1.16	-3.9576	0.8923	0.2677
-3.3	-1.0071	1.226	-4.2471	0.9461	0.2799
-3.2	-1.0893	1.2958	-4.5638	1.0025	0.2933

-3.1	-1.1803	1.3697	-4.9106	1.0614	0.3083
-3	-1.2813	1.4471	-5.2909	1.122	0.3251
-2.9	-1.3935	1.5277	-5.7082	1.1835	0.3442
-2.8	-1.5187	1.6106	-6.1667	1.2444	0.3662
-2.7	-1.6587	1.6943	-6.6705	1.3026	0.3917
-2.6	-1.816	1.7765	-7.2244	1.3551	0.4214
-2.5	-1.9931	1.8539	-7.8331	1.3978	0.4561
-2.4	-2.1932	1.9221	-8.5017	1.4253	0.4968
-2.3	-2.4199	1.9751	-9.2349	1.4308	0.5443
-2.2	-2.6771	2.0058	-10.0371	1.4058	0.6
-2.1	-2.9688	2.0053	-10.9116	1.34	0.6653
-2	-3.2988	1.9636	-11.8601	1.2214	0.7422
-1.9	-3.6708	1.869	-12.8814	1.036	0.833
-1.8	-4.0873	1.7082	-13.9703	0.7678	0.9404
-1.7	-4.5495	1.4659	-15.1145	0.3986	1.0673
-1.6	-5.0565	1.1228	-16.2924	-0.0926	1.2154
-1.5	-5.6048	0.6537	-17.468	-0.7297	1.3834
-1.4	-6.1871	0.0246	-18.5857	-1.5394	1.564
-1.3	-6.7915	-0.8114	-19.563	-2.5497	1.7383
-1.2	-7.3998	-1.9161	-20.2834	-3.7859	1.8698
-1.1	-7.9851	-3.3653	-20.59	-5.2625	1.8972
-1	-8.5085	-5.2407	-20.2849	-6.9698	1.7291
-0.9	-8.9152	-7.6083	-19.1373	-8.8553	1.247
-0.8	-9.1318	-10.487	-16.9084	-10.8056	0.3186
-0.7	-9.0698	-13.8111	-13.3984	-12.6391	-1.172
-0.6	-8.6412	-17.4051	-8.5186	-14.1238	-3.2813
-0.5	-7.7919	-20.9925	-2.3831	-15.0332	-5.9593
-0.4	-6.5485	-24.25	4.6044	-15.2365	-9.0135
-0.3	-5.0617	-26.8965	11.7113	-14.7906	-12.1059
-0.2	-3.6103	-28.7726	17.9416	-13.9756	-14.797
-0.1	-2.5407	-29.8586	22.2365	-13.2193	-16.6393
0	-2.146	-30.2103	23.7723	-12.9146	-17.2957
0.1	-2.5417	-29.8617	22.2366	-13.2211	-16.6406
0.2	-3.6123	-28.7785	17.9417	-13.9789	-14.7996
0.3	-5.0645	-26.9048	11.7112	-14.795	-12.1098
0.4	-6.5521	-24.2602	4.604	-15.2417	-9.0185
0.5	-7.7958	-21.0037	-2.3838	-15.0388	-5.9649
0.6	-8.6453	-17.4162	-8.5195	-14.1292	-3.287
0.7	-9.0736	-13.8214	-13.3994	-12.6442	-1.1772
0.8	-9.1351	-10.496	-16.9094	-10.8101	0.3141
0.9	-8.9179	-7.6156	-19.1381	-8.8592	1.2436
1	-8.5106	-5.2464	-20.2855	-6.9732	1.7268
1.1	-7.9866	-3.3695	-20.5903	-5.2654	1.8959
1.2	-7.4007	-1.9189	-20.2833	-3.7883	1.8694
1.3	-6.7919	-0.8132	-19.5627	-2.5518	1.7386
1.4	-6.1871	0.0237	-18.5851	-1.5412	1.5649
1.5	-5.6046	0.6535	-17.4671	-0.7313	1.3848
1.6	-5.0561	1.123	-16.2913	-0.094	1.217
1.7	-4.5489	1.4666	-15.1133	0.3974	1.0692

1.8	-4.0866	1.7091	-13.9689	0.7667	0.9424
1.9	-3.67	1.8699	-12.8801	1.035	0.8349
2	-3.298	1.9646	-11.8586	1.2205	0.7441
2.1	-2.9679	2.0064	-10.9101	1.3392	0.6672
2.2	-2.6763	2.0068	-10.0356	1.405	0.6018
2.3	-2.4191	1.9761	-9.2335	1.4301	0.546
2.4	-2.1924	1.9231	-8.5003	1.4247	0.4984
2.5	-1.9923	1.8548	-7.8318	1.3972	0.4576
2.6	-1.8153	1.7773	-7.2231	1.3545	0.4228
2.7	-1.6581	1.695	-6.6693	1.3021	0.3929
2.8	-1.5181	1.6113	-6.1655	1.244	0.3673
2.9	-1.393	1.5283	-5.7071	1.1831	0.3452
3	-1.2808	1.4476	-5.2898	1.1216	0.326
3.1	-1.1799	1.3701	-4.9096	1.061	0.3091
3.2	-1.0889	1.2962	-4.5629	1.0022	0.294
3.3	-1.0066	1.2263	-4.2462	0.9458	0.2805
3.4	-0.9322	1.1603	-3.9568	0.8921	0.2682
3.5	-0.8645	1.0982	-3.6918	0.8413	0.2569
3.6	-0.8031	1.0398	-3.449	0.7934	0.2464
3.7	-0.7471	0.9848	-3.2261	0.7483	0.2365
3.8	-0.696	0.9333	-3.0212	0.7061	0.2272
3.9	-0.6493	0.8849	-2.8328	0.6665	0.2184
4	-0.6065	0.8395	-2.6591	0.6295	0.21
4.1	-0.5673	0.7968	-2.4988	0.5948	0.202
4.2	-0.5314	0.7568	-2.3508	0.5624	0.1944
4.3	-0.4983	0.719	-2.2138	0.532	0.187
4.4	-0.4678	0.6836	-2.087	0.5036	0.18
4.5	-0.4397	0.6504	-1.9694	0.4771	0.1733
4.6	-0.4137	0.6191	-1.8602	0.4522	0.1669
4.7	-0.3897	0.5897	-1.7588	0.429	0.1607
4.8	-0.3675	0.5619	-1.6644	0.4071	0.1548
4.9	-0.3469	0.5358	-1.5764	0.3867	0.1491
5	-0.3278	0.5111	-1.4944	0.3675	0.1436

o-benzyne diradical, $^1A_1$ (C_{2v})

```
Charge =  0 Multiplicity = 1
 C,0,-0.7026250139,1.0572200238,0.0000417353
 C,0,-1.4584472488,-0.1337253268,0.0000059006
 C,0,-0.6224101244,-1.2351834872,-0.0000590145
 C,0,0.6222709581,-1.2352326707,-0.0000590145
 C,0,1.4584375134,-0.1338792353,0.0000058984
 C,0,0.702739721,1.0571470344,0.0000417327
 H,0,-1.228631082,2.0077158498,0.000069835
 H,0,-2.541608554,-0.1365540654,-0.0000015491
 H,0,2.5415980916,-0.1368269748,-0.000001551
 H,0,1.2288467118,2.0075871612,0.0000698378
```

Sum of electronic and zero-point Energies= -230.890737
Sum of electronic and thermal Energies= -230.886264
Sum of electronic and thermal Enthalpies= -230.885320
Sum of electronic and thermal Free Energies= -230.918088

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.4371	0.7479	-2.0593	0.3853	0.3626
-4.9	-0.4635	0.7846	-2.1753	0.4043	0.3803
-4.8	-0.4921	0.8236	-2.3	0.4245	0.3991
-4.7	-0.523	0.8649	-2.434	0.4459	0.419
-4.6	-0.5566	0.9086	-2.5783	0.4685	0.4401
-4.5	-0.593	0.9549	-2.7338	0.4925	0.4624
-4.4	-0.6326	1.0038	-2.9016	0.5179	0.4859
-4.3	-0.6757	1.0557	-3.0829	0.5449	0.5108
-4.2	-0.7228	1.1105	-3.279	0.5734	0.5371
-4.1	-0.7743	1.1685	-3.4914	0.6036	0.5649
-4	-0.8307	1.2296	-3.7216	0.6355	0.5941
-3.9	-0.8925	1.2939	-3.9715	0.6691	0.6248
-3.8	-0.9605	1.3615	-4.2431	0.7045	0.657
-3.7	-1.0354	1.4325	-4.5385	0.7418	0.6907
-3.6	-1.118	1.5066	-4.8604	0.7809	0.7257
-3.5	-1.2093	1.5837	-5.2115	0.8217	0.762
-3.4	-1.3104	1.6635	-5.5947	0.8641	0.7994
-3.3	-1.4226	1.7456	-6.0136	0.9081	0.8375
-3.2	-1.5475	1.8294	-6.4718	0.9533	0.8761
-3.1	-1.6865	1.914	-6.9735	0.9994	0.9146
-3	-1.8417	1.9982	-7.5232	1.046	0.9522
-2.9	-2.0152	2.0803	-8.1258	1.0923	0.988
-2.8	-2.2094	2.1584	-8.7867	1.1376	1.0208
-2.7	-2.4273	2.2297	-9.5115	1.1807	1.049
-2.6	-2.6718	2.2907	-10.3062	1.2203	1.0704
-2.5	-2.9466	2.3371	-11.177	1.2546	1.0825
-2.4	-3.2555	2.3635	-12.13	1.2814	1.0821
-2.3	-3.6026	2.3635	-13.1713	1.2983	1.0652
-2.2	-3.9924	2.3291	-14.3062	1.302	1.0271
-2.1	-4.4293	2.2513	-15.5391	1.2891	0.9622
-2	-4.9177	2.1195	-16.8725	1.2555	0.864
-1.9	-5.4615	1.9221	-18.3066	1.1969	0.7252
-1.8	-6.0639	1.6461	-19.8379	1.1085	0.5376
-1.7	-6.727	1.2772	-21.4581	0.9854	0.2918
-1.6	-7.4507	0.8001	-23.1523	0.8223	-0.0222
-1.5	-8.2331	0.1986	-24.8978	0.6142	-0.4156
-1.4	-9.0689	-0.545	-26.6617	0.3555	-0.9005
-1.3	-9.9498	-1.4492	-28.4001	0.0405	-1.4897
-1.2	-10.8635	-2.5335	-30.0568	-0.337	-2.1965
-1.1	-11.7942	-3.8174	-31.5652	-0.7842	-3.0332
-1	-12.7229	-5.3178	-32.8507	-1.3084	-4.0094
-0.9	-13.6282	-7.0458	-33.8388	-1.917	-5.1288
-0.8	-14.4881	-8.9995	-34.4647	-2.6145	-6.385
-0.7	-15.2814	-11.1558	-34.6883	-3.3989	-7.7569
-0.6	-15.9896	-13.4606	-34.5082	-4.2569	-9.2037
-0.5	-16.5985	-15.8214	-33.9743	-5.1583	-10.6631
-0.4	-17.0988	-18.1053	-33.1912	-6.0527	-12.0526
-0.3	-17.4862	-20.1485	-32.3101	-6.8716	-13.2769
-0.2	-17.7603	-21.7747	-31.5062	-7.536	-14.2387
-0.1	-17.9232	-22.8254	-30.9443	-7.9712	-14.8542
0	-17.9772	-23.1887	-30.7428	-8.1228	-15.0659
0.1	-17.9231	-22.8246	-30.9448	-7.971	-14.8536
0.2	-17.7602	-21.7735	-31.5071	-7.5358	-14.2377
0.3	-17.4861	-20.1468	-32.3114	-6.8713	-13.2755
0.4	-17.0987	-18.1033	-33.1927	-6.0524	-12.0509
0.5	-16.5984	-15.8192	-33.9758	-5.1581	-10.6611
0.6	-15.9894	-13.4587	-34.5097	-4.257	-9.2017

0.7	-15.2812	-11.154	-34.6896	-3.3991	-7.7549
0.8	-14.4879	-8.9979	-34.4658	-2.6148	-6.3831
0.9	-13.628	-7.0444	-33.8396	-1.9175	-5.1269
1	-12.7227	-5.3166	-32.8513	-1.3089	-4.0077
1.1	-11.794	-3.8164	-31.5655	-0.7847	-3.0317
1.2	-10.8632	-2.5328	-30.057	-0.3376	-2.1952
1.3	-9.9495	-1.4486	-28.4	0.04	-1.4886
1.4	-9.0687	-0.5445	-26.6615	0.355	-0.8995
1.5	-8.2328	0.199	-24.8975	0.6137	-0.4147
1.6	-7.4505	0.8004	-23.152	0.8219	-0.0215
1.7	-6.7267	1.2774	-21.4576	0.985	0.2924
1.8	-6.0637	1.6462	-19.8374	1.1082	0.538
1.9	-5.4613	1.9222	-18.3061	1.1966	0.7256
2	-4.9175	2.1196	-16.872	1.2553	0.8643
2.1	-4.4291	2.2513	-15.5386	1.2889	0.9624
2.2	-3.9922	2.3291	-14.3058	1.3018	1.0273
2.3	-3.6025	2.3634	-13.1709	1.2981	1.0653
2.4	-3.2554	2.3635	-12.1296	1.2813	1.0822
2.5	-2.9465	2.337	-11.1766	1.2544	1.0826
2.6	-2.6717	2.2906	-10.3058	1.2201	1.0705
2.7	-2.4272	2.2296	-9.5111	1.1806	1.049
2.8	-2.2094	2.1583	-8.7864	1.1374	1.0209
2.9	-2.0151	2.0803	-8.1255	1.0922	0.9881
3	-1.8416	1.9981	-7.5229	1.0459	0.9522
3.1	-1.6865	1.9139	-6.9732	0.9993	0.9146
3.2	-1.5474	1.8293	-6.4716	0.9532	0.8761
3.3	-1.4226	1.7455	-6.0134	0.908	0.8375
3.4	-1.3104	1.6635	-5.5945	0.8641	0.7994
3.5	-1.2092	1.5836	-5.2113	0.8216	0.762
3.6	-1.1179	1.5065	-4.8603	0.7808	0.7257
3.7	-1.0353	1.4323	-4.5384	0.7417	0.6906
3.8	-0.9605	1.3615	-4.2429	0.7045	0.657
3.9	-0.8925	1.2938	-3.9714	0.669	0.6248
4	-0.8307	1.2295	-3.7215	0.6354	0.5941
4.1	-0.7743	1.1684	-3.4913	0.6035	0.5649
4.2	-0.7228	1.1104	-3.2789	0.5733	0.5371
4.3	-0.6757	1.0556	-3.0828	0.5448	0.5108
4.4	-0.6326	1.0038	-2.9015	0.5179	0.4859
4.5	-0.593	0.9549	-2.7337	0.4925	0.4624
4.6	-0.5566	0.9086	-2.5782	0.4685	0.4401
4.7	-0.523	0.8648	-2.4339	0.4458	0.419
4.8	-0.4921	0.8236	-2.2999	0.4245	0.3991
4.9	-0.4635	0.7846	-2.1753	0.4043	0.3803
5	-0.4371	0.7479	-2.0593	0.3853	0.3626

o-benzyne diradical, $^3A_1$ (C_{2v})

```
Charge =  0 Multiplicity = 3
 C,0,-1.3924633571,-0.0170713447,0.0000192104
 C,0,-0.7130958557,1.2128282222,0.0001116428
 C,0,0.6626172483,1.2046630531,0.0001307777
 C,0,1.3748968133,0.0045209519,0.0001307705
 C,0,0.7231119534,-1.207009485,0.0001116582
 C,0,-0.6819356327,-1.2142712304,0.0000192142
 H,0,-2.4767730918,-0.0284240267,-0.0000403141
 H,0,-1.2610081016,2.1506799901,0.0000786787
 H,0,1.2839627411,-2.1371847477,0.0000786805
 H,0,-1.2113127172,-2.1606313829,-0.0000403188
```

Sum of electronic and zero-point Energies= -230.847931

Sum of electronic and thermal Energies= -230.843526
Sum of electronic and thermal Enthalpies= -230.842581
Sum of electronic and thermal Free Energies= -230.876314

NICS-scan

Distance	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.4569	0.5903	-1.9609	0.2247	0.3656
-4.9	-0.4845	0.6186	-2.0719	0.2346	0.384
-4.8	-0.5142	0.6485	-2.1912	0.245	0.4035
-4.7	-0.5465	0.6801	-2.3196	0.2559	0.4242
-4.6	-0.5814	0.7135	-2.4578	0.2673	0.4462
-4.5	-0.6194	0.7487	-2.6068	0.2792	0.4695
-4.4	-0.6606	0.7859	-2.7676	0.2915	0.4944
-4.3	-0.7055	0.8249	-2.9415	0.3042	0.5207
-4.2	-0.7545	0.866	-3.1296	0.3173	0.5487
-4.1	-0.808	0.9092	-3.3334	0.3308	0.5784
-4	-0.8666	0.9544	-3.5544	0.3446	0.6098
-3.9	-0.9309	1.0017	-3.7943	0.3586	0.6431
-3.8	-1.0014	1.051	-4.0552	0.3726	0.6784
-3.7	-1.0791	1.1019	-4.3391	0.3864	0.7155
-3.6	-1.1647	1.1544	-4.6485	0.3998	0.7546
-3.5	-1.2593	1.2083	-4.986	0.4126	0.7957
-3.4	-1.3639	1.2628	-5.3546	0.4242	0.8386
-3.3	-1.48	1.3175	-5.7575	0.4343	0.8832
-3.2	-1.6089	1.3714	-6.1982	0.442	0.9294
-3.1	-1.7524	1.4234	-6.6807	0.4467	0.9767
-3	-1.9124	1.4719	-7.2093	0.4472	1.0247
-2.9	-2.0911	1.5151	-7.7886	0.4423	1.0728
-2.8	-2.291	1.5504	-8.4235	0.4304	1.12
-2.7	-2.5149	1.5746	-9.1192	0.4095	1.1651
-2.6	-2.7658	1.5837	-9.8812	0.377	1.2067
-2.5	-3.0474	1.5727	-10.7148	0.33	1.2427
-2.4	-3.3632	1.5356	-11.6253	0.2648	1.2708
-2.3	-3.7174	1.4649	-12.6172	0.177	1.2879
-2.2	-4.1141	1.3522	-13.6945	0.0616	1.2906
-2.1	-4.5574	1.1871	-14.8593	-0.0876	1.2747
-2	-5.051	0.9584	-16.1115	-0.2772	1.2356
-1.9	-5.5981	0.6533	-17.4476	-0.5151	1.1684
-1.8	-6.2008	0.2573	-18.8596	-0.8101	1.0674
-1.7	-6.8593	-0.2445	-20.3335	-1.1716	0.9271
-1.6	-7.5719	-0.8686	-21.8471	-1.6103	0.7417
-1.5	-8.3335	-1.632	-23.3684	-2.1374	0.5054
-1.4	-9.1353	-2.552	-24.8539	-2.765	0.213
-1.3	-9.9642	-3.6459	-26.2465	-3.5055	-0.1404
-1.2	-10.8019	-4.9297	-27.4759	-4.371	-0.5587
-1.1	-11.6253	-6.4161	-28.4598	-5.3722	-1.0439
-1	-12.407	-8.1114	-29.1095	-6.5161	-1.5953
-0.9	-13.1169	-10.0117	-29.3392	-7.8036	-2.2081
-0.8	-13.7256	-12.0966	-29.0801	-9.2249	-2.8717
-0.7	-14.2079	-14.3238	-28.2999	-10.7554	-3.5684
-0.6	-14.5487	-16.6241	-27.0221	-12.3512	-4.2729
-0.5	-14.7474	-18.9001	-25.342	-13.9467	-4.9534
-0.4	-14.821	-21.0305	-23.4326	-15.4564	-5.5741
-0.3	-14.8038	-22.8805	-21.5311	-16.7811	-6.0994
-0.2	-14.7415	-24.3175	-19.9069	-17.8194	-6.4981
-0.1	-14.6805	-25.2301	-18.8113	-18.4831	-6.747
0	-14.6557	-25.5431	-18.4241	-18.7115	-6.8316
0.1	-14.6803	-25.2305	-18.8105	-18.4832	-6.7473

0.2	-14.7412	-24.3183	-19.9054	-17.8195	-6.4988
0.3	-14.8036	-22.8814	-21.5292	-16.7811	-6.1003
0.4	-14.8207	-21.0317	-23.4305	-15.4564	-5.5753
0.5	-14.7471	-18.9015	-25.3399	-13.9466	-4.9549
0.6	-14.5486	-16.6255	-27.0202	-12.351	-4.2745
0.7	-14.2079	-14.3253	-28.2984	-10.7552	-3.5701
0.8	-13.7257	-12.098	-29.079	-9.2246	-2.8734
0.9	-13.1172	-10.0131	-29.3385	-7.8033	-2.2098
1	-12.4073	-8.1126	-29.1092	-6.5157	-1.5969
1.1	-11.6257	-6.4171	-28.4599	-5.3718	-1.0453
1.2	-10.8023	-4.9306	-27.4763	-4.3706	-0.56
1.3	-9.9646	-3.6467	-26.2471	-3.5051	-0.1416
1.4	-9.1358	-2.5526	-24.8546	-2.7646	0.212
1.5	-8.3339	-1.6326	-23.3693	-2.1371	0.5045
1.6	-7.5723	-0.8691	-21.848	-1.61	0.7409
1.7	-6.8598	-0.2449	-20.3344	-1.1713	0.9264
1.8	-6.2012	0.2571	-18.8605	-0.8098	1.0669
1.9	-5.5985	0.653	-17.4485	-0.5149	1.1679
2	-5.0513	0.9583	-16.1123	-0.277	1.2353
2.1	-4.5577	1.1871	-14.8601	-0.0873	1.2744
2.2	-4.1144	1.3521	-13.6953	0.0617	1.2904
2.3	-3.7177	1.4649	-12.618	0.1772	1.2877
2.4	-3.3634	1.5356	-11.6259	0.2649	1.2707
2.5	-3.0476	1.5727	-10.7154	0.3301	1.2426
2.6	-2.766	1.5837	-9.8818	0.3771	1.2066
2.7	-2.515	1.5747	-9.1197	0.4096	1.1651
2.8	-2.2911	1.5505	-8.424	0.4306	1.1199
2.9	-2.0913	1.5153	-7.789	0.4425	1.0728
3	-1.9125	1.472	-7.2097	0.4473	1.0247
3.1	-1.7525	1.4235	-6.6811	0.4468	0.9767
3.2	-1.609	1.3715	-6.1985	0.4421	0.9294
3.3	-1.4801	1.3175	-5.7578	0.4343	0.8832
3.4	-1.364	1.2629	-5.3549	0.4243	0.8386
3.5	-1.2593	1.2084	-4.9863	0.4127	0.7957
3.6	-1.1647	1.1545	-4.6488	0.3999	0.7546
3.7	-1.0791	1.102	-4.3394	0.3865	0.7155
3.8	-1.0015	1.051	-4.0554	0.3726	0.6784
3.9	-0.9309	1.0018	-3.7945	0.3586	0.6432
4	-0.8667	0.9545	-3.5545	0.3447	0.6098
4.1	-0.8081	0.9093	-3.3335	0.3309	0.5784
4.2	-0.7545	0.8661	-3.1297	0.3174	0.5487
4.3	-0.7056	0.825	-2.9416	0.3043	0.5207
4.4	-0.6606	0.7859	-2.7678	0.2915	0.4944
4.5	-0.6194	0.7488	-2.6069	0.2792	0.4696
4.6	-0.5814	0.7136	-2.4579	0.2674	0.4462
4.7	-0.5465	0.6802	-2.3197	0.256	0.4242
4.8	-0.5143	0.6486	-2.1913	0.2451	0.4035
4.9	-0.4845	0.6187	-2.072	0.2347	0.384
5	-0.4569	0.5903	-1.961	0.2247	0.3656

m-benzyne diradical, $^1A_1$ (C_{2v})

```
Charge =  0 Multiplicity = 1
 C,0,1.551356813,-0.0000000109,0.0000798454
 C,0,0.7577962667,-1.1656893714,0.0001105697
 C,0,-0.5745274182,-0.8094753161,0.0000083591
 C,0,-1.6515739845,0.0000000261,-0.0000625538
 C,0,-0.5745274094,0.8094753412,-0.0001022227
 C,0,0.7577963103,1.1656893728,-0.0000441972
```

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H,0,2.6393804981,-0.0000000235,0.0001585911
H,0,1.1347432658,-2.1803636176,0.0002078984
H,0,-2.7368876617,0.0000000196,-0.0000745338
H,0,1.1347433199,2.1803636257,-0.0000817562
```

Sum of electronic and zero-point Energies= -230.870640
Sum of electronic and thermal Energies= -230.865996
Sum of electronic and thermal Enthalpies= -230.865052
Sum of electronic and thermal Free Energies= -230.898070

NICS-scan

Distance(Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.4256	0.6125	-1.8892	0.2335	0.379
-4.9	-0.4493	0.642	-1.9899	0.2436	0.3984
-4.8	-0.4748	0.6733	-2.0977	0.2542	0.4191
-4.7	-0.5022	0.7066	-2.2131	0.2654	0.4412
-4.6	-0.5317	0.7419	-2.3369	0.2772	0.4647
-4.5	-0.5634	0.7795	-2.4698	0.2896	0.4899
-4.4	-0.5977	0.8195	-2.6126	0.3027	0.5168
-4.3	-0.6347	0.8621	-2.7663	0.3165	0.5456
-4.2	-0.6748	0.9075	-2.9318	0.3311	0.5764
-4.1	-0.7182	0.9559	-3.1103	0.3465	0.6094
-4	-0.7652	1.0075	-3.3031	0.3627	0.6448
-3.9	-0.8163	1.0627	-3.5116	0.3799	0.6828
-3.8	-0.8719	1.1217	-3.7373	0.3981	0.7236
-3.7	-0.9325	1.1847	-3.9822	0.4173	0.7674
-3.6	-0.9985	1.2525	-4.2481	0.4378	0.8147
-3.5	-1.0707	1.3251	-4.5373	0.4596	0.8655
-3.4	-1.1498	1.403	-4.8524	0.4828	0.9202
-3.3	-1.2365	1.4868	-5.1964	0.5076	0.9792
-3.2	-1.3319	1.5769	-5.5725	0.5341	1.0428
-3.1	-1.437	1.6735	-5.9844	0.5624	1.1111
-3	-1.5532	1.7771	-6.4366	0.5927	1.1844
-2.9	-1.6821	1.8877	-6.9339	0.625	1.2627
-2.8	-1.8257	2.0047	-7.4819	0.6591	1.3456
-2.7	-1.9866	2.1272	-8.087	0.6946	1.4326
-2.6	-2.1678	2.2534	-8.7567	0.7309	1.5225
-2.5	-2.3731	2.3799	-9.4993	0.7666	1.6133
-2.4	-2.6074	2.5023	-10.3245	0.8	1.7023
-2.3	-2.8763	2.6142	-11.2431	0.8287	1.7855
-2.2	-3.1868	2.7071	-12.2677	0.8491	1.858
-2.1	-3.5473	2.7707	-13.4125	0.8571	1.9136
-2	-3.9674	2.7917	-14.6939	0.8472	1.9445
-1.9	-4.4589	2.7538	-16.1304	0.8124	1.9414
-1.8	-5.0356	2.6363	-17.743	0.7434	1.8929
-1.7	-5.7148	2.4113	-19.5557	0.6271	1.7842
-1.6	-6.5184	2.0396	-21.5947	0.4443	1.5953
-1.5	-7.4749	1.4634	-23.8882	0.1652	1.2982
-1.4	-8.6222	0.5976	-26.4643	-0.2557	0.8533
-1.3	-10.0096	-0.6812	-29.3477	-0.8867	0.2055
-1.2	-11.6993	-2.5436	-32.5541	-1.8256	-0.718
-1.1	-13.7627	-5.2055	-36.0824	-3.2017	-2.0038
-1	-16.2698	-8.9055	-39.904	-5.1675	-3.738
-0.9	-19.2673	-13.8508	-43.951	-7.8732	-5.9776
-0.8	-22.7451	-20.1299	-48.1055	-11.4215	-8.7084
-0.7	-26.5996	-27.6065	-52.1922	-15.8068	-11.7997
-0.6	-30.6054	-35.8334	-55.9828	-20.8579	-14.9755
-0.5	-34.4221	-44.0435	-59.2228	-26.2099	-17.8336
-0.4	-37.661	-51.2923	-61.6907	-31.3454	-19.9469

-0.3	-40.0179	-56.7694	-63.2842	-35.7198	-21.0496
-0.2	-41.417	-60.1602	-64.0908	-38.9326	-21.2276
-0.1	-42.0485	-61.7731	-64.3723	-40.8316	-20.9415
0	-42.2112	-62.2101	-64.4236	-41.4501	-20.76
0.1	-42.0492	-61.7732	-64.3742	-40.8314	-20.9418
0.2	-41.4182	-60.1605	-64.0941	-38.9323	-21.2282
0.3	-40.0194	-56.7698	-63.2886	-35.7195	-21.0503
0.4	-37.6628	-51.2927	-61.6955	-31.3451	-19.9476
0.5	-34.4238	-44.0438	-59.2277	-26.2097	-17.8341
0.6	-30.607	-35.8337	-55.9873	-20.8579	-14.9758
0.7	-26.6011	-27.6069	-52.1963	-15.807	-11.7999
0.8	-22.7464	-20.1302	-48.109	-11.4218	-8.7084
0.9	-19.2684	-13.8512	-43.954	-7.8737	-5.9775
1	-16.2708	-8.906	-39.9066	-5.1681	-3.7379
1.1	-13.7635	-5.206	-36.0846	-3.2024	-2.0036
1.2	-11.7001	-2.5441	-32.556	-1.8263	-0.7178
1.3	-10.0104	-0.6818	-29.3493	-0.8875	0.2057
1.4	-8.6229	0.597	-26.4657	-0.2565	0.8535
1.5	-7.4755	1.4628	-23.8894	0.1644	1.2984
1.6	-6.519	2.0389	-21.5958	0.4435	1.5954
1.7	-5.7153	2.4107	-19.5567	0.6264	1.7843
1.8	-5.0361	2.6357	-17.7439	0.7427	1.893
1.9	-4.4593	2.7533	-16.1312	0.8118	1.9415
2	-3.9678	2.7912	-14.6947	0.8466	1.9446
2.1	-3.5477	2.7702	-13.4133	0.8566	1.9136
2.2	-3.1872	2.7067	-12.2684	0.8486	1.8581
2.3	-2.8767	2.6138	-11.2437	0.8282	1.7856
2.4	-2.6077	2.5019	-10.325	0.7996	1.7023
2.5	-2.3734	2.3796	-9.4999	0.7662	1.6134
2.6	-2.1681	2.2531	-8.7572	0.7305	1.5226
2.7	-1.9868	2.127	-8.0875	0.6943	1.4327
2.8	-1.8259	2.0045	-7.4823	0.6588	1.3457
2.9	-1.6823	1.8874	-6.9343	0.6247	1.2627
3	-1.5534	1.777	-6.437	0.5925	1.1845
3.1	-1.4372	1.6734	-5.9848	0.5622	1.1112
3.2	-1.332	1.5766	-5.5728	0.5338	1.0428
3.3	-1.2367	1.4867	-5.1967	0.5074	0.9793
3.4	-1.1499	1.4029	-4.8527	0.4826	0.9203
3.5	-1.0709	1.3249	-4.5376	0.4594	0.8655
3.6	-0.9987	1.2523	-4.2483	0.4376	0.8147
3.7	-0.9326	1.1847	-3.9824	0.4172	0.7675
3.8	-0.872	1.1215	-3.7376	0.3979	0.7236
3.9	-0.8164	1.0626	-3.5118	0.3798	0.6828
4	-0.7653	1.0074	-3.3033	0.3626	0.6448
4.1	-0.7182	0.9558	-3.1105	0.3464	0.6094
4.2	-0.6749	0.9074	-2.932	0.331	0.5764
4.3	-0.6348	0.862	-2.7664	0.3164	0.5456
4.4	-0.5978	0.8194	-2.6128	0.3026	0.5168
4.5	-0.5635	0.7795	-2.4699	0.2896	0.4899
4.6	-0.5317	0.7419	-2.337	0.2771	0.4648
4.7	-0.5022	0.7066	-2.2133	0.2654	0.4412
4.8	-0.4748	0.6733	-2.0978	0.2542	0.4191
4.9	-0.4493	0.642	-1.99	0.2435	0.3985
5	-0.4256	0.6124	-1.8893	0.2334	0.379

m-benzyne diradical, $^3A_1$ (C_{2v})

```
Charge =  0 Multiplicity = 3
```

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C,0,-1.3879181648,-0.0167904742,0.0000250087
C,0,-0.7162599632,1.2155763709,0.0001023398
C,0,0.6607088813,1.1722257037,0.0000340401
C,0,1.417693818,0.0171432235,-0.0001280621
C,0,0.6888676563,-1.1559100211,-0.0001299754
C,0,-0.6866513309,-1.2325505688,-0.0000786766
H,0,-2.4734844811,-0.0299181709,0.0000780128
H,0,-1.2681661516,2.1480169229,0.0002068262
H,0,2.503650636,0.0302754467,-0.0001051301
H,0,-1.2158409001,-2.1780684325,-0.0001043833
```

Sum of electronic and zero-point Energies= -230.855189
Sum of electronic and thermal Energies= -230.850792
Sum of electronic and thermal Enthalpies= -230.849848
Sum of electronic and thermal Free Energies= -230.883565

NICS-scan

Distance	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.4413	0.6618	-1.9857	0.2942	0.3676
-4.9	-0.468	0.694	-2.098	0.3081	0.3859
-4.8	-0.4968	0.7281	-2.2186	0.3227	0.4054
-4.7	-0.528	0.7642	-2.3483	0.3382	0.426
-4.6	-0.5619	0.8024	-2.488	0.3545	0.4479
-4.5	-0.5986	0.8428	-2.6386	0.3716	0.4712
-4.4	-0.6386	0.8854	-2.8012	0.3896	0.4958
-4.3	-0.6821	0.9305	-2.9768	0.4085	0.522
-4.2	-0.7296	0.9781	-3.1669	0.4284	0.5497
-4.1	-0.7815	1.0282	-3.3727	0.4491	0.5791
-4	-0.8383	1.081	-3.5959	0.4708	0.6102
-3.9	-0.9006	1.1363	-3.8382	0.4933	0.643
-3.8	-0.9691	1.1944	-4.1016	0.5167	0.6777
-3.7	-1.0445	1.2549	-4.3883	0.5407	0.7142
-3.6	-1.1276	1.3178	-4.7006	0.5653	0.7525
-3.5	-1.2195	1.3829	-5.0413	0.5903	0.7926
-3.4	-1.3212	1.4497	-5.4133	0.6153	0.8344
-3.3	-1.4341	1.5177	-5.8198	0.64	0.8777
-3.2	-1.5595	1.5861	-6.2645	0.6639	0.9222
-3.1	-1.6992	1.6538	-6.7514	0.6863	0.9675
-3	-1.855	1.7196	-7.2848	0.7064	1.0132
-2.9	-2.0292	1.7816	-7.8693	0.7231	1.0585
-2.8	-2.2242	1.8376	-8.51	0.7351	1.1025
-2.7	-2.4427	1.8843	-9.2123	0.7405	1.1438
-2.6	-2.6879	1.918	-9.9816	0.7372	1.1808
-2.5	-2.9632	1.934	-10.8236	0.7225	1.2115
-2.4	-3.2724	1.9266	-11.7437	0.6933	1.2333
-2.3	-3.6195	1.8886	-12.747	0.6455	1.2431
-2.2	-4.0087	1.8118	-13.8378	0.5747	1.2371
-2.1	-4.4441	1.6866	-15.0189	0.4754	1.2112
-2	-4.9296	1.5022	-16.2911	0.3418	1.1604
-1.9	-5.4686	1.2465	-17.6522	0.1672	1.0793
-1.8	-6.0632	0.9063	-19.0959	-0.0559	0.9622
-1.7	-6.714	0.468	-20.6101	-0.335	0.803
-1.6	-7.4197	-0.0834	-22.1757	-0.6786	0.5952
-1.5	-8.1757	-0.7624	-23.7648	-1.0949	0.3325
-1.4	-8.9742	-1.584	-25.3386	-1.5923	0.0083
-1.3	-9.8029	-2.5619	-26.8467	-2.1786	-0.3833
-1.2	-10.645	-3.7086	-28.2265	-2.8607	-0.8479
-1.1	-11.4793	-5.0324	-29.4053	-3.643	-1.3894
-1	-12.2802	-6.5364	-30.3043	-4.5268	-2.0096
-0.9	-13.0201	-8.213	-30.8472	-5.5071	-2.7059

-0.8	-13.6712	-10.0411	-30.9726	-6.5713	-3.4698
-0.7	-14.2096	-11.9798	-30.6491	-7.6956	-4.2842
-0.6	-14.6195	-13.9667	-29.8918	-8.8441	-5.1226
-0.5	-14.8973	-15.9167	-28.7753	-9.9686	-5.9481
-0.4	-15.0546	-17.7272	-27.4364	-11.0108	-6.7164
-0.3	-15.1173	-19.2876	-26.0644	-11.9082	-7.3794
-0.2	-15.1216	-20.4918	-24.8731	-12.6004	-7.8914
-0.1	-15.1051	-21.2527	-24.0625	-13.0377	-8.215
0	-15.096	-21.5131	-23.7749	-13.1873	-8.3258
0.1	-15.105	-21.2531	-24.062	-13.0378	-8.2153
0.2	-15.1216	-20.4924	-24.8722	-12.6005	-7.8919
0.3	-15.1172	-19.2884	-26.0631	-11.9083	-7.3801
0.4	-15.0544	-17.7283	-27.435	-11.011	-6.7173
0.5	-14.8972	-15.9179	-28.7738	-9.9687	-5.9492
0.6	-14.6194	-13.9679	-29.8905	-8.8442	-5.1237
0.7	-14.2096	-11.981	-30.6479	-7.6956	-4.2854
0.8	-13.6713	-10.0422	-30.9717	-6.5712	-3.471
0.9	-13.0202	-8.2141	-30.8465	-5.507	-2.7071
1	-12.2804	-6.5373	-30.3038	-4.5266	-2.0107
1.1	-11.4794	-5.0333	-29.4051	-3.6429	-1.3904
1.2	-10.6452	-3.7092	-28.2265	-2.8605	-0.8487
1.3	-9.8031	-2.5625	-26.8468	-2.1784	-0.3841
1.4	-8.9744	-1.5844	-25.3388	-1.5921	0.0077
1.5	-8.176	-0.7628	-23.7651	-1.0947	0.3319
1.6	-7.4199	-0.0837	-22.1761	-0.6784	0.5947
1.7	-6.7142	0.4678	-20.6105	-0.3348	0.8026
1.8	-6.0633	0.9062	-19.0963	-0.0557	0.9619
1.9	-5.4688	1.2465	-17.6527	0.1674	1.0791
2	-4.9298	1.5021	-16.2916	0.342	1.1601
2.1	-4.4442	1.6866	-15.0193	0.4756	1.211
2.2	-4.0088	1.8118	-13.8382	0.5748	1.237
2.3	-3.6196	1.8887	-12.7474	0.6457	1.243
2.4	-3.2725	1.9266	-11.744	0.6934	1.2332
2.5	-2.9632	1.9342	-10.8239	0.7227	1.2115
2.6	-2.6879	1.9181	-9.9819	0.7373	1.1808
2.7	-2.4427	1.8844	-9.2126	0.7406	1.1438
2.8	-2.2242	1.8377	-8.5103	0.7352	1.1025
2.9	-2.0292	1.7819	-7.8695	0.7233	1.0586
3	-1.8551	1.7198	-7.285	0.7065	1.0133
3.1	-1.6992	1.654	-6.7516	0.6864	0.9676
3.2	-1.5595	1.5862	-6.2647	0.664	0.9222
3.3	-1.4341	1.5178	-5.82	0.6401	0.8777
3.4	-1.3212	1.4498	-5.4134	0.6154	0.8344
3.5	-1.2195	1.3831	-5.0415	0.5904	0.7927
3.6	-1.1276	1.318	-4.7008	0.5654	0.7526
3.7	-1.0445	1.255	-4.3884	0.5408	0.7142
3.8	-0.9691	1.1945	-4.1018	0.5168	0.6777
3.9	-0.9006	1.1365	-3.8383	0.4934	0.6431
4	-0.8383	1.0811	-3.596	0.4709	0.6102
4.1	-0.7815	1.0283	-3.3728	0.4492	0.5791
4.2	-0.7296	0.9781	-3.1669	0.4284	0.5497
4.3	-0.6821	0.9306	-2.9769	0.4086	0.522
4.4	-0.6386	0.8856	-2.8013	0.3897	0.4959
4.5	-0.5986	0.8428	-2.6387	0.3716	0.4712
4.6	-0.5619	0.8024	-2.4881	0.3545	0.4479
4.7	-0.528	0.7642	-2.3484	0.3382	0.426
4.8	-0.4968	0.7282	-2.2186	0.3228	0.4054
4.9	-0.468	0.694	-2.098	0.3081	0.3859

5	-0.4413	0.6618	-1.9858	0.2942	0.3676

p-benzyne diradical, ^1A_g (D_{2h})

```
Charge =  0 Multiplicity = 1
 C,0,1.1932193426,0.7400024546,-0.0000260999
 C,0,0.0000211944,1.3550552465,-0.0000267279
 C,0,-1.1931988035,0.7400414886,-0.0000037011
 C,0,-1.1932193426,-0.7400024546,0.0000260999
 C,0,-0.0000211944,-1.3550552465,0.0000267279
 C,0,1.1931988035,-0.7400414886,0.0000037011
 H,0,2.1749773488,1.1968913183,-0.0000685753
 H,0,-2.1749419164,1.1969611594,0.0000195621
 H,0,-2.1749773488,-1.1968913183,0.0000685753
 H,0,2.1749419164,-1.1969611594,-0.0000195621
```

Sum of electronic and zero-point Energies= -230.832458
Sum of electronic and thermal Energies= -230.827565
Sum of electronic and thermal Enthalpies= -230.826620
Sum of electronic and thermal Free Energies= -230.860082

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.6326	0.6115	-2.5094	0.2036	0.4079
-4.9	-0.6702	0.6402	-2.6507	0.2117	0.4285
-4.8	-0.7107	0.6705	-2.8026	0.2201	0.4504
-4.7	-0.7545	0.7024	-2.9659	0.2288	0.4736
-4.6	-0.8019	0.7361	-3.1418	0.2377	0.4984
-4.5	-0.8533	0.7715	-3.3314	0.2468	0.5247
-4.4	-0.9091	0.8088	-3.5361	0.2561	0.5527
-4.3	-0.9697	0.8479	-3.7572	0.2654	0.5825
-4.2	-1.0358	0.8891	-3.9964	0.2748	0.6143
-4.1	-1.1078	0.9322	-4.2556	0.2841	0.6481
-4	-1.1865	0.9772	-4.5366	0.2932	0.684
-3.9	-1.2726	1.024	-4.8419	0.3018	0.7222
-3.8	-1.367	1.0727	-5.1738	0.3099	0.7628
-3.7	-1.4707	1.123	-5.5352	0.317	0.806
-3.6	-1.5849	1.1746	-5.9292	0.3229	0.8517
-3.5	-1.7107	1.2273	-6.3593	0.3272	0.9001
-3.4	-1.8497	1.2804	-6.8294	0.3292	0.9512
-3.3	-2.0035	1.3334	-7.3439	0.3282	1.0052
-3.2	-2.1741	1.3853	-7.9075	0.3235	1.0618
-3.1	-2.3637	1.4349	-8.5259	0.3138	1.1211
-3	-2.5747	1.4806	-9.2049	0.2978	1.1828
-2.9	-2.8102	1.5206	-9.9512	0.2739	1.2467
-2.8	-3.0734	1.552	-10.7722	0.2398	1.3122
-2.7	-3.3681	1.5717	-11.676	0.193	1.3787
-2.6	-3.6986	1.5754	-12.6713	0.1301	1.4453
-2.5	-4.0699	1.5579	-13.7677	0.0474	1.5105
-2.4	-4.4875	1.5129	-14.9753	-0.0599	1.5728
-2.3	-4.9574	1.4326	-16.3047	-0.1974	1.63
-2.2	-5.4865	1.3075	-17.7668	-0.3717	1.6792
-2.1	-6.0819	1.1269	-19.3727	-0.5904	1.7173
-2	-6.7516	0.878	-21.1327	-0.862	1.74
-1.9	-7.5032	0.5468	-23.0564	-1.1958	1.7426
-1.8	-8.3446	0.1175	-25.1512	-1.6019	1.7194
-1.7	-9.283	-0.4272	-27.4219	-2.0908	1.6636

-1.6	-10.3247	-1.1055	-29.8686	-2.6729	1.5674
-1.5	-11.4738	-1.9359	-32.4855	-3.3574	1.4215
-1.4	-12.732	-2.937	-35.2589	-4.1518	1.2148
-1.3	-14.0969	-4.1258	-38.165	-5.0602	0.9344
-1.2	-15.5611	-5.5152	-41.1681	-6.0809	0.5657
-1.1	-17.1104	-7.112	-44.2192	-7.2047	0.0927
-1	-18.7227	-8.9117	-47.2565	-8.4113	-0.5004
-0.9	-20.3672	-10.8944	-50.207	-9.6682	-1.2262
-0.8	-22.0038	-13.0197	-52.9918	-10.9298	-2.0899
-0.7	-23.5856	-15.2238	-55.5331	-12.14	-3.0838
-0.6	-25.0614	-17.4207	-57.7634	-13.2392	-4.1815
-0.5	-26.381	-19.5084	-59.6347	-14.1746	-5.3338
-0.4	-27.5015	-21.3801	-61.1243	-14.9116	-6.4685
-0.3	-28.3912	-22.9376	-62.236	-15.4418	-7.4958
-0.2	-29.032	-24.1023	-62.9936	-15.7824	-8.3199
-0.1	-29.4168	-24.8206	-63.4297	-15.966	-8.8546
0	-29.5449	-25.0632	-63.5716	-16.0231	-9.0401
0.1	-29.4168	-24.8206	-63.4297	-15.966	-8.8546
0.2	-29.032	-24.1023	-62.9936	-15.7824	-8.3199
0.3	-28.3912	-22.9376	-62.236	-15.4418	-7.4958
0.4	-27.5015	-21.3801	-61.1243	-14.9116	-6.4685
0.5	-26.381	-19.5084	-59.6347	-14.1746	-5.3338
0.6	-25.0614	-17.4207	-57.7634	-13.2392	-4.1815
0.7	-23.5856	-15.2238	-55.5331	-12.14	-3.0838
0.8	-22.0038	-13.0197	-52.9918	-10.9298	-2.0899
0.9	-20.3672	-10.8944	-50.207	-9.6682	-1.2262
1	-18.7227	-8.9117	-47.2565	-8.4113	-0.5004
1.1	-17.1104	-7.112	-44.2192	-7.2047	0.0927
1.2	-15.5611	-5.5152	-41.1681	-6.0809	0.5657
1.3	-14.0969	-4.1258	-38.165	-5.0602	0.9344
1.4	-12.732	-2.937	-35.2589	-4.1518	1.2148
1.5	-11.4738	-1.9359	-32.4855	-3.3574	1.4215
1.6	-10.3247	-1.1055	-29.8686	-2.6729	1.5674
1.7	-9.283	-0.4272	-27.4219	-2.0908	1.6636
1.8	-8.3446	0.1175	-25.1512	-1.6019	1.7194
1.9	-7.5032	0.5468	-23.0564	-1.1958	1.7426
2	-6.7516	0.878	-21.1327	-0.862	1.74
2.1	-6.0819	1.1269	-19.3727	-0.5904	1.7173
2.2	-5.4865	1.3075	-17.7668	-0.3717	1.6792
2.3	-4.9574	1.4326	-16.3047	-0.1974	1.63
2.4	-4.4875	1.5129	-14.9753	-0.0599	1.5728
2.5	-4.0699	1.5579	-13.7677	0.0474	1.5105
2.6	-3.6986	1.5754	-12.6713	0.1301	1.4453
2.7	-3.3681	1.5717	-11.676	0.193	1.3787
2.8	-3.0734	1.552	-10.7722	0.2398	1.3122
2.9	-2.8102	1.5206	-9.9512	0.2739	1.2467
3	-2.5747	1.4806	-9.2049	0.2978	1.1828
3.1	-2.3637	1.4349	-8.5259	0.3138	1.1211
3.2	-2.1741	1.3853	-7.9075	0.3235	1.0618
3.3	-2.0035	1.3334	-7.3439	0.3282	1.0052
3.4	-1.8497	1.2804	-6.8294	0.3292	0.9512
3.5	-1.7107	1.2273	-6.3593	0.3272	0.9001
3.6	-1.5849	1.1746	-5.9292	0.3229	0.8517
3.7	-1.4707	1.123	-5.5352	0.317	0.806
3.8	-1.367	1.0727	-5.1738	0.3099	0.7628
3.9	-1.2726	1.024	-4.8419	0.3018	0.7222
4	-1.1865	0.9772	-4.5366	0.2932	0.684
4.1	-1.1078	0.9322	-4.2556	0.2841	0.6481

4.2	-1.0358	0.8891	-3.9964	0.2748	0.6143
4.3	-0.9697	0.8479	-3.7572	0.2654	0.5825
4.4	-0.9091	0.8088	-3.5361	0.2561	0.5527
4.5	-0.8533	0.7715	-3.3314	0.2468	0.5247
4.6	-0.8019	0.7361	-3.1418	0.2377	0.4984
4.7	-0.7545	0.7024	-2.9659	0.2288	0.4736
4.8	-0.7107	0.6705	-2.8026	0.2201	0.4504
4.9	-0.6702	0.6402	-2.6507	0.2117	0.4285
5	-0.6326	0.6115	-2.5094	0.2036	0.4079

p-benzyne diradical, ^{3}A (C_1)

```
Charge =  0 Multiplicity = 3
 C,0,-1.4191961629,-0.0239939525,-0.0000303923
 C,0,-0.6732312301,1.1338914657,-0.000055852
 C,0,0.7004637362,1.234494045,-0.0000930199
 C,0,1.4191768939,0.0239935707,-0.000108506
 C,0,0.6732108824,-1.1338905048,-0.0000841386
 C,0,-0.7004847754,-1.2344944586,-0.000044603
 H,0,-2.5042630393,-0.0153021216,0.0000000064
 H,0,1.2122766281,2.1913101887,-0.0001148436
 H,0,2.5042433952,0.0153024696,-0.0001423362
 H,0,-1.2122963281,-2.1913107021,-0.0000263146
```

Sum of electronic and zero-point Energies= -230.857049
Sum of electronic and thermal Energies= -230.852659
Sum of electronic and thermal Enthalpies= -230.851714
Sum of electronic and thermal Free Energies= -230.885423

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.41	0.648	-1.8779	0.257	0.391
-4.9	-0.4349	0.6796	-1.9842	0.2687	0.4109
-4.8	-0.4618	0.713	-2.0985	0.2809	0.4321
-4.7	-0.491	0.7484	-2.2214	0.2938	0.4546
-4.6	-0.5227	0.7858	-2.3539	0.3072	0.4786
-4.5	-0.5571	0.8254	-2.4966	0.3213	0.5041
-4.4	-0.5945	0.8673	-2.6508	0.3361	0.5312
-4.3	-0.6353	0.9116	-2.8173	0.3515	0.5601
-4.2	-0.6798	0.9583	-2.9976	0.3675	0.5908
-4.1	-0.7284	1.0076	-3.1929	0.3841	0.6235
-4	-0.7817	1.0594	-3.4047	0.4012	0.6582
-3.9	-0.8402	1.114	-3.6347	0.4188	0.6952
-3.8	-0.9045	1.1711	-3.8847	0.4368	0.7343
-3.7	-0.9753	1.231	-4.1569	0.4551	0.7759
-3.6	-1.0535	1.2932	-4.4536	0.4734	0.8198
-3.5	-1.1398	1.3577	-4.7772	0.4915	0.8662
-3.4	-1.2355	1.4242	-5.1306	0.5092	0.915
-3.3	-1.3416	1.4921	-5.5169	0.5259	0.9662
-3.2	-1.4596	1.561	-5.9397	0.5413	1.0197
-3.1	-1.5909	1.6297	-6.4025	0.5546	1.0751
-3	-1.7375	1.6973	-6.9097	0.5651	1.1322
-2.9	-1.9012	1.762	-7.4655	0.5716	1.1904
-2.8	-2.0843	1.8221	-8.0749	0.5731	1.249
-2.7	-2.2894	1.8745	-8.7428	0.5677	1.3068
-2.6	-2.5194	1.9162	-9.4744	0.5537	1.3625
-2.5	-2.7774	1.9428	-10.275	0.5286	1.4142
-2.4	-3.0669	1.9491	-11.1497	0.4895	1.4596
-2.3	-3.3914	1.9289	-12.1031	0.433	1.4959
-2.2	-3.7549	1.8742	-13.1389	0.3548	1.5194

-2.1	-4.161	1.7763	-14.2593	0.2502	1.5261
-2	-4.6133	1.6248	-15.4646	0.1135	1.5113
-1.9	-5.1146	1.408	-16.7518	-0.0616	1.4696
-1.8	-5.6668	1.1131	-18.1136	-0.2822	1.3953
-1.7	-6.2704	0.7258	-19.5371	-0.5564	1.2822
-1.6	-6.9236	0.2311	-21.0019	-0.8929	1.124
-1.5	-7.622	-0.3874	-22.4787	-1.3017	0.9143
-1.4	-8.3579	-1.1468	-23.9271	-1.7935	0.6467
-1.3	-9.1196	-2.0644	-25.2945	-2.3801	0.3157
-1.2	-9.8914	-3.1578	-26.5163	-3.0747	-0.0831
-1.1	-10.6532	-4.4428	-27.5168	-3.8908	-0.552
-1	-11.3819	-5.9309	-28.2149	-4.8416	-1.0893
-0.9	-12.0525	-7.6257	-28.5319	-5.9375	-1.6882
-0.8	-12.6407	-9.5165	-28.4056	-7.1822	-2.3343
-0.7	-13.1261	-11.5718	-27.8063	-8.5661	-3.0057
-0.6	-13.4959	-13.7329	-26.7548	-10.0601	-3.6728
-0.5	-13.7484	-15.9091	-25.3361	-11.6077	-4.3014
-0.4	-13.8946	-17.9804	-23.7036	-13.1229	-4.8575
-0.3	-13.9578	-19.806	-22.0673	-14.4937	-5.3123
-0.2	-13.9689	-21.2418	-20.6648	-15.5955	-5.6463
-0.1	-13.9595	-22.1613	-19.7172	-16.3123	-5.849
0	-13.9535	-22.4781	-19.3823	-16.5613	-5.9168
0.1	-13.9595	-22.1613	-19.7172	-16.3123	-5.849
0.2	-13.9689	-21.2418	-20.6648	-15.5955	-5.6463
0.3	-13.9578	-19.806	-22.0673	-14.4937	-5.3123
0.4	-13.8946	-17.9804	-23.7036	-13.1229	-4.8575
0.5	-13.7484	-15.9091	-25.3361	-11.6077	-4.3014
0.6	-13.4959	-13.7329	-26.7548	-10.0601	-3.6728
0.7	-13.1261	-11.5718	-27.8063	-8.5661	-3.0057
0.8	-12.6407	-9.5165	-28.4056	-7.1822	-2.3343
0.9	-12.0525	-7.6257	-28.5319	-5.9375	-1.6882
1	-11.3819	-5.9309	-28.2149	-4.8416	-1.0893
1.1	-10.6532	-4.4428	-27.5168	-3.8908	-0.552
1.2	-9.8914	-3.1578	-26.5163	-3.0747	-0.0831
1.3	-9.1196	-2.0644	-25.2945	-2.3801	0.3157
1.4	-8.3579	-1.1468	-23.9271	-1.7935	0.6467
1.5	-7.622	-0.3874	-22.4787	-1.3017	0.9143
1.6	-6.9236	0.2311	-21.0019	-0.8929	1.124
1.7	-6.2704	0.7258	-19.5371	-0.5564	1.2822
1.8	-5.6668	1.1131	-18.1136	-0.2822	1.3953
1.9	-5.1146	1.408	-16.7518	-0.0616	1.4696
2	-4.6133	1.6248	-15.4646	0.1135	1.5113
2.1	-4.161	1.7763	-14.2593	0.2502	1.5261
2.2	-3.7549	1.8742	-13.1389	0.3548	1.5194
2.3	-3.3914	1.9289	-12.1031	0.433	1.4959
2.4	-3.0669	1.9491	-11.1497	0.4895	1.4596
2.5	-2.7774	1.9428	-10.275	0.5286	1.4142
2.6	-2.5194	1.9162	-9.4744	0.5537	1.3625
2.7	-2.2894	1.8745	-8.7428	0.5677	1.3068
2.8	-2.0843	1.8221	-8.0749	0.5731	1.249
2.9	-1.9012	1.762	-7.4655	0.5716	1.1904
3	-1.7375	1.6973	-6.9097	0.5651	1.1322
3.1	-1.5909	1.6297	-6.4025	0.5546	1.0751
3.2	-1.4596	1.561	-5.9397	0.5413	1.0197
3.3	-1.3416	1.4921	-5.5169	0.5259	0.9662
3.4	-1.2355	1.4242	-5.1306	0.5092	0.915
3.5	-1.1398	1.3577	-4.7772	0.4915	0.8662
3.6	-1.0535	1.2932	-4.4536	0.4734	0.8198

3.7	-0.9753	1.231	-4.1569	0.4551	0.7759
3.8	-0.9045	1.1711	-3.8847	0.4368	0.7343
3.9	-0.8402	1.114	-3.6347	0.4188	0.6952
4	-0.7817	1.0594	-3.4047	0.4012	0.6582
4.1	-0.7284	1.0076	-3.1929	0.3841	0.6235
4.2	-0.6798	0.9583	-2.9976	0.3675	0.5908
4.3	-0.6353	0.9116	-2.8173	0.3515	0.5601
4.4	-0.5945	0.8673	-2.6508	0.3361	0.5312
4.5	-0.5571	0.8254	-2.4966	0.3213	0.5041
4.6	-0.5227	0.7858	-2.3539	0.3072	0.4786
4.7	-0.491	0.7484	-2.2214	0.2938	0.4546
4.8	-0.4618	0.713	-2.0985	0.2809	0.4321
4.9	-0.4349	0.6796	-1.9842	0.2687	0.4109
5	-0.41	0.648	-1.8779	0.257	0.391

cis-bicyclobutadienylene (C_{2v}), 6

```
C,0,-0.0269248321,1.2863284261,-1.1174201578
 C,0,-1.1625912168,0.4958393056,-1.1315046768
 C,0,-0.8843289485,-0.0358479099,0.2214963086
 C,0,0.352731471,0.8250486639,0.2368703208
 C,0,-0.220922397,-1.0028014324,0.9480458527
 C,0,1.0164624983,-0.142325201,0.962687956
 C,0,0.6739308206,-2.1797756523,0.8777783696
 C,0,1.8099431172,-1.3897787419,0.8920892925
 H,0,0.4898324427,1.8167753396,-1.9061751544
 H,0,-1.8267435959,0.2050775924,-1.9345502206
 H,0,0.5279806308,-3.2255762999,0.6420743922
 H,0,2.8446300098,-1.6140640901,0.6693077172
```

Sum of electronic and zero-point Energies= -306.893045
Sum of electronic and thermal Energies= -306.887099
Sum of electronic and thermal Enthalpies= -306.886155
Sum of electronic and thermal Free Energies= -306.922988

NICS-scan (central ring)

Distance (Å)	NICSiso	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.0419	0.7296	-0.8552	0.3495	0.3801
-4.9	-0.0444	0.7663	-0.8996	0.3674	0.3989
-4.8	-0.0473	0.8052	-0.947	0.3864	0.4188
-4.7	-0.0504	0.8466	-0.9978	0.4067	0.4399
-4.6	-0.0539	0.8907	-1.0522	0.4285	0.4622
-4.5	-0.0577	0.9377	-1.1107	0.4518	0.4859
-4.4	-0.0619	0.9877	-1.1735	0.4768	0.5109
-4.3	-0.0666	1.0411	-1.241	0.5037	0.5374
-4.2	-0.0719	1.0982	-1.3138	0.5327	0.5655
-4.1	-0.0777	1.1591	-1.3923	0.5639	0.5952
-4	-0.0843	1.2241	-1.477	0.5976	0.6265
-3.9	-0.0916	1.2937	-1.5685	0.634	0.6597
-3.8	-0.0998	1.3682	-1.6676	0.6736	0.6946
-3.7	-0.1089	1.448	-1.7748	0.7165	0.7315
-3.6	-0.1192	1.5336	-1.8912	0.7632	0.7704
-3.5	-0.1307	1.6253	-2.0174	0.8141	0.8112
-3.4	-0.1436	1.7237	-2.1545	0.8696	0.8541
-3.3	-0.158	1.8294	-2.3036	0.9304	0.899

-3.2	-0.1742	1.943	-2.4656	0.9971	0.9459
-3.1	-0.1924	2.0647	-2.6418	1.0701	0.9946
-3	-0.2128	2.1949	-2.8334	1.1502	1.0447
-2.9	-0.236	2.3335	-3.0414	1.2378	1.0957
-2.8	-0.2623	2.4801	-3.2671	1.3335	1.1466
-2.7	-0.2927	2.6333	-3.5112	1.4373	1.196
-2.6	-0.3279	2.7908	-3.7745	1.5492	1.2416
-2.5	-0.3694	2.949	-4.0572	1.6683	1.2807
-2.4	-0.4186	3.1026	-4.3585	1.7934	1.3092
-2.3	-0.4774	3.2444	-4.6767	1.922	1.3224
-2.2	-0.5478	3.3653	-5.0087	2.0509	1.3144
-2.1	-0.6316	3.454	-5.3487	2.1755	1.2785
-2	-0.73	3.4981	-5.6881	2.2904	1.2077
-1.9	-0.8435	3.4834	-6.0138	2.3885	1.0949
-1.8	-0.9705	3.3954	-6.3069	2.4614	0.934
-1.7	-1.1075	3.2184	-6.5407	2.4983	0.7201
-1.6	-1.2478	2.9354	-6.6788	2.4845	0.4509
-1.5	-1.3817	2.5272	-6.6723	2.3995	0.1277
-1.4	-1.4964	1.9696	-6.4587	2.213	-0.2434
-1.3	-1.5766	1.2314	-5.9614	1.881	-0.6496
-1.2	-1.6068	0.2718	-5.0922	1.3409	-1.0691
-1.1	-1.5735	-0.9597	-3.7606	0.5098	-1.4695
-1	-1.47	-2.5204	-1.8897	-0.7117	-1.8087
-0.9	-1.3028	-4.4656	0.557	-2.4252	-2.0404
-0.8	-1.1001	-6.84	3.5396	-4.708	-2.132
-0.7	-0.9234	-9.6714	6.9012	-7.5752	-2.0962
-0.6	-0.8807	-12.9761	10.3341	-10.9406	-2.0355
-0.5	-1.1343	-16.7769	13.3741	-14.5915	-2.1854
-0.4	-1.8898	-21.1157	15.4461	-18.195	-2.9207
-0.3	-3.3495	-26.0286	15.9803	-21.3462	-4.6824
-0.2	-5.6251	-31.4615	14.5862	-23.6553	-7.8062
-0.1	-8.6386	-37.1424	11.2266	-24.8469	-12.2955
0	-12.0679	-42.5025	6.2989	-24.8357	-17.6668
0.1	-15.396	-46.7449	0.5568	-23.7433	-23.0016
0.2	-18.0659	-49.0883	-5.1095	-21.8548	-27.2335
0.3	-19.6684	-49.0728	-9.9324	-19.5367	-29.5361
0.4	-20.0644	-46.749	-13.4442	-17.151	-29.598
0.5	-19.3884	-42.6472	-15.5181	-14.9898	-27.6574
0.6	-17.9537	-37.5654	-16.2958	-13.2389	-24.3265
0.7	-16.1248	-32.3047	-16.0696	-11.97	-20.3347
0.8	-14.2149	-27.4723	-15.1725	-11.1563	-16.316
0.9	-12.4361	-23.4028	-13.9055	-10.7045	-12.6983
1	-10.8946	-20.1817	-12.5023	-10.4917	-9.69
1.1	-9.6157	-17.7245	-11.1225	-10.3973	-7.3272
1.2	-8.5751	-15.8653	-9.8601	-10.324	-5.5413
1.3	-7.7277	-14.4234	-8.7596	-10.2048	-4.2186
1.4	-7.0249	-13.2434	-7.8314	-10.0027	-3.2407
1.5	-6.425	-12.2091	-7.0661	-9.7035	-2.5056
1.6	-5.8956	-11.2432	-6.4437	-9.309	-1.9342

1.7	-5.4141	-10.3013	-5.9408	-8.8309	-1.4704
1.8	-4.9656	-9.3626	-5.5341	-8.286	-1.0766
1.9	-4.5418	-8.4228	-5.2025	-7.6931	-0.7297
2	-4.1386	-7.4879	-4.928	-7.0711	-0.4168
2.1	-3.7551	-6.5695	-4.696	-6.4376	-0.1319
2.2	-3.3921	-5.6816	-4.4948	-5.8082	0.1266
2.3	-3.0511	-4.8378	-4.3155	-5.1962	0.3584
2.4	-2.7338	-4.0501	-4.1513	-4.6121	0.562
2.5	-2.4416	-3.3273	-3.9976	-4.0638	0.7365
2.6	-2.1752	-2.6748	-3.8507	-3.5564	0.8816
2.7	-1.9345	-2.0948	-3.7086	-3.0928	0.998
2.8	-1.7187	-1.5866	-3.5696	-2.6739	1.0873
2.9	-1.5267	-1.1472	-3.433	-2.2992	1.152
3	-1.3567	-0.7716	-3.2985	-1.9665	1.1949
3.1	-1.2068	-0.4543	-3.166	-1.6734	1.2191
3.2	-1.0748	-0.1888	-3.0356	-1.4165	1.2277
3.3	-0.9589	0.031	-2.9077	-1.1925	1.2235
3.4	-0.8571	0.2112	-2.7825	-0.998	1.2092
3.5	-0.7676	0.3576	-2.6605	-0.8295	1.1871
3.6	-0.6889	0.475	-2.5418	-0.684	1.159
3.7	-0.6195	0.5681	-2.4267	-0.5586	1.1267
3.8	-0.5583	0.6406	-2.3156	-0.4508	1.0914
3.9	-0.5042	0.696	-2.2084	-0.3582	1.0542
4	-0.4562	0.737	-2.1055	-0.2789	1.0159
4.1	-0.4136	0.7661	-2.0067	-0.211	0.9771
4.2	-0.3756	0.7854	-1.9122	-0.153	0.9384
4.3	-0.3418	0.7964	-1.8219	-0.1037	0.9001
4.4	-0.3116	0.8008	-1.7357	-0.0617	0.8625
4.5	-0.2846	0.7997	-1.6536	-0.0261	0.8258
4.6	-0.2604	0.7942	-1.5755	0.004	0.7902
4.7	-0.2387	0.7852	-1.5013	0.0293	0.7559
4.8	-0.2191	0.7733	-1.4307	0.0506	0.7227
4.9	-0.2015	0.7591	-1.3637	0.0682	0.6909
5	-0.1857	0.7432	-1.3002	0.0829	0.6603

NICS-scan (terminal ring)

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.0165	0.6995	-0.7492	0.3297	0.3698
-4.9	-0.0167	0.7349	-0.7851	0.3458	0.3891
-4.8	-0.0168	0.7727	-0.8231	0.363	0.4097
-4.7	-0.0168	0.8129	-0.8635	0.3812	0.4317
-4.6	-0.0168	0.8559	-0.9063	0.4007	0.4552
-4.5	-0.0166	0.9019	-0.9516	0.4214	0.4805
-4.4	-0.0162	0.9512	-0.9998	0.4436	0.5076
-4.3	-0.0156	1.0038	-1.0508	0.4672	0.5366
-4.2	-0.0148	1.0604	-1.1049	0.4925	0.5679
-4.1	-0.0137	1.1211	-1.1622	0.5195	0.6016
-4	-0.0122	1.1863	-1.2229	0.5485	0.6378

-3.9	-0.0103	1.2564	-1.2871	0.5795	0.6769
-3.8	-0.0077	1.3319	-1.355	0.6128	0.7191
-3.7	-0.0045	1.4131	-1.4265	0.6485	0.7646
-3.6	-0.0004	1.5007	-1.5018	0.6868	0.8139
-3.5	0.0048	1.5953	-1.5808	0.7281	0.8672
-3.4	0.0113	1.6973	-1.6633	0.7724	0.9249
-3.3	0.0195	1.8075	-1.7491	0.8201	0.9874
-3.2	0.0296	1.9264	-1.8377	0.8714	1.055
-3.1	0.0421	2.0548	-1.9284	0.9265	1.1283
-3	0.0576	2.193	-2.0203	0.9856	1.2074
-2.9	0.0764	2.3413	-2.1119	1.0485	1.2928
-2.8	0.0994	2.4997	-2.2014	1.1151	1.3846
-2.7	0.1271	2.6675	-2.2863	1.1848	1.4827
-2.6	0.1602	2.8436	-2.3631	1.2566	1.587
-2.5	0.1994	3.0256	-2.4274	1.3287	1.6969
-2.4	0.2454	3.2099	-2.4737	1.3986	1.8113
-2.3	0.2992	3.392	-2.4944	1.4629	1.9291
-2.2	0.3617	3.5653	-2.4802	1.5168	2.0485
-2.1	0.4343	3.7219	-2.4189	1.5546	2.1673
-2	0.5193	3.8529	-2.2949	1.5693	2.2836
-1.9	0.6197	3.9476	-2.0885	1.5527	2.3949
-1.8	0.74	3.9943	-1.7743	1.4952	2.4991
-1.7	0.8863	3.9796	-1.3208	1.386	2.5936
-1.6	1.0662	3.8876	-0.6891	1.212	2.6756
-1.5	1.2883	3.6978	0.167	0.9574	2.7404
-1.4	1.561	3.3829	1.3001	0.6026	2.7803
-1.3	1.8902	2.906	2.7647	0.1237	2.7823
-1.2	2.2756	2.2169	4.6099	-0.5079	2.7248
-1.1	2.7064	1.253	6.8664	-1.3221	2.5751
-1	3.1566	-0.0583	9.5281	-2.3448	2.2865
-0.9	3.5808	-1.7885	12.5309	-3.5865	1.798
-0.8	3.9125	-3.9944	15.732	-5.0305	1.0361
-0.7	4.0663	-6.7019	18.9008	-6.6226	-0.0793
-0.6	3.9429	-9.8995	21.7281	-8.2732	-1.6263
-0.5	3.4403	-13.5467	23.8675	-9.8783	-3.6684
-0.4	2.4718	-17.5924	25.0077	-11.3579	-6.2345
-0.3	0.9933	-21.9839	24.9639	-12.6954	-9.2885
-0.2	-0.9623	-26.6392	23.7524	-13.9489	-12.6903
-0.1	-3.2577	-31.3761	21.603	-15.2097	-16.1664
0	-5.6519	-35.8401	18.8845	-16.5208	-19.3193
0.1	-7.845	-39.5071	15.972	-17.8058	-21.7013
0.2	-9.5604	-41.8094	13.1283	-18.8687	-22.9407
0.3	-10.6263	-42.3397	10.4607	-19.4751	-22.8646
0.4	-11.0191	-41.0176	7.9602	-19.4628	-21.5548
0.5	-10.8476	-38.1209	5.5782	-18.8115	-19.3094
0.6	-10.2959	-34.1749	3.2871	-17.6388	-16.5361
0.7	-9.5575	-29.7764	1.1037	-16.1417	-13.6347
0.8	-8.7861	-25.4381	-0.92	-14.5257	-10.9124
0.9	-8.0749	-21.5048	-2.7199	-12.954	-8.5508

1	-7.4616	-18.1434	-4.2412	-11.528	-6.6154
1.1	-6.9448	-15.3826	-5.4517	-10.2927	-5.0899
1.2	-6.504	-13.1668	-6.3454	-9.2533	-3.9135
1.3	-6.1145	-11.4044	-6.9391	-8.3931	-3.0113
1.4	-5.7551	-10.0003	-7.2651	-7.6872	-2.3131
1.5	-5.4115	-8.8701	-7.3643	-7.1093	-1.7608
1.6	-5.0755	-7.9467	-7.2799	-6.6356	-1.3111
1.7	-4.744	-7.1782	-7.0537	-6.2453	-0.9329
1.8	-4.4165	-6.5256	-6.7238	-5.9202	-0.6054
1.9	-4.0944	-5.9599	-6.3233	-5.6446	-0.3153
2	-3.7799	-5.459	-5.8806	-5.4045	-0.0545
2.1	-3.4751	-5.0064	-5.4189	-5.1878	0.1814
2.2	-3.1823	-4.5894	-4.9574	-4.9841	0.3947
2.3	-2.9032	-4.1989	-4.5107	-4.7851	0.5862
2.4	-2.6394	-3.8281	-4.09	-4.5841	0.756
2.5	-2.3918	-3.4725	-3.7028	-4.3767	0.9042
2.6	-2.161	-3.1293	-3.3538	-4.1602	1.0309
2.7	-1.9474	-2.7972	-3.0449	-3.9339	1.1367
2.8	-1.7508	-2.4763	-2.7761	-3.6985	1.2222
2.9	-1.5708	-2.167	-2.5455	-3.4556	1.2886
3	-1.407	-1.8708	-2.3502	-3.2081	1.3373
3.1	-1.2585	-1.5891	-2.1864	-2.9589	1.3698
3.2	-1.1245	-1.3234	-2.05	-2.7112	1.3878
3.3	-1.004	-1.0754	-1.9368	-2.4683	1.3929
3.4	-0.8961	-0.8458	-1.8426	-2.2328	1.387
3.5	-0.7997	-0.6356	-1.7637	-2.0071	1.3715
3.6	-0.7139	-0.4449	-1.6967	-1.7931	1.3482
3.7	-0.6376	-0.2739	-1.6389	-1.5923	1.3184
3.8	-0.5698	-0.1217	-1.5877	-1.4053	1.2836
3.9	-0.5098	0.0121	-1.5414	-1.2327	1.2448
4	-0.4565	0.1288	-1.4984	-1.0745	1.2033
4.1	-0.4093	0.2295	-1.4575	-0.9304	1.1599
4.2	-0.3675	0.3155	-1.418	-0.7999	1.1154
4.3	-0.3304	0.3881	-1.3793	-0.6824	1.0705
4.4	-0.2974	0.4487	-1.341	-0.5771	1.0258
4.5	-0.2681	0.4985	-1.3028	-0.4831	0.9816
4.6	-0.242	0.5389	-1.2648	-0.3995	0.9384
4.7	-0.2187	0.5708	-1.2269	-0.3255	0.8963
4.8	-0.1979	0.5953	-1.1891	-0.2602	0.8555
4.9	-0.1793	0.6135	-1.1516	-0.2028	0.8163
5	-0.1627	0.6262	-1.1142	-0.1524	0.7786

trans-bicyclobutadienylene (C_{2h})

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Charge =  0 Multiplicity = 1
 C,0,-0.5130959458,1.8592584675,1.0929436274
 C,0,-1.614852863,1.0779566775,1.1018800625
 C,0,-0.9242237786,-0.110718653,0.5064875612
 C,0,0.3741798083,0.8096781676,0.4965553985
 C,0,-0.2880524548,-0.9985004222,1.4067897598
 C,0,1.0105880991,-0.0779656056,1.3968781692
 C,0,0.5987622742,-2.0475415031,0.8090060243
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C,0,1.7005867474,-1.2662837516,0.8001883151
H,0,-0.2427319362,2.7615856676,1.621330033
H,0,-2.550110867,1.1252159636,1.6399812419
H,0,0.3277941479,-2.949114773,0.2796555
H,0,2.6358567685,-1.3132702352,0.2621043071
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Sum of electronic and zero-point Energies= -306.840113
Sum of electronic and thermal Energies= -306.833966
Sum of electronic and thermal Enthalpies= -306.833022
Sum of electronic and thermal Free Energies= -306.869588

NICS-scan (central ring)

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.0467	1.4252	-1.5652	0.7552	0.67
-4.9	-0.0528	1.4977	-1.6563	0.7896	0.7081
-4.8	-0.06	1.5738	-1.7539	0.8251	0.7487
-4.7	-0.0684	1.6533	-1.8586	0.8614	0.7919
-4.6	-0.0783	1.7359	-1.9708	0.8981	0.8378
-4.5	-0.0899	1.8214	-2.0912	0.9349	0.8865
-4.4	-0.1038	1.9091	-2.2204	0.971	0.9381
-4.3	-0.1202	1.9983	-2.359	1.0059	0.9924
-4.2	-0.14	2.0877	-2.5077	1.0383	1.0494
-4.1	-0.1638	2.1757	-2.6672	1.067	1.1087
-4	-0.1927	2.2602	-2.8383	1.0902	1.17
-3.9	-0.228	2.3378	-3.0219	1.1054	1.2324
-3.8	-0.2713	2.4048	-3.2188	1.1098	1.295
-3.7	-0.3247	2.4559	-3.43	1.0996	1.3563
-3.6	-0.3906	2.4848	-3.6566	1.0703	1.4145
-3.5	-0.4722	2.4831	-3.8998	1.0161	1.467
-3.4	-0.5733	2.4412	-4.1611	0.9304	1.5108
-3.3	-0.6982	2.3474	-4.442	0.8053	1.5421
-3.2	-0.8521	2.1883	-4.7445	0.6317	1.5566
-3.1	-1.0406	1.949	-5.0709	0.3998	1.5492
-3	-1.2701	1.6133	-5.4237	0.0989	1.5144
-2.9	-1.5473	1.1642	-5.806	-0.2822	1.4464
-2.8	-1.8788	0.5851	-6.2215	-0.754	1.3391
-2.7	-2.2713	-0.1398	-6.6743	-1.3264	1.1866
-2.6	-2.7308	-1.0232	-7.169	-2.0066	0.9834
-2.5	-3.2617	-2.0739	-7.7112	-2.7986	0.7247
-2.4	-3.8666	-3.293	-8.3068	-3.7003	0.4073
-2.3	-4.5449	-4.672	-8.9627	-4.7019	0.0299
-2.2	-5.2918	-6.1891	-9.6862	-5.7834	-0.4057
-2.1	-6.0972	-7.8069	-10.4848	-6.9129	-0.894
-2	-6.9455	-9.471	-11.3656	-8.0458	-1.4252
-1.9	-7.8156	-11.1119	-12.335	-9.1269	-1.985
-1.8	-8.6827	-12.6509	-13.3973	-10.0955	-2.5554
-1.7	-9.5222	-14.0112	-14.5554	-10.894	-3.1172
-1.6	-10.3149	-15.1333	-15.8114	-11.4797	-3.6536
-1.5	-11.0545	-15.9938	-17.1698	-11.8379	-4.1559

-1.4	-11.755	-16.6232	-18.6419	-11.9928	-4.6304
-1.3	-12.4583	-17.1226	-20.2523	-12.0159	-5.1067
-1.2	-13.2397	-17.6742	-22.0451	-12.028	-5.6462
-1.1	-14.2118	-18.5473	-24.0882	-12.1962	-6.3511
-1	-15.523	-20.0959	-26.4732	-12.7264	-7.3695
-0.9	-17.3499	-22.743	-29.3067	-13.8485	-8.8945
-0.8	-19.8781	-26.9407	-32.6935	-15.7923	-11.1484
-0.7	-23.2657	-33.0905	-36.7067	-18.7475	-14.343
-0.6	-27.5874	-41.4154	-41.3467	-22.8034	-18.612
-0.5	-32.7622	-51.7926	-46.494	-27.8739	-23.9187
-0.4	-38.4859	-63.591	-51.8668	-33.6273	-29.9637
-0.3	-44.2024	-75.5982	-57.0091	-39.4606	-36.1376
-0.2	-49.1562	-86.1341	-61.3344	-44.5594	-41.5747
-0.1	-52.5468	-93.4013	-64.2392	-48.0657	-45.3356
0	-53.7541	-95.9996	-65.2626	-49.3172	-46.6824
0.1	-52.5434	-93.3981	-64.232	-48.0635	-45.3346
0.2	-49.1494	-86.1272	-61.321	-44.5546	-41.5726
0.3	-44.1926	-75.5868	-56.991	-39.4526	-36.1342
0.4	-38.4733	-63.574	-51.8459	-33.6153	-29.9587
0.5	-32.747	-51.7693	-46.4718	-27.8573	-23.912
0.6	-27.57	-41.3855	-41.3244	-22.7819	-18.6036
0.7	-23.2463	-33.0542	-36.6848	-18.7211	-14.3331
0.8	-19.8568	-26.8981	-32.6723	-15.7611	-11.137
0.9	-17.3269	-22.6945	-29.286	-13.8128	-8.8817
1	-15.4983	-20.0421	-26.4528	-12.6867	-7.3554
1.1	-14.1857	-18.489	-24.068	-12.1532	-6.3358
1.2	-13.2125	-17.6125	-22.0249	-11.9824	-5.6301
1.3	-12.4304	-17.0589	-20.2323	-11.969	-5.0899
1.4	-11.7272	-16.5594	-18.6223	-11.946	-4.6134
1.5	-11.0275	-15.9318	-17.1509	-11.7926	-4.1392
1.6	-10.2895	-15.075	-15.7934	-11.4374	-3.6376
1.7	-9.4989	-13.9581	-14.5385	-10.8559	-3.1022
1.8	-8.662	-12.6044	-13.3816	-10.0626	-2.5418
1.9	-7.7978	-11.0727	-12.3207	-9.0997	-1.973
2	-6.9306	-9.4392	-11.3526	-8.0244	-1.4148
2.1	-6.0851	-7.7822	-10.473	-6.897	-0.8852
2.2	-5.2822	-6.171	-9.6756	-5.7726	-0.3984
2.3	-4.5376	-4.6595	-8.9532	-4.6953	0.0358
2.4	-3.8612	-3.2854	-8.2982	-3.6973	0.4119
2.5	-3.2578	-2.0701	-7.7034	-2.7984	0.7283
2.6	-2.7282	-1.0225	-7.162	-2.0086	0.9861
2.7	-2.2697	-0.1412	-6.668	-1.3299	1.1887
2.8	-1.878	0.582	-6.2158	-0.7586	1.3406
2.9	-1.547	1.1599	-5.8009	-0.2875	1.4474
3	-1.2703	1.6082	-5.419	0.0932	1.515
3.1	-1.0411	1.9435	-5.0667	0.394	1.5495
3.2	-0.8527	2.1825	-4.7407	0.6259	1.5566
3.3	-0.699	2.3416	-4.4386	0.7996	1.542
3.4	-0.5742	2.4354	-4.1579	0.9249	1.5105

3.5	-0.4731	2.4775	-3.897	1.0109	1.4666
3.6	-0.3915	2.4795	-3.654	1.0654	1.4141
3.7	-0.3255	2.451	-3.4276	1.0951	1.3559
3.8	-0.2722	2.4002	-3.2166	1.1056	1.2946
3.9	-0.2288	2.3335	-3.0199	1.1015	1.232
4	-0.1935	2.2562	-2.8366	1.0866	1.1696
4.1	-0.1645	2.1721	-2.6656	1.0638	1.1083
4.2	-0.1406	2.0844	-2.5062	1.0354	1.049
4.3	-0.1208	1.9953	-2.3577	1.0032	0.9921
4.4	-0.1043	1.9064	-2.2192	0.9686	0.9378
4.5	-0.0904	1.8189	-2.0902	0.9326	0.8863
4.6	-0.0787	1.7336	-1.9698	0.896	0.8376
4.7	-0.0688	1.6512	-1.8577	0.8595	0.7917
4.8	-0.0604	1.5719	-1.7531	0.8234	0.7485
4.9	-0.0532	1.496	-1.6555	0.7881	0.7079
5	-0.047	1.4235	-1.5645	0.7537	0.6698

NICS-scan (terminal ring)

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.007	0.9288	-0.9079	0.5123	0.4165
-4.9	0.0075	0.9755	-0.953	0.5375	0.438
-4.8	0.0081	1.0252	-1.001	0.5643	0.4609
-4.7	0.0087	1.0784	-1.0523	0.5929	0.4855
-4.6	0.0094	1.1351	-1.1069	0.6233	0.5118
-4.5	0.0101	1.1957	-1.1653	0.6557	0.54
-4.4	0.011	1.2607	-1.2277	0.6904	0.5703
-4.3	0.0119	1.3302	-1.2945	0.7273	0.6029
-4.2	0.013	1.4048	-1.366	0.7668	0.638
-4.1	0.0141	1.4848	-1.4426	0.809	0.6758
-4	0.0154	1.5708	-1.5247	0.8541	0.7167
-3.9	0.0168	1.6631	-1.6128	0.9023	0.7608
-3.8	0.0183	1.7624	-1.7073	0.9538	0.8086
-3.7	0.0201	1.8691	-1.8088	1.0088	0.8603
-3.6	0.022	1.9839	-1.9179	1.0675	0.9164
-3.5	0.0241	2.1074	-2.0351	1.13	0.9774
-3.4	0.0263	2.24	-2.161	1.1964	1.0436
-3.3	0.0288	2.3827	-2.2963	1.2669	1.1158
-3.2	0.0313	2.5356	-2.4416	1.3411	1.1945
-3.1	0.034	2.6993	-2.5975	1.419	1.2803
-3	0.0365	2.874	-2.7645	1.4999	1.3741
-2.9	0.0387	3.0594	-2.9433	1.5828	1.4766
-2.8	0.0402	3.2548	-3.1342	1.6662	1.5886
-2.7	0.0405	3.4589	-3.3374	1.7479	1.711
-2.6	0.0388	3.6691	-3.5529	1.8245	1.8446
-2.5	0.0339	3.8821	-3.7803	1.8917	1.9904
-2.4	0.0245	4.0925	-4.0189	1.9432	2.1493
-2.3	0.0088	4.2935	-4.267	1.9715	2.322
-2.2	-0.0153	4.4761	-4.5221	1.9665	2.5096
-2.1	-0.0504	4.6297	-4.7807	1.9164	2.7133

-2	-0.0987	4.7413	-5.0374	1.8068	2.9345
-1.9	-0.1629	4.7961	-5.2848	1.6209	3.1752
-1.8	-0.2453	4.777	-5.5128	1.3392	3.4378
-1.7	-0.348	4.664	-5.708	0.9393	3.7247
-1.6	-0.4736	4.4328	-5.8535	0.3951	4.0377
-1.5	-0.6252	4.0529	-5.9286	-0.3235	4.3764
-1.4	-0.8085	3.4845	-5.9099	-1.251	4.7355
-1.3	-1.0328	2.6752	-5.7736	-2.4255	5.1007
-1.2	-1.3142	1.5568	-5.4994	-3.8859	5.4427
-1.1	-1.6775	0.0452	-5.0778	-5.6653	5.7105
-1	-2.1581	-1.9558	-4.5187	-7.7797	5.8239
-0.9	-2.8015	-4.544	-3.8604	-10.2131	5.6691
-0.8	-3.6596	-7.8023	-3.1767	-12.9016	5.0993
-0.7	-4.7849	-11.7797	-2.5749	-15.7261	3.9464
-0.6	-6.2201	-16.4777	-2.1825	-18.5238	2.0461
-0.5	-7.9884	-21.8472	-2.1181	-21.128	-0.7192
-0.4	-10.0817	-27.7953	-2.4497	-23.4305	-4.3648
-0.3	-12.4471	-34.1865	-3.1549	-25.4425	-8.744
-0.2	-14.9738	-40.8184	-4.1031	-27.3083	-13.5101
-0.1	-17.4852	-47.3719	-5.0838	-29.2378	-18.1341
0	-19.7502	-53.3693	-5.8814	-31.3715	-21.9978
0.1	-21.5235	-58.2081	-6.3623	-33.6564	-24.5517
0.2	-22.6095	-61.3019	-6.5268	-35.8244	-25.4775
0.3	-22.9241	-62.28	-6.4924	-37.4993	-24.7807
0.4	-22.5201	-61.1344	-6.4261	-38.3646	-22.7698
0.5	-21.5638	-58.2236	-6.4677	-38.2851	-19.9385
0.6	-20.2753	-54.1422	-6.6837	-37.3295	-16.8127
0.7	-18.864	-49.5306	-7.0614	-35.7064	-13.8242
0.8	-17.4826	-44.9176	-7.5303	-33.6711	-11.2465
0.9	-16.2118	-40.6398	-7.9956	-31.4489	-9.1909
1	-15.0684	-36.8385	-8.3667	-29.196	-7.6425
1.1	-14.0281	-33.5059	-8.5784	-26.9943	-6.5116
1.2	-13.0491	-30.5474	-8.5998	-24.8675	-5.6799
1.3	-12.0904	-27.8374	-8.4337	-22.8042	-5.0332
1.4	-11.1229	-25.2595	-8.1092	-20.7804	-4.4791
1.5	-10.133	-22.7279	-7.671	-18.7749	-3.953
1.6	-9.1217	-20.1966	-7.1686	-16.7789	-3.4177
1.7	-8.1012	-17.6571	-6.6465	-14.7988	-2.8583
1.8	-7.0902	-15.1312	-6.1395	-12.8542	-2.277
1.9	-6.1099	-12.6594	-5.6703	-10.9731	-1.6863
2	-5.1802	-10.2903	-5.2502	-9.1864	-1.1039
2.1	-4.3175	-8.0707	-4.8817	-7.5225	-0.5482
2.2	-3.5336	-6.0392	-4.5617	-6.0036	-0.0356
2.3	-2.8354	-4.2222	-4.2838	-4.644	0.4218
2.4	-2.2249	-2.634	-4.0408	-3.4502	0.8162
2.5	-1.7009	-1.2769	-3.8258	-2.4212	1.1443
2.6	-1.2588	-0.1439	-3.6327	-1.5504	1.4065
2.7	-0.8925	0.7791	-3.4567	-0.827	1.6061
2.8	-0.5945	1.5107	-3.2941	-0.2377	1.7484

2.9	-0.3565	2.0726	-3.1421	0.2326	1.84
3	-0.1704	2.4875	-2.9986	0.5993	1.8882
3.1	-0.0281	2.7779	-2.8624	0.8774	1.9005
3.2	0.0778	2.9657	-2.7323	1.0816	1.8841
3.3	0.1541	3.0702	-2.6079	1.2248	1.8454
3.4	0.207	3.1094	-2.4886	1.319	1.7904
3.5	0.2414	3.0985	-2.3742	1.3745	1.724
3.6	0.2618	3.0501	-2.2646	1.3998	1.6503
3.7	0.2717	2.9749	-2.1597	1.4024	1.5725
3.8	0.2739	2.8811	-2.0595	1.3879	1.4932
3.9	0.2705	2.7755	-1.9638	1.3612	1.4143
4	0.2634	2.6629	-1.8727	1.3258	1.3371
4.1	0.2537	2.5472	-1.786	1.2847	1.2625
4.2	0.2425	2.431	-1.7035	1.2399	1.1911
4.3	0.2304	2.3164	-1.6253	1.1931	1.1233
4.4	0.2179	2.2047	-1.551	1.1455	1.0592
4.5	0.2054	2.0967	-1.4805	1.0978	0.9989
4.6	0.1931	1.9931	-1.4137	1.0509	0.9422
4.7	0.1812	1.894	-1.3504	1.0049	0.8891
4.8	0.1698	1.7998	-1.2904	0.9604	0.8394
4.9	0.159	1.7104	-1.2335	0.9175	0.7929
5	0.1487	1.6256	-1.1795	0.8762	0.7494

(1*Z*,5*Z*)-cycloocta-1,5-dien-3,7-diyne (D_{2h}), **7**

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Charge =  0 Multiplicity = 1
 C,0,1.9038527402,0.6776309203,0.
 C,0,1.9038527402,-0.6776309203,0.
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 C,0,0.6058105338,-1.3126771614,0.
 C,0,-0.6058105338,1.3126771614,0.
 C,0,-0.6058105338,-1.3126771614,0.
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 C,0,-1.9038527402,-0.6776309203,0.
 H,0,2.8266343903,1.2439270525,0.
 H,0,2.8266343903,-1.2439270525,0.
 H,0,-2.8266343903,1.2439270525,0.
 H,0,-2.8266343903,-1.2439270525,0.
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Sum of electronic and zero-point Energies= -307.036965
Sum of electronic and thermal Energies= -307.030570
Sum of electronic and thermal Enthalpies= -307.029626
Sum of electronic and thermal Free Energies= -307.065629

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	1.037	0.9585	2.1526	0.4684	0.4901
-4.9	1.098	1.0027	2.2913	0.4897	0.513
-4.8	1.1636	1.0492	2.4417	0.512	0.5372
-4.7	1.2344	1.0984	2.605	0.5356	0.5628
-4.6	1.3109	1.1501	2.7826	0.5603	0.5898
-4.5	1.3935	1.2047	2.9759	0.5862	0.6185
-4.4	1.483	1.2622	3.1867	0.6134	0.6488
-4.3	1.5799	1.3227	3.4169	0.6418	0.6809

-4.2	1.685	1.3863	3.6686	0.6715	0.7148
-4.1	1.7991	1.4532	3.9441	0.7024	0.7508
-4	1.9232	1.5235	4.2462	0.7346	0.7889
-3.9	2.0583	1.5972	4.5778	0.7679	0.8293
-3.8	2.2056	1.6743	4.9424	0.8023	0.872
-3.7	2.3662	1.7549	5.3438	0.8376	0.9173
-3.6	2.5417	1.8389	5.7862	0.8737	0.9652
-3.5	2.7336	1.9263	6.2745	0.9103	1.016
-3.4	2.9436	2.0167	6.8141	0.947	1.0697
-3.3	3.1737	2.11	7.411	0.9835	1.1265
-3.2	3.4259	2.2056	8.072	1.0191	1.1865
-3.1	3.7026	2.303	8.8047	1.0532	1.2498
-3	4.0063	2.4014	9.6175	1.0849	1.3165
-2.9	4.3398	2.4997	10.5197	1.1131	1.3866
-2.8	4.7058	2.5961	11.5214	1.1362	1.4599
-2.7	5.1075	2.6885	12.634	1.1525	1.536
-2.6	5.5478	2.774	13.8695	1.1594	1.6146
-2.5	6.0298	2.8484	15.2411	1.1539	1.6945
-2.4	6.5564	2.9068	16.7625	1.1321	1.7747
-2.3	7.1302	2.9421	18.4484	1.0889	1.8532
-2.2	7.753	2.9457	20.3135	1.0178	1.9279
-2.1	8.4264	2.9066	22.3727	0.9109	1.9957
-2	9.1507	2.8117	24.6403	0.7582	2.0535
-1.9	9.9248	2.6452	27.1292	0.5479	2.0973
-1.8	10.7463	2.389	29.8498	0.2655	2.1235
-1.7	11.6106	2.0227	32.809	-0.1056	2.1283
-1.6	12.5107	1.524	36.0082	-0.5846	2.1086
-1.5	13.4369	0.8692	39.4413	-1.1929	2.0621
-1.4	14.3756	0.0346	43.0922	-1.9531	1.9877
-1.3	15.3099	-1.0027	46.9325	-2.8887	1.886
-1.2	16.2188	-2.2623	50.9188	-4.0214	1.7591
-1.1	17.0779	-3.7573	54.9911	-5.3688	1.6115
-1	17.8606	-5.4906	59.0724	-6.9402	1.4496
-0.9	18.5403	-7.4499	63.0709	-8.7321	1.2822
-0.8	19.094	-9.6024	66.8843	-10.7222	1.1198
-0.7	19.5059	-11.8908	70.4084	-12.8647	0.9739
-0.6	19.7719	-14.2322	73.5478	-15.0872	0.855
-0.5	19.9024	-16.5198	76.2271	-17.2903	0.7705
-0.4	19.9228	-18.6317	78.4001	-19.3535	0.7218
-0.3	19.8709	-20.4408	80.0535	-21.1448	0.704
-0.2	19.7903	-21.8299	81.201	-22.536	0.7061
-0.1	19.7223	-22.7044	81.8713	-23.4191	0.7147
0	19.6961	-23.003	82.0912	-23.7219	0.7189
0.1	19.7223	-22.7044	81.8713	-23.4191	0.7147
0.2	19.7903	-21.8299	81.201	-22.536	0.7061
0.3	19.8709	-20.4408	80.0535	-21.1448	0.704
0.4	19.9228	-18.6317	78.4001	-19.3535	0.7218
0.5	19.9024	-16.5198	76.2271	-17.2903	0.7705
0.6	19.7719	-14.2322	73.5478	-15.0872	0.855

0.7	19.5059	-11.8908	70.4084	-12.8647	0.9739
0.8	19.094	-9.6024	66.8843	-10.7222	1.1198
0.9	18.5403	-7.4499	63.0709	-8.7321	1.2822
1	17.8606	-5.4906	59.0724	-6.9402	1.4496
1.1	17.0779	-3.7573	54.9911	-5.3688	1.6115
1.2	16.2188	-2.2623	50.9188	-4.0214	1.7591
1.3	15.3099	-1.0027	46.9325	-2.8887	1.886
1.4	14.3756	0.0346	43.0922	-1.9531	1.9877
1.5	13.4369	0.8692	39.4413	-1.1929	2.0621
1.6	12.5107	1.524	36.0082	-0.5846	2.1086
1.7	11.6106	2.0227	32.809	-0.1056	2.1283
1.8	10.7463	2.389	29.8498	0.2655	2.1235
1.9	9.9248	2.6452	27.1292	0.5479	2.0973
2	9.1507	2.8117	24.6403	0.7582	2.0535
2.1	8.4264	2.9066	22.3727	0.9109	1.9957
2.2	7.753	2.9457	20.3135	1.0178	1.9279
2.3	7.1302	2.9421	18.4484	1.0889	1.8532
2.4	6.5564	2.9068	16.7625	1.1321	1.7747
2.5	6.0298	2.8484	15.2411	1.1539	1.6945
2.6	5.5478	2.774	13.8695	1.1594	1.6146
2.7	5.1075	2.6885	12.634	1.1525	1.536
2.8	4.7058	2.5961	11.5214	1.1362	1.4599
2.9	4.3398	2.4997	10.5197	1.1131	1.3866
3	4.0063	2.4014	9.6175	1.0849	1.3165
3.1	3.7026	2.303	8.8047	1.0532	1.2498
3.2	3.4259	2.2056	8.072	1.0191	1.1865
3.3	3.1737	2.11	7.411	0.9835	1.1265
3.4	2.9436	2.0167	6.8141	0.947	1.0697
3.5	2.7336	1.9263	6.2745	0.9103	1.016
3.6	2.5417	1.8389	5.7862	0.8737	0.9652
3.7	2.3662	1.7549	5.3438	0.8376	0.9173
3.8	2.2056	1.6743	4.9424	0.8023	0.872
3.9	2.0583	1.5972	4.5778	0.7679	0.8293
4	1.9232	1.5235	4.2462	0.7346	0.7889
4.1	1.7991	1.4532	3.9441	0.7024	0.7508
4.2	1.685	1.3863	3.6686	0.6715	0.7148
4.3	1.5799	1.3227	3.4169	0.6418	0.6809
4.4	1.483	1.2622	3.1867	0.6134	0.6488
4.5	1.3935	1.2047	2.9759	0.5862	0.6185
4.6	1.3109	1.1501	2.7826	0.5603	0.5898
4.7	1.2344	1.0984	2.605	0.5356	0.5628
4.8	1.1636	1.0492	2.4417	0.512	0.5372
4.9	1.098	1.0027	2.2913	0.4897	0.513
5	1.037	0.9585	2.1526	0.4684	0.4901

[bicyclo[3.2.0]hepta-1,3,6-trienyl]$^-$ (C_{2v}), 8

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Charge = -1 Multiplicity = 1
 C,0,0.,0.8237666747,-1.6912561867
 C,0,0.,-0.8237666747,-1.6912561867
 C,0,0.,-0.7703462603,-0.3319584645
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C,0,0.,0.7703462603,-0.3319584645
C,0,0.,-1.2015511591,1.0398578159
C,0,0.,0.,1.7906158482
C,0,0.,1.2015511591,1.0398578159
H,0,0.,1.6026941201,-2.44631553
H,0,0.,-1.6026941201,-2.44631553
H,0,0.,-2.203035464,1.4485857019
H,0,0.,2.203035464,1.4485857019
H,0,0.,0.,2.8812510186
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Sum of electronic and zero-point Energies= -269.556091
Sum of electronic and thermal Energies= -269.549634
Sum of electronic and thermal Enthalpies= -269.548689
Sum of electronic and thermal Free Energies= -269.584980

NICS-scan (cyclobutadiene ring)

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	4.3797	0.7889	12.3503	0.3782	0.4107
-4.9	4.6366	0.8282	13.0816	0.3963	0.4319
-4.8	4.9137	0.8704	13.8707	0.4157	0.4547
-4.7	5.213	0.9154	14.7235	0.4364	0.479
-4.6	5.5367	0.9638	15.6463	0.4586	0.5052
-4.5	5.8874	1.0158	16.6464	0.4825	0.5333
-4.4	6.2679	1.0717	17.7319	0.5081	0.5636
-4.3	6.6813	1.1319	18.9119	0.5357	0.5962
-4.2	7.1313	1.197	20.1968	0.5655	0.6315
-4.1	7.6219	1.2673	21.5984	0.5977	0.6696
-4	8.1578	1.3434	23.13	0.6326	0.7108
-3.9	8.7443	1.4259	24.8068	0.6705	0.7554
-3.8	9.3873	1.5154	26.6464	0.7116	0.8038
-3.7	10.0938	1.6127	28.6687	0.7563	0.8564
-3.6	10.8717	1.7184	30.8967	0.805	0.9134
-3.5	11.7302	1.8334	33.3572	0.858	0.9754
-3.4	12.6799	1.9587	36.0808	0.9159	1.0428
-3.3	13.7328	2.0952	39.1033	0.9792	1.116
-3.2	14.9033	2.2438	42.4661	1.0482	1.1956
-3.1	16.2076	2.4055	46.2173	1.1237	1.2818
-3	17.6648	2.5813	50.4131	1.2061	1.3752
-2.9	19.2968	2.7719	55.1185	1.2961	1.4758
-2.8	21.1289	2.9778	60.409	1.394	1.5838
-2.7	23.1904	3.1991	66.3722	1.5004	1.6987
-2.6	25.5147	3.4351	73.1092	1.6156	1.8195
-2.5	28.1401	3.684	80.7364	1.7395	1.9445
-2.4	31.1102	3.9432	89.3874	1.8721	2.0711
-2.3	34.4744	4.2083	99.215	2.0129	2.1954
-2.2	38.2888	4.4732	110.3932	2.1613	2.3119
-2.1	42.6167	4.7301	123.1201	2.3166	2.4135
-2	47.5297	4.9689	137.6202	2.4778	2.4911
-1.9	53.1078	5.1775	154.146	2.6439	2.5336
-1.8	59.44	5.3407	172.9793	2.8135	2.5272
-1.7	66.6221	5.4399	194.4265	2.9847	2.4552

-1.6	74.7526	5.451	218.8068	3.1537	2.2973
-1.5	83.9221	5.3416	246.4247	3.3129	2.0287
-1.4	94.196	5.0675	277.5204	3.4479	1.6196
-1.3	105.585	4.5681	312.1868	3.5329	1.0352
-1.2	118.0038	3.7624	350.249	3.5249	0.2375
-1.1	131.2187	2.5488	391.1073	3.358	-0.8092
-1	144.793	0.8108	433.5683	2.9392	-2.1284
-0.9	158.0495	-1.5651	475.7135	2.1513	-3.7164
-0.8	170.0774	-4.6592	514.8914	0.8663	-5.5255
-0.7	179.8195	-8.4776	547.9362	-1.0258	-7.4518
-0.6	186.2637	-12.9123	571.7033	-3.5741	-9.3382
-0.5	188.7373	-17.7181	583.9299	-6.7164	-11.0017
-0.4	187.2452	-22.5252	584.2609	-10.2402	-12.285
-0.3	182.7155	-26.89	575.0364	-13.7748	-13.1152
-0.2	176.9624	-30.3728	561.26	-16.8359	-13.5369
-0.1	172.2325	-32.6147	549.3122	-18.9266	-13.6881
0	170.4099	-33.3876	544.6174	-19.6704	-13.7172
0.1	172.2325	-32.6147	549.3122	-18.9266	-13.6881
0.2	176.9624	-30.3728	561.26	-16.8359	-13.5369
0.3	182.7155	-26.89	575.0364	-13.7748	-13.1152
0.4	187.2452	-22.5252	584.2609	-10.2402	-12.285
0.5	188.7373	-17.7181	583.9299	-6.7164	-11.0017
0.6	186.2637	-12.9123	571.7033	-3.5741	-9.3382
0.7	179.8195	-8.4776	547.9362	-1.0258	-7.4518
0.8	170.0774	-4.6592	514.8914	0.8663	-5.5255
0.9	158.0495	-1.5651	475.7135	2.1513	-3.7164
1	144.793	0.8108	433.5683	2.9392	-2.1284
1.1	131.2187	2.5488	391.1073	3.358	-0.8092
1.2	118.0038	3.7624	350.249	3.5249	0.2375
1.3	105.585	4.5681	312.1868	3.5329	1.0352
1.4	94.196	5.0675	277.5204	3.4479	1.6196
1.5	83.9221	5.3416	246.4247	3.3129	2.0287
1.6	74.7526	5.451	218.8068	3.1537	2.2973
1.7	66.6221	5.4399	194.4265	2.9847	2.4552
1.8	59.44	5.3407	172.9793	2.8135	2.5272
1.9	53.1078	5.1775	154.146	2.6439	2.5336
2	47.5297	4.9689	137.6202	2.4778	2.4911
2.1	42.6167	4.7301	123.1201	2.3166	2.4135
2.2	38.2888	4.4732	110.3932	2.1613	2.3119
2.3	34.4744	4.2083	99.215	2.0129	2.1954
2.4	31.1102	3.9432	89.3874	1.8721	2.0711
2.5	28.1401	3.684	80.7364	1.7395	1.9445
2.6	25.5147	3.4351	73.1092	1.6156	1.8195
2.7	23.1904	3.1991	66.3722	1.5004	1.6987
2.8	21.1289	2.9778	60.409	1.394	1.5838
2.9	19.2968	2.7719	55.1185	1.2961	1.4758
3	17.6648	2.5813	50.4131	1.2061	1.3752
3.1	16.2076	2.4055	46.2173	1.1237	1.2818
3.2	14.9033	2.2438	42.4661	1.0482	1.1956

3.3	13.7328	2.0952	39.1033	0.9792	1.116
3.4	12.6799	1.9587	36.0808	0.9159	1.0428
3.5	11.7302	1.8334	33.3572	0.858	0.9754
3.6	10.8717	1.7184	30.8967	0.805	0.9134
3.7	10.0938	1.6127	28.6687	0.7563	0.8564
3.8	9.3873	1.5154	26.6464	0.7116	0.8038
3.9	8.7443	1.4259	24.8068	0.6705	0.7554
4	8.1578	1.3434	23.13	0.6326	0.7108
4.1	7.6219	1.2673	21.5984	0.5977	0.6696
4.2	7.1313	1.197	20.1968	0.5655	0.6315
4.3	6.6813	1.1319	18.9119	0.5357	0.5962
4.4	6.2679	1.0717	17.7319	0.5081	0.5636
4.5	5.8874	1.0158	16.6464	0.4825	0.5333
4.6	5.5367	0.9638	15.6463	0.4586	0.5052
4.7	5.213	0.9154	14.7235	0.4364	0.479
4.8	4.9137	0.8704	13.8707	0.4157	0.4547
4.9	4.6366	0.8282	13.0816	0.3963	0.4319
5	4.3797	0.7889	12.3503	0.3782	0.4107

NICS-scan (cyclopentadienyl ring

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	4.3279	0.828	12.1557	0.423	0.405
-4.9	4.5764	0.8702	12.859	0.4446	0.4256
-4.8	4.8437	0.9153	13.6157	0.4677	0.4476
-4.7	5.1315	0.9637	14.4308	0.4925	0.4712
-4.6	5.4417	1.0154	15.3097	0.519	0.4964
-4.5	5.7766	1.0711	16.2587	0.5475	0.5236
-4.4	6.1385	1.1308	17.2846	0.5781	0.5527
-4.3	6.53	1.1951	18.395	0.6111	0.584
-4.2	6.9543	1.2644	19.5984	0.6466	0.6178
-4.1	7.4145	1.339	20.9043	0.6848	0.6542
-4	7.9144	1.4196	22.3235	0.7261	0.6935
-3.9	8.4582	1.5066	23.8679	0.7706	0.736
-3.8	9.0506	1.6007	25.5511	0.8187	0.782
-3.7	9.6969	1.7025	27.3884	0.8707	0.8318
-3.6	10.4032	1.8124	29.3971	0.9267	0.8857
-3.5	11.176	1.9313	31.5967	0.9872	0.9441
-3.4	12.0231	2.0598	34.0094	1.0524	1.0074
-3.3	12.953	2.1986	36.6605	1.1227	1.0759
-3.2	13.9756	2.3483	39.5785	1.1982	1.1501
-3.1	15.1019	2.5097	42.7961	1.2793	1.2304
-3	16.3444	2.683	46.3502	1.366	1.317
-2.9	17.7171	2.8685	50.2829	1.4585	1.41
-2.8	19.2359	3.0663	54.6416	1.5568	1.5095
-2.7	20.9185	3.2755	59.4801	1.6605	1.615
-2.6	22.7846	3.4952	64.8586	1.7692	1.726
-2.5	24.8558	3.7228	70.8446	1.882	1.8408
-2.4	27.1561	3.9554	77.5128	1.998	1.9574
-2.3	29.7111	4.188	84.9455	2.1154	2.0726

-2.2	32.5488	4.4141	93.2323	2.2323	2.1818
-2.1	35.6985	4.6258	102.4697	2.3465	2.2793
-2	39.1909	4.8124	112.7602	2.4551	2.3573
-1.9	43.0573	4.9618	124.21	2.5552	2.4066
-1.8	47.3284	5.0589	136.9262	2.6434	2.4155
-1.7	52.0321	5.0862	151.0101	2.7159	2.3703
-1.6	57.1903	5.023	166.5477	2.7683	2.2547
-1.5	62.8126	4.8445	183.5932	2.7948	2.0497
-1.4	68.8884	4.5212	202.144	2.7876	1.7336
-1.3	75.3748	4.0186	222.1057	2.7359	1.2827
-1.2	82.1813	3.2978	243.2461	2.625	0.6728
-1.1	89.1536	2.3171	265.1437	2.4352	-0.1181
-1	96.06	1.0382	287.1419	2.1427	-1.1045
-0.9	102.5886	-0.565	308.3307	1.7219	-2.2869
-0.8	108.3639	-2.4942	327.5858	1.1502	-3.6444
-0.7	112.9945	-4.7131	343.6966	0.4161	-5.1292
-0.6	116.1532	-7.1368	355.5964	-0.4709	-6.6659
-0.5	117.6792	-9.6309	362.6686	-1.4718	-8.1591
-0.4	117.6735	-12.0224	365.0428	-2.5146	-9.5078
-0.3	116.5396	-14.1234	363.7422	-3.4992	-10.6242
-0.2	114.9278	-15.7604	360.5439	-4.3126	-11.4478
-0.1	113.5692	-16.7981	357.5058	-4.8502	-11.9479
0	113.0428	-17.1533	356.2818	-5.0383	-12.115
0.1	113.5692	-16.7981	357.5058	-4.8502	-11.9479
0.2	114.9278	-15.7604	360.5439	-4.3126	-11.4478
0.3	116.5396	-14.1234	363.7422	-3.4992	-10.6242
0.4	117.6735	-12.0224	365.0428	-2.5146	-9.5078
0.5	117.6792	-9.6309	362.6686	-1.4718	-8.1591
0.6	116.1532	-7.1368	355.5964	-0.4709	-6.6659
0.7	112.9945	-4.7131	343.6966	0.4161	-5.1292
0.8	108.3639	-2.4942	327.5858	1.1502	-3.6444
0.9	102.5886	-0.565	308.3307	1.7219	-2.2869
1	96.06	1.0382	287.1419	2.1427	-1.1045
1.1	89.1536	2.3171	265.1437	2.4352	-0.1181
1.2	82.1813	3.2978	243.2461	2.625	0.6728
1.3	75.3748	4.0186	222.1057	2.7359	1.2827
1.4	68.8884	4.5212	202.144	2.7876	1.7336
1.5	62.8126	4.8445	183.5932	2.7948	2.0497
1.6	57.1903	5.023	166.5477	2.7683	2.2547
1.7	52.0321	5.0862	151.0101	2.7159	2.3703
1.8	47.3284	5.0589	136.9262	2.6434	2.4155
1.9	43.0573	4.9618	124.21	2.5552	2.4066
2	39.1909	4.8124	112.7602	2.4551	2.3573
2.1	35.6985	4.6258	102.4697	2.3465	2.2793
2.2	32.5488	4.4141	93.2323	2.2323	2.1818
2.3	29.7111	4.188	84.9455	2.1154	2.0726
2.4	27.1561	3.9554	77.5128	1.998	1.9574
2.5	24.8558	3.7228	70.8446	1.882	1.8408
2.6	22.7846	3.4952	64.8586	1.7692	1.726

2.7	20.9185	3.2755	59.4801	1.6605	1.615
2.8	19.2359	3.0663	54.6416	1.5568	1.5095
2.9	17.7171	2.8685	50.2829	1.4585	1.41
3	16.3444	2.683	46.3502	1.366	1.317
3.1	15.1019	2.5097	42.7961	1.2793	1.2304
3.2	13.9756	2.3483	39.5785	1.1982	1.1501
3.3	12.953	2.1986	36.6605	1.1227	1.0759
3.4	12.0231	2.0598	34.0094	1.0524	1.0074
3.5	11.176	1.9313	31.5967	0.9872	0.9441
3.6	10.4032	1.8124	29.3971	0.9267	0.8857
3.7	9.6969	1.7025	27.3884	0.8707	0.8318
3.8	9.0506	1.6007	25.5511	0.8187	0.782
3.9	8.4582	1.5066	23.8679	0.7706	0.736
4	7.9144	1.4196	22.3235	0.7261	0.6935
4.1	7.4145	1.339	20.9043	0.6848	0.6542
4.2	6.9543	1.2644	19.5984	0.6466	0.6178
4.3	6.53	1.1951	18.395	0.6111	0.584
4.4	6.1385	1.1308	17.2846	0.5781	0.5527
4.5	5.7766	1.0711	16.2587	0.5475	0.5236
4.6	5.4417	1.0154	15.3097	0.519	0.4964
4.7	5.1315	0.9637	14.4308	0.4925	0.4712
4.8	4.8437	0.9153	13.6157	0.4677	0.4476
4.9	4.5764	0.8702	12.859	0.4446	0.4256
5	4.3279	0.828	12.1557	0.423	0.405

cubane (O_h), 9

```
Charge =  0 Multiplicity = 1
 C,0,0.7853,0.7853,0.
 C,0,-0.7853,-0.7853,-1.5706
 C,0,0.7853,-0.7853,0.
 C,0,0.7853,0.7853,-1.5706
 C,0,0.7853,-0.7853,-1.5706
 C,0,-0.7853,0.7853,-1.5706
 C,0,-0.7853,-0.7853,0.
 C,0,-0.7853,0.7853,0.
 H,0,1.4144,1.4144,0.6291
 H,0,-1.4144,-1.4144,-2.1997
 H,0,1.4144,-1.4144,0.6291
 H,0,1.4144,1.4144,-2.1997
 H,0,1.4144,-1.4144,-2.1997
 H,0,-1.4144,1.4144,-2.1997
 H,0,-1.4144,-1.4144,0.6291
 H,0,-1.4144,1.4144,0.6291
```

Sum of electronic and zero-point Energies= -309.399896
Sum of electronic and thermal Energies= -309.395335
Sum of electronic and thermal Enthalpies= -309.394391
Sum of electronic and thermal Free Energies= -309.425099

NICS-Scan(center)

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.0443	1.0782	-1.2111	0.5391	0.5391
-4.9	-0.0485	1.133	-1.2785	0.5665	0.5665
-4.8	-0.0531	1.191	-1.3503	0.5955	0.5955
-4.7	-0.0583	1.252	-1.4269	0.626	0.626

-4.6	-0.064	1.3166	-1.5086	0.6583	0.6583
-4.5	-0.0704	1.3846	-1.5957	0.6923	0.6923
-4.4	-0.0774	1.456	-1.6884	0.728	0.728
-4.3	-0.0853	1.5312	-1.787	0.7656	0.7656
-4.2	-0.0939	1.6098	-1.8917	0.8049	0.8049
-4.1	-0.1035	1.6922	-2.0027	0.8461	0.8461
-4	-0.114	1.7782	-2.12	0.8891	0.8891
-3.9	-0.1254	1.8674	-2.2436	0.9337	0.9337
-3.8	-0.1378	1.9598	-2.3733	0.9799	0.9799
-3.7	-0.151	2.0552	-2.5084	1.0276	1.0276
-3.6	-0.165	2.1532	-2.6481	1.0766	1.0766
-3.5	-0.1793	2.253	-2.791	1.1265	1.1265
-3.4	-0.1936	2.3542	-2.9351	1.1771	1.1771
-3.3	-0.2072	2.4558	-3.0775	1.2279	1.2279
-3.2	-0.2191	2.5568	-3.214	1.2784	1.2784
-3.1	-0.2278	2.6556	-3.339	1.3278	1.3278
-3	-0.2313	2.7508	-3.4446	1.3754	1.3754
-2.9	-0.2267	2.8404	-3.5204	1.4202	1.4202
-2.8	-0.2101	2.9218	-3.5522	1.4609	1.4609
-2.7	-0.1761	2.9926	-3.5209	1.4963	1.4963
-2.6	-0.1175	3.0486	-3.4011	1.5243	1.5243
-2.5	-0.0246	3.0852	-3.1588	1.5426	1.5426
-2.4	0.1153	3.095	-2.7492	1.5475	1.5475
-2.3	0.318	3.0676	-2.1135	1.5338	1.5338
-2.2	0.6036	2.987	-1.1762	1.4935	1.4935
-2.1	0.9954	2.8284	0.1579	1.4142	1.4142
-2	1.5194	2.5544	2.0038	1.2772	1.2772
-1.9	2.2014	2.1106	4.4937	1.0553	1.0553
-1.8	3.0629	1.4222	7.7665	0.7111	0.7111
-1.7	4.1147	0.3962	11.9479	0.1981	0.1981
-1.6	5.3498	-1.0682	17.1175	-0.5341	-0.5341
-1.5	6.737	-3.0522	23.2632	-1.5261	-1.5261
-1.4	8.2184	-5.5728	30.228	-2.7864	-2.7864
-1.3	9.714	-8.5208	37.6629	-4.2604	-4.2604
-1.2	11.1363	-11.5988	45.0077	-5.7994	-5.7994
-1.1	12.4139	-14.2862	51.5279	-7.1431	-7.1431
-1	13.5192	-15.868	56.4255	-7.934	-7.934
-0.9	14.4873	-15.5544	59.0162	-7.7772	-7.7772
-0.8	15.4132	-12.6838	58.9232	-6.3419	-6.3419
-0.7	16.4193	-6.952	56.21	-3.476	-3.476
-0.6	17.6033	1.4226	51.3873	0.7113	0.7113
-0.5	18.9878	11.6774	45.2861	5.8387	5.8387
-0.4	20.4987	22.6394	38.8568	11.3197	11.3197
-0.3	21.9791	32.9606	32.9765	16.4803	16.4803
-0.2	23.2317	41.3646	28.3306	20.6823	20.6823
-0.1	24.0708	46.8356	25.3768	23.4178	23.4178
0	24.366	48.732	24.366	24.366	24.366
0.1	24.0708	46.8356	25.3768	23.4178	23.4178
0.2	23.2317	41.3646	28.3306	20.6823	20.6823

0.3	21.9791	32.9606	32.9765	16.4803	16.4803
0.4	20.4987	22.6394	38.8568	11.3197	11.3197
0.5	18.9878	11.6774	45.2861	5.8387	5.8387
0.6	17.6033	1.4226	51.3873	0.7113	0.7113
0.7	16.4193	-6.952	56.21	-3.476	-3.476
0.8	15.4132	-12.6838	58.9232	-6.3419	-6.3419
0.9	14.4873	-15.5544	59.0162	-7.7772	-7.7772
1	13.5192	-15.868	56.4255	-7.934	-7.934
1.1	12.4139	-14.2862	51.5279	-7.1431	-7.1431
1.2	11.1363	-11.5988	45.0077	-5.7994	-5.7994
1.3	9.714	-8.5208	37.6629	-4.2604	-4.2604
1.4	8.2184	-5.5728	30.228	-2.7864	-2.7864
1.5	6.737	-3.0522	23.2632	-1.5261	-1.5261
1.6	5.3498	-1.0682	17.1175	-0.5341	-0.5341
1.7	4.1147	0.3962	11.9479	0.1981	0.1981
1.8	3.0629	1.4222	7.7665	0.7111	0.7111
1.9	2.2014	2.1106	4.4937	1.0553	1.0553
2	1.5194	2.5544	2.0038	1.2772	1.2772
2.1	0.9954	2.8284	0.1579	1.4142	1.4142
2.2	0.6036	2.987	-1.1762	1.4935	1.4935
2.3	0.318	3.0676	-2.1135	1.5338	1.5338
2.4	0.1153	3.095	-2.7492	1.5475	1.5475
2.5	-0.0246	3.0852	-3.1588	1.5426	1.5426
2.6	-0.1175	3.0486	-3.4011	1.5243	1.5243
2.7	-0.1761	2.9926	-3.5209	1.4963	1.4963
2.8	-0.2101	2.9218	-3.5522	1.4609	1.4609
2.9	-0.2267	2.8404	-3.5204	1.4202	1.4202
3	-0.2313	2.7508	-3.4446	1.3754	1.3754
3.1	-0.2278	2.6556	-3.339	1.3278	1.3278
3.2	-0.2191	2.5568	-3.214	1.2784	1.2784
3.3	-0.2072	2.4558	-3.0775	1.2279	1.2279
3.4	-0.1936	2.3542	-2.9351	1.1771	1.1771
3.5	-0.1793	2.253	-2.791	1.1265	1.1265
3.6	-0.165	2.1532	-2.6481	1.0766	1.0766
3.7	-0.151	2.0552	-2.5084	1.0276	1.0276
3.8	-0.1378	1.9598	-2.3733	0.9799	0.9799
3.9	-0.1254	1.8674	-2.2436	0.9337	0.9337
4	-0.114	1.7782	-2.12	0.8891	0.8891
4.1	-0.1035	1.6922	-2.0027	0.8461	0.8461
4.2	-0.0939	1.6098	-1.8917	0.8049	0.8049
4.3	-0.0853	1.5312	-1.787	0.7656	0.7656
4.4	-0.0774	1.456	-1.6884	0.728	0.728
4.5	-0.0704	1.3846	-1.5957	0.6923	0.6923
4.6	-0.064	1.3166	-1.5086	0.6583	0.6583
4.7	-0.0583	1.252	-1.4269	0.626	0.626
4.8	-0.0531	1.191	-1.3503	0.5955	0.5955
4.9	-0.0485	1.133	-1.2785	0.5665	0.5665
5	-0.0443	1.0782	-1.2111	0.5391	0.5391

NICS-Scan(face)

Distance(Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.1042	1.5632	-1.8759	0.7816	0.7816
-4.9	-0.114	1.644	-1.986	0.822	0.822
-4.8	-0.1247	1.7282	-2.1024	0.8641	0.8641
-4.7	-0.1365	1.8156	-2.2251	0.9078	0.9078
-4.6	-0.1493	1.906	-2.3538	0.953	0.953
-4.5	-0.163	1.9992	-2.4882	0.9996	0.9996
-4.4	-0.1776	2.0946	-2.6273	1.0473	1.0473
-4.3	-0.1928	2.1916	-2.7699	1.0958	1.0958
-4.2	-0.2082	2.2894	-2.914	1.1447	1.1447
-4.1	-0.2232	2.3874	-3.0568	1.1937	1.1937
-4	-0.2368	2.484	-3.1945	1.242	1.242
-3.9	-0.2478	2.578	-3.3216	1.289	1.289
-3.8	-0.2543	2.6678	-3.4307	1.3339	1.3339
-3.7	-0.2535	2.7512	-3.5117	1.3756	1.3756
-3.6	-0.2418	2.8258	-3.551	1.4129	1.4129
-3.5	-0.214	2.8884	-3.5304	1.4442	1.4442
-3.4	-0.1634	2.9352	-3.4255	1.4676	1.4676
-3.3	-0.0808	2.9612	-3.2037	1.4806	1.4806
-3.2	0.0457	2.959	-2.822	1.4795	1.4795
-3.1	0.2314	2.9182	-2.2239	1.4591	1.4591
-3	0.4955	2.8228	-1.3363	1.4114	1.4114
-2.9	0.8605	2.6488	-0.0673	1.3244	1.3244
-2.8	1.352	2.3606	1.6954	1.1803	1.1803
-2.7	1.9961	1.9064	4.0819	0.9532	0.9532
-2.6	2.8156	1.2158	7.2311	0.6079	0.6079
-2.5	3.8243	0.2004	11.2724	0.1002	0.1002
-2.4	5.0195	-1.2364	16.2947	-0.6182	-0.6182
-2.3	6.3757	-3.1756	22.3027	-1.5878	-1.5878
-2.2	7.8408	-5.6414	29.164	-2.8207	-2.8207
-2.1	9.3389	-8.5432	36.5599	-4.2716	-4.2716
-2	10.7822	-11.614	43.9607	-5.807	-5.807
-1.9	12.0937	-14.3712	50.6524	-7.1856	-7.1856
-1.8	13.2347	-16.1324	55.8363	-8.0662	-8.0662
-1.7	14.227	-16.1182	58.7991	-8.0591	-8.0591
-1.6	15.156	-13.64	59.1079	-6.82	-6.82
-1.5	16.1437	-8.3268	56.7578	-4.1634	-4.1634
-1.4	17.2979	-0.3048	52.1986	-0.1524	-0.1524
-1.3	18.6591	9.751	46.2263	4.8755	4.8755
-1.2	20.1705	20.7248	39.7867	10.3624	10.3624
-1.1	21.6858	31.28	33.7774	15.64	15.64
-1	23.0088	40.1104	28.916	20.0552	20.0552
-0.9	23.9462	46.1454	25.6931	23.0727	23.0727
-0.8	24.3553	48.6778	24.388	24.3389	24.3389
-0.7	24.1751	47.4226	25.1027	23.7113	23.7113
-0.6	23.4377	42.531	27.7822	21.2655	21.2655
-0.5	22.2607	34.5794	32.2027	17.2897	17.2897
-0.4	20.8216	24.5258	37.939	12.2629	12.2629
-0.3	19.317	13.612	44.339	6.806	6.806

-0.2	17.9126	3.1896	50.5481	1.5948	1.5948
-0.1	16.6991	-5.5188	55.6161	-2.7594	-2.7594
0	15.6716	-11.6662	58.681	-5.8331	-5.8331
0.1	14.7448	-14.94	59.1745	-7.47	-7.47
0.2	13.7977	-15.5712	56.9643	-7.7856	-7.7856
0.3	12.727	-14.1872	52.3682	-7.0936	-7.0936
0.4	11.4847	-11.583	46.037	-5.7915	-5.7915
0.5	10.0866	-8.5044	38.7642	-4.2522	-4.2522
0.6	8.5972	-5.511	31.3026	-2.7555	-2.7555
0.7	7.103	-2.9328	24.2417	-1.4664	-1.4664
0.8	5.6872	-0.9	17.9616	-0.45	-0.45
0.9	4.4134	0.5954	12.6449	0.2977	0.2977
1	3.3187	1.6346	8.3216	0.8173	0.8173
1.1	2.4148	2.322	4.9224	1.161	1.161
1.2	1.694	2.7558	2.3261	1.3779	1.3779
1.3	1.1364	3.0152	0.3941	1.5076	1.5076
1.4	0.7167	3.1576	-1.0075	1.5788	1.5788
1.5	0.4086	3.2224	-1.9967	1.6112	1.6112
1.6	0.188	3.2354	-2.6715	1.6177	1.6177
1.7	0.0342	3.213	-3.1103	1.6065	1.6065
1.8	-0.0696	3.1654	-3.3741	1.5827	1.5827
1.9	-0.1366	3.0996	-3.5096	1.5498	1.5498
2	-0.1772	3.0206	-3.5521	1.5103	1.5103
2.1	-0.1989	2.9316	-3.5283	1.4658	1.4658
2.2	-0.2075	2.8356	-3.4579	1.4178	1.4178
2.3	-0.2071	2.7346	-3.3559	1.3673	1.3673
2.4	-0.2008	2.6308	-3.2333	1.3154	1.3154
2.5	-0.1909	2.5254	-3.098	1.2627	1.2627
2.6	-0.1787	2.42	-2.9562	1.21	1.21
2.7	-0.1656	2.3154	-2.8122	1.1577	1.1577
2.8	-0.1521	2.2126	-2.6689	1.1063	1.1063
2.9	-0.1389	2.112	-2.5286	1.056	1.056
3	-0.1262	2.0144	-2.3928	1.0072	1.0072
3.1	-0.1142	1.9198	-2.2623	0.9599	0.9599
3.2	-0.1031	1.8286	-2.1378	0.9143	0.9143
3.3	-0.0929	1.7408	-2.0195	0.8704	0.8704
3.4	-0.0836	1.657	-1.9076	0.8285	0.8285
3.5	-0.0751	1.5766	-1.802	0.7883	0.7883
3.6	-0.0675	1.5	-1.7025	0.75	0.75
3.7	-0.0606	1.4272	-1.6089	0.7136	0.7136
3.8	-0.0544	1.3578	-1.5211	0.6789	0.6789
3.9	-0.0489	1.292	-1.4386	0.646	0.646
4	-0.0439	1.2296	-1.3613	0.6148	0.6148
4.1	-0.0394	1.1706	-1.2887	0.5853	0.5853
4.2	-0.0354	1.1146	-1.2207	0.5573	0.5573
4.3	-0.0318	1.0618	-1.157	0.5309	0.5309
4.4	-0.0285	1.0116	-1.0973	0.5058	0.5058
4.5	-0.0256	0.9644	-1.0412	0.4822	0.4822
4.6	-0.023	0.9196	-0.9887	0.4598	0.4598

4.7	-0.0207	0.8774	-0.9394	0.4387	0.4387
4.8	-0.0185	0.8374	-0.8931	0.4187	0.4187
4.9	-0.0166	0.7996	-0.8496	0.3998	0.3998
5	-0.0149	0.764	-0.8087	0.382	0.382

$[C_5H_5]^+$ (C_{2v}), 10

```
Charge =  1 Multiplicity = 1
 C,0,-0.1181991498,0.0033184759,0.0214174057
 C,0,-0.1143305861,-0.0025151717,1.3663334453
 C,0,1.2790276691,-0.0069798065,1.7679520809
 C,0,2.168102031,-0.0025995445,0.6268707648
 C,0,1.3794738891,0.0032993249,-0.4643784702
 H,0,-0.9682151912,0.0075568664,-0.64915246
 H,0,-0.9566555261,-0.003978268,2.0410271492
 H,0,1.614717906,-0.0122620486,2.8028555177
 H,0,3.2462222508,-0.0040757759,0.675765176
 H,0,1.6746891338,0.00760909,-1.5062196445
```

Sum of electronic and zero-point Energies= -193.118125
Sum of electronic and thermal Energies= -193.113614
Sum of electronic and thermal Enthalpies= -193.112670
Sum of electronic and thermal Free Energies= -193.144945

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	1.141	0.2844	3.1388	0.1423	0.1421
-4.9	1.2158	0.2979	3.3494	0.1485	0.1494
-4.8	1.2971	0.3123	3.5792	0.1551	0.1572
-4.7	1.3859	0.3275	3.8304	0.1619	0.1656
-4.6	1.483	0.3436	4.1055	0.169	0.1746
-4.5	1.5893	0.3606	4.4074	0.1764	0.1842
-4.4	1.706	0.3787	4.7394	0.1841	0.1946
-4.3	1.8344	0.3979	5.1053	0.1921	0.2058
-4.2	1.9759	0.4182	5.5094	0.2003	0.2179
-4.1	2.1322	0.4397	5.9567	0.2087	0.231
-4	2.3052	0.4626	6.4532	0.2173	0.2453
-3.9	2.4974	0.4866	7.0054	0.2259	0.2607
-3.8	2.7112	0.5122	7.6214	0.2346	0.2776
-3.7	2.9498	0.5392	8.3103	0.2431	0.2961
-3.6	3.2168	0.5676	9.0829	0.2513	0.3163
-3.5	3.5165	0.5976	9.9518	0.2591	0.3385
-3.4	3.8537	0.6291	10.9321	0.2661	0.363
-3.3	4.2345	0.662	12.0414	0.2719	0.3901
-3.2	4.6656	0.6964	13.3005	0.2761	0.4203
-3.1	5.1555	0.7319	14.7344	0.2779	0.454
-3	5.7137	0.7684	16.3727	0.2765	0.4919
-2.9	6.3518	0.8051	18.2503	0.2705	0.5346
-2.8	7.0835	0.8413	20.4091	0.2583	0.583
-2.7	7.9247	0.8757	22.8985	0.2374	0.6383
-2.6	8.8944	0.9061	25.7771	0.2045	0.7016
-2.5	10.0144	0.9293	29.1138	0.1549	0.7744
-2.4	11.31	0.941	32.9889	0.0826	0.8584
-2.3	12.8101	0.9349	37.4955	-0.0207	0.9556
-2.2	14.5476	0.9026	42.7402	-0.1655	1.0681
-2.1	16.5589	0.8335	48.8433	-0.365	1.1985
-2	18.8844	0.7145	55.9386	-0.6352	1.3497
-1.9	21.5676	0.531	64.1718	-0.9943	1.5253
-1.8	24.655	0.267	73.6981	-1.4626	1.7296

-1.7	28.1942	-0.0933	84.6759	-2.061	1.9677
-1.6	32.2315	-0.5635	97.258	-2.8095	2.246
-1.5	36.8072	-1.1529	111.5746	-3.7248	2.5719
-1.4	41.9479	-1.8639	127.7076	-4.8174	2.9535
-1.3	47.6537	-2.6885	145.6496	-6.0869	3.3984
-1.2	53.8813	-3.605	165.249	-7.5168	3.9118
-1.1	60.522	-4.573	186.139	-9.0669	4.4939
-1	67.3793	-5.5296	207.6675	-10.6659	5.1363
-0.9	74.1542	-6.3862	228.8487	-12.2048	5.8186
-0.8	80.4508	-7.0309	248.3833	-13.538	6.5071
-0.7	85.8172	-7.3405	264.7922	-14.4972	7.1567
-0.6	89.8303	-7.2067	276.6975	-14.9247	7.718
-0.5	92.2158	-6.5763	283.2237	-14.7261	8.1498
-0.4	92.9708	-5.4964	284.4087	-13.9284	8.432
-0.3	92.4297	-4.1427	281.4317	-12.7176	8.5749
-0.2	91.2199	-2.8052	276.4648	-11.4225	8.6173
-0.1	90.0862	-1.8189	272.0776	-10.4314	8.6125
0	89.6335	-1.4543	270.3548	-10.0602	8.6059
0.1	90.094	-1.8155	272.0976	-10.431	8.6155
0.2	91.2343	-2.7986	276.5014	-11.4217	8.6231
0.3	92.4486	-4.1331	281.4789	-12.7165	8.5834
0.4	92.9919	-5.4845	284.4601	-13.9273	8.4428
0.5	92.2369	-6.5626	283.2734	-14.7251	8.1625
0.6	89.8497	-7.1922	276.7414	-14.9241	7.7319
0.7	85.8341	-7.3259	264.8282	-14.4971	7.1712
0.8	80.4647	-7.0168	248.411	-13.5384	6.5216
0.9	74.1652	-6.3731	228.8688	-12.2057	5.8326
1	67.3878	-5.5178	207.6811	-10.6673	5.1495
1.1	60.5284	-4.5626	186.1476	-9.0687	4.5061
1.2	53.886	-3.5959	165.2538	-7.5188	3.9229
1.3	47.657	-2.6807	145.6519	-6.089	3.4083
1.4	41.9502	-1.8572	127.708	-4.8195	2.9623
1.5	36.8089	-1.1472	111.5739	-3.7269	2.5797
1.6	32.2326	-0.5587	97.2565	-2.8115	2.2528
1.7	28.1949	-0.0893	84.674	-2.0629	1.9736
1.8	24.6555	0.2704	73.696	-1.4644	1.7348
1.9	21.5679	0.5341	64.1697	-0.9959	1.53
2	18.8846	0.7172	55.9365	-0.6367	1.3539
2.1	16.559	0.8358	48.8413	-0.3664	1.2022
2.2	14.5477	0.9047	42.7384	-0.1667	1.0714
2.3	12.8102	0.9368	37.4938	-0.0218	0.9586
2.4	11.31	0.9428	32.9873	0.0817	0.8611
2.5	10.0144	0.9309	29.1124	0.1541	0.7768
2.6	8.8945	0.9076	25.7758	0.2038	0.7038
2.7	7.9248	0.8771	22.8974	0.2368	0.6403
2.8	7.0836	0.8427	20.408	0.2578	0.5849
2.9	6.3519	0.8063	18.2494	0.2701	0.5362
3	5.7138	0.7695	16.3718	0.2761	0.4934
3.1	5.1556	0.733	14.7337	0.2776	0.4554
3.2	4.6658	0.6974	13.2999	0.2758	0.4216
3.3	4.2346	0.6631	12.0408	0.2717	0.3914
3.4	3.8539	0.63	10.9316	0.2659	0.3641
3.5	3.5166	0.5984	9.9513	0.2589	0.3395
3.6	3.217	0.5684	9.0824	0.2512	0.3172
3.7	2.9499	0.54	8.3099	0.243	0.297
3.8	2.7113	0.5129	7.6211	0.2344	0.2785
3.9	2.4975	0.4873	7.0051	0.2258	0.2615
4	2.3053	0.4632	6.4529	0.2172	0.246

4.1	2.1323	0.4403	5.9565	0.2086	0.2317
4.2	1.976	0.4188	5.5091	0.2002	0.2186
4.3	1.8345	0.3984	5.105	0.192	0.2064
4.4	1.7061	0.3793	4.7392	0.1841	0.1952
4.5	1.5895	0.3611	4.4072	0.1764	0.1847
4.6	1.4831	0.3441	4.1053	0.169	0.1751
4.7	1.386	0.328	3.8302	0.1619	0.1661
4.8	1.2972	0.3128	3.579	0.1551	0.1577
4.9	1.2159	0.2983	3.3492	0.1485	0.1498
5	1.1411	0.2848	3.1386	0.1423	0.1425

pentalene (C_{2h}), 11

```
Charge =  0 Multiplicity = 1
C,0,-0.1554296745,0.7122599236,0.
 C,0,-1.623582189,0.843440045,0.
 C,0,-2.1314222002,-0.4115197612,0.
 C,0,-1.0093217399,-1.4017378585,0.
 H,0,-2.1839343669,1.7672126433,0.
 H,0,-3.1780913137,-0.6826104985,0.
 H,0,-1.1471313711,-2.4758063601,0.
 C,0,0.1554296745,-0.7122599236,0.
 C,0,1.623582189,-0.843440045,0.
 C,0,2.1314222002,0.4115197612,0.
 C,0,1.0093217399,1.4017378585,0.
 H,0,2.1839343669,-1.7672126433,0.
 H,0,3.1780913137,0.6826104985,0.
 H,0,1.1471313711,2.4758063601,0.
```

Sum of electronic and zero-point Energies= -308.337912
Sum of electronic and thermal Energies= -308.332214
Sum of electronic and thermal Enthalpies= -308.331270
Sum of electronic and thermal Free Energies= -308.366776

NICS-scan

Distance	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.4455	0.7215	0.6152	0.3201	0.4014
-4.9	0.472	0.7539	0.662	0.3333	0.4206
-4.8	0.5005	0.7882	0.7133	0.3472	0.441
-4.7	0.5314	0.8245	0.7697	0.3619	0.4626
-4.6	0.5649	0.863	0.8317	0.3774	0.4856
-4.5	0.6013	0.9038	0.9001	0.3937	0.5101
-4.4	0.6409	0.9471	0.9756	0.411	0.5361
-4.3	0.6841	0.9932	1.0592	0.4293	0.5639
-4.2	0.7313	1.042	1.1519	0.4486	0.5934
-4.1	0.783	1.094	1.2549	0.4691	0.6249
-4	0.8397	1.1494	1.3697	0.4909	0.6585
-3.9	0.9021	1.2085	1.4978	0.5141	0.6944
-3.8	0.9709	1.2713	1.6414	0.5387	0.7326
-3.7	1.0469	1.3383	1.8025	0.5649	0.7734
-3.6	1.1312	1.4097	1.984	0.5928	0.8169
-3.5	1.2249	1.4856	2.189	0.6225	0.8631
-3.4	1.3293	1.5664	2.4214	0.654	0.9124
-3.3	1.4459	1.6521	2.6856	0.6875	0.9646
-3.2	1.5767	1.743	2.9871	0.7231	1.0199
-3.1	1.7238	1.839	3.3325	0.7608	1.0782
-3	1.8898	1.9398	3.7295	0.8004	1.1394
-2.9	2.0777	2.0453	4.1878	0.842	1.2033
-2.8	2.2909	2.1543	4.7185	0.8851	1.2692
-2.7	2.5338	2.2658	5.3356	0.9293	1.3365

-2.6	2.8109	2.3775	6.0553	0.9736	1.4039
-2.5	3.1279	2.4864	6.8974	1.0168	1.4696
-2.4	3.491	2.5879	7.885	1.0568	1.5311
-2.3	3.9072	2.6757	9.0457	1.0908	1.5849
-2.2	4.3843	2.7416	10.4113	1.115	1.6266
-2.1	4.9311	2.7743	12.019	1.124	1.6503
-2	5.5571	2.7606	13.9109	1.1117	1.6489
-1.9	6.2729	2.6841	16.1347	1.07	1.6141
-1.8	7.0898	2.5261	18.7433	0.9897	1.5364
-1.7	8.0202	2.266	21.7945	0.8606	1.4054
-1.6	9.0768	1.8817	25.3488	0.6714	1.2103
-1.5	10.2723	1.3502	29.4667	0.4102	0.94
-1.4	11.6168	0.6487	34.2018	0.0647	0.584
-1.3	13.1153	-0.2448	39.5908	-0.3775	0.1327
-1.2	14.7624	-1.3499	45.637	-0.9282	-0.4217
-1.1	16.5357	-2.6822	52.2893	-1.598	-1.0842
-1	18.389	-4.2495	59.4165	-2.3944	-1.8551
-0.9	20.2465	-6.0467	66.7863	-3.319	-2.7277
-0.8	22.0029	-8.0491	74.0576	-4.3638	-3.6853
-0.7	23.533	-10.205	80.8041	-5.5063	-4.6987
-0.6	24.7152	-12.4319	86.5775	-6.7064	-5.7255
-0.5	25.4645	-14.6183	91.0117	-7.9059	-6.7124
-0.4	25.7684	-16.6341	93.9392	-9.032	-7.6021
-0.3	25.7072	-18.3491	95.4707	-10.0073	-8.3418
-0.2	25.4437	-19.6521	95.983	-10.7602	-8.8919
-0.1	25.1756	-20.4636	95.9904	-11.2349	-9.2287
0	25.0653	-20.7388	95.9348	-11.397	-9.3418
0.1	25.1756	-20.4636	95.9904	-11.2349	-9.2287
0.2	25.4437	-19.6521	95.983	-10.7602	-8.8919
0.3	25.7072	-18.3491	95.4707	-10.0073	-8.3418
0.4	25.7684	-16.6341	93.9392	-9.032	-7.6021
0.5	25.4645	-14.6183	91.0117	-7.9059	-6.7124
0.6	24.7152	-12.4319	86.5775	-6.7064	-5.7255
0.7	23.533	-10.205	80.8041	-5.5063	-4.6987
0.8	22.0029	-8.0491	74.0576	-4.3638	-3.6853
0.9	20.2465	-6.0467	66.7863	-3.319	-2.7277
1	18.389	-4.2495	59.4165	-2.3944	-1.8551
1.1	16.5357	-2.6822	52.2893	-1.598	-1.0842
1.2	14.7624	-1.3499	45.637	-0.9282	-0.4217
1.3	13.1153	-0.2448	39.5908	-0.3775	0.1327
1.4	11.6168	0.6487	34.2018	0.0647	0.584
1.5	10.2723	1.3502	29.4667	0.4102	0.94
1.6	9.0768	1.8817	25.3488	0.6714	1.2103
1.7	8.0202	2.266	21.7945	0.8606	1.4054
1.8	7.0898	2.5261	18.7433	0.9897	1.5364
1.9	6.2729	2.6841	16.1347	1.07	1.6141
2	5.5571	2.7606	13.9109	1.1117	1.6489
2.1	4.9311	2.7743	12.019	1.124	1.6503
2.2	4.3843	2.7416	10.4113	1.115	1.6266
2.3	3.9072	2.6757	9.0457	1.0908	1.5849
2.4	3.491	2.5879	7.885	1.0568	1.5311
2.5	3.1279	2.4864	6.8974	1.0168	1.4696
2.6	2.8109	2.3775	6.0553	0.9736	1.4039
2.7	2.5338	2.2658	5.3356	0.9293	1.3365
2.8	2.2909	2.1543	4.7185	0.8851	1.2692
2.9	2.0777	2.0453	4.1878	0.842	1.2033
3	1.8898	1.9398	3.7295	0.8004	1.1394
3.1	1.7238	1.839	3.3325	0.7608	1.0782

3.2	1.5767	1.743	2.9871	0.7231	1.0199
3.3	1.4459	1.6521	2.6856	0.6875	0.9646
3.4	1.3293	1.5664	2.4214	0.654	0.9124
3.5	1.2249	1.4856	2.189	0.6225	0.8631
3.6	1.1312	1.4097	1.984	0.5928	0.8169
3.7	1.0469	1.3383	1.8025	0.5649	0.7734
3.8	0.9709	1.2713	1.6414	0.5387	0.7326
3.9	0.9021	1.2085	1.4978	0.5141	0.6944
4	0.8397	1.1494	1.3697	0.4909	0.6585
4.1	0.783	1.094	1.2549	0.4691	0.6249
4.2	0.7313	1.042	1.1519	0.4486	0.5934
4.3	0.6841	0.9932	1.0592	0.4293	0.5639
4.4	0.6409	0.9471	0.9756	0.411	0.5361
4.5	0.6013	0.9038	0.9001	0.3937	0.5101
4.6	0.5649	0.863	0.8317	0.3774	0.4856
4.7	0.5314	0.8245	0.7697	0.3619	0.4626
4.8	0.5005	0.7882	0.7133	0.3472	0.441
4.9	0.472	0.7539	0.662	0.3333	0.4206
5	0.4455	0.7215	0.6152	0.3201	0.4014

acepentalene (C_{2h}), 12

```
Charge =  0 Multiplicity = 1
 C,0,1.1893,0.0055,0.2911
 C,0,0.4692,-1.1126,-0.0096
 C,0,-0.9542,-0.7069,-0.2669
 C,0,-0.9542,0.6431,-0.3057
 C,0,0.25,1.171,0.2911
 C,0,-2.1584,1.171,0.2911
 C,0,-1.7101,2.1168,1.1694
 C,0,-0.1984,2.1168,1.1694
 C,0,-2.3777,-1.1126,-0.0096
 C,0,-3.0978,0.0055,0.2911
 H,0,2.2496,0.0314,0.5033
 H,0,0.8654,-2.1182,-0.0631
 H,0,-2.2833,2.6134,1.9435
 H,0,0.3748,2.6134,1.9435
 H,0,-2.7739,-2.1182,-0.0631
 H,0,-4.1581,0.0314,0.5033
```

Sum of electronic and zero-point Energies= -384.464450
Sum of electronic and thermal Energies= -384.457943
Sum of electronic and thermal Enthalpies= -384.456998
Sum of electronic and thermal Free Energies= -384.495120

NICS-scan

Distance	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.2804	0.6258	0.2154	0.3657	0.2601
-4.9	0.2953	0.6544	0.2314	0.3823	0.2721
-4.8	0.3113	0.6848	0.249	0.3999	0.2849
-4.7	0.3284	0.717	0.2682	0.4184	0.2986
-4.6	0.3468	0.7511	0.2892	0.4381	0.313
-4.5	0.3665	0.7874	0.3123	0.4589	0.3285
-4.4	0.3878	0.8259	0.3376	0.4809	0.345
-4.3	0.4108	0.8667	0.3656	0.5041	0.3626
-4.2	0.4356	0.9102	0.3965	0.5288	0.3814
-4.1	0.4624	0.9565	0.4306	0.5548	0.4017
-4	0.4914	1.0058	0.4685	0.5824	0.4234
-3.9	0.523	1.0584	0.5107	0.6115	0.4469

-3.8	0.5574	1.1143	0.5577	0.6421	0.4722
-3.7	0.5948	1.174	0.6104	0.6743	0.4997
-3.6	0.6357	1.2375	0.6695	0.708	0.5295
-3.5	0.6804	1.3051	0.7362	0.7431	0.562
-3.4	0.7295	1.3768	0.8117	0.7792	0.5976
-3.3	0.7833	1.4525	0.8976	0.816	0.6365
-3.2	0.8425	1.532	0.9956	0.8528	0.6792
-3.1	0.9075	1.6147	1.108	0.8886	0.7261
-3	0.979	1.6994	1.2376	0.9218	0.7776
-2.9	1.0574	1.7847	1.3876	0.9506	0.8341
-2.8	1.1433	1.8677	1.5622	0.972	0.8957
-2.7	1.237	1.945	1.7661	0.9825	0.9625
-2.6	1.339	2.0116	2.0054	0.9773	1.0343
-2.5	1.4495	2.0614	2.2872	0.9507	1.1107
-2.4	1.5689	2.0866	2.6201	0.8957	1.1909
-2.3	1.6975	2.0781	3.0144	0.8042	1.2739
-2.2	1.8361	2.0259	3.4826	0.6673	1.3586
-2.1	1.9862	1.919	4.0395	0.4754	1.4436
-2	2.1497	1.7463	4.7029	0.2186	1.5277
-1.9	2.3303	1.4972	5.4936	-0.1124	1.6096
-1.8	2.5327	1.162	6.4362	-0.5259	1.6879
-1.7	2.764	0.7332	7.5588	-1.0281	1.7613
-1.6	3.0331	0.2063	8.8929	-1.6213	1.8276
-1.5	3.3514	-0.4183	10.4725	-2.302	1.8837
-1.4	3.7328	-1.1339	12.3322	-3.0583	1.9244
-1.3	4.1929	-1.9261	14.5048	-3.8672	1.9411
-1.2	4.7486	-2.7721	17.018	-4.693	1.9209
-1.1	5.4157	-3.6434	19.8904	-5.4881	1.8447
-1	6.2055	-4.5116	23.1282	-6.1978	1.6862
-0.9	7.1202	-5.3606	26.7212	-6.7721	1.4115
-0.8	8.147	-6.1998	30.6407	-7.1812	0.9814
-0.7	9.2538	-7.0738	34.8353	-7.4314	0.3576
-0.6	10.3897	-8.059	39.2282	-7.5723	-0.4867
-0.5	11.4915	-9.2389	43.7133	-7.6877	-1.5512
-0.4	12.4978	-10.6609	48.1542	-7.8662	-2.7947
-0.3	13.3656	-12.2924	52.3892	-8.1631	-4.1293
-0.2	14.0798	-14.0024	56.2417	-8.5709	-5.4315
-0.1	14.6499	-15.5867	59.5363	-9.0177	-6.569
0	15.0945	-16.8301	62.1136	-9.3956	-7.4345
0.1	15.421	-17.5756	63.8386	-9.6031	-7.9725
0.2	15.6132	-17.7648	64.6045	-9.5785	-8.1863
0.3	15.6348	-17.4339	64.3383	-9.3088	-8.1251
0.4	15.4458	-16.6774	63.0148	-8.8198	-7.8576
0.5	15.0237	-15.6046	60.6757	-8.1558	-7.4488
0.6	14.377	-14.3122	57.4433	-7.3656	-6.9466
0.7	13.5465	-12.8759	53.5154	-6.4951	-6.3808
0.8	12.5941	-11.358	49.1403	-5.5872	-5.7708
0.9	11.588	-9.8141	44.578	-4.6813	-5.1328
1	10.5882	-8.2975	40.0623	-3.8131	-4.4844

1.1	9.6394	-6.8568	35.7748	-3.0116	-3.8452
1.2	8.7679	-5.5304	31.8342	-2.2965	-3.2339
1.3	7.9851	-4.3442	28.2993	-1.6775	-2.6667
1.4	7.2905	-3.3094	25.181	-1.1549	-2.1545
1.5	6.6774	-2.425	22.4572	-0.7219	-1.7031
1.6	6.1355	-1.681	20.0873	-0.3677	-1.3133
1.7	5.6538	-1.0622	18.0235	-0.0799	-0.9823
1.8	5.2221	-0.5517	16.2181	0.1532	-0.7049
1.9	4.8317	-0.1334	14.6284	0.3416	-0.475
2	4.4753	0.2076	13.2181	0.4935	-0.2859
2.1	4.1472	0.4834	11.9581	0.6148	-0.1314
2.2	3.8432	0.7044	10.8253	0.7103	-0.0059
2.3	3.5604	0.879	9.802	0.7835	0.0955
2.4	3.2964	1.0145	8.8747	0.8375	0.177
2.5	3.0499	1.117	8.0326	0.8747	0.2423
2.6	2.8198	1.1921	7.2673	0.8977	0.2944
2.7	2.6054	1.2445	6.5719	0.9087	0.3358
2.8	2.4062	1.2783	5.9403	0.9097	0.3686
2.9	2.2216	1.2972	5.3674	0.9028	0.3944
3	2.0509	1.3042	4.8485	0.8896	0.4146
3.1	1.8935	1.3017	4.3789	0.8716	0.4301
3.2	1.7489	1.2919	3.9547	0.8501	0.4418
3.3	1.6161	1.2764	3.572	0.8261	0.4503
3.4	1.4945	1.2565	3.2271	0.8005	0.456
3.5	1.3833	1.2334	2.9164	0.774	0.4594
3.6	1.2816	1.2077	2.637	0.747	0.4607
3.7	1.1886	1.1803	2.3857	0.7201	0.4602
3.8	1.1037	1.1514	2.1598	0.6933	0.4581
3.9	1.0261	1.1217	1.9568	0.6671	0.4546
4	0.9552	1.0913	1.7743	0.6415	0.4498
4.1	0.8903	1.0605	1.6103	0.6165	0.444
4.2	0.8309	1.0297	1.4629	0.5924	0.4373
4.3	0.7764	0.9989	1.3303	0.5691	0.4298
4.4	0.7264	0.9682	1.211	0.5466	0.4216
4.5	0.6805	0.9379	1.1035	0.525	0.4129
4.6	0.6382	0.908	1.0067	0.5042	0.4038
4.7	0.5993	0.8785	0.9194	0.4842	0.3943
4.8	0.5634	0.8496	0.8406	0.4651	0.3845
4.9	0.5303	0.8213	0.7695	0.4467	0.3746
5	0.4996	0.7937	0.7052	0.4291	0.3646

[fluorenyl]$^{+}$ (C_{2v}), 13

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H,0,0.,-4.5214741991,-0.4406640735
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H,0,0.,-1.4076974817,2.5425632296
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Sum of electronic and zero-point Energies= -500.478722
Sum of electronic and thermal Energies= -500.469833
Sum of electronic and thermal Enthalpies= -500.468889
Sum of electronic and thermal Free Energies= -500.512158

NICS-scan (Cp ring)

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.2606	0.7221	0.0595	0.3391	0.383
-4.9	0.2796	0.749	0.0898	0.3507	0.3983
-4.8	0.3004	0.7771	0.1243	0.3627	0.4144
-4.7	0.3233	0.8063	0.1637	0.3751	0.4312
-4.6	0.3485	0.8368	0.2086	0.3879	0.4489
-4.5	0.3761	0.8687	0.2597	0.4012	0.4675
-4.4	0.4067	0.9021	0.318	0.415	0.4871
-4.3	0.4405	0.9369	0.3846	0.4292	0.5077
-4.2	0.4779	0.9733	0.4605	0.4439	0.5294
-4.1	0.5195	1.0114	0.5472	0.4591	0.5523
-4	0.5658	1.0511	0.6464	0.4747	0.5764
-3.9	0.6176	1.0928	0.7599	0.4908	0.602
-3.8	0.6754	1.1362	0.89	0.5073	0.6289
-3.7	0.7404	1.1818	1.0395	0.5243	0.6575
-3.6	0.8136	1.2294	1.2114	0.5416	0.6878
-3.5	0.8961	1.2789	1.4095	0.5591	0.7198
-3.4	0.9896	1.3306	1.6383	0.5768	0.7538
-3.3	1.0958	1.3843	1.9031	0.5945	0.7898
-3.2	1.2167	1.4397	2.2104	0.6118	0.8279
-3.1	1.3548	1.4966	2.5678	0.6285	0.8681
-3	1.5129	1.5541	2.9847	0.6437	0.9104
-2.9	1.6944	1.6113	3.4719	0.6568	0.9545
-2.8	1.9031	1.6664	4.0429	0.6662	1.0002
-2.7	2.1435	1.7171	4.7133	0.6704	1.0467
-2.6	2.4206	1.76	5.5019	0.6668	1.0932
-2.5	2.7404	1.7903	6.4309	0.652	1.1383
-2.4	3.1095	1.8021	7.5264	0.6218	1.1803
-2.3	3.5354	1.7874	8.8188	0.5706	1.2168
-2.2	4.0267	1.7367	10.3434	0.4917	1.245
-2.1	4.5932	1.6386	12.1411	0.3771	1.2615
-2	5.2462	1.4802	14.2585	0.2175	1.2627
-1.9	5.9985	1.2469	16.7488	0.0026	1.2443
-1.8	6.8648	0.9233	19.6713	-0.2787	1.202
-1.7	7.8616	0.4934	23.0912	-0.6379	1.1313

-1.6	9.0062	-0.0589	27.0775	-1.0866	1.0277
-1.5	10.3161	-0.7497	31.6981	-1.6359	0.8862
-1.4	11.8059	-1.5936	37.0115	-2.2953	0.7017
-1.3	13.4834	-2.6032	43.0534	-3.0717	0.4685
-1.2	15.3437	-3.7857	49.8168	-3.9664	0.1807
-1.1	17.3622	-5.1398	57.2264	-4.972	-0.1678
-1	19.4874	-6.6498	65.112	-6.0678	-0.582
-0.9	21.6365	-8.2783	73.188	-7.215	-1.0633
-0.8	23.6973	-9.9613	81.0531	-8.3542	-1.6071
-0.7	25.5396	-11.6066	88.2253	-9.4078	-2.1988
-0.6	27.0388	-13.1035	94.22	-10.2909	-2.8126
-0.5	28.1075	-14.344	98.6663	-10.9319	-3.4121
-0.4	28.7251	-15.2546	101.43	-11.2979	-3.9567
-0.3	28.9552	-15.8239	102.6895	-11.4146	-4.4093
-0.2	28.9338	-16.1095	102.9107	-11.366	-4.7435
-0.1	28.8278	-16.2146	102.6981	-11.2683	-4.9463
0	28.7748	-16.2364	102.5609	-11.2224	-5.014
0.1	28.8278	-16.2146	102.6981	-11.2683	-4.9463
0.2	28.9338	-16.1095	102.9107	-11.366	-4.7435
0.3	28.9552	-15.8239	102.6895	-11.4146	-4.4093
0.4	28.7251	-15.2546	101.43	-11.2979	-3.9567
0.5	28.1075	-14.344	98.6663	-10.9319	-3.4121
0.6	27.0388	-13.1035	94.22	-10.2909	-2.8126
0.7	25.5396	-11.6066	88.2253	-9.4078	-2.1988
0.8	23.6973	-9.9613	81.0531	-8.3542	-1.6071
0.9	21.6365	-8.2783	73.188	-7.215	-1.0633
1	19.4874	-6.6498	65.112	-6.0678	-0.582
1.1	17.3622	-5.1398	57.2264	-4.972	-0.1678
1.2	15.3437	-3.7857	49.8168	-3.9664	0.1807
1.3	13.4834	-2.6032	43.0534	-3.0717	0.4685
1.4	11.8059	-1.5936	37.0115	-2.2953	0.7017
1.5	10.3161	-0.7497	31.6981	-1.6359	0.8862
1.6	9.0062	-0.0589	27.0775	-1.0866	1.0277
1.7	7.8616	0.4934	23.0912	-0.6379	1.1313
1.8	6.8648	0.9233	19.6713	-0.2787	1.202
1.9	5.9985	1.2469	16.7488	0.0026	1.2443
2	5.2462	1.4802	14.2585	0.2175	1.2627
2.1	4.5932	1.6386	12.1411	0.3771	1.2615
2.2	4.0267	1.7367	10.3434	0.4917	1.245
2.3	3.5354	1.7874	8.8188	0.5706	1.2168
2.4	3.1095	1.8021	7.5264	0.6218	1.1803
2.5	2.7404	1.7903	6.4309	0.652	1.1383
2.6	2.4206	1.76	5.5019	0.6668	1.0932
2.7	2.1435	1.7171	4.7133	0.6704	1.0467
2.8	1.9031	1.6664	4.0429	0.6662	1.0002
2.9	1.6944	1.6113	3.4719	0.6568	0.9545
3	1.5129	1.5541	2.9847	0.6437	0.9104
3.1	1.3548	1.4966	2.5678	0.6285	0.8681
3.2	1.2167	1.4397	2.2104	0.6118	0.8279

3.3	1.0958	1.3843	1.9031	0.5945	0.7898
3.4	0.9896	1.3306	1.6383	0.5768	0.7538
3.5	0.8961	1.2789	1.4095	0.5591	0.7198
3.6	0.8136	1.2294	1.2114	0.5416	0.6878
3.7	0.7404	1.1818	1.0395	0.5243	0.6575
3.8	0.6754	1.1362	0.89	0.5073	0.6289
3.9	0.6176	1.0928	0.7599	0.4908	0.602
4	0.5658	1.0511	0.6464	0.4747	0.5764
4.1	0.5195	1.0114	0.5472	0.4591	0.5523
4.2	0.4779	0.9733	0.4605	0.4439	0.5294
4.3	0.4405	0.9369	0.3846	0.4292	0.5077
4.4	0.4067	0.9021	0.318	0.415	0.4871
4.5	0.3761	0.8687	0.2597	0.4012	0.4675
4.6	0.3485	0.8368	0.2086	0.3879	0.4489
4.7	0.3233	0.8063	0.1637	0.3751	0.4312
4.8	0.3004	0.7771	0.1243	0.3627	0.4144
4.9	0.2796	0.749	0.0898	0.3507	0.3983
5	0.2606	0.7221	0.0595	0.3391	0.383

NICS-scan (benzene ring)

Distance(Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.145	0.7109	-0.2759	0.3155	0.3954
-4.9	0.1526	0.7401	-0.2822	0.3285	0.4116
-4.8	0.1608	0.7709	-0.2885	0.3422	0.4287
-4.7	0.1695	0.8032	-0.2948	0.3567	0.4465
-4.6	0.1787	0.8373	-0.3011	0.3721	0.4652
-4.5	0.1886	0.8732	-0.3073	0.3885	0.4847
-4.4	0.1992	0.9109	-0.3132	0.4059	0.505
-4.3	0.2105	0.9506	-0.319	0.4244	0.5262
-4.2	0.2226	0.9923	-0.3243	0.4441	0.5482
-4.1	0.2356	1.0361	-0.3292	0.465	0.5711
-4	0.2496	1.0821	-0.3333	0.4874	0.5947
-3.9	0.2646	1.1302	-0.3365	0.5112	0.619
-3.8	0.2807	1.1806	-0.3383	0.5366	0.644
-3.7	0.2982	1.2331	-0.3385	0.5636	0.6695
-3.6	0.3171	1.2877	-0.3365	0.5924	0.6953
-3.5	0.3375	1.3442	-0.3316	0.6229	0.7213
-3.4	0.3599	1.4025	-0.3229	0.6553	0.7472
-3.3	0.3843	1.4621	-0.3093	0.6894	0.7727
-3.2	0.4111	1.5225	-0.2894	0.7251	0.7974
-3.1	0.4407	1.5832	-0.2612	0.7623	0.8209
-3	0.4735	1.6431	-0.2226	0.8004	0.8427
-2.9	0.5101	1.7007	-0.1704	0.8388	0.8619
-2.8	0.5512	1.7544	-0.1009	0.8765	0.8779
-2.7	0.5975	1.8018	-0.0093	0.9122	0.8896
-2.6	0.6501	1.84	0.1102	0.9441	0.8959
-2.5	0.7099	1.8649	0.2649	0.9696	0.8953
-2.4	0.7785	1.8718	0.4637	0.9858	0.886
-2.3	0.8575	1.8549	0.7177	0.9889	0.866

-2.2	0.9489	1.8069	1.0397	0.9744	0.8325
-2.1	1.0552	1.72	1.4457	0.9372	0.7828
-2	1.1798	1.5851	1.9542	0.8718	0.7133
-1.9	1.3267	1.3928	2.5874	0.7725	0.6203
-1.8	1.5014	1.1331	3.371	0.6334	0.4997
-1.7	1.7103	0.7966	4.3343	0.4492	0.3474
-1.6	1.9616	0.3746	5.5103	0.2154	0.1592
-1.5	2.2647	-0.1401	6.9341	-0.0716	-0.0685
-1.4	2.6296	-0.7524	8.6411	-0.4135	-0.3389
-1.3	3.0662	-1.4641	10.6628	-0.8102	-0.6539
-1.2	3.5823	-2.2734	13.0204	-1.2589	-1.0145
-1.1	4.1814	-3.1735	15.7178	-1.7538	-1.4197
-1	4.86	-4.1511	18.7311	-2.2852	-1.8659
-0.9	5.6051	-5.1858	22.0012	-2.8391	-2.3467
-0.8	6.3929	-6.2494	25.4281	-3.3975	-2.8519
-0.7	7.1896	-7.3055	28.8743	-3.9388	-3.3667
-0.6	7.9549	-8.3127	32.1775	-4.4401	-3.8726
-0.5	8.6483	-9.2279	35.1728	-4.88	-4.3479
-0.4	9.2357	-10.0129	37.7201	-5.2425	-4.7704
-0.3	9.6956	-10.6386	39.7253	-5.519	-5.1196
-0.2	10.0196	-11.0891	41.1479	-5.7095	-5.3796
-0.1	10.21	-11.3589	41.989	-5.8194	-5.5395
0	10.2726	-11.4484	42.2662	-5.8551	-5.5933
0.1	10.21	-11.3589	41.989	-5.8194	-5.5395
0.2	10.0196	-11.0891	41.1479	-5.7095	-5.3796
0.3	9.6956	-10.6386	39.7253	-5.519	-5.1196
0.4	9.2357	-10.0129	37.7201	-5.2425	-4.7704
0.5	8.6483	-9.2279	35.1728	-4.88	-4.3479
0.6	7.9549	-8.3127	32.1775	-4.4401	-3.8726
0.7	7.1896	-7.3055	28.8743	-3.9388	-3.3667
0.8	6.3929	-6.2494	25.4281	-3.3975	-2.8519
0.9	5.6051	-5.1858	22.0012	-2.8391	-2.3467
1	4.86	-4.1511	18.7311	-2.2852	-1.8659
1.1	4.1814	-3.1735	15.7178	-1.7538	-1.4197
1.2	3.5823	-2.2734	13.0204	-1.2589	-1.0145
1.3	3.0662	-1.4641	10.6628	-0.8102	-0.6539
1.4	2.6296	-0.7524	8.6411	-0.4135	-0.3389
1.5	2.2647	-0.1401	6.9341	-0.0716	-0.0685
1.6	1.9616	0.3746	5.5103	0.2154	0.1592
1.7	1.7103	0.7966	4.3343	0.4492	0.3474
1.8	1.5014	1.1331	3.371	0.6334	0.4997
1.9	1.3267	1.3928	2.5874	0.7725	0.6203
2	1.1798	1.5851	1.9542	0.8718	0.7133
2.1	1.0552	1.72	1.4457	0.9372	0.7828
2.2	0.9489	1.8069	1.0397	0.9744	0.8325
2.3	0.8575	1.8549	0.7177	0.9889	0.866
2.4	0.7785	1.8718	0.4637	0.9858	0.886
2.5	0.7099	1.8649	0.2649	0.9696	0.8953
2.6	0.6501	1.84	0.1102	0.9441	0.8959

2.7	0.5975	1.8018	-0.0093	0.9122	0.8896
2.8	0.5512	1.7544	-0.1009	0.8765	0.8779
2.9	0.5101	1.7007	-0.1704	0.8388	0.8619
3	0.4735	1.6431	-0.2226	0.8004	0.8427
3.1	0.4407	1.5832	-0.2612	0.7623	0.8209
3.2	0.4111	1.5225	-0.2894	0.7251	0.7974
3.3	0.3843	1.4621	-0.3093	0.6894	0.7727
3.4	0.3599	1.4025	-0.3229	0.6553	0.7472
3.5	0.3375	1.3442	-0.3316	0.6229	0.7213
3.6	0.3171	1.2877	-0.3365	0.5924	0.6953
3.7	0.2982	1.2331	-0.3385	0.5636	0.6695
3.8	0.2807	1.1806	-0.3383	0.5366	0.644
3.9	0.2646	1.1302	-0.3365	0.5112	0.619
4	0.2496	1.0821	-0.3333	0.4874	0.5947
4.1	0.2356	1.0361	-0.3292	0.465	0.5711
4.2	0.2226	0.9923	-0.3243	0.4441	0.5482
4.3	0.2105	0.9506	-0.319	0.4244	0.5262
4.4	0.1992	0.9109	-0.3132	0.4059	0.505
4.5	0.1886	0.8732	-0.3073	0.3885	0.4847
4.6	0.1787	0.8373	-0.3011	0.3721	0.4652
4.7	0.1695	0.8032	-0.2948	0.3567	0.4465
4.8	0.1608	0.7709	-0.2885	0.3422	0.4287
4.9	0.1526	0.7401	-0.2822	0.3285	0.4116
5	0.145	0.7109	-0.2759	0.3155	0.3954

[tetrabenzo[5.5]fulvalene]$^{2+}$ (D_2), 14

```
Charge =  2 Multiplicity = 1
 H,0,-4.9008744645,-1.0582673681,1.1591722668
 C,0,-3.8463194805,-1.2969271615,1.2282274141
 C,0,-1.1043257807,-2.0145061054,1.4834995365
 C,0,-2.8838589147,-0.5231842156,0.6332755231
 C,0,-3.4336630718,-2.4443930778,1.9585573396
 C,0,-2.0905912923,-2.7957298014,2.0858228479
 C,0,-1.5040636484,-0.8848050379,0.7476502904
 H,0,0.0580742032,-2.2768898785,-1.5895746917
 H,0,-4.1896768435,-3.0589318153,2.4342742174
 H,0,-1.8150774685,-3.6722952059,2.6582188606
 C,0,-0.7281142638,0.0982222214,0.0575060459
 H,0,-0.0580742062,-2.2768902984,1.5895721777
 C,0,0.7281142151,0.0982222495,-0.0575078803
 C,0,-1.6029182843,1.0810807391,-0.5023754608
 C,0,1.602918224,1.0810806094,0.502373915
 C,0,1.5040636126,-0.8848048053,-0.7476524102
 C,0,-3.6990122571,2.640704016,-1.3946620608
 C,0,-1.3239175265,2.2109181144,-1.2917318997
 C,0,-2.9475999144,0.7193843407,-0.1725584493
 C,0,-3.991663133,1.4931326454,-0.6086777095
 C,0,-2.3926508388,2.9921460064,-1.7313887627
 H,0,-0.3073833944,2.4734331577,-1.5609309296
 H,0,1.8150774793,-3.6722943531,-2.658221875
 H,0,-5.0222252914,1.2543648141,-0.3747056682
 H,0,-2.2105480928,3.8687834264,-2.3398786801
 H,0,-4.520432074,3.2552179871,-1.7456052573
 C,0,3.6990121749,2.6407036572,1.3946609709
 C,0,2.9475998586,0.7193843131,0.1725568138
 C,0,1.3239174479,2.210917778,1.2917306463
 C,0,2.392650747,2.9921455565,1.7313877374
```

```
C,0,3.9916630647,1.4931325029,0.6086763104
H,0,4.9008744378,-1.0582670345,-1.1591743647
H,0,0.3073833074,2.4734327511,1.5609297109
H,0,2.2105479854,3.8687828196,2.3398778762
H,0,5.0222252308,1.2543647479,0.3747042179
H,0,4.5204319822,3.2552175413,1.7456043469
C,0,3.4336630649,-2.4443923953,-1.9585600001
C,0,2.8838588707,-0.523184008,-0.6332775238
C,0,1.1043257646,-2.0145056524,-1.4835020106
C,0,2.090591289,-2.7957291243,-2.0858255843
C,0,3.8463194533,-1.2969267616,-1.228229648
H,0,4.1896768279,-3.0589308948,-2.4342771987
```

Sum of electronic and zero-point Energies= -999.691233
Sum of electronic and thermal Energies= -999.672624
Sum of electronic and thermal Enthalpies= -999.671679
Sum of electronic and thermal Free Energies= -999.737248

NICS-scan(Cp ring)

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.359	0.5625	0.5146	0.1207	0.4418
-4.9	0.3834	0.5699	0.5802	0.1158	0.4541
-4.8	0.4098	0.5768	0.6527	0.1104	0.4664
-4.7	0.4386	0.583	0.7326	0.1044	0.4786
-4.6	0.4699	0.5887	0.8211	0.0979	0.4908
-4.5	0.5042	0.5937	0.9188	0.0909	0.5028
-4.4	0.5416	0.5978	1.027	0.0832	0.5146
-4.3	0.5826	0.601	1.1468	0.075	0.526
-4.2	0.6276	0.6032	1.2796	0.0661	0.5371
-4.1	0.677	0.6041	1.427	0.0565	0.5476
-4	0.7315	0.6039	1.5906	0.0463	0.5576
-3.9	0.7916	0.6023	1.7725	0.0354	0.5669
-3.8	0.858	0.5992	1.9749	0.0238	0.5754
-3.7	0.9317	0.5946	2.2006	0.0115	0.5831
-3.6	1.0136	0.5881	2.4527	-0.0016	0.5897
-3.5	1.105	0.5799	2.7349	-0.0153	0.5952
-3.4	1.2071	0.5697	3.0516	-0.0298	0.5995
-3.3	1.3218	0.5573	3.408	-0.045	0.6023
-3.2	1.451	0.5426	3.8104	-0.0609	0.6035
-3.1	1.5973	0.5252	4.2666	-0.0775	0.6027
-3	1.7636	0.5049	4.7858	-0.0948	0.5997
-2.9	1.9535	0.4812	5.3792	-0.1126	0.5938
-2.8	2.1712	0.4534	6.0604	-0.1308	0.5842
-2.7	2.422	0.4202	6.8457	-0.1494	0.5696
-2.6	2.7116	0.3802	7.7546	-0.1682	0.5484
-2.5	3.047	0.3307	8.8104	-0.1872	0.5179
-2.4	3.4361	0.2682	10.0403	-0.2065	0.4747
-2.3	3.8879	0.1872	11.4764	-0.2266	0.4138
-2.2	4.4122	0.081	13.1558	-0.2482	0.3292
-2.1	5.0205	-0.0597	15.1212	-0.2726	0.2129
-2	5.7253	-0.2457	17.4217	-0.3015	0.0558
-1.9	6.5406	-0.4907	20.1125	-0.3375	-0.1532
-1.8	7.4819	-0.8099	23.2555	-0.3838	-0.4261
-1.7	8.566	-1.2199	26.918	-0.4442	-0.7757
-1.6	9.8106	-1.7389	31.1708	-0.5235	-1.2154
-1.5	11.2326	-2.3849	36.0828	-0.6271	-1.7578
-1.4	12.8454	-3.1759	41.7122	-0.762	-2.4139
-1.3	14.6545	-4.1282	48.0918	-0.9366	-3.1916
-1.2	16.6511	-5.2543	55.2077	-1.1613	-4.093

-1.1	18.8043	-6.5599	62.9726	-1.4488	-5.1111
-1	21.0533	-8.0376	71.1974	-1.8126	-6.225
-0.9	23.303	-9.6614	79.5704	-2.2652	-7.3962
-0.8	25.4264	-11.3796	87.6588	-2.8141	-8.5655
-0.7	27.2783	-13.1127	94.9477	-3.4563	-9.6564
-0.6	28.7228	-14.7592	100.9274	-4.174	-10.5852
-0.5	29.6692	-16.212	105.2196	-4.9313	-11.2807
-0.4	30.1085	-17.3845	107.71	-5.6762	-11.7083
-0.3	30.1311	-18.2351	108.6283	-6.3468	-11.8883
-0.2	29.9133	-18.7767	108.5165	-6.8802	-11.8965
-0.1	29.6663	-19.0624	108.0614	-7.2238	-11.8386
0	29.5622	-19.1499	107.8363	-7.3426	-11.8073
0.1	29.6671	-19.0633	108.0645	-7.2242	-11.8391
0.2	29.9147	-18.7783	108.5223	-6.881	-11.8973
0.3	30.133	-18.2373	108.6361	-6.3479	-11.8894
0.4	30.1107	-17.3871	107.7191	-5.6776	-11.7095
0.5	29.6715	-16.2148	105.2291	-4.9328	-11.282
0.6	28.7249	-14.762	100.9366	-4.1755	-10.5865
0.7	27.2802	-13.1156	94.9562	-3.4579	-9.6577
0.8	25.428	-11.3824	87.6663	-2.8156	-8.5668
0.9	23.3043	-9.6641	79.5769	-2.2666	-7.3975
1	21.0543	-8.0401	71.2029	-1.8138	-6.2263
1.1	18.805	-6.5622	62.9772	-1.4498	-5.1124
1.2	16.6517	-5.2564	55.2115	-1.1621	-4.0943
1.3	14.6549	-4.1301	48.0949	-0.9372	-3.1929
1.4	12.8457	-3.1777	41.7148	-0.7625	-2.4152
1.5	11.2328	-2.3864	36.085	-0.6274	-1.759
1.6	9.8108	-1.7402	31.1727	-0.5236	-1.2166
1.7	8.5662	-1.2211	26.9196	-0.4442	-0.7769
1.8	7.482	-0.8109	23.2569	-0.3837	-0.4272
1.9	6.5407	-0.4915	20.1138	-0.3373	-0.1542
2	5.7255	-0.2464	17.4228	-0.3012	0.0548
2.1	5.0207	-0.0601	15.1222	-0.2722	0.2121
2.2	4.4124	0.0806	13.1566	-0.2478	0.3284
2.3	3.888	0.1869	11.4771	-0.2262	0.4131
2.4	3.4363	0.2679	10.041	-0.2061	0.474
2.5	3.0472	0.3305	8.811	-0.1868	0.5173
2.6	2.7117	0.38	7.7551	-0.1678	0.5478
2.7	2.4221	0.4201	6.8461	-0.149	0.5691
2.8	2.1713	0.4532	6.0608	-0.1305	0.5837
2.9	1.9535	0.481	5.3795	-0.1123	0.5933
3	1.7636	0.5048	4.7861	-0.0945	0.5993
3.1	1.5973	0.5251	4.2669	-0.0773	0.6024
3.2	1.451	0.5424	3.8107	-0.0607	0.6031
3.3	1.3218	0.5572	3.4082	-0.0448	0.602
3.4	1.2071	0.5696	3.0518	-0.0296	0.5992
3.5	1.105	0.5798	2.7351	-0.0151	0.5949
3.6	1.0137	0.588	2.4529	-0.0014	0.5894
3.7	0.9317	0.5944	2.2008	0.0116	0.5828
3.8	0.8581	0.5991	1.9751	0.0239	0.5752
3.9	0.7916	0.6022	1.7726	0.0355	0.5667
4	0.7315	0.6038	1.5907	0.0464	0.5574
4.1	0.677	0.604	1.4271	0.0566	0.5474
4.2	0.6276	0.6031	1.2797	0.0662	0.5369
4.3	0.5826	0.601	1.1469	0.0751	0.5259
4.4	0.5416	0.5977	1.0271	0.0833	0.5144
4.5	0.5042	0.5937	0.9189	0.091	0.5027
4.6	0.4699	0.5887	0.8211	0.098	0.4907

4.7	0.4386	0.583	0.7327	0.1045	0.4785
4.8	0.4098	0.5767	0.6527	0.1104	0.4663
4.9	0.3834	0.5698	0.5803	0.1158	0.454
5	0.359	0.5625	0.5146	0.1208	0.4417

NICS-scan (benzene ring)

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.0298	0.5454	-0.4559	0.3521	0.1933
-4.9	0.0285	0.5639	-0.4783	0.3669	0.197
-4.8	0.027	0.583	-0.5019	0.3825	0.2005
-4.7	0.0253	0.6028	-0.5268	0.3991	0.2037
-4.6	0.0234	0.6233	-0.5531	0.4167	0.2066
-4.5	0.0213	0.6445	-0.5807	0.4355	0.209
-4.4	0.0189	0.6663	-0.6097	0.4554	0.2109
-4.3	0.0162	0.6886	-0.64	0.4766	0.212
-4.2	0.0133	0.7114	-0.6714	0.4992	0.2122
-4.1	0.0101	0.7345	-0.704	0.5232	0.2113
-4	0.0067	0.7574	-0.7374	0.5486	0.2088
-3.9	0.0029	0.7801	-0.7713	0.5756	0.2045
-3.8	-0.0011	0.8019	-0.8053	0.6041	0.1978
-3.7	-0.0055	0.8223	-0.8388	0.6342	0.1881
-3.6	-0.0102	0.8403	-0.871	0.6657	0.1746
-3.5	-0.0154	0.8546	-0.9009	0.6984	0.1562
-3.4	-0.0212	0.8634	-0.927	0.7319	0.1315
-3.3	-0.0278	0.8644	-0.9477	0.7656	0.0988
-3.2	-0.0355	0.8541	-0.9605	0.7984	0.0557
-3.1	-0.0448	0.8281	-0.9625	0.8289	-0.0008
-3	-0.0563	0.781	-0.95	0.8551	-0.0741
-2.9	-0.0708	0.7056	-0.918	0.8743	-0.1687
-2.8	-0.0891	0.5933	-0.8605	0.883	-0.2897
-2.7	-0.112	0.4338	-0.7697	0.8768	-0.443
-2.6	-0.1401	0.2156	-0.6358	0.8506	-0.635
-2.5	-0.1736	-0.074	-0.4467	0.7983	-0.8723
-2.4	-0.2118	-0.4482	-0.1872	0.7132	-1.1614
-2.3	-0.2529	-0.92	0.1615	0.5881	-1.5081
-2.2	-0.2931	-1.5013	0.622	0.4151	-1.9164
-2.1	-0.3265	-2.2007	1.2211	0.1864	-2.3871
-2	-0.3441	-3.0217	1.9893	-0.1053	-2.9164
-1.9	-0.3332	-3.9599	2.9601	-0.4668	-3.4931
-1.8	-0.2766	-4.9976	4.1678	-0.9025	-4.0951
-1.7	-0.152	-6.0996	5.6438	-1.4137	-4.6859
-1.6	0.0679	-7.2075	7.4113	-1.9963	-5.2112
-1.5	0.4147	-8.2349	9.4792	-2.6381	-5.5968
-1.4	0.9219	-9.0692	11.8348	-3.3175	-5.7517
-1.3	1.6201	-9.578	14.4383	-4.0015	-5.5765
-1.2	2.5306	-9.6283	17.22	-4.6474	-4.9809
-1.1	3.6566	-9.1143	20.0841	-5.207	-3.9073
-1	4.9757	-7.9909	22.9181	-5.6351	-2.3558
-0.9	6.4359	-6.3003	25.6079	-5.8997	-0.4006
-0.8	7.958	-4.18	28.0541	-5.9916	1.8116

-0.7	9.4471	-1.842	30.1835	-5.9291	4.0871
-0.6	10.809	0.4735	31.9536	-5.7543	6.2278
-0.5	11.9675	2.5544	33.3482	-5.5226	8.077
-0.4	12.8764	4.2603	34.3691	-5.2891	9.5494
-0.3	13.5218	5.5373	35.0282	-5.0972	10.6345
-0.2	13.9147	6.4013	35.3427	-4.9735	11.3748
-0.1	14.0774	6.8997	35.3326	-4.9297	11.8294
0	14.0291	7.07	35.0172	-4.9688	12.0388
0.1	13.7747	6.9144	34.4098	-5.0907	12.0051
0.2	13.3035	6.4003	33.5101	-5.293	11.6933
0.3	12.5954	5.4863	32.2999	-5.5677	11.054
0.4	11.6368	4.1637	30.7466	-5.8942	10.0579
0.5	10.4384	2.4972	28.8181	-6.2335	8.7307
0.6	9.049	0.6418	26.5052	-6.5294	7.1712
0.7	7.5577	-1.172	23.8452	-6.7161	5.5441
0.8	6.0818	-2.6875	20.9329	-6.7337	4.0462
0.9	4.743	-3.6847	17.9138	-6.5429	2.8582
1	3.641	-4.0361	14.9591	-6.1363	2.1002
1.1	2.8337	-3.7317	12.2329	-5.5393	1.8076
1.2	2.3311	-2.8692	9.8625	-4.803	1.9338
1.3	2.1015	-1.617	7.9215	-3.9913	2.3743
1.4	2.0866	-0.1679	6.4277	-3.1677	2.9998
1.5	2.2178	1.3002	5.3531	-2.3859	3.6861
1.6	2.4299	2.6504	4.6391	-1.6837	4.3341
1.7	2.6691	3.794	4.2131	-1.0834	4.8774
1.8	2.8963	4.6881	4.0007	-0.593	5.2811
1.9	3.0864	5.3247	3.9344	-0.2104	5.5351
2	3.226	5.7201	3.9578	0.0737	5.6464
2.1	3.3103	5.904	4.0269	0.2721	5.6319
2.2	3.3406	5.9128	4.1092	0.3996	5.5132
2.3	3.3219	5.7836	4.182	0.4707	5.3129
2.4	3.261	5.5517	4.2313	0.4991	5.0526
2.5	3.166	5.2491	4.2489	0.4972	4.7519
2.6	3.0449	4.903	4.2317	0.4754	4.4276
2.7	2.9054	4.5363	4.1797	0.4425	4.0938
2.8	2.7542	4.1668	4.0957	0.4051	3.7617
2.9	2.5971	3.808	3.9834	0.3681	3.4399
3	2.4389	3.4691	3.8477	0.3346	3.1345
3.1	2.2832	3.156	3.6935	0.3066	2.8494
3.2	2.1324	2.8715	3.5257	0.2847	2.5868
3.3	1.9884	2.6163	3.3489	0.2689	2.3474
3.4	1.8521	2.3893	3.167	0.2585	2.1308
3.5	1.7241	2.1887	2.9836	0.2528	1.9359
3.6	1.6044	2.0119	2.8014	0.2506	1.7613
3.7	1.4929	1.8563	2.6226	0.2511	1.6052
3.8	1.3893	1.7189	2.449	0.2533	1.4656
3.9	1.2931	1.5976	2.2818	0.2566	1.341
4	1.2039	1.4898	2.1219	0.2603	1.2295
4.1	1.1212	1.3937	1.9698	0.264	1.1297

4.2	1.0445	1.3076	1.8258	0.2674	1.0402
4.3	0.9734	1.2302	1.69	0.2704	0.9598
4.4	0.9075	1.1601	1.5623	0.2727	0.8874
4.5	0.8464	1.0966	1.4425	0.2744	0.8222
4.6	0.7897	1.0387	1.3303	0.2755	0.7632
4.7	0.7371	0.9858	1.2256	0.276	0.7098
4.8	0.6884	0.9373	1.1278	0.2758	0.6615
4.9	0.6431	0.8928	1.0366	0.2752	0.6176
5	0.6012	0.8517	0.9517	0.274	0.5777

$[C_6H_6]$ (T_1) (D_{2h}), 15

```
Charge =  0 Multiplicity = 3
 C,0,0.7593884119,1.207416114,0.
 C,0,-0.7593884119,1.207416114,0.
 C,0,-1.4419756276,0.,0.
 C,0,-0.7593884119,-1.207416114,0.
 C,0,0.7593884119,-1.207416114,0.
 C,0,1.4419756276,0.,0.
 H,0,1.2869878528,2.152353689,0.
 H,0,-1.2869878528,2.152353689,0.
 H,0,-2.526784901,0.,0.
 H,0,-1.2869878528,-2.152353689,0.
 H,0,1.2869878528,-2.152353689,0.
 H,0,2.526784901,0.,0.
```

Sum of electronic and zero-point Energies= -232.078058
Sum of electronic and thermal Energies= -232.072040
Sum of electronic and thermal Enthalpies= -232.071095
Sum of electronic and thermal Free Energies= -232.106749

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.6857	0.7098	1.3473	0.3574	0.3524
-4.9	0.7295	0.746	1.4424	0.3751	0.3709
-4.8	0.777	0.7845	1.5464	0.3939	0.3906
-4.7	0.8286	0.8256	1.6602	0.4139	0.4117
-4.6	0.8848	0.8694	1.785	0.4351	0.4343
-4.5	0.9461	0.9161	1.9221	0.4576	0.4585
-4.4	1.013	0.9661	2.0729	0.4816	0.4845
-4.3	1.0862	1.0193	2.2392	0.507	0.5123
-4.2	1.1664	1.0763	2.4228	0.534	0.5423
-4.1	1.2543	1.137	2.626	0.5626	0.5744
-4	1.3511	1.202	2.8512	0.593	0.609
-3.9	1.4576	1.2714	3.1013	0.6251	0.6463
-3.8	1.5751	1.3456	3.3796	0.6592	0.6864
-3.7	1.7049	1.4249	3.6899	0.6952	0.7297
-3.6	1.8486	1.5095	4.0365	0.7331	0.7764
-3.5	2.008	1.5996	4.4244	0.7729	0.8267
-3.4	2.1851	1.6957	4.8595	0.8146	0.8811
-3.3	2.382	1.7977	5.3484	0.858	0.9397
-3.2	2.6015	1.9059	5.8988	0.9029	1.003
-3.1	2.8465	2.02	6.5194	0.9488	1.0712
-3	3.1202	2.14	7.2206	0.9953	1.1447
-2.9	3.4264	2.2652	8.014	1.0415	1.2237
-2.8	3.7691	2.3946	8.9128	1.0861	1.3085
-2.7	4.153	2.5266	9.9324	1.1276	1.399
-2.6	4.583	2.6591	11.0898	1.1638	1.4953
-2.5	5.0644	2.7887	12.4046	1.1918	1.5969

-2.4	5.6031	2.911	13.8983	1.2079	1.7031
-2.3	6.205	3.0202	15.5948	1.2074	1.8128
-2.2	6.8765	3.1093	17.5202	1.1849	1.9244
-2.1	7.6241	3.1696	19.7027	1.1339	2.0357
-2	8.4542	3.1908	22.1719	1.0472	2.1436
-1.9	9.3732	3.1612	24.9585	0.9168	2.2444
-1.8	10.387	3.0685	28.0926	0.735	2.3335
-1.7	11.5007	2.8994	31.6028	0.494	2.4054
-1.6	12.7178	2.6406	35.5127	0.1872	2.4534
-1.5	14.0391	2.2792	39.838	-0.1904	2.4696
-1.4	15.4614	1.8033	44.581	-0.6413	2.4446
-1.3	16.9758	1.2026	49.7248	-1.1645	2.3671
-1.2	18.5651	0.4699	55.2255	-1.7543	2.2242
-1.1	20.2026	-0.3974	61.0051	-2.3989	2.0015
-1	21.8504	-1.3952	66.9462	-3.0796	1.6844
-0.9	23.4603	-2.5099	72.891	-3.7699	1.26
-0.8	24.9771	-3.7162	78.6477	-4.4369	0.7207
-0.7	26.3441	-4.9754	84.0076	-5.0439	0.0685
-0.6	27.5118	-6.236	88.7713	-5.5566	-0.6794
-0.5	28.4476	-7.4379	92.7807	-5.9499	-1.488
-0.4	29.1431	-8.5183	95.9475	-6.2158	-2.3025
-0.3	29.6157	-9.4193	98.2664	-6.3665	-3.0528
-0.2	29.9034	-10.0945	99.8045	-6.4321	-3.6624
-0.1	30.0513	-10.5115	100.6654	-6.4501	-4.0614
0	30.096	-10.6525	100.9403	-6.4518	-4.2007
0.1	30.0512	-10.5116	100.6653	-6.4492	-4.0624
0.2	29.9033	-10.0945	99.8043	-6.4303	-3.6642
0.3	29.6156	-9.4195	98.2663	-6.3641	-3.0554
0.4	29.1431	-8.5183	95.9475	-6.2127	-2.3056
0.5	28.4477	-7.4379	92.781	-5.9464	-1.4915
0.6	27.512	-6.2359	88.7719	-5.5528	-0.6831
0.7	26.3445	-4.9751	84.0085	-5.04	0.0649
0.8	24.9777	-3.7158	78.6489	-4.433	0.7172
0.9	23.461	-2.5093	72.8924	-3.7661	1.2568
1	21.8511	-1.3945	66.9478	-3.076	1.6815
1.1	20.2034	-0.3966	61.0068	-2.3956	1.999
1.2	18.566	0.4707	55.2272	-1.7512	2.2219
1.3	16.9767	1.2034	49.7265	-1.1617	2.3651
1.4	15.4623	1.8042	44.5827	-0.6387	2.4429
1.5	14.0399	2.2801	39.8395	-0.1881	2.4682
1.6	12.7186	2.6416	35.5142	0.1893	2.4523
1.7	11.5015	2.9003	31.6041	0.4958	2.4045
1.8	10.3877	3.0693	28.0939	0.7366	2.3327
1.9	9.3739	3.1621	24.9596	0.9183	2.2438
2	8.4548	3.1916	22.173	1.0485	2.1431
2.1	7.6247	3.1704	19.7036	1.1351	2.0353
2.2	6.8771	3.1101	17.521	1.186	1.9241
2.3	6.2055	3.0209	15.5955	1.2083	1.8126
2.4	5.6035	2.9116	13.8989	1.2087	1.7029
2.5	5.0648	2.7892	12.4052	1.1925	1.5967
2.6	4.5833	2.6597	11.0904	1.1645	1.4952
2.7	4.1533	2.5272	9.9328	1.1282	1.399
2.8	3.7694	2.3951	8.9132	1.0866	1.3085
2.9	3.4267	2.2657	8.0143	1.0419	1.2238
3	3.1205	2.1404	7.221	0.9957	1.1447
3.1	2.8467	2.0205	6.5197	0.9492	1.0713
3.2	2.6018	1.9063	5.899	0.9032	1.0031
3.3	2.3822	1.7981	5.3486	0.8583	0.9398

3.4	2.1852	1.696	4.8597	0.8148	0.8812
3.5	2.0082	1.5999	4.4246	0.7731	0.8268
3.6	1.8488	1.5098	4.0366	0.7333	0.7765
3.7	1.7051	1.4252	3.69	0.6954	0.7298
3.8	1.5752	1.3459	3.3797	0.6594	0.6865
3.9	1.4577	1.2717	3.1014	0.6253	0.6464
4	1.3512	1.2022	2.8513	0.5931	0.6091
4.1	1.2545	1.1372	2.6261	0.5627	0.5745
4.2	1.1665	1.0765	2.4229	0.5341	0.5424
4.3	1.0863	1.0195	2.2393	0.5071	0.5124
4.4	1.0131	0.9663	2.073	0.4817	0.4846
4.5	0.9462	0.9163	1.9221	0.4577	0.4586
4.6	0.8849	0.8696	1.7851	0.4352	0.4344
4.7	0.8287	0.8258	1.6602	0.414	0.4118
4.8	0.7771	0.7847	1.5464	0.394	0.3907
4.9	0.7296	0.7462	1.4425	0.3752	0.371
5	0.6858	0.7099	1.3474	0.3574	0.3525

$[C_6H_6]^+$ (D_{2h}), 16

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Charge =  1 Multiplicity = 2
C,0,0.,-0.0052837069,1.3817819
 C,0,0.,1.2449726554,0.6899345749
 C,0,0.,1.250220023,-0.6790135523
 C,0,0.,0.0052837069,-1.3817819
 C,0,0.,-1.2449726554,-0.6899345749
 C,0,0.,-1.250220023,0.6790135523
 H,0,0.,-0.009727386,2.4670635068
 H,0,0.,2.1672096112,1.2577710144
 H,0,0.,2.1767999712,-1.2398615021
 H,0,0.,0.009727386,-2.4670635068
 H,0,0.,-2.1672096112,-1.2577710144
 H,0,0.,-2.1767999712,1.2398615021
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Sum of electronic and zero-point Energies= -231.878359
Sum of electronic and thermal Energies= -231.873141
Sum of electronic and thermal Enthalpies= -231.872197
Sum of electronic and thermal Free Energies= -231.906483

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.1908	0.4327	0.1397	0.2088	0.2239
-4.9	0.2053	0.4537	0.1623	0.2185	0.2352
-4.8	0.2213	0.4758	0.1881	0.2287	0.2471
-4.7	0.2389	0.4993	0.2175	0.2395	0.2598
-4.6	0.2584	0.5242	0.2511	0.2509	0.2733
-4.5	0.28	0.5504	0.2895	0.2628	0.2876
-4.4	0.3039	0.5783	0.3336	0.2754	0.3029
-4.3	0.3306	0.6076	0.3841	0.2885	0.3191
-4.2	0.3603	0.6386	0.4421	0.3022	0.3364
-4.1	0.3934	0.6715	0.5088	0.3166	0.3549
-4	0.4306	0.706	0.5858	0.3315	0.3745
-3.9	0.4723	0.7423	0.6746	0.347	0.3953
-3.8	0.5193	0.7804	0.7774	0.3629	0.4175
-3.7	0.5723	0.8204	0.8966	0.3793	0.4411
-3.6	0.6323	0.8621	1.0349	0.3959	0.4662
-3.5	0.7005	0.9055	1.196	0.4127	0.4928
-3.4	0.778	0.9503	1.3838	0.4293	0.521

-3.3	0.8666	0.9964	1.6033	0.4455	0.5509
-3.2	0.9679	1.0434	1.8604	0.4608	0.5826
-3.1	1.0843	1.0906	2.1621	0.4746	0.616
-3	1.2181	1.1374	2.5169	0.4862	0.6512
-2.9	1.3724	1.1825	2.9348	0.4944	0.6881
-2.8	1.5507	1.2244	3.4277	0.4977	0.7267
-2.7	1.7569	1.261	4.0097	0.4943	0.7667
-2.6	1.9956	1.2894	4.6974	0.4815	0.8079
-2.5	2.2721	1.3062	5.5101	0.4562	0.85
-2.4	2.5922	1.3065	6.4703	0.4142	0.8923
-2.3	2.9626	1.2846	7.6033	0.3504	0.9342
-2.2	3.3907	1.2338	8.9382	0.2589	0.9749
-2.1	3.8845	1.1464	10.5072	0.1329	1.0135
-2	4.4532	1.0138	12.3458	-0.0352	1.049
-1.9	5.1066	0.8277	14.4922	-0.253	1.0807
-1.8	5.8555	0.5797	16.9867	-0.5282	1.1079
-1.7	6.7111	0.263	19.8701	-0.8673	1.1303
-1.6	7.6848	-0.1267	23.1811	-1.2751	1.1484
-1.5	8.7871	-0.5909	26.9522	-1.7536	1.1627
-1.4	10.0258	-1.1261	31.2034	-2.3008	1.1747
-1.3	11.4032	-1.7235	35.933	-2.9094	1.1859
-1.2	12.9131	-2.3674	41.1067	-3.5653	1.1979
-1.1	14.5368	-3.0342	46.6446	-4.2458	1.2116
-1	16.2395	-3.6918	52.4103	-4.9193	1.2275
-0.9	17.9684	-4.3007	58.2059	-5.5456	1.2449
-0.8	19.6545	-4.8161	63.7795	-6.0783	1.2622
-0.7	21.2192	-5.1941	68.8516	-6.4715	1.2774
-0.6	22.5862	-5.4009	73.1595	-6.6896	1.2887
-0.5	23.6967	-5.4247	76.5149	-6.7197	1.295
-0.4	24.5239	-5.2847	78.8565	-6.5815	1.2968
-0.3	25.0794	-5.0359	80.2741	-6.3312	1.2953
-0.2	25.4082	-4.7604	80.9852	-6.053	1.2926
-0.1	25.571	-4.548	81.2609	-5.8382	1.2902
0	25.6186	-4.4683	81.3241	-5.7576	1.2893
0.1	25.571	-4.548	81.2609	-5.8382	1.2902
0.2	25.4082	-4.7604	80.9852	-6.053	1.2926
0.3	25.0794	-5.0359	80.2741	-6.3312	1.2953
0.4	24.5239	-5.2847	78.8565	-6.5815	1.2968
0.5	23.6967	-5.4247	76.5149	-6.7197	1.295
0.6	22.5862	-5.4009	73.1595	-6.6896	1.2887
0.7	21.2192	-5.1941	68.8516	-6.4715	1.2774
0.8	19.6545	-4.8161	63.7795	-6.0783	1.2622
0.9	17.9684	-4.3007	58.2059	-5.5456	1.2449
1	16.2395	-3.6918	52.4103	-4.9193	1.2275
1.1	14.5368	-3.0342	46.6446	-4.2458	1.2116
1.2	12.9131	-2.3674	41.1067	-3.5653	1.1979
1.3	11.4032	-1.7235	35.933	-2.9094	1.1859
1.4	10.0258	-1.1261	31.2034	-2.3008	1.1747
1.5	8.7871	-0.5909	26.9522	-1.7536	1.1627

1.6	7.6848	-0.1267	23.1811	-1.2751	1.1484
1.7	6.7111	0.263	19.8701	-0.8673	1.1303
1.8	5.8555	0.5797	16.9867	-0.5282	1.1079
1.9	5.1066	0.8277	14.4922	-0.253	1.0807
2	4.4532	1.0138	12.3458	-0.0352	1.049
2.1	3.8845	1.1464	10.5072	0.1329	1.0135
2.2	3.3907	1.2338	8.9382	0.2589	0.9749
2.3	2.9626	1.2846	7.6033	0.3504	0.9342
2.4	2.5922	1.3065	6.4703	0.4142	0.8923
2.5	2.2721	1.3062	5.5101	0.4562	0.85
2.6	1.9956	1.2894	4.6974	0.4815	0.8079
2.7	1.7569	1.261	4.0097	0.4943	0.7667
2.8	1.5507	1.2244	3.4277	0.4977	0.7267
2.9	1.3724	1.1825	2.9348	0.4944	0.6881
3	1.2181	1.1374	2.5169	0.4862	0.6512
3.1	1.0843	1.0906	2.1621	0.4746	0.616
3.2	0.9679	1.0434	1.8604	0.4608	0.5826
3.3	0.8666	0.9964	1.6033	0.4455	0.5509
3.4	0.778	0.9503	1.3838	0.4293	0.521
3.5	0.7005	0.9055	1.196	0.4127	0.4928
3.6	0.6323	0.8621	1.0349	0.3959	0.4662
3.7	0.5723	0.8204	0.8966	0.3793	0.4411
3.8	0.5193	0.7804	0.7774	0.3629	0.4175
3.9	0.4723	0.7423	0.6746	0.347	0.3953
4	0.4306	0.706	0.5858	0.3315	0.3745
4.1	0.3934	0.6715	0.5088	0.3166	0.3549
4.2	0.3603	0.6386	0.4421	0.3022	0.3364
4.3	0.3306	0.6076	0.3841	0.2885	0.3191
4.4	0.3039	0.5783	0.3336	0.2754	0.3029
4.5	0.28	0.5504	0.2895	0.2628	0.2876
4.6	0.2584	0.5242	0.2511	0.2509	0.2733
4.7	0.2389	0.4993	0.2175	0.2395	0.2598
4.8	0.2213	0.4758	0.1881	0.2287	0.2471
4.9	0.2053	0.4537	0.1623	0.2185	0.2352
5	0.1908	0.4327	0.1397	0.2088	0.2239

$[C_6H_6]^-$ (D_{2h}), 17

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Charge = -1 Multiplicity = 2
C,0,0.,1.397846724,0.
 C,0,1.2261885129,0.727612737,0.
 C,0,1.2261885129,-0.727612737,0.
 C,0,0.,-1.397846724,0.
 C,0,-1.2261885129,-0.727612737,0.
 C,0,-1.2261885129,0.727612737,0.
 H,0,0.,2.4888528945,0.
 H,0,2.1587809313,1.2844176774,0.
 H,0,2.1587809313,-1.2844176774,0.
 H,0,0.,-2.4888528945,0.
 H,0,-2.1587809313,-1.2844176774,0.
 H,0,-2.1587809313,1.2844176774,0.
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Sum of electronic and zero-point Energies= -232.172678
Sum of electronic and thermal Energies= -232.166971
Sum of electronic and thermal Enthalpies= -232.166027

Sum of electronic and thermal Free Energies= -232.200318

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	2.1978	0.9118	5.6815	0.463	0.4488
-4.9	2.3341	0.9681	6.0342	0.4914	0.4767
-4.8	2.4814	1.0292	6.415	0.5223	0.5069
-4.7	2.6408	1.0956	6.8267	0.5558	0.5398
-4.6	2.8134	1.1678	7.2722	0.5923	0.5755
-4.5	3.0005	1.2465	7.7549	0.6321	0.6144
-4.4	3.2035	1.3322	8.2783	0.6754	0.6568
-4.3	3.4241	1.4258	8.8464	0.7227	0.7031
-4.2	3.6639	1.5279	9.4639	0.7743	0.7536
-4.1	3.9251	1.6395	10.1357	0.8308	0.8087
-4	4.2096	1.7614	10.8674	0.8925	0.8689
-3.9	4.52	1.8947	11.6652	0.96	0.9347
-3.8	4.8588	2.0404	12.536	1.0338	1.0066
-3.7	5.2291	2.1995	13.4877	1.1145	1.085
-3.6	5.634	2.3731	14.529	1.2026	1.1705
-3.5	6.0772	2.5622	15.6694	1.2986	1.2636
-3.4	6.5627	2.7681	16.9199	1.4033	1.3648
-3.3	7.0947	2.9916	18.2925	1.517	1.4746
-3.2	7.6782	3.2339	19.8008	1.6404	1.5935
-3.1	8.3183	3.4953	21.4596	1.7737	1.7216
-3	9.0208	3.7766	23.2857	1.9173	1.8593
-2.9	9.7918	4.0778	25.2976	2.0714	2.0064
-2.8	10.638	4.3984	27.5156	2.2357	2.1627
-2.7	11.5665	4.7373	29.9621	2.4098	2.3275
-2.6	12.5847	5.0925	32.6617	2.5928	2.4997
-2.5	13.7006	5.4609	35.6409	2.7834	2.6775
-2.4	14.9221	5.838	38.9284	2.9794	2.8586
-2.3	16.2576	6.2178	42.555	3.178	3.0398
-2.2	17.7152	6.5927	46.5529	3.3758	3.2169
-2.1	19.3028	6.953	50.9556	3.5682	3.3848
-2	21.0279	7.2871	55.7967	3.7497	3.5374
-1.9	22.8968	7.5816	61.1087	3.914	3.6676
-1.8	24.914	7.821	66.921	4.054	3.767
-1.7	27.0816	7.9879	73.2569	4.1614	3.8265
-1.6	29.3977	8.0634	80.1296	4.2276	3.8358
-1.5	31.8546	8.0269	87.5369	4.243	3.7839
-1.4	34.4371	7.8571	95.4543	4.198	3.6591
-1.3	37.1199	7.5318	103.828	4.0826	3.4492
-1.2	39.8655	7.0297	112.5667	3.8876	3.1421
-1.1	42.6225	6.3318	121.5357	3.6048	2.727
-1	45.3263	5.4245	130.5544	3.2289	2.1956
-0.9	47.9012	4.3038	139.3997	2.7591	1.5447
-0.8	50.2664	2.9803	147.8188	2.2011	0.7792
-0.7	52.3455	1.4845	155.5521	1.5695	-0.085
-0.6	54.0786	-0.1288	162.3647	0.8891	-1.0179

-0.5	55.4338	-1.7789	168.0804	0.1951	-1.974
-0.4	56.4155	-3.3629	172.6094	-0.4683	-2.8946
-0.3	57.0644	-4.7648	175.9579	-1.0529	-3.7119
-0.2	57.4476	-5.8685	178.2113	-1.5113	-4.3572
-0.1	57.6389	-6.5754	179.4921	-1.804	-4.7714
0	57.6955	-6.819	179.9053	-1.9047	-4.9143
0.1	57.6389	-6.5754	179.4921	-1.804	-4.7714
0.2	57.4476	-5.8685	178.2113	-1.5113	-4.3572
0.3	57.0644	-4.7648	175.9579	-1.0529	-3.7119
0.4	56.4155	-3.3629	172.6094	-0.4683	-2.8946
0.5	55.4338	-1.7789	168.0804	0.1951	-1.974
0.6	54.0786	-0.1288	162.3647	0.8891	-1.0179
0.7	52.3455	1.4845	155.5521	1.5695	-0.085
0.8	50.2664	2.9803	147.8188	2.2011	0.7792
0.9	47.9012	4.3038	139.3997	2.7591	1.5447
1	45.3263	5.4245	130.5544	3.2289	2.1956
1.1	42.6225	6.3318	121.5357	3.6048	2.727
1.2	39.8655	7.0297	112.5667	3.8876	3.1421
1.3	37.1199	7.5318	103.828	4.0826	3.4492
1.4	34.4371	7.8571	95.4543	4.198	3.6591
1.5	31.8546	8.0269	87.5369	4.243	3.7839
1.6	29.3977	8.0634	80.1296	4.2276	3.8358
1.7	27.0816	7.9879	73.2569	4.1614	3.8265
1.8	24.914	7.821	66.921	4.054	3.767
1.9	22.8968	7.5816	61.1087	3.914	3.6676
2	21.0279	7.2871	55.7967	3.7497	3.5374
2.1	19.3028	6.953	50.9556	3.5682	3.3848
2.2	17.7152	6.5927	46.5529	3.3758	3.2169
2.3	16.2576	6.2178	42.555	3.178	3.0398
2.4	14.9221	5.838	38.9284	2.9794	2.8586
2.5	13.7006	5.4609	35.6409	2.7834	2.6775
2.6	12.5847	5.0925	32.6617	2.5928	2.4997
2.7	11.5665	4.7373	29.9621	2.4098	2.3275
2.8	10.638	4.3984	27.5156	2.2357	2.1627
2.9	9.7918	4.0778	25.2976	2.0714	2.0064
3	9.0208	3.7766	23.2857	1.9173	1.8593
3.1	8.3183	3.4953	21.4596	1.7737	1.7216
3.2	7.6782	3.2339	19.8008	1.6404	1.5935
3.3	7.0947	2.9916	18.2925	1.517	1.4746
3.4	6.5627	2.7681	16.9199	1.4033	1.3648
3.5	6.0772	2.5622	15.6694	1.2986	1.2636
3.6	5.634	2.3731	14.529	1.2026	1.1705
3.7	5.2291	2.1995	13.4877	1.1145	1.085
3.8	4.8588	2.0404	12.536	1.0338	1.0066
3.9	4.52	1.8947	11.6652	0.96	0.9347
4	4.2096	1.7614	10.8674	0.8925	0.8689
4.1	3.9251	1.6395	10.1357	0.8308	0.8087
4.2	3.6639	1.5279	9.4639	0.7743	0.7536
4.3	3.4241	1.4258	8.8464	0.7227	0.7031

4.4	3.2035	1.3322	8.2783	0.6754	0.6568
4.5	3.0005	1.2465	7.7549	0.6321	0.6144
4.6	2.8134	1.1678	7.2722	0.5923	0.5755
4.7	2.6408	1.0956	6.8267	0.5558	0.5398
4.8	2.4814	1.0292	6.415	0.5223	0.5069
4.9	2.3341	0.9681	6.0342	0.4914	0.4767
5	2.1978	0.9118	5.6815	0.463	0.4488

cycloheptatrienyl (C_{2v}), 18

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Charge =  0 Multiplicity = 2
 C,0,-1.4681862,-0.679368,0.
 C,0,-1.4681862,0.679368,0.
 C,0,-0.3408422,1.587131,0.
 C,0,0.9966128,1.266766,0.
 C,0,1.6247918,0.,0.
 C,0,0.9966128,-1.266766,0.
 C,0,-0.3408422,-1.587131,0.
 H,0,-2.4427932,-1.159492,0.
 H,0,-2.4427932,1.159492,0.
 H,0,-0.5899092,2.642921,0.
 H,0,1.6784208,2.114346,0.
 H,0,2.7087998,0.,0.
 H,0,1.6784208,-2.114346,0.
 H,0,-0.5899092,-2.642921,0.
```

Sum of electronic and zero-point Energies= -270.848791
Sum of electronic and thermal Energies= -270.842227
Sum of electronic and thermal Enthalpies= -270.841283
Sum of electronic and thermal Free Energies= -270.879791

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	1.3643	0.8288	3.2641	0.4148	0.414
-4.9	1.4467	0.8687	3.4714	0.4348	0.4339
-4.8	1.5358	0.9112	3.6962	0.4561	0.4551
-4.7	1.6321	0.9562	3.9401	0.4786	0.4776
-4.6	1.7363	1.0037	4.2052	0.5024	0.5013
-4.5	1.8493	1.0542	4.4937	0.5277	0.5265
-4.4	1.9719	1.1076	4.8082	0.5544	0.5532
-4.3	2.1052	1.1643	5.1514	0.5828	0.5815
-4.2	2.2503	1.2242	5.5266	0.6128	0.6114
-4.1	2.4083	1.2877	5.9373	0.6446	0.6431
-4	2.5807	1.3548	6.3874	0.6782	0.6766
-3.9	2.7691	1.4258	6.8817	0.7138	0.712
-3.8	2.9752	1.5006	7.425	0.7513	0.7493
-3.7	3.2009	1.5795	8.0233	0.7908	0.7887
-3.6	3.4485	1.6624	8.683	0.8323	0.8301
-3.5	3.7202	1.7494	9.4114	0.8759	0.8735
-3.4	4.019	1.8403	10.2166	0.9215	0.9188
-3.3	4.3477	1.935	11.1081	0.969	0.966
-3.2	4.7097	2.033	12.0961	1.0181	1.0149
-3.1	5.1088	2.1339	13.1923	1.0687	1.0652
-3	5.5489	2.237	14.4097	1.1204	1.1166

-2.9	6.0345	2.3409	15.7627	1.1725	1.1684
-2.8	6.5705	2.4445	17.2672	1.2245	1.22
-2.7	7.1621	2.5457	18.9407	1.2753	1.2704
-2.6	7.8148	2.6419	20.8025	1.3236	1.3183
-2.5	8.5344	2.7302	22.8729	1.368	1.3622
-2.4	9.327	2.8068	25.1742	1.4066	1.4002
-2.3	10.1987	2.8667	27.7292	1.4368	1.4299
-2.2	11.1555	2.9047	30.5619	1.4561	1.4486
-2.1	12.2034	2.9143	33.6959	1.4612	1.4531
-2	13.3476	2.8885	37.1543	1.4486	1.4399
-1.9	14.5925	2.8199	40.9578	1.4146	1.4053
-1.8	15.9413	2.7007	45.1234	1.3553	1.3454
-1.7	17.3952	2.5235	49.6622	1.267	1.2565
-1.6	18.9527	2.2816	54.5765	1.1463	1.1353
-1.5	20.6088	1.9698	59.8566	0.9907	0.9791
-1.4	22.354	1.5849	65.4771	0.7985	0.7864
-1.3	24.1729	1.126	71.3927	0.5693	0.5567
-1.2	26.0438	0.5961	77.5353	0.3045	0.2916
-1.1	27.9376	0.0016	83.8112	0.0074	-0.0058
-1	29.8185	-0.6465	90.1018	-0.3165	-0.33
-0.9	31.6448	-1.3325	96.2669	-0.6594	-0.6731
-0.8	33.3719	-2.037	102.1528	-1.0116	-1.0254
-0.7	34.956	-2.7364	107.6045	-1.3613	-1.3751
-0.6	36.3584	-3.4053	112.4806	-1.6958	-1.7095
-0.5	37.5502	-4.018	116.6687	-2.0023	-2.0157
-0.4	38.515	-4.551	120.096	-2.269	-2.282
-0.3	39.2494	-4.9844	122.7326	-2.486	-2.4984
-0.2	39.7604	-5.3034	124.5845	-2.6458	-2.6576
-0.1	40.0598	-5.4982	125.6777	-2.7437	-2.7545
0	40.1583	-5.5637	126.0385	-2.7769	-2.7868
0.1	40.0599	-5.4982	125.6778	-2.7447	-2.7535
0.2	39.7605	-5.3032	124.5848	-2.6478	-2.6554
0.3	39.2496	-4.9842	122.7329	-2.4888	-2.4954
0.4	38.5152	-4.5507	120.0964	-2.2725	-2.2782
0.5	37.5505	-4.0177	116.6691	-2.0064	-2.0113
0.6	36.3587	-3.4049	112.4811	-1.7002	-1.7047
0.7	34.9563	-2.736	107.6049	-1.3659	-1.3701
0.8	33.3722	-2.0366	102.1532	-1.0163	-1.0203
0.9	31.645	-1.3322	96.2673	-0.664	-0.6682
1	29.8187	-0.6462	90.1022	-0.3209	-0.3253
1.1	27.9378	0.0019	83.8115	0.0033	-0.0014
1.2	26.044	0.5964	77.5356	0.3007	0.2957
1.3	24.1731	1.1263	71.393	0.5658	0.5605
1.4	22.3541	1.5851	65.4773	0.7953	0.7898
1.5	20.6089	1.97	59.8568	0.9879	0.9821
1.6	18.9528	2.2818	54.5766	1.1438	1.138
1.7	17.3953	2.5235	49.6622	1.2647	1.2588
1.8	15.9414	2.7007	45.1234	1.3533	1.3474
1.9	14.5926	2.8199	40.9578	1.4128	1.4071

2	13.3476	2.8886	37.1543	1.4471	1.4415
2.1	12.2034	2.9143	33.6959	1.4598	1.4545
2.2	11.1555	2.9047	30.5619	1.4549	1.4498
2.3	10.1987	2.8667	27.7292	1.4358	1.4309
2.4	9.327	2.8068	25.1741	1.4057	1.4011
2.5	8.5344	2.7303	22.8729	1.3673	1.363
2.6	7.8148	2.6419	20.8024	1.323	1.3189
2.7	7.1621	2.5456	18.9407	1.2747	1.2709
2.8	6.5705	2.4444	17.2671	1.224	1.2204
2.9	6.0345	2.3409	15.7626	1.1721	1.1688
3	5.5489	2.2369	14.4097	1.12	1.1169
3.1	5.1087	2.1339	13.1923	1.0684	1.0655
3.2	4.7097	2.033	12.0961	1.0178	1.0152
3.3	4.3477	1.935	11.1081	0.9687	0.9663
3.4	4.019	1.8403	10.2166	0.9213	0.919
3.5	3.7202	1.7493	9.4113	0.8757	0.8736
3.6	3.4484	1.6624	8.683	0.8322	0.8302
3.7	3.2009	1.5794	8.0233	0.7906	0.7888
3.8	2.9752	1.5005	7.425	0.7511	0.7494
3.9	2.7691	1.4256	6.8816	0.7136	0.712
4	2.5807	1.3547	6.3874	0.6781	0.6766
4.1	2.4083	1.2876	5.9372	0.6445	0.6431
4.2	2.2502	1.2241	5.5266	0.6127	0.6114
4.3	2.1052	1.1642	5.1514	0.5827	0.5815
4.4	1.9719	1.1076	4.8082	0.5544	0.5532
4.5	1.8493	1.0541	4.4937	0.5276	0.5265
4.6	1.7363	1.0037	4.2052	0.5024	0.5013
4.7	1.6321	0.9561	3.9401	0.4785	0.4776
4.8	1.5358	0.9111	3.6961	0.456	0.4551
4.9	1.4467	0.8687	3.4714	0.4348	0.4339
5	1.3643	0.8287	3.2641	0.4148	0.4139

cyclooctatetraene (D_{2d}), 19

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Charge =  0 Multiplicity = 1
 C,0,-8.3558565309,0.5809290751,1.2555225943
 C,0,-8.0913964362,-0.8669027868,1.2871898085
 C,0,-7.0080090199,-1.5070747491,0.8283889765
 C,0,-5.8247088576,-0.9151374112,0.1830899537
 C,0,-5.7982019544,-0.1057186315,-0.8837834199
 C,0,-6.9460210061,0.3845740271,-1.6642538884
 C,0,-8.0291168142,1.0250520177,-1.2051816076
 C,0,-8.329072366,1.3906580661,0.188910438
 H,0,-8.6797971401,1.0092279864,2.2028806594
 H,0,-8.8389375949,-1.4588366343,1.8131385418
 H,0,-6.9436421918,-2.5787746918,1.0106088357
 H,0,-4.8685428161,-1.2441459424,0.5872438171
 H,0,-4.8221614399,0.1715856045,-1.2791479809
 H,0,-6.8505449724,0.2696117842,-2.7429200457
 H,0,-8.7451432737,1.3903467827,-1.9398411827
 H,0,-8.6327475858,2.4259055033,0.3368545003
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Sum of electronic and zero-point Energies= -309.537020
Sum of electronic and thermal Energies= -309.530276
Sum of electronic and thermal Enthalpies= -309.529331

Sum of electronic and thermal Free Energies= -309.567502

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.1608	1.0924	-0.6101	0.4213	0.6711
-4.9	0.1698	1.1442	-0.6349	0.4369	0.7073
-4.8	0.1794	1.1987	-0.6606	0.4528	0.7459
-4.7	0.1897	1.2562	-0.6872	0.469	0.7872
-4.6	0.2007	1.3168	-0.7146	0.4853	0.8315
-4.5	0.2125	1.3804	-0.7428	0.5016	0.8788
-4.4	0.2252	1.4474	-0.7717	0.5179	0.9295
-4.3	0.2389	1.5178	-0.8011	0.5338	0.984
-4.2	0.2535	1.5916	-0.831	0.5492	1.0424
-4.1	0.2693	1.6689	-0.861	0.5638	1.1051
-4	0.2863	1.7497	-0.8908	0.5773	1.1724
-3.9	0.3046	1.8339	-0.9202	0.5891	1.2448
-3.8	0.3242	1.9214	-0.9487	0.5988	1.3226
-3.7	0.3454	2.0119	-0.9757	0.6056	1.4063
-3.6	0.3681	2.1048	-1.0004	0.6087	1.4961
-3.5	0.3924	2.1994	-1.0222	0.607	1.5924
-3.3	0.4459	2.3895	-1.0518	0.5837	1.8058
-3.2	0.4749	2.4814	-1.0568	0.5584	1.923
-3.1	0.505	2.5677	-1.0527	0.5207	2.047
-3	0.536	2.6449	-1.0371	0.4676	2.1773
-2.9	0.5671	2.7084	-1.0072	0.3953	2.3131
-2.8	0.5975	2.7521	-0.9596	0.2993	2.4528
-2.7	0.6261	2.7685	-0.8901	0.174	2.5945
-2.6	0.6516	2.7488	-0.7941	0.0134	2.7354
-2.5	0.6722	2.6824	-0.6658	-0.1898	2.8722
-2.4	0.6863	2.5575	-0.4988	-0.4433	3.0008
-2.3	0.6919	2.3611	-0.2855	-0.7553	3.1164
-2.2	0.6874	2.0799	-0.0175	-1.1342	3.2141
-2.1	0.6719	1.7008	0.3149	-1.5876	3.2884
-2	0.6451	1.2129	0.7224	-2.1216	3.3345
-1.9	0.6081	0.6076	1.2165	-2.7401	3.3477
-1.8	0.5636	-0.1189	1.8096	-3.4434	3.3245
-1.7	0.5164	-0.9646	2.5139	-4.227	3.2624
-1.6	0.4737	-1.92	3.3411	-5.0803	3.1603
-1.5	0.4449	-2.9668	4.3014	-5.9853	3.0185
-1.4	0.4413	-4.0773	5.4013	-6.9155	2.8382
-1.3	0.4762	-5.2143	6.643	-7.836	2.6217
-1.2	0.5632	-6.3321	8.0217	-8.7035	2.3714
-1.1	0.7151	-7.3795	9.5248	-9.4688	2.0893
-1	0.9422	-8.3038	11.1303	-10.08	1.7762
-0.9	1.2497	-9.0573	12.8065	-10.4884	1.4311
-0.8	1.6361	-9.6044	14.5129	-10.6544	1.05
-0.7	2.091	-9.9285	16.2014	-10.5542	0.6257
-0.6	2.5941	-10.0367	17.8189	-10.1846	0.1479
-0.5	3.1162	-9.9615	19.3101	-9.5651	-0.3964

-0.4	3.621	-9.7575	20.6205	-8.736	-1.0215
-0.3	4.0688	-9.4931	21.6996	-7.7529	-1.7402
-0.2	4.4215	-9.2397	22.5042	-6.6788	-2.5609
-0.1	4.6473	-9.0592	23.001	-5.5756	-3.4836
0	4.725	-8.9942	23.169	-4.4971	-4.4971
0.1	4.6473	-9.0592	23.001	-3.4836	-5.5756
0.2	4.4215	-9.2397	22.5042	-2.5609	-6.6788
0.3	4.0688	-9.4931	21.6996	-1.7402	-7.7529
0.4	3.621	-9.7575	20.6205	-1.0215	-8.736
0.5	3.1162	-9.9615	19.3101	-0.3964	-9.5651
0.6	2.5941	-10.0367	17.8189	0.1479	-10.1846
0.7	2.091	-9.9285	16.2014	0.6257	-10.5542
0.8	1.6361	-9.6044	14.5129	1.05	-10.6544
0.9	1.2497	-9.0573	12.8065	1.4311	-10.4884
1	0.9422	-8.3038	11.1303	1.7762	-10.08
1.1	0.7151	-7.3795	9.5248	2.0893	-9.4688
1.2	0.5632	-6.3321	8.0217	2.3714	-8.7035
1.3	0.4762	-5.2143	6.643	2.6217	-7.836
1.4	0.4413	-4.0773	5.4013	2.8382	-6.9155
1.5	0.4449	-2.9668	4.3014	3.0185	-5.9853
1.6	0.4737	-1.92	3.3411	3.1603	-5.0803
1.7	0.5164	-0.9646	2.5139	3.2624	-4.227
1.8	0.5636	-0.1189	1.8096	3.3245	-3.4434
1.9	0.6081	0.6076	1.2165	3.3477	-2.7401
2	0.6451	1.2129	0.7224	3.3345	-2.1216
2.1	0.6719	1.7008	0.3149	3.2884	-1.5876
2.2	0.6874	2.0799	-0.0175	3.2141	-1.1342
2.3	0.6919	2.3611	-0.2855	3.1164	-0.7553
2.4	0.6863	2.5575	-0.4988	3.0008	-0.4433
2.5	0.6722	2.6824	-0.6658	2.8722	-0.1898
2.6	0.6516	2.7488	-0.7941	2.7354	0.0134
2.7	0.6261	2.7685	-0.8901	2.5945	0.174
2.8	0.5975	2.7521	-0.9596	2.4528	0.2993
2.9	0.5671	2.7084	-1.0072	2.3131	0.3953
3	0.536	2.6449	-1.0371	2.1773	0.4676
3.1	0.505	2.5677	-1.0527	2.047	0.5207
3.2	0.4749	2.4814	-1.0568	1.923	0.5584
3.3	0.4459	2.3895	-1.0518	1.8058	0.5837
3.4	0.4184	2.2948	-1.0397	1.6956	0.5992
3.5	0.3924	2.1994	-1.0222	1.5924	0.607
3.6	0.3681	2.1048	-1.0004	1.4961	0.6087
3.7	0.3454	2.0119	-0.9757	1.4063	0.6056
3.8	0.3242	1.9214	-0.9487	1.3226	0.5988
3.9	0.3046	1.8339	-0.9202	1.2448	0.5891
4	0.2863	1.7497	-0.8908	1.1724	0.5773
4.1	0.2693	1.6689	-0.861	1.1051	0.5638
4.2	0.2535	1.5916	-0.831	1.0424	0.5492
4.3	0.2389	1.5178	-0.8011	0.984	0.5338
4.4	0.2252	1.4474	-0.7717	0.9295	0.5179

4.5	0.2125	1.3804	-0.7428	0.8788	0.5016
4.6	0.2007	1.3168	-0.7146	0.8315	0.4853
4.7	0.1897	1.2562	-0.6872	0.7872	0.469
4.8	0.1794	1.1987	-0.6606	0.7459	0.4528
4.9	0.1698	1.1442	-0.6349	0.7073	0.4369
5	0.1608	1.0924	-0.6101	0.6711	0.4213

Cyclooctatetraene, $^1A_{1g}$ (D_{8h})

```
Charge =  0 Multiplicity = 1
 C,0,0.,1.8148192514,0.
 C,0,1.3087110246,1.3087110246,0.
 C,0,1.8148192514,0.,0.
 C,0,1.3087110246,-1.3087110246,0.
 C,0,0.,-1.8148192514,0.
 C,0,-1.3087110246,-1.3087110246,0.
 C,0,-1.8148192514,0.,0.
 C,0,-1.3087110246,1.3087110246,0.
 H,0,0.,2.9045842264,0.
 H,0,2.0749619171,2.0749619171,0.
 H,0,2.9045842264,0.,0.
 H,0,2.0749619171,-2.0749619171,0.
 H,0,0.,-2.9045842264,0.
 H,0,-2.0749619171,-2.0749619171,0.
 H,0,-2.9045842264,0.,0.
 H,0,-2.0749619171,2.0749619171,0.
```

Sum of electronic and zero-point Energies= -309.483327
Sum of electronic and thermal Energies= -309.476434
Sum of electronic and thermal Enthalpies= -309.475489
Sum of electronic and thermal Free Energies= -309.512769

NICS-scan

Distance(Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-5.9183	0.8808	-18.6357	0.4404	0.4404
-4.9	-6.2579	0.9212	-19.695	0.4606	0.4606
-4.8	-6.6231	0.9638	-20.833	0.4819	0.4819
-4.7	-7.0161	1.0086	-22.0568	0.5043	0.5043
-4.6	-7.4395	1.0558	-23.3743	0.5279	0.5279
-4.5	-7.8961	1.1056	-24.794	0.5528	0.5528
-4.4	-8.3891	1.158	-26.3255	0.579	0.579
-4.3	-8.922	1.2132	-27.9792	0.6066	0.6066
-4.2	-9.4984	1.2714	-29.7667	0.6357	0.6357
-4.1	-10.1228	1.3326	-31.7009	0.6663	0.6663
-4	-10.7997	1.3966	-33.7959	0.6983	0.6983
-3.9	-11.5344	1.464	-36.0672	0.732	0.732
-3.8	-12.3325	1.5344	-38.532	0.7672	0.7672
-3.7	-13.2004	1.608	-41.2093	0.804	0.804
-3.6	-14.145	1.6848	-44.1198	0.8424	0.8424
-3.5	-15.174	1.7644	-47.2864	0.8822	0.8822
-3.4	-16.2957	1.847	-50.734	0.9235	0.9235
-3.3	-17.5193	1.932	-54.49	0.966	0.966
-3.2	-18.8549	2.0192	-58.5837	1.0096	1.0096
-3.1	-20.3131	2.1078	-63.047	1.0539	1.0539
-3	-21.9056	2.1972	-67.9141	1.0986	1.0986
-2.9	-23.6448	2.2866	-73.221	1.1433	1.1433

-2.8	-25.5437	2.3746	-79.0056	1.1873	1.1873
-2.7	-27.6157	2.4598	-85.307	1.2299	1.2299
-2.6	-29.8747	2.5402	-92.1643	1.2701	1.2701
-2.5	-32.3342	2.6136	-99.6163	1.3068	1.3068
-2.4	-35.0073	2.6772	-107.699	1.3386	1.3386
-2.3	-37.9058	2.7278	-116.445	1.3639	1.3639
-2.2	-41.0394	2.7614	-125.88	1.3807	1.3807
-2.1	-44.4146	2.7738	-136.018	1.3869	1.3869
-2	-48.0338	2.7604	-146.862	1.3802	1.3802
-1.9	-51.8933	2.716	-158.396	1.358	1.358
-1.8	-55.9821	2.6358	-170.582	1.3179	1.3179
-1.7	-60.28	2.5152	-183.355	1.2576	1.2576
-1.6	-64.7555	2.3498	-196.617	1.1749	1.1749
-1.5	-69.3648	2.137	-210.232	1.0685	1.0685
-1.4	-74.0502	1.8756	-224.026	0.9378	0.9378
-1.3	-78.7401	1.5664	-237.787	0.7832	0.7832
-1.2	-83.3502	1.2126	-251.263	0.6063	0.6063
-1.1	-87.7864	0.8206	-264.18	0.4103	0.4103
-1	-91.9502	0.3992	-276.25	0.1996	0.1996
-0.9	-95.7458	-0.0398	-287.198	-0.0199	-0.0199
-0.8	-99.0899	-0.483	-296.787	-0.2415	-0.2415
-0.7	-101.922	-0.9158	-304.849	-0.4579	-0.4579
-0.6	-104.212	-1.3226	-311.312	-0.6613	-0.6613
-0.5	-105.967	-1.6898	-316.212	-0.8449	-0.8449
-0.4	-107.233	-2.005	-319.693	-1.0025	-1.0025
-0.3	-108.081	-2.2586	-321.983	-1.1293	-1.1293
-0.2	-108.599	-2.4438	-323.352	-1.2219	-1.2219
-0.1	-108.869	-2.5566	-324.052	-1.2783	-1.2783
0	-108.953	-2.5944	-324.263	-1.2972	-1.2972
0.1	-108.869	-2.5566	-324.052	-1.2783	-1.2783
0.2	-108.599	-2.4438	-323.352	-1.2219	-1.2219
0.3	-108.081	-2.2586	-321.983	-1.1293	-1.1293
0.4	-107.233	-2.005	-319.693	-1.0025	-1.0025
0.5	-105.967	-1.6898	-316.212	-0.8449	-0.8449
0.6	-104.212	-1.3226	-311.312	-0.6613	-0.6613
0.7	-101.922	-0.9158	-304.849	-0.4579	-0.4579
0.8	-99.0899	-0.483	-296.787	-0.2415	-0.2415
0.9	-95.7458	-0.0398	-287.198	-0.0199	-0.0199
1	-91.9502	0.3992	-276.25	0.1996	0.1996
1.1	-87.7864	0.8206	-264.18	0.4103	0.4103
1.2	-83.3502	1.2126	-251.263	0.6063	0.6063
1.3	-78.7401	1.5664	-237.787	0.7832	0.7832
1.4	-74.0502	1.8756	-224.026	0.9378	0.9378
1.5	-69.3648	2.137	-210.232	1.0685	1.0685
1.6	-64.7555	2.3498	-196.617	1.1749	1.1749
1.7	-60.28	2.5152	-183.355	1.2576	1.2576
1.8	-55.9821	2.6358	-170.582	1.3179	1.3179
1.9	-51.8933	2.716	-158.396	1.358	1.358
2	-48.0338	2.7604	-146.862	1.3802	1.3802

2.1	-44.4146	2.7738	-136.018	1.3869	1.3869
2.2	-41.0394	2.7614	-125.88	1.3807	1.3807
2.3	-37.9058	2.7278	-116.445	1.3639	1.3639
2.4	-35.0073	2.6772	-107.699	1.3386	1.3386
2.5	-32.3342	2.6136	-99.6163	1.3068	1.3068
2.6	-29.8747	2.5402	-92.1643	1.2701	1.2701
2.7	-27.6157	2.4598	-85.307	1.2299	1.2299
2.8	-25.5437	2.3746	-79.0056	1.1873	1.1873
2.9	-23.6448	2.2866	-73.221	1.1433	1.1433
3	-21.9056	2.1972	-67.9141	1.0986	1.0986
3.1	-20.3131	2.1078	-63.047	1.0539	1.0539
3.2	-18.8549	2.0192	-58.5837	1.0096	1.0096
3.3	-17.5193	1.932	-54.49	0.966	0.966
3.4	-16.2957	1.847	-50.734	0.9235	0.9235
3.5	-15.174	1.7644	-47.2864	0.8822	0.8822
3.6	-14.145	1.6848	-44.1198	0.8424	0.8424
3.7	-13.2004	1.608	-41.2093	0.804	0.804
3.8	-12.3325	1.5344	-38.532	0.7672	0.7672
3.9	-11.5344	1.464	-36.0672	0.732	0.732
4	-10.7997	1.3966	-33.7959	0.6983	0.6983
4.1	-10.1228	1.3326	-31.7009	0.6663	0.6663
4.2	-9.4984	1.2714	-29.7667	0.6357	0.6357
4.3	-8.922	1.2132	-27.9792	0.6066	0.6066
4.4	-8.3891	1.158	-26.3255	0.579	0.579
4.5	-7.8961	1.1056	-24.794	0.5528	0.5528
4.6	-7.4395	1.0558	-23.3743	0.5279	0.5279
4.7	-7.0161	1.0086	-22.0568	0.5043	0.5043
4.8	-6.6231	0.9638	-20.833	0.4819	0.4819
4.9	-6.2579	0.9212	-19.695	0.4606	0.4606
5	-5.9183	0.8808	-18.6357	0.4404	0.4404

Cyclooctatetraene, $^3A_{1g}$ (D_{8h})

```
Charge =  0 Multiplicity = 3
 C,0,0.,1.8335,0.
 C,0,1.2965,1.2965,0.
 C,0,1.8335,0.,0.
 C,0,1.2965,-1.2965,0.
 C,0,0.,-1.8335,0.
 C,0,-1.2965,-1.2965,0.
 C,0,-1.8335,0.,0.
 C,0,-1.2965,1.2965,0.
 H,0,0.,2.9203,0.
 H,0,2.065,2.065,0.
 H,0,2.9203,0.,0.
 H,0,2.065,-2.065,0.
 H,0,0.,-2.9203,0.
 H,0,-2.065,-2.065,0.
 H,0,-2.9203,0.,0.
 H,0,-2.065,2.065,0.
```

Sum of electronic and zero-point Energies= -309.512074
Sum of electronic and thermal Energies= -309.505391
Sum of electronic and thermal Enthalpies= -309.504447
Sum of electronic and thermal Free Energies= -309.541888

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.8886	0.9018	-3.5676	0.4509	0.4509
-4.9	-0.9379	0.9426	-3.7563	0.4713	0.4713
-4.8	-0.9908	0.9854	-3.9577	0.4927	0.4927
-4.7	-1.0475	1.0306	-4.173	0.5153	0.5153
-4.6	-1.1084	1.078	-4.4032	0.539	0.539
-4.5	-1.1739	1.1278	-4.6495	0.5639	0.5639
-4.4	-1.2443	1.1804	-4.9133	0.5902	0.5902
-4.3	-1.3202	1.2354	-5.196	0.6177	0.6177
-4.2	-1.402	1.2932	-5.4992	0.6466	0.6466
-4.1	-1.4902	1.3538	-5.8244	0.6769	0.6769
-4	-1.5855	1.4172	-6.1736	0.7086	0.7086
-3.9	-1.6884	1.4834	-6.5487	0.7417	0.7417
-3.8	-1.7997	1.5524	-6.9517	0.7762	0.7762
-3.7	-1.9202	1.6242	-7.3849	0.8121	0.8121
-3.6	-2.0507	1.6986	-7.8508	0.8493	0.8493
-3.5	-2.1922	1.7752	-8.3518	0.8876	0.8876
-3.4	-2.3455	1.8542	-8.8906	0.9271	0.9271
-3.3	-2.5118	1.9346	-9.4701	0.9673	0.9673
-3.2	-2.6923	2.0164	-10.0932	1.0082	1.0082
-3.1	-2.8881	2.0984	-10.7627	1.0492	1.0492
-3	-3.1005	2.18	-11.4816	1.09	1.09
-2.9	-3.3309	2.26	-12.2527	1.13	1.13
-2.8	-3.5805	2.337	-13.0786	1.1685	1.1685
-2.7	-3.8509	2.409	-13.9617	1.2045	1.2045
-2.6	-4.1432	2.474	-14.9036	1.237	1.237
-2.5	-4.4587	2.5292	-15.9054	1.2646	1.2646
-2.4	-4.7985	2.5716	-16.967	1.2858	1.2858
-2.3	-5.1631	2.5978	-18.0871	1.2989	1.2989
-2.2	-5.5531	2.6032	-19.2623	1.3016	1.3016
-2.1	-5.968	2.5832	-20.4874	1.2916	1.2916
-2	-6.407	2.533	-21.7541	1.2665	1.2665
-1.9	-6.868	2.4472	-23.0511	1.2236	1.2236
-1.8	-7.3476	2.3206	-24.3634	1.1603	1.1603
-1.7	-7.8411	2.1484	-25.6718	1.0742	1.0742
-1.6	-8.3421	1.9266	-26.9528	0.9633	0.9633
-1.5	-8.8422	1.6522	-28.1788	0.8261	0.8261
-1.4	-9.3313	1.3244	-29.3184	0.6622	0.6622
-1.3	-9.7977	0.9446	-30.3375	0.4723	0.4723
-1.2	-10.2283	0.5168	-31.2016	0.2584	0.2584
-1.1	-10.6099	0.048	-31.8778	0.024	0.024
-1	-10.9302	-0.4516	-32.3391	-0.2258	-0.2258
-0.9	-11.1791	-0.9694	-32.5679	-0.4847	-0.4847
-0.8	-11.3503	-1.49	-32.5608	-0.745	-0.745
-0.7	-11.4432	-1.9974	-32.3321	-0.9987	-0.9987
-0.6	-11.4636	-2.4746	-31.9163	-1.2373	-1.2373
-0.5	-11.4245	-2.9058	-31.3677	-1.4529	-1.4529
-0.4	-11.3447	-3.2768	-30.7573	-1.6384	-1.6384

-0.3	-11.2472	-3.5762	-30.1653	-1.7881	-1.7881
-0.2	-11.1558	-3.7958	-29.6717	-1.8979	-1.8979
-0.1	-11.0914	-3.9294	-29.3447	-1.9647	-1.9647
0	-11.0682	-3.9744	-29.2303	-1.9872	-1.9872
0.1	-11.0914	-3.9294	-29.3447	-1.9647	-1.9647
0.2	-11.1558	-3.7958	-29.6717	-1.8979	-1.8979
0.3	-11.2472	-3.5762	-30.1653	-1.7881	-1.7881
0.4	-11.3447	-3.2768	-30.7573	-1.6384	-1.6384
0.5	-11.4245	-2.9058	-31.3677	-1.4529	-1.4529
0.6	-11.4636	-2.4746	-31.9163	-1.2373	-1.2373
0.7	-11.4432	-1.9974	-32.3321	-0.9987	-0.9987
0.8	-11.3503	-1.49	-32.5608	-0.745	-0.745
0.9	-11.1791	-0.9694	-32.5679	-0.4847	-0.4847
1	-10.9302	-0.4516	-32.3391	-0.2258	-0.2258
1.1	-10.6099	0.048	-31.8778	0.024	0.024
1.2	-10.2283	0.5168	-31.2016	0.2584	0.2584
1.3	-9.7977	0.9446	-30.3375	0.4723	0.4723
1.4	-9.3313	1.3244	-29.3184	0.6622	0.6622
1.5	-8.8422	1.6522	-28.1788	0.8261	0.8261
1.6	-8.3421	1.9266	-26.9528	0.9633	0.9633
1.7	-7.8411	2.1484	-25.6718	1.0742	1.0742
1.8	-7.3476	2.3206	-24.3634	1.1603	1.1603
1.9	-6.868	2.4472	-23.0511	1.2236	1.2236
2	-6.407	2.533	-21.7541	1.2665	1.2665
2.1	-5.968	2.5832	-20.4874	1.2916	1.2916
2.2	-5.5531	2.6032	-19.2623	1.3016	1.3016
2.3	-5.1631	2.5978	-18.0871	1.2989	1.2989
2.4	-4.7985	2.5716	-16.967	1.2858	1.2858
2.5	-4.4587	2.5292	-15.9054	1.2646	1.2646
2.6	-4.1432	2.474	-14.9036	1.237	1.237
2.7	-3.8509	2.409	-13.9617	1.2045	1.2045
2.8	-3.5805	2.337	-13.0786	1.1685	1.1685
2.9	-3.3309	2.26	-12.2527	1.13	1.13
3	-3.1005	2.18	-11.4816	1.09	1.09
3.1	-2.8881	2.0984	-10.7627	1.0492	1.0492
3.2	-2.6923	2.0164	-10.0932	1.0082	1.0082
3.3	-2.5118	1.9346	-9.4701	0.9673	0.9673
3.4	-2.3455	1.8542	-8.8906	0.9271	0.9271
3.5	-2.1922	1.7752	-8.3518	0.8876	0.8876
3.6	-2.0507	1.6986	-7.8508	0.8493	0.8493
3.7	-1.9202	1.6242	-7.3849	0.8121	0.8121
3.8	-1.7997	1.5524	-6.9517	0.7762	0.7762
3.9	-1.6884	1.4834	-6.5487	0.7417	0.7417
4	-1.5855	1.4172	-6.1736	0.7086	0.7086
4.1	-1.4902	1.3538	-5.8244	0.6769	0.6769
4.2	-1.402	1.2932	-5.4992	0.6466	0.6466
4.3	-1.3202	1.2354	-5.196	0.6177	0.6177
4.4	-1.2443	1.1804	-4.9133	0.5902	0.5902
4.5	-1.1739	1.1278	-4.6495	0.5639	0.5639

4.6	-1.1084	1.078	-4.4032	0.539	0.539
4.7	-1.0475	1.0306	-4.173	0.5153	0.5153
4.8	-0.9908	0.9854	-3.9577	0.4927	0.4927
4.9	-0.9379	0.9426	-3.7563	0.4713	0.4713
5	-0.8886	0.9018	-3.5676	0.4509	0.4509

[*c*-C_4H_8] (D_{2d}), 20

```
Charge =  0 Multiplicity = 1
 C,0,-0.7673908458,0.7673908458,0.1231789953
 C,0,-0.7673908458,-0.7673908458,-0.1231789953
 C,0,0.7673908458,-0.7673908458,0.1231789953
 C,0,0.7673908458,0.7673908458,-0.1231789953
 H,0,-1.0079769888,1.0079769888,1.1620062945
 H,0,-1.3868180384,1.3868180384,-0.5288770589
 H,0,-1.0079769888,-1.0079769888,-1.1620062945
 H,0,-1.3868180384,-1.3868180384,0.5288770589
 H,0,1.3868180384,-1.3868180384,-0.5288770589
 H,0,1.0079769888,-1.0079769888,1.1620062945
 H,0,1.3868180384,1.3868180384,0.5288770589
 H,0,1.0079769888,1.0079769888,-1.1620062945
```

Sum of electronic and zero-point Energies= -157.146945
Sum of electronic and thermal Energies= -157.142796
Sum of electronic and thermal Enthalpies= -157.141852
Sum of electronic and thermal Free Energies= -157.171785

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.1089	1.1094	-0.7826	0.5462	0.5632
-4.9	0.1148	1.1698	-0.8254	0.5745	0.5953
-4.8	0.1211	1.2346	-0.8713	0.6047	0.6299
-4.7	0.1278	1.3038	-0.9204	0.6367	0.6671
-4.6	0.135	1.3779	-0.973	0.6707	0.7072
-4.5	0.1426	1.4572	-1.0294	0.7068	0.7504
-4.4	0.1508	1.5424	-1.0898	0.7452	0.7972
-4.3	0.1596	1.6337	-1.1547	0.7859	0.8478
-4.2	0.169	1.7314	-1.2244	0.8289	0.9025
-4.1	0.179	1.8363	-1.2992	0.8745	0.9618
-4	0.1897	1.9487	-1.3795	0.9225	1.0262
-3.9	0.2011	2.0691	-1.4658	0.9731	1.096
-3.8	0.2132	2.1979	-1.5584	1.026	1.1719
-3.7	0.226	2.3357	-1.6578	1.0814	1.2543
-3.6	0.2394	2.4826	-1.7643	1.1387	1.3439
-3.5	0.2535	2.639	-1.8785	1.1978	1.4412
-3.4	0.2681	2.8049	-2.0007	1.2581	1.5468
-3.3	0.2831	2.9804	-2.1311	1.3188	1.6616
-3.2	0.2983	3.1648	-2.2699	1.3789	1.7859
-3.1	0.3134	3.3575	-2.4173	1.4369	1.9206
-3	0.328	3.557	-2.5731	1.491	2.066
-2.9	0.3415	3.7614	-2.7368	1.5387	2.2227
-2.8	0.3533	3.9676	-2.9076	1.5767	2.3909
-2.7	0.3624	4.1715	-3.0842	1.6009	2.5706
-2.6	0.3677	4.3679	-3.2648	1.6062	2.7617
-2.5	0.3677	4.5498	-3.4466	1.5863	2.9635
-2.4	0.3609	4.7086	-3.6258	1.5336	3.175
-2.3	0.3454	4.8339	-3.7976	1.439	3.3949
-2.2	0.3194	4.9135	-3.9555	1.2923	3.6212

-2.1	0.281	4.9339	-4.0907	1.082	3.8519
-2	0.2291	4.8797	-4.1924	0.7955	4.0842
-1.9	0.1629	4.7347	-4.2461	0.4196	4.3151
-1.8	0.0826	4.4808	-4.233	-0.0597	4.5405
-1.7	-0.0103	4.0977	-4.1285	-0.6571	4.7548
-1.6	-0.1129	3.5612	-3.9	-1.3882	4.9494
-1.5	-0.2213	2.8403	-3.5043	-2.2703	5.1106
-1.4	-0.3299	1.8942	-2.8838	-3.3233	5.2175
-1.3	-0.4321	0.6664	-1.9628	-4.5713	5.2377
-1.2	-0.521	-0.9187	-0.6442	-6.0431	5.1244
-1.1	-0.5893	-2.961	1.193	-7.7723	4.8113
-1	-0.6314	-5.5836	3.6893	-9.7937	4.2101
-0.9	-0.6436	-8.9243	6.9935	-12.1346	3.2103
-0.8	-0.6258	-13.1148	11.2375	-14.8005	1.6857
-0.7	-0.5817	-18.2405	16.4953	-17.7528	-0.4877
-0.6	-0.519	-24.2846	22.7275	-20.8842	-3.4004
-0.5	-0.4477	-31.0631	29.7201	-23.9971	-7.066
-0.4	-0.378	-38.1725	37.0385	-26.7978	-11.3747
-0.3	-0.3186	-44.9821	44.0264	-28.9201	-16.062
-0.2	-0.2747	-50.7025	49.8783	-29.9866	-20.7159
-0.1	-0.2485	-54.5382	53.7928	-29.7012	-24.837
0	-0.2398	-55.8912	55.1717	-27.9456	-27.9456
0.1	-0.2485	-54.5382	53.7928	-24.837	-29.7012
0.2	-0.2747	-50.7025	49.8783	-20.7159	-29.9866
0.3	-0.3186	-44.9821	44.0264	-16.062	-28.9201
0.4	-0.378	-38.1725	37.0385	-11.3747	-26.7978
0.5	-0.4477	-31.0631	29.7201	-7.066	-23.9971
0.6	-0.519	-24.2846	22.7275	-3.4004	-20.8842
0.7	-0.5817	-18.2405	16.4953	-0.4877	-17.7528
0.8	-0.6258	-13.1148	11.2375	1.6857	-14.8005
0.9	-0.6436	-8.9243	6.9935	3.2103	-12.1346
1	-0.6314	-5.5836	3.6893	4.2101	-9.7937
1.1	-0.5893	-2.961	1.193	4.8113	-7.7723
1.2	-0.521	-0.9187	-0.6442	5.1244	-6.0431
1.3	-0.4321	0.6664	-1.9628	5.2377	-4.5713
1.4	-0.3299	1.8942	-2.8838	5.2175	-3.3233
1.5	-0.2213	2.8403	-3.5043	5.1106	-2.2703
1.6	-0.1129	3.5612	-3.9	4.9494	-1.3882
1.7	-0.0103	4.0977	-4.1285	4.7548	-0.6571
1.8	0.0826	4.4808	-4.233	4.5405	-0.0597
1.9	0.1629	4.7347	-4.2461	4.3151	0.4196
2	0.2291	4.8797	-4.1924	4.0842	0.7955
2.1	0.281	4.9339	-4.0907	3.8519	1.082
2.2	0.3194	4.9135	-3.9555	3.6212	1.2923
2.3	0.3454	4.8339	-3.7976	3.3949	1.439
2.4	0.3609	4.7086	-3.6258	3.175	1.5336
2.5	0.3677	4.5498	-3.4466	2.9635	1.5863
2.6	0.3677	4.3679	-3.2648	2.7617	1.6062
2.7	0.3624	4.1715	-3.0842	2.5706	1.6009
2.8	0.3533	3.9676	-2.9076	2.3909	1.5767
2.9	0.3415	3.7614	-2.7368	2.2227	1.5387
3	0.328	3.557	-2.5731	2.066	1.491
3.1	0.3134	3.3575	-2.4173	1.9206	1.4369
3.2	0.2983	3.1648	-2.2699	1.7859	1.3789
3.3	0.2831	2.9804	-2.1311	1.6616	1.3188
3.4	0.2681	2.8049	-2.0007	1.5468	1.2581
3.5	0.2535	2.639	-1.8785	1.4412	1.1978
3.6	0.2394	2.4826	-1.7643	1.3439	1.1387

3.7	0.226	2.3357	-1.6578	1.2543	1.0814
3.8	0.2132	2.1979	-1.5584	1.1719	1.026
3.9	0.2011	2.0691	-1.4658	1.096	0.9731
4	0.1897	1.9487	-1.3795	1.0262	0.9225
4.1	0.179	1.8363	-1.2992	0.9618	0.8745
4.2	0.169	1.7314	-1.2244	0.9025	0.8289
4.3	0.1596	1.6337	-1.1547	0.8478	0.7859
4.4	0.1508	1.5424	-1.0898	0.7972	0.7452
4.5	0.1426	1.4572	-1.0294	0.7504	0.7068
4.6	0.135	1.3779	-0.973	0.7072	0.6707
4.7	0.1278	1.3038	-0.9204	0.6671	0.6367
4.8	0.1211	1.2346	-0.8713	0.6299	0.6047
4.9	0.1148	1.1698	-0.8254	0.5953	0.5745
5	0.1089	1.1094	-0.7826	0.5632	0.5462

[2.2.0]bicyclohexane (C_2), 21

```
Charge =  0 Multiplicity = 1
 C,0,-0.2006875012,1.7879938007,-0.5568329365
 C,0,-1.4285877291,0.8327326916,-0.6796149879
 C,0,-1.1097367635,0.2288477565,0.717845345
 C,0,0.1833977739,1.1256394308,0.7895065956
 C,0,-0.2270017316,-1.0436763593,0.6981279679
 C,0,1.0564857775,-0.156079012,0.6691403173
 H,0,-0.3794259849,-1.7150141986,-0.1516775736
 H,0,1.6491908686,-0.2136880496,-0.247961402
 H,0,-0.4935592382,2.8348059141,-0.4477374375
 H,0,0.5512925138,1.7260861831,-1.3486814613
 H,0,-1.386598214,0.1134896549,-1.5023154608
 H,0,-2.3874818459,1.3520240832,-0.7347407589
 H,0,-1.9097665322,0.2712964444,1.458248047
 H,0,0.4073703657,1.787757723,1.6270443926
 H,0,-0.3086194394,-1.6321173415,1.6148925146
 H,0,1.7269276804,-0.3223987215,1.5146568384
```

Sum of electronic and zero-point Energies= -234.515166
Sum of electronic and thermal Energies= -234.509657
Sum of electronic and thermal Enthalpies= -234.508713
Sum of electronic and thermal Free Energies= -234.544577

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.1199	1.8227	-1.4632	0.8272	0.9955
-4.9	0.1285	1.9202	-1.5348	0.8723	1.0479
-4.8	0.1379	2.0228	-1.6093	0.92	1.1028
-4.7	0.1481	2.1308	-1.6864	0.9705	1.1603
-4.6	0.1594	2.2438	-1.7658	1.0237	1.2201
-4.5	0.1716	2.3617	-1.8469	1.0797	1.282
-4.4	0.185	2.4841	-1.929	1.1384	1.3457
-4.3	0.1996	2.6101	-2.0113	1.1997	1.4104
-4.2	0.2155	2.7388	-2.0924	1.2634	1.4754
-4.1	0.2327	2.8687	-2.1708	1.3291	1.5396
-4	0.2512	2.9978	-2.2443	1.3962	1.6016
-3.9	0.2709	3.1232	-2.3105	1.4637	1.6595
-3.8	0.2917	3.2415	-2.3663	1.5305	1.711
-3.7	0.3134	3.348	-2.4079	1.5948	1.7532
-3.6	0.3354	3.4369	-2.4309	1.6542	1.7827
-3.5	0.3571	3.5014	-2.4302	1.7058	1.7956

-3.4	0.3777	3.5332	-2.4	1.7457	1.7875
-3.3	0.3963	3.5234	-2.3344	1.7692	1.7542
-3.2	0.4118	3.4621	-2.2267	1.7706	1.6915
-3.1	0.423	3.3398	-2.0709	1.7435	1.5963
-3	0.4288	3.148	-1.8615	1.6807	1.4673
-2.9	0.4287	2.8804	-1.5944	1.5749	1.3055
-2.8	0.4221	2.534	-1.2679	1.4187	1.1153
-2.7	0.4093	2.1113	-0.8834	1.2059	0.9054
-2.6	0.3915	1.621	-0.4465	0.9323	0.6887
-2.5	0.3707	1.0794	0.0328	0.5973	0.4821
-2.4	0.3501	0.5108	0.5395	0.2051	0.3057
-2.3	0.3341	-0.0525	1.0547	-0.2333	0.1808
-2.2	0.3284	-0.5718	1.557	-0.6989	0.1271
-2.1	0.34	-1.0042	2.0243	-1.1641	0.1599
-2	0.3769	-1.3064	2.4371	-1.5933	0.2869
-1.9	0.4472	-1.4398	2.7813	-1.9454	0.5056
-1.8	0.5584	-1.3768	3.0521	-2.1781	0.8013
-1.7	0.7164	-1.1083	3.2576	-2.2543	1.146
-1.6	0.9235	-0.6521	3.4225	-2.1499	1.4978
-1.5	1.177	-0.0607	3.5918	-1.8622	1.8015
-1.4	1.4688	0.5723	3.834	-1.4166	1.9889
-1.3	1.7843	1.1088	4.2442	-0.8717	1.9805
-1.2	2.1043	1.3671	4.9458	-0.3204	1.6875
-1.1	2.4062	1.1279	6.0906	0.1129	1.015
-1	2.6676	0.1499	7.8527	0.2807	-0.1308
-0.9	2.8699	-1.8068	10.4166	0.0257	-1.8325
-0.8	3.0021	-4.9446	13.9508	-0.8	-4.1446
-0.7	3.0631	-9.3785	18.5679	-2.3077	-7.0708
-0.6	3.0634	-15.0776	24.2679	-4.5406	-10.537
-0.5	3.0223	-21.8079	30.8747	-7.4412	-14.3667
-0.4	2.9626	-29.0961	37.984	-10.8265	-18.2696
-0.3	2.9029	-36.243	44.9518	-14.3853	-21.8577
-0.2	2.8497	-42.4088	50.9578	-17.7098	-24.699
-0.1	2.7943	-46.77	55.1528	-20.3659	-26.4041
0	2.7164	-48.7145	56.8638	-21.989	-26.7255
0.1	2.5934	-48.0031	55.7834	-22.3743	-25.6288
0.2	2.4102	-44.829	52.0596	-21.5246	-23.3044
0.3	2.166	-39.7479	46.2458	-19.6366	-20.1113
0.4	1.8739	-33.513	39.1347	-17.034	-16.479
0.5	1.556	-26.8869	31.555	-14.0785	-12.8084
0.6	1.2371	-20.4961	24.2073	-11.0926	-9.4035
0.7	0.9392	-14.76	17.5777	-8.3131	-6.4469
0.8	0.679	-9.8908	11.9278	-5.8802	-4.0106
0.9	0.4661	-5.9349	7.3334	-3.8497	-2.0852
1	0.304	-2.8306	3.7426	-2.2169	-0.6137
1.1	0.1904	-0.4608	1.0321	-0.942	0.4812
1.2	0.1194	1.3073	-0.9491	0.0298	1.2775
1.3	0.0826	2.599	-2.3511	0.755	1.844
1.4	0.0712	3.5208	-3.3073	1.2845	2.2363

1.5	0.0766	4.1582	-3.9285	1.6607	2.4975
1.6	0.0918	4.5776	-4.3023	1.9179	2.6597
1.7	0.1111	4.8296	-4.4964	2.0828	2.7468
1.8	0.1306	4.9532	-4.5616	2.1766	2.7766
1.9	0.1477	4.9787	-4.5356	2.2158	2.7629
2	0.1612	4.9298	-4.4464	2.2136	2.7162
2.1	0.1705	4.8258	-4.3144	2.1806	2.6452
2.2	0.1758	4.6821	-4.1547	2.1252	2.5569
2.3	0.1776	4.5111	-3.9782	2.0543	2.4568
2.4	0.1767	4.3229	-3.7928	1.9733	2.3496
2.5	0.1735	4.125	-3.6044	1.8863	2.2387
2.6	0.1689	3.9237	-3.4171	1.7966	2.1271
2.7	0.1632	3.7232	-3.2335	1.7065	2.0167
2.8	0.157	3.5267	-3.0558	1.6178	1.9089
2.9	0.1504	3.3364	-2.8851	1.5315	1.8049
3	0.1438	3.1537	-2.7223	1.4484	1.7053
3.1	0.1372	2.9794	-2.5677	1.369	1.6104
3.2	0.1308	2.8138	-2.4215	1.2935	1.5203
3.3	0.1245	2.6571	-2.2836	1.2219	1.4352
3.4	0.1185	2.5094	-2.1539	1.1544	1.355
3.5	0.1127	2.3702	-2.032	1.0907	1.2795
3.6	0.1072	2.2393	-1.9176	1.0308	1.2085
3.7	0.102	2.1163	-1.8104	0.9745	1.1418
3.8	0.0969	2.0009	-1.71	0.9216	1.0793
3.9	0.0922	1.8925	-1.616	0.8719	1.0206
4	0.0876	1.7909	-1.528	0.8253	0.9656
4.1	0.0833	1.6957	-1.4456	0.7816	0.9141
4.2	0.0793	1.6063	-1.3685	0.7406	0.8657
4.3	0.0754	1.5225	-1.2963	0.7021	0.8204
4.4	0.0717	1.444	-1.2287	0.666	0.778
4.5	0.0683	1.3702	-1.1654	0.6321	0.7381
4.6	0.065	1.3012	-1.1061	0.6004	0.7008
4.7	0.0619	1.2362	-1.0505	0.5705	0.6657
4.8	0.059	1.1753	-0.9984	0.5425	0.6328
4.9	0.0562	1.118	-0.9494	0.5161	0.6019
5	0.0536	1.0642	-0.9035	0.4914	0.5728

[3]ladderane (C_{2h}), 22

```
Charge =  0 Multiplicity = 1
 C,0,-1.6207201922,0.8223211727,-0.5624778211
 C,0,-1.4807302521,-0.7270744597,-0.701833773
 C,0,-0.7649603183,-0.7914809023,0.6826027893
 C,0,-0.7982023649,0.7745164707,0.7500701128
 C,0,0.7982023649,-0.7745164707,0.7500701128
 C,0,0.7649603183,0.7914809023,0.6826027893
 C,0,1.6207201922,-0.8223211727,-0.5624778211
 C,0,1.4807302521,0.7270744597,-0.701833773
 H,0,-2.6527722257,1.1349741075,-0.3880264558
 H,0,-1.2209768327,1.4303017484,-1.37725966
 H,0,-0.8886034162,-1.0671050231,-1.5537162504
 H,0,-2.4336535639,-1.2592350284,-0.7270501736
 H,0,-1.2548310628,-1.4131765588,1.4336396459
 H,0,-1.2097348228,1.3073305216,1.6092075859
 H,0,1.2097348228,-1.3073305216,1.6092075859
```

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H,0,1.2548310628,1.4131765588,1.4336396459
H,0,1.2209768327,-1.4303017484,-1.37725966
H,0,2.6527722257,-1.1349741075,-0.3880264558
H,0,2.4336535639,1.2592350284,-0.7270501736
H,0,0.8886034162,1.0671050231,-1.5537162504
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Sum of electronic and zero-point Energies= -311.887278
Sum of electronic and thermal Energies= -311.880517
Sum of electronic and thermal Enthalpies= -311.879573
Sum of electronic and thermal Free Energies= -311.918401

NICS-scan(central ring)

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.0455	1.8336	-1.6971	0.7882	1.0454
-4.9	0.0499	1.9292	-1.7793	0.8304	1.0988
-4.8	0.0549	2.0296	-1.865	0.8749	1.1547
-4.7	0.0603	2.1349	-1.9539	0.9219	1.213
-4.6	0.0664	2.245	-2.0457	0.9715	1.2735
-4.5	0.0731	2.3594	-2.14	1.0234	1.336
-4.4	0.0806	2.4778	-2.2361	1.0778	1.4
-4.3	0.0888	2.5994	-2.333	1.1345	1.4649
-4.2	0.0978	2.723	-2.4296	1.1931	1.5299
-4.1	0.1077	2.8473	-2.5243	1.2534	1.5939
-4	0.1183	2.9701	-2.615	1.3146	1.6555
-3.9	0.1298	3.0887	-2.6994	1.3759	1.7128
-3.8	0.1418	3.1996	-2.7744	1.436	1.7636
-3.7	0.1541	3.2985	-2.8363	1.4933	1.8052
-3.6	0.1664	3.3798	-2.8807	1.5454	1.8344
-3.5	0.178	3.4368	-2.9027	1.5894	1.8474
-3.4	0.1884	3.4619	-2.8967	1.6215	1.8404
-3.3	0.1966	3.4465	-2.8567	1.6372	1.8093
-3.2	0.2016	3.3812	-2.7764	1.6307	1.7505
-3.1	0.2023	3.2567	-2.6498	1.5956	1.6611
-3	0.1976	3.0644	-2.4716	1.5245	1.5399
-2.9	0.1865	2.7972	-2.2376	1.4093	1.3879
-2.8	0.1683	2.4509	-1.946	1.2419	1.209
-2.7	0.1425	2.0252	-1.5978	1.0145	1.0107
-2.6	0.1091	1.5256	-1.1982	0.7212	0.8044
-2.5	0.0691	0.964	-0.7568	0.3589	0.6051
-2.4	0.024	0.36	-0.2879	-0.0705	0.4305
-2.3	-0.0232	-0.2588	0.1893	-0.5584	0.2996
-2.2	-0.0682	-0.8566	0.6522	-1.0871	0.2305
-2.1	-0.1051	-1.3917	1.0765	-1.6294	0.2377
-2	-0.1263	-1.8182	1.4392	-2.1478	0.3296
-1.9	-0.1232	-2.0916	1.7219	-2.5974	0.5058
-1.8	-0.0867	-2.1751	1.9152	-2.9302	0.7551
-1.7	-0.0084	-2.0483	2.0231	-3.1024	1.0541
-1.6	0.1171	-1.7159	2.0673	-3.0827	1.3668
-1.5	0.2913	-1.218	2.092	-2.8623	1.6443
-1.4	0.51	-0.6366	2.1666	-2.462	1.8254
-1.3	0.7631	-0.1	2.3892	-1.9375	1.8375
-1.2	1.035	0.2182	2.8868	-1.3792	1.5974

-1.1	1.3068	0.106	3.8145	-0.9077	1.0137
-1	1.5583	-0.6731	5.3481	-0.6636	-0.0095
-0.9	1.771	-2.3567	7.6696	-0.7922	-1.5645
-0.8	1.9306	-5.1485	10.9402	-1.4223	-3.7262
-0.7	2.0296	-9.171	15.2597	-2.6405	-6.5305
-0.6	2.0687	-14.4054	20.6115	-4.4612	-9.9442
-0.5	2.057	-20.6326	26.8035	-6.7998	-13.8328
-0.4	2.0103	-27.3927	33.4236	-9.456	-17.9367
-0.3	1.948	-33.9942	39.8382	-12.1216	-21.8726
-0.2	1.8889	-39.5966	45.2631	-14.4208	-25.1758
-0.1	1.8475	-43.3716	48.9142	-15.9841	-27.3875
0	1.8328	-44.7057	50.204	-16.5388	-28.1669
0.1	1.8475	-43.3716	48.9142	-15.9841	-27.3875
0.2	1.8889	-39.5966	45.2631	-14.4208	-25.1758
0.3	1.948	-33.9942	39.8382	-12.1216	-21.8726
0.4	2.0103	-27.3927	33.4236	-9.456	-17.9367
0.5	2.057	-20.6326	26.8035	-6.7998	-13.8328
0.6	2.0687	-14.4054	20.6115	-4.4612	-9.9442
0.7	2.0296	-9.171	15.2597	-2.6405	-6.5305
0.8	1.9306	-5.1485	10.9402	-1.4223	-3.7262
0.9	1.771	-2.3567	7.6696	-0.7922	-1.5645
1	1.5583	-0.6731	5.3481	-0.6636	-0.0095
1.1	1.3068	0.106	3.8145	-0.9077	1.0137
1.2	1.035	0.2182	2.8868	-1.3792	1.5974
1.3	0.7631	-0.1	2.3892	-1.9375	1.8375
1.4	0.51	-0.6366	2.1666	-2.462	1.8254
1.5	0.2913	-1.218	2.092	-2.8623	1.6443
1.6	0.1171	-1.7159	2.0673	-3.0827	1.3668
1.7	-0.0084	-2.0483	2.0231	-3.1024	1.0541
1.8	-0.0867	-2.1751	1.9152	-2.9302	0.7551
1.9	-0.1232	-2.0916	1.7219	-2.5974	0.5058
2	-0.1263	-1.8182	1.4392	-2.1478	0.3296
2.1	-0.1051	-1.3917	1.0765	-1.6294	0.2377
2.2	-0.0682	-0.8566	0.6522	-1.0871	0.2305
2.3	-0.0232	-0.2588	0.1893	-0.5584	0.2996
2.4	0.024	0.36	-0.2879	-0.0705	0.4305
2.5	0.0691	0.964	-0.7568	0.3589	0.6051
2.6	0.1091	1.5256	-1.1982	0.7212	0.8044
2.7	0.1425	2.0252	-1.5978	1.0145	1.0107
2.8	0.1683	2.4509	-1.946	1.2419	1.209
2.9	0.1865	2.7972	-2.2376	1.4093	1.3879
3	0.1976	3.0644	-2.4716	1.5245	1.5399
3.1	0.2023	3.2567	-2.6498	1.5956	1.6611
3.2	0.2016	3.3812	-2.7764	1.6307	1.7505
3.3	0.1966	3.4465	-2.8567	1.6372	1.8093
3.4	0.1884	3.4619	-2.8967	1.6215	1.8404
3.5	0.178	3.4368	-2.9027	1.5894	1.8474
3.6	0.1664	3.3798	-2.8807	1.5454	1.8344
3.7	0.1541	3.2985	-2.8363	1.4933	1.8052

3.8	0.1418	3.1996	-2.7744	1.436	1.7636
3.9	0.1298	3.0887	-2.6994	1.3759	1.7128
4	0.1183	2.9701	-2.615	1.3146	1.6555
4.1	0.1077	2.8473	-2.5243	1.2534	1.5939
4.2	0.0978	2.723	-2.4296	1.1931	1.5299
4.3	0.0888	2.5994	-2.333	1.1345	1.4649
4.4	0.0806	2.4778	-2.2361	1.0778	1.4
4.5	0.0731	2.3594	-2.14	1.0234	1.336
4.6	0.0664	2.245	-2.0457	0.9715	1.2735
4.7	0.0603	2.1349	-1.9539	0.9219	1.213
4.8	0.0549	2.0296	-1.865	0.8749	1.1547
4.9	0.0499	1.9292	-1.7793	0.8304	1.0988
5	0.0455	1.8336	-1.6971	0.7882	1.0454

NICS-scan(terminal ring)

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.105	1.2104	-0.8954	0.537	0.6734
-4.9	0.1097	1.2682	-0.9392	0.5622	0.706
-4.8	0.1146	1.3296	-0.9857	0.5889	0.7407
-4.7	0.1199	1.3948	-1.0351	0.6173	0.7775
-4.6	0.1254	1.4641	-1.0877	0.6475	0.8166
-4.5	0.1313	1.5377	-1.1437	0.6795	0.8582
-4.4	0.1375	1.616	-1.2033	0.7135	0.9025
-4.3	0.1441	1.6992	-1.2668	0.7496	0.9496
-4.2	0.1511	1.7877	-1.3344	0.788	0.9997
-4.1	0.1585	1.8818	-1.4064	0.8288	1.053
-4	0.1663	1.982	-1.4831	0.8722	1.1098
-3.9	0.1745	2.0885	-1.5649	0.9183	1.1702
-3.8	0.1833	2.2018	-1.6519	0.9673	1.2345
-3.7	0.1926	2.3224	-1.7446	1.0194	1.303
-3.6	0.2024	2.4505	-1.8432	1.0747	1.3758
-3.5	0.2128	2.5866	-1.9481	1.1334	1.4532
-3.4	0.2239	2.731	-2.0594	1.1956	1.5354
-3.3	0.2356	2.884	-2.1774	1.2615	1.6225
-3.2	0.2479	3.046	-2.3022	1.3311	1.7149
-3.1	0.261	3.2168	-2.4339	1.4044	1.8124
-3	0.2747	3.3966	-2.5724	1.4813	1.9153
-2.9	0.2892	3.5848	-2.7172	1.5616	2.0232
-2.8	0.3043	3.7807	-2.8679	1.6448	2.1359
-2.7	0.3199	3.9831	-3.0234	1.7302	2.2529
-2.6	0.3359	4.1899	-3.1822	1.8167	2.3732
-2.5	0.3519	4.3979	-3.3421	1.9025	2.4954
-2.4	0.3677	4.6031	-3.4998	1.9854	2.6177
-2.3	0.3829	4.7995	-3.6509	2.0623	2.7372
-2.2	0.3968	4.9798	-3.7892	2.1291	2.8507
-2.1	0.4093	5.1341	-3.9063	2.1806	2.9535
-2	0.4199	5.2503	-3.9905	2.2102	3.0401
-1.9	0.4289	5.313	-4.0263	2.2095	3.1035
-1.8	0.437	5.3032	-3.9924	2.1682	3.135

-1.7	0.4457	5.1972	-3.86	2.0734	3.1238
-1.6	0.4579	4.9643	-3.5905	1.9084	3.0559
-1.5	0.4777	4.5652	-3.132	1.6522	2.913
-1.4	0.5107	3.9485	-2.4163	1.2775	2.671
-1.3	0.564	3.047	-1.3549	0.7496	2.2974
-1.2	0.6455	1.7734	0.1629	0.0246	1.7488
-1.1	0.7631	0.0195	2.2696	-0.9501	0.9696
-1	0.9234	-2.3426	5.1129	-2.2337	-0.1089
-0.9	1.1301	-5.4487	8.8389	-3.8845	-1.5642
-0.8	1.3816	-9.4188	13.5637	-5.9462	-3.4726
-0.7	1.6702	-14.318	19.3285	-8.4274	-5.8906
-0.6	1.9807	-20.1022	26.0445	-11.2751	-8.8271
-0.5	2.2917	-26.5603	33.4355	-14.3496	-12.2107
-0.4	2.577	-33.2712	41.0023	-17.4103	-15.8609
-0.3	2.8102	-39.6052	48.0359	-20.1274	-19.4778
-0.2	2.9708	-44.7945	53.7071	-22.128	-22.6665
-0.1	3.0509	-48.0797	57.2326	-23.0758	-25.0039
0	3.0592	-48.8998	58.0773	-22.7635	-26.1363
0.1	3.0191	-47.0583	56.1155	-21.1828	-25.8755
0.2	2.9607	-42.7932	51.6752	-18.5398	-24.2534
0.3	2.9083	-36.7177	45.4425	-15.2067	-21.511
0.4	2.8708	-29.6577	38.27	-11.6301	-18.0276
0.5	2.8384	-22.4588	30.9739	-8.2332	-14.2256
0.6	2.7872	-15.8274	24.1889	-5.343	-10.4844
0.7	2.6882	-10.2456	18.3101	-3.1567	-7.0889
0.8	2.5171	-5.9554	13.5067	-1.7427	-4.2127
0.9	2.2611	-2.9923	9.7756	-1.0633	-1.929
1	1.9219	-1.2397	7.0055	-1.006	-0.2337
1.1	1.5153	-0.4862	5.0322	-1.4148	0.9286
1.2	1.0675	-0.4761	3.6786	-2.1176	1.6415
1.3	0.6103	-0.9476	2.7786	-2.9473	1.9997
1.4	0.1764	-1.6603	2.1896	-3.758	2.0977
1.5	-0.2059	-2.4146	1.7967	-4.4367	2.0221
1.6	-0.5162	-3.0615	1.5128	-4.9089	1.8474
1.7	-0.7434	-3.5058	1.2757	-5.1395	1.6337
1.8	-0.8856	-3.7018	1.0451	-5.1282	1.4264
1.9	-0.9491	-3.646	0.7986	-4.9023	1.2563
2	-0.9457	-3.3646	0.5275	-4.5061	1.1415
2.1	-0.89	-2.9028	0.2327	-3.9916	1.0888
2.2	-0.7974	-2.3137	-0.0786	-3.41	1.0963
2.3	-0.6822	-1.6506	-0.3958	-2.8065	1.1559
2.4	-0.5565	-0.9614	-0.7079	-2.2169	1.2555
2.5	-0.43	-0.2857	-1.0044	-1.6669	1.3812
2.6	-0.3099	0.347	-1.2768	-1.1724	1.5194
2.7	-0.2009	0.9158	-1.5186	-0.7418	1.6576
2.8	-0.1058	1.4087	-1.7262	-0.3771	1.7858
2.9	-0.0257	1.8205	-1.8975	-0.076	1.8965
3	0.0396	2.1516	-2.0329	0.1666	1.985
3.1	0.0909	2.4065	-2.1339	0.3574	2.0491

3.2	0.1298	2.5923	-2.2031	0.5037	2.0886
3.3	0.158	2.7176	-2.2437	0.6127	2.1049
3.4	0.1774	2.7916	-2.2593	0.6913	2.1003
3.5	0.1899	2.8234	-2.2538	0.7455	2.0779
3.6	0.1969	2.8214	-2.2308	0.7805	2.0409
3.7	0.1998	2.793	-2.1936	0.8007	1.9923
3.8	0.1998	2.7445	-2.1453	0.8096	1.9349
3.9	0.1976	2.6813	-2.0886	0.81	1.8713
4	0.194	2.6078	-2.0258	0.8041	1.8037
4.1	0.1894	2.5273	-1.9589	0.7936	1.7337
4.2	0.1843	2.4424	-1.8895	0.7797	1.6627
4.3	0.1788	2.3553	-1.8189	0.7634	1.5919
4.4	0.1731	2.2675	-1.7482	0.7455	1.522
4.5	0.1673	2.18	-1.678	0.7264	1.4536
4.6	0.1616	2.094	-1.6091	0.7067	1.3873
4.7	0.156	2.0098	-1.5419	0.6866	1.3232
4.8	0.1504	1.9279	-1.4766	0.6663	1.2616
4.9	0.145	1.8487	-1.4136	0.646	1.2027
5	0.1398	1.7722	-1.3529	0.6259	1.1463

1,2-dihydrocyclobutabenzene (C_2), 23

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Charge =  0 Multiplicity = 1
 C,0,-3.1257,-0.7004,0.
 C,0,-3.1257,0.7004,0.
 C,0,-1.932,1.4364,0.
 C,0,-0.7599,0.6966,0.
 C,0,-0.7599,-0.6966,0.
 C,0,-1.932,-1.4364,0.
 C,0,0.7599,0.7918,0.
 C,0,0.7599,-0.7918,0.
 H,0,-4.0753,-1.2243,0.
 H,0,-4.0753,1.2243,0.
 H,0,-1.9482,2.521,0.
 H,0,-1.9482,-2.521,0.
 H,0,1.2055,1.2463,0.8884
 H,0,1.2055,1.2463,-0.8884
 H,0,1.2055,-1.2463,-0.8884
 H,0,1.2055,-1.2463,0.8884
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Sum of electronic and zero-point Energies= -309.574703
Sum of electronic and thermal Energies= -309.568697
Sum of electronic and thermal Enthalpies= -309.567753
Sum of electronic and thermal Free Energies= -309.603900

NICS-scan (cyclobutane ring)

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.2895	0.9554	-1.8239	0.4417	0.5137
-4.9	-0.3026	0.9981	-1.9059	0.4605	0.5376
-4.8	-0.3164	1.043	-1.9924	0.4802	0.5628
-4.7	-0.331	1.0905	-2.0836	0.501	0.5895
-4.6	-0.3464	1.1406	-2.1798	0.5228	0.6178
-4.5	-0.3627	1.1934	-2.2814	0.5458	0.6476
-4.4	-0.3798	1.2491	-2.3885	0.5699	0.6792
-4.3	-0.3979	1.3079	-2.5016	0.5952	0.7127
-4.2	-0.417	1.3698	-2.6208	0.6218	0.748

-4.1	-0.4372	1.4351	-2.7466	0.6497	0.7854
-4	-0.4584	1.5038	-2.8792	0.6789	0.8249
-3.9	-0.4809	1.5763	-3.019	0.7096	0.8667
-3.8	-0.5046	1.6526	-3.1662	0.7417	0.9109
-3.7	-0.5295	1.7327	-3.3211	0.7752	0.9575
-3.6	-0.5557	1.8168	-3.484	0.8101	1.0067
-3.5	-0.5833	1.905	-3.655	0.8465	1.0585
-3.4	-0.6123	1.9974	-3.8342	0.8843	1.1131
-3.3	-0.6426	2.0939	-4.0216	0.9234	1.1705
-3.2	-0.6742	2.1945	-4.2171	0.9637	1.2308
-3.1	-0.7071	2.2991	-4.4203	1.0051	1.294
-3	-0.7411	2.4073	-4.6306	1.0472	1.3601
-2.9	-0.7761	2.5188	-4.847	1.0897	1.4291
-2.8	-0.8119	2.6326	-5.0683	1.1319	1.5007
-2.7	-0.8484	2.7473	-5.2926	1.1727	1.5746
-2.6	-0.8854	2.8609	-5.5172	1.2107	1.6502
-2.5	-0.9228	2.9703	-5.7387	1.2437	1.7266
-2.4	-0.9605	3.0711	-5.9525	1.2689	1.8022
-2.3	-0.9985	3.1571	-6.1526	1.2822	1.8749
-2.2	-1.0369	3.2205	-6.3311	1.2786	1.9419
-2.1	-1.0757	3.2507	-6.4778	1.2516	1.9991
-2	-1.1147	3.2348	-6.5791	1.1931	2.0417
-1.9	-1.1535	3.1568	-6.6173	1.0936	2.0632
-1.8	-1.1909	2.9966	-6.5693	0.9413	2.0553
-1.7	-1.2247	2.7303	-6.4045	0.7225	2.0078
-1.6	-1.2518	2.3276	-6.083	0.4203	1.9073
-1.5	-1.2677	1.7503	-5.5534	0.0142	1.7361
-1.4	-1.2666	0.9503	-4.75	-0.5209	1.4712
-1.3	-1.2416	-0.1334	-3.5913	-1.2151	1.0817
-1.2	-1.1848	-1.5745	-1.9798	-2.1029	0.5284
-1.1	-1.0875	-3.458	0.1954	-3.2204	-0.2376
-1	-0.94	-5.8706	3.0504	-4.5989	-1.2717
-0.9	-0.731	-8.8846	6.6915	-6.2547	-2.6299
-0.8	-0.4467	-12.5312	11.1912	-8.1754	-4.3558
-0.7	-0.0713	-16.7696	16.5557	-10.3066	-6.463
-0.6	0.4085	-21.4592	22.6847	-12.5454	-8.9138
-0.5	0.9946	-26.3495	29.3333	-14.7471	-11.6024
-0.4	1.6638	-31.0968	36.0881	-16.749	-14.3478
-0.3	2.3564	-35.311	42.3801	-18.405	-16.906
-0.2	2.9764	-38.6199	47.5489	-19.6174	-19.0025
-0.1	3.4111	-40.7278	50.9612	-20.3455	-20.3823
0	3.5681	-41.4509	52.1552	-20.5867	-20.8642
0.1	3.4111	-40.7278	50.9612	-20.3455	-20.3823
0.2	2.9764	-38.6199	47.5489	-19.6174	-19.0025
0.3	2.3564	-35.311	42.3801	-18.405	-16.906
0.4	1.6638	-31.0968	36.0881	-16.749	-14.3478
0.5	0.9946	-26.3495	29.3333	-14.7471	-11.6024
0.6	0.4085	-21.4592	22.6847	-12.5454	-8.9138
0.7	-0.0713	-16.7696	16.5557	-10.3066	-6.463

0.8	-0.4467	-12.5312	11.1912	-8.1754	-4.3558
0.9	-0.731	-8.8846	6.6915	-6.2547	-2.6299
1	-0.94	-5.8706	3.0504	-4.5989	-1.2717
1.1	-1.0875	-3.458	0.1954	-3.2204	-0.2376
1.2	-1.1848	-1.5745	-1.9798	-2.1029	0.5284
1.3	-1.2416	-0.1334	-3.5913	-1.2151	1.0817
1.4	-1.2666	0.9503	-4.75	-0.5209	1.4712
1.5	-1.2677	1.7503	-5.5534	0.0142	1.7361
1.6	-1.2518	2.3276	-6.083	0.4203	1.9073
1.7	-1.2247	2.7303	-6.4045	0.7225	2.0078
1.8	-1.1909	2.9966	-6.5693	0.9413	2.0553
1.9	-1.1535	3.1568	-6.6173	1.0936	2.0632
2	-1.1147	3.2348	-6.5791	1.1931	2.0417
2.1	-1.0757	3.2507	-6.4778	1.2516	1.9991
2.2	-1.0369	3.2205	-6.3311	1.2786	1.9419
2.3	-0.9985	3.1571	-6.1526	1.2822	1.8749
2.4	-0.9605	3.0711	-5.9525	1.2689	1.8022
2.5	-0.9228	2.9703	-5.7387	1.2437	1.7266
2.6	-0.8854	2.8609	-5.5172	1.2107	1.6502
2.7	-0.8484	2.7473	-5.2926	1.1727	1.5746
2.8	-0.8119	2.6326	-5.0683	1.1319	1.5007
2.9	-0.7761	2.5188	-4.847	1.0897	1.4291
3	-0.7411	2.4073	-4.6306	1.0472	1.3601
3.1	-0.7071	2.2991	-4.4203	1.0051	1.294
3.2	-0.6742	2.1945	-4.2171	0.9637	1.2308
3.3	-0.6426	2.0939	-4.0216	0.9234	1.1705
3.4	-0.6123	1.9974	-3.8342	0.8843	1.1131
3.5	-0.5833	1.905	-3.655	0.8465	1.0585
3.6	-0.5557	1.8168	-3.484	0.8101	1.0067
3.7	-0.5295	1.7327	-3.3211	0.7752	0.9575
3.8	-0.5046	1.6526	-3.1662	0.7417	0.9109
3.9	-0.4809	1.5763	-3.019	0.7096	0.8667
4	-0.4584	1.5038	-2.8792	0.6789	0.8249
4.1	-0.4372	1.4351	-2.7466	0.6497	0.7854
4.2	-0.417	1.3698	-2.6208	0.6218	0.748
4.3	-0.3979	1.3079	-2.5016	0.5952	0.7127
4.4	-0.3798	1.2491	-2.3885	0.5699	0.6792
4.5	-0.3627	1.1934	-2.2814	0.5458	0.6476
4.6	-0.3464	1.1406	-2.1798	0.5228	0.6178
4.7	-0.331	1.0905	-2.0836	0.501	0.5895
4.8	-0.3164	1.043	-1.9924	0.4802	0.5628
4.9	-0.3026	0.9981	-1.9059	0.4605	0.5376
5	-0.2895	0.9554	-1.8239	0.4417	0.5137

NICS-scan (benzene ring)

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.4471	0.9311	-2.2724	0.3998	0.5313
-4.9	-0.4739	0.9719	-2.3934	0.4153	0.5566
-4.8	-0.5028	1.0148	-2.523	0.4315	0.5833

-4.7	-0.534	1.0598	-2.6618	0.4483	0.6115
-4.6	-0.5678	1.1074	-2.8107	0.4659	0.6415
-4.5	-0.6044	1.1575	-2.9706	0.4843	0.6732
-4.4	-0.6441	1.2102	-3.1425	0.5035	0.7067
-4.3	-0.6873	1.2657	-3.3275	0.5234	0.7423
-4.2	-0.7342	1.3241	-3.5268	0.5442	0.7799
-4.1	-0.7854	1.3855	-3.7417	0.5658	0.8197
-4	-0.8413	1.4501	-3.9738	0.5883	0.8618
-3.9	-0.9023	1.5178	-4.2248	0.6115	0.9063
-3.8	-0.9692	1.5889	-4.4965	0.6356	0.9533
-3.7	-1.0426	1.6632	-4.7909	0.6605	1.0027
-3.6	-1.1232	1.7408	-5.1103	0.6861	1.0547
-3.5	-1.2119	1.8215	-5.4573	0.7122	1.1093
-3.4	-1.3098	1.9051	-5.8346	0.7388	1.1663
-3.3	-1.418	1.9914	-6.2452	0.7657	1.2257
-3.2	-1.5377	2.0796	-6.6926	0.7924	1.2872
-3.1	-1.6705	2.1689	-7.1804	0.8185	1.3504
-3	-1.818	2.2585	-7.7125	0.8436	1.4149
-2.9	-1.9822	2.3467	-8.2933	0.8668	1.4799
-2.8	-2.1652	2.4317	-8.9273	0.8871	1.5446
-2.7	-2.3694	2.5107	-9.6191	0.9031	1.6076
-2.6	-2.5976	2.5807	-10.3736	0.9132	1.6675
-2.5	-2.8527	2.6374	-11.1955	0.9152	1.7222
-2.4	-3.1378	2.6758	-12.0892	0.9064	1.7694
-2.3	-3.4561	2.6902	-13.0585	0.8838	1.8064
-2.2	-3.8108	2.6734	-14.1058	0.8434	1.83
-2.1	-4.2047	2.6178	-15.232	0.7812	1.8366
-2	-4.64	2.5152	-16.4353	0.6925	1.8227
-1.9	-5.1178	2.357	-17.7102	0.5725	1.7845
-1.8	-5.6373	2.1344	-19.0463	0.416	1.7184
-1.7	-6.1958	1.8393	-20.4266	0.2182	1.6211
-1.6	-6.787	1.4647	-21.8258	-0.0254	1.4901
-1.5	-7.4013	1.0047	-23.2085	-0.3186	1.3233
-1.4	-8.0241	0.455	-24.5273	-0.6645	1.1195
-1.3	-8.6362	-0.1864	-25.7222	-1.0647	0.8783
-1.2	-9.2132	-0.9194	-26.7201	-1.5191	0.5997
-1.1	-9.7265	-1.7413	-27.4383	-2.0254	0.2841
-1	-10.1451	-2.6456	-27.7897	-2.5777	-0.0679
-0.9	-10.4384	-3.6217	-27.6935	-3.1663	-0.4554
-0.8	-10.581	-4.653	-27.0901	-3.7765	-0.8765
-0.7	-10.5583	-5.7152	-25.9597	-4.3884	-1.3268
-0.6	-10.3721	-6.7754	-24.3408	-4.9783	-1.7971
-0.5	-10.0459	-7.7923	-22.3453	-5.5204	-2.2719
-0.4	-9.6264	-8.7184	-20.1609	-5.9907	-2.7277
-0.3	-9.1803	-9.5039	-18.0368	-6.3698	-3.1341
-0.2	-8.7843	-10.1028	-16.2501	-6.6454	-3.4574
-0.1	-8.5114	-10.478	-15.0563	-6.8117	-3.6663
0	-8.4141	-10.6057	-14.6366	-6.8671	-3.7386
0.1	-8.5114	-10.478	-15.0563	-6.8117	-3.6663

0.2	-8.7843	-10.1028	-16.2501	-6.6454	-3.4574
0.3	-9.1803	-9.5039	-18.0368	-6.3698	-3.1341
0.4	-9.6264	-8.7184	-20.1609	-5.9907	-2.7277
0.5	-10.0459	-7.7923	-22.3453	-5.5204	-2.2719
0.6	-10.3721	-6.7754	-24.3408	-4.9783	-1.7971
0.7	-10.5583	-5.7152	-25.9597	-4.3884	-1.3268
0.8	-10.581	-4.653	-27.0901	-3.7765	-0.8765
0.9	-10.4384	-3.6217	-27.6935	-3.1663	-0.4554
1	-10.1451	-2.6456	-27.7897	-2.5777	-0.0679
1.1	-9.7265	-1.7413	-27.4383	-2.0254	0.2841
1.2	-9.2132	-0.9194	-26.7201	-1.5191	0.5997
1.3	-8.6362	-0.1864	-25.7222	-1.0647	0.8783
1.4	-8.0241	0.455	-24.5273	-0.6645	1.1195
1.5	-7.4013	1.0047	-23.2085	-0.3186	1.3233
1.6	-6.787	1.4647	-21.8258	-0.0254	1.4901
1.7	-6.1958	1.8393	-20.4266	0.2182	1.6211
1.8	-5.6373	2.1344	-19.0463	0.416	1.7184
1.9	-5.1178	2.357	-17.7102	0.5725	1.7845
2	-4.64	2.5152	-16.4353	0.6925	1.8227
2.1	-4.2047	2.6178	-15.232	0.7812	1.8366
2.2	-3.8108	2.6734	-14.1058	0.8434	1.83
2.3	-3.4561	2.6902	-13.0585	0.8838	1.8064
2.4	-3.1378	2.6758	-12.0892	0.9064	1.7694
2.5	-2.8527	2.6374	-11.1955	0.9152	1.7222
2.6	-2.5976	2.5807	-10.3736	0.9132	1.6675
2.7	-2.3694	2.5107	-9.6191	0.9031	1.6076
2.8	-2.1652	2.4317	-8.9273	0.8871	1.5446
2.9	-1.9822	2.3467	-8.2933	0.8668	1.4799
3	-1.818	2.2585	-7.7125	0.8436	1.4149
3.1	-1.6705	2.1689	-7.1804	0.8185	1.3504
3.2	-1.5377	2.0796	-6.6926	0.7924	1.2872
3.3	-1.418	1.9914	-6.2452	0.7657	1.2257
3.4	-1.3098	1.9051	-5.8346	0.7388	1.1663
3.5	-1.2119	1.8215	-5.4573	0.7122	1.1093
3.6	-1.1232	1.7408	-5.1103	0.6861	1.0547
3.7	-1.0426	1.6632	-4.7909	0.6605	1.0027
3.8	-0.9692	1.5889	-4.4965	0.6356	0.9533
3.9	-0.9023	1.5178	-4.2248	0.6115	0.9063
4	-0.8413	1.4501	-3.9738	0.5883	0.8618
4.1	-0.7854	1.3855	-3.7417	0.5658	0.8197
4.2	-0.7342	1.3241	-3.5268	0.5442	0.7799
4.3	-0.6873	1.2657	-3.3275	0.5234	0.7423
4.4	-0.6441	1.2102	-3.1425	0.5035	0.7067
4.5	-0.6044	1.1575	-2.9706	0.4843	0.6732
4.6	-0.5678	1.1074	-2.8107	0.4659	0.6415
4.7	-0.534	1.0598	-2.6618	0.4483	0.6115
4.8	-0.5028	1.0148	-2.523	0.4315	0.5833
4.9	-0.4739	0.9719	-2.3934	0.4153	0.5566
5	-0.4471	0.9311	-2.2724	0.3998	0.5313

pyrrolyl nitrenium ion (C_1), 24

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Charge =  1 Multiplicity = 1
C,0,0.051504854,1.1173504787,-0.1729461993
 C,0,-1.1757412863,0.3440189709,-0.0288422748
 C,0,-0.7683750383,-0.9345057223,-0.0305223142
 C,0,0.8014627907,-0.8518856222,-0.0391561787
 N,0,1.211385939,0.3738200525,-0.0936441747
 H,0,1.4807021693,-1.6981570081,0.0287219484
 H,0,0.1165444032,2.1825342853,-0.3899220644
 H,0,-2.1770961348,0.747849794,-0.0313226396
 H,0,-1.3456296968,-1.8497812289,-0.0058331028
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Sum of electronic and zero-point Energies= -209.161982
Sum of electronic and thermal Energies= -209.157428
Sum of electronic and thermal Enthalpies= -209.156484
Sum of electronic and thermal Free Energies= -209.189110

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.2471	0.2052	0.5361	0.1083	0.0969
-4.9	0.2648	0.2146	0.5799	0.1128	0.1018
-4.8	0.2844	0.2247	0.6284	0.1176	0.1071
-4.7	0.3058	0.2352	0.6822	0.1225	0.1127
-4.6	0.3295	0.2464	0.742	0.1276	0.1188
-4.5	0.3556	0.2581	0.8087	0.1329	0.1252
-4.4	0.3845	0.2705	0.8831	0.1383	0.1322
-4.3	0.4166	0.2834	0.9664	0.1438	0.1396
-4.2	0.4523	0.297	1.06	0.1494	0.1476
-4.1	0.4921	0.3112	1.1652	0.155	0.1562
-4	0.5367	0.3261	1.2839	0.1607	0.1654
-3.9	0.5866	0.3416	1.4183	0.1662	0.1754
-3.8	0.6428	0.3577	1.5707	0.1715	0.1862
-3.7	0.7062	0.3744	1.7441	0.1765	0.1979
-3.6	0.7779	0.3916	1.9421	0.181	0.2106
-3.5	0.8593	0.4091	2.1687	0.1847	0.2244
-3.4	0.952	0.4269	2.4291	0.1874	0.2395
-3.3	1.058	0.4448	2.7292	0.1888	0.256
-3.2	1.1795	0.4624	3.0761	0.1882	0.2742
-3.1	1.3193	0.4792	3.4786	0.1849	0.2943
-3	1.4807	0.4949	3.9471	0.1782	0.3167
-2.9	1.6674	0.5081	4.4942	0.1665	0.3416
-2.8	1.8843	0.5177	5.1351	0.1481	0.3696
-2.7	2.1365	0.5217	5.8878	0.1206	0.4011
-2.6	2.4306	0.5174	6.7744	0.0806	0.4368
-2.5	2.7738	0.5008	7.8207	0.0234	0.4774
-2.4	3.1749	0.467	9.0579	-0.0569	0.5239
-2.3	3.644	0.4096	10.5224	-0.1681	0.5777
-2.2	4.1927	0.321	12.2572	-0.3198	0.6408
-2.1	4.8347	0.1918	14.3123	-0.5238	0.7156
-2	5.586	0.0123	16.7458	-0.7938	0.8061
-1.9	6.4653	-0.2282	19.624	-1.1454	0.9172
-1.8	7.494	-0.5401	23.022	-1.5957	1.0556
-1.7	8.6967	-0.9323	27.0225	-2.1624	1.2301

-1.6	10.1008	-1.4117	31.7142	-2.8629	1.4512
-1.5	11.7347	-1.9815	37.1857	-3.713	1.7315
-1.4	13.6254	-2.6398	43.5161	-4.7243	2.0845
-1.3	15.7937	-3.3772	50.7582	-5.901	2.5238
-1.2	18.2467	-4.1735	58.9137	-7.2348	3.0613
-1.1	20.9689	-4.9934	67.9002	-8.6979	3.7045
-1	23.9108	-5.7806	77.5131	-10.234	4.4534
-0.9	26.9804	-6.453	87.3942	-11.751	5.298
-0.8	30.0403	-6.9018	97.0227	-13.1183	6.2165
-0.7	32.917	-7.0016	105.7525	-14.1764	7.1748
-0.6	35.4251	-6.6387	112.9141	-14.767	8.1283
-0.5	37.4069	-5.7577	117.9784	-14.7837	9.026
-0.4	38.7753	-4.4198	120.7458	-14.2331	9.8133
-0.3	39.5459	-2.842	121.4796	-13.2781	10.4361
-0.2	39.8355	-1.3859	120.8922	-12.2296	10.8437
-0.1	39.8209	-0.4684	119.9313	-11.4634	10.995
0	39.6667	-0.4178	119.4179	-11.284	10.8662
0.1	39.4537	-1.3343	119.6954	-11.7941	10.4598
0.2	39.1466	-3.037	120.4767	-12.8442	9.8072
0.3	38.6153	-5.1307	120.9767	-14.093	8.9623
0.4	37.6995	-7.1545	120.2532	-15.1447	7.9902
0.5	36.2797	-8.7339	117.5731	-15.6888	6.9549
0.6	34.3238	-9.6675	112.6391	-15.5803	5.9128
0.7	31.8949	-9.9317	105.6164	-14.8413	4.9096
0.8	29.1266	-9.6285	97.0082	-13.6093	3.9808
0.9	26.1842	-8.9178	87.4704	-12.0694	3.1516
1	23.228	-7.9619	77.646	-10.399	2.4371
1.1	20.3881	-6.8959	68.0602	-8.7383	1.8424
1.2	17.754	-5.8171	59.0792	-7.1813	1.3642
1.3	15.3755	-4.7892	50.9156	-5.7816	0.9924
1.4	13.2698	-3.8493	43.6587	-4.5623	0.713
1.5	11.4317	-3.0164	37.3115	-3.5265	0.5101
1.6	9.8421	-2.2977	31.8238	-2.6652	0.3675
1.7	8.4753	-1.6918	27.1178	-1.9627	0.2709
1.8	7.304	-1.1929	23.105	-1.4005	0.2076
1.9	6.3018	-0.7914	19.6968	-0.9589	0.1675
2	5.4446	-0.4758	16.8097	-0.6188	0.143
2.1	4.7116	-0.2336	14.3685	-0.3618	0.1282
2.2	4.0847	-0.0523	12.3065	-0.1716	0.1193
2.3	3.5485	0.08	10.5655	-0.0339	0.1139
2.4	3.0898	0.1741	9.0954	0.0638	0.1103
2.5	2.6973	0.2388	7.8531	0.1312	0.1076
2.6	2.3613	0.2818	6.802	0.1764	0.1054
2.7	2.0734	0.309	5.9113	0.2055	0.1035
2.8	1.8265	0.3248	5.1548	0.2231	0.1017
2.9	1.6144	0.3326	4.5107	0.2327	0.0999
3	1.4318	0.3347	3.9607	0.2366	0.0981
3.1	1.2742	0.3327	3.4898	0.2365	0.0962
3.2	1.1378	0.3281	3.0852	0.2338	0.0943

3.3	1.0193	0.3215	2.7364	0.2292	0.0923
3.4	0.9162	0.3135	2.4349	0.2233	0.0902
3.5	0.826	0.3048	2.1732	0.2167	0.0881
3.6	0.7469	0.2953	1.9455	0.2095	0.0858
3.7	0.6774	0.2854	1.7467	0.202	0.0834
3.8	0.6159	0.2754	1.5725	0.1944	0.081
3.9	0.5616	0.2652	1.4195	0.1867	0.0785
4	0.5133	0.2551	1.2846	0.1791	0.076
4.1	0.4703	0.2453	1.1655	0.1717	0.0736
4.2	0.4318	0.2356	1.0599	0.1645	0.0711
4.3	0.3974	0.2261	0.9661	0.1575	0.0686
4.4	0.3665	0.2169	0.8826	0.1507	0.0662
4.5	0.3387	0.2081	0.8079	0.1442	0.0639
4.6	0.3135	0.1994	0.7412	0.1379	0.0615
4.7	0.2908	0.1912	0.6812	0.1319	0.0593
4.8	0.2702	0.1833	0.6273	0.1262	0.0571
4.9	0.2515	0.1757	0.5788	0.1207	0.055
5	0.2345	0.1684	0.5349	0.1155	0.0529

Carbazolyl nitrenium ion (C_{2v}), 25

```
Charge =  1 Multiplicity = 1
 C,0,3.3679,0.6321,0.
 C,0,2.8432,1.9207,0.
 C,0,1.4582,2.1115,0.
 C,0,0.642,0.9665,0.
 C,0,1.1883,-0.3614,0.
 C,0,2.5417,-0.5372,0.
 N,0,-0.714,0.9665,0.
 C,0,-1.1125,-0.3296,0.
 C,0,-0.0038,-1.242,0.
 C,0,-0.2335,-2.5873,0.
 C,0,-1.594,-3.0334,0.
 C,0,-2.6715,-2.1532,0.
 C,0,-2.4468,-0.7733,0.
 H,0,4.4442,0.5014,0.
 H,0,3.5102,2.7732,0.
 H,0,1.011,3.0986,0.
 H,0,3.0043,-1.5169,0.
 H,0,0.567,-3.3174,0.
 H,0,-1.7853,-4.1005,0.
 H,0,-3.6823,-2.5401,0.
 H,0,-3.2588,-0.0557,0.
```

Sum of electronic and zero-point Energies= -516.507091
Sum of electronic and thermal Energies= -516.498257
Sum of electronic and thermal Enthalpies= -516.497312
Sum of electronic and thermal Free Energies= -516.541120

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.7888	0.5455	1.8208	0.2439	0.3016
-4.9	0.8327	0.5626	1.9353	0.2506	0.312
-4.8	0.8798	0.5802	2.0592	0.2574	0.3228
-4.7	0.9305	0.5981	2.1934	0.2642	0.3339
-4.6	0.9851	0.6163	2.3389	0.271	0.3453
-4.5	1.0439	0.6348	2.4971	0.2777	0.3571

-4.4	1.1075	0.6532	2.6692	0.2842	0.369
-4.3	1.1762	0.6718	2.8567	0.2906	0.3812
-4.2	1.2507	0.6904	3.0616	0.2968	0.3936
-4.1	1.3315	0.7086	3.2857	0.3025	0.4061
-4	1.4193	0.7265	3.5314	0.3078	0.4187
-3.9	1.515	0.7437	3.8014	0.3125	0.4312
-3.8	1.6196	0.76	4.0988	0.3164	0.4436
-3.7	1.734	0.7749	4.4272	0.3193	0.4556
-3.6	1.8596	0.788	4.7907	0.3209	0.4671
-3.5	1.9977	0.7989	5.1943	0.321	0.4779
-3.4	2.1502	0.8067	5.6439	0.3191	0.4876
-3.3	2.3191	0.8108	6.1463	0.3149	0.4959
-3.2	2.5067	0.8103	6.7097	0.3078	0.5025
-3.1	2.7159	0.8038	7.3439	0.2971	0.5067
-3	2.9502	0.79	8.0605	0.282	0.508
-2.9	3.2136	0.7673	8.8736	0.2616	0.5057
-2.8	3.5111	0.7335	9.7997	0.2346	0.4989
-2.7	3.8484	0.6862	10.8591	0.1996	0.4866
-2.6	4.2326	0.6223	12.0755	0.1547	0.4676
-2.5	4.6718	0.5379	13.4775	0.0975	0.4404
-2.4	5.1757	0.4283	15.0988	0.0253	0.403
-2.3	5.7555	0.2877	16.979	-0.0655	0.3532
-2.2	6.4244	0.1086	19.1646	-0.1794	0.288
-2.1	7.1973	-0.1176	21.7096	-0.3215	0.2039
-2	8.0914	-0.4014	24.6758	-0.498	0.0966
-1.9	9.1262	-0.7553	28.1339	-0.7163	-0.039
-1.8	10.3234	-1.1927	32.1629	-0.9841	-0.2086
-1.7	11.7069	-1.7287	36.8494	-1.3102	-0.4185
-1.6	13.3021	-2.3785	42.2849	-1.7034	-0.6751
-1.5	15.1343	-3.1571	48.5599	-2.1719	-0.9852
-1.4	17.2255	-4.0772	55.7536	-2.7227	-1.3545
-1.3	19.5895	-5.1477	63.916	-3.3597	-1.788
-1.2	22.2243	-6.3697	73.0426	-4.0814	-2.2883
-1.1	25.102	-7.7328	83.0389	-4.8779	-2.8549
-1	28.1579	-9.2079	93.6816	-5.7262	-3.4817
-0.9	31.2813	-10.7416	104.5854	-6.5866	-4.155
-0.8	34.3142	-12.2508	115.1936	-7.4002	-4.8506
-0.7	37.0645	-13.625	124.8184	-8.0923	-5.5327
-0.6	39.3367	-14.7399	132.75	-8.5838	-6.1561
-0.5	40.9806	-15.489	138.4309	-8.814	-6.675
-0.4	41.944	-15.8239	141.6558	-8.7683	-7.0556
-0.3	42.3064	-15.7909	142.7101	-8.5006	-7.2903
-0.2	42.2706	-15.5361	142.3478	-8.1329	-7.4032
-0.1	42.0989	-15.2623	141.559	-7.8218	-7.4405
0	42.0128	-15.1475	141.1859	-7.7007	-7.4468
0.1	42.0989	-15.2623	141.559	-7.8218	-7.4405
0.2	42.2706	-15.5361	142.3478	-8.1329	-7.4032
0.3	42.3064	-15.7909	142.7101	-8.5006	-7.2903
0.4	41.944	-15.8239	141.6558	-8.7683	-7.0556

0.5	40.9806	-15.489	138.4309	-8.814	-6.675
0.6	39.3367	-14.7399	132.75	-8.5838	-6.1561
0.7	37.0645	-13.625	124.8184	-8.0923	-5.5327
0.8	34.3142	-12.2508	115.1936	-7.4002	-4.8506
0.9	31.2813	-10.7416	104.5854	-6.5866	-4.155
1	28.1579	-9.2079	93.6816	-5.7262	-3.4817
1.1	25.102	-7.7328	83.0389	-4.8779	-2.8549
1.2	22.2243	-6.3697	73.0426	-4.0814	-2.2883
1.3	19.5895	-5.1477	63.916	-3.3597	-1.788
1.4	17.2255	-4.0772	55.7536	-2.7227	-1.3545
1.5	15.1343	-3.1571	48.5599	-2.1719	-0.9852
1.6	13.3021	-2.3785	42.2849	-1.7034	-0.6751
1.7	11.7069	-1.7287	36.8494	-1.3102	-0.4185
1.8	10.3234	-1.1927	32.1629	-0.9841	-0.2086
1.9	9.1262	-0.7553	28.1339	-0.7163	-0.039
2	8.0914	-0.4014	24.6758	-0.498	0.0966
2.1	7.1973	-0.1176	21.7096	-0.3215	0.2039
2.2	6.4244	0.1086	19.1646	-0.1794	0.288
2.3	5.7555	0.2877	16.979	-0.0655	0.3532
2.4	5.1757	0.4283	15.0988	0.0253	0.403
2.5	4.6718	0.5379	13.4775	0.0975	0.4404
2.6	4.2326	0.6223	12.0755	0.1547	0.4676
2.7	3.8484	0.6862	10.8591	0.1996	0.4866
2.8	3.5111	0.7335	9.7997	0.2346	0.4989
2.9	3.2136	0.7673	8.8736	0.2616	0.5057
3	2.9502	0.79	8.0605	0.282	0.508
3.1	2.7159	0.8038	7.3439	0.2971	0.5067
3.2	2.5067	0.8103	6.7097	0.3078	0.5025
3.3	2.3191	0.8108	6.1463	0.3149	0.4959
3.4	2.1502	0.8067	5.6439	0.3191	0.4876
3.5	1.9977	0.7989	5.1943	0.321	0.4779
3.6	1.8596	0.788	4.7907	0.3209	0.4671
3.7	1.734	0.7749	4.4272	0.3193	0.4556
3.8	1.6196	0.76	4.0988	0.3164	0.4436
3.9	1.515	0.7437	3.8014	0.3125	0.4312
4	1.4193	0.7265	3.5314	0.3078	0.4187
4.1	1.3315	0.7086	3.2857	0.3025	0.4061
4.2	1.2507	0.6904	3.0616	0.2968	0.3936
4.3	1.1762	0.6718	2.8567	0.2906	0.3812
4.4	1.1075	0.6532	2.6692	0.2842	0.369
4.5	1.0439	0.6348	2.4971	0.2777	0.3571
4.6	0.9851	0.6163	2.3389	0.271	0.3453
4.7	0.9305	0.5981	2.1934	0.2642	0.3339
4.8	0.8798	0.5802	2.0592	0.2574	0.3228
4.9	0.8327	0.5626	1.9353	0.2506	0.312
5	0.7888	0.5455	1.8208	0.2439	0.3016

borole (C_s), 26

```
Charge =  0 Multiplicity = 1
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```
C,0,-0.0779828783,1.0168640522,0.0605263821
C,0,1.2282829665,0.2813105037,-0.0717007905
C,0,0.7940412051,-0.9740871732,-0.0912181402
C,0,-0.6888021089,-0.7490238393,0.0329858609
B,0,-1.3298679802,0.470729673,-0.5575154228
H,0,-1.2361822872,-1.2772021206,0.8171174799
H,0,-0.1895033576,1.747836127,0.8647455211
H,0,2.2109535227,0.7213217241,-0.1733107021
H,0,1.2961012502,-1.9240887533,-0.2139662709
H,0,-2.4474403323,0.8571398065,-0.5629639175
```

Sum of electronic and zero-point Energies= -180.127444
Sum of electronic and thermal Energies= -180.122975
Sum of electronic and thermal Enthalpies= -180.122031
Sum of electronic and thermal Free Energies= -180.154083

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.0322	0.5611	-0.6578	0.2399	0.3212
-4.9	-0.0339	0.5887	-0.6904	0.2507	0.338
-4.8	-0.0356	0.6181	-0.7249	0.2621	0.356
-4.7	-0.0374	0.6493	-0.7615	0.2741	0.3752
-4.6	-0.0393	0.6824	-0.8004	0.2867	0.3957
-4.5	-0.0413	0.7175	-0.8415	0.2998	0.4177
-4.4	-0.0434	0.7548	-0.8852	0.3135	0.4413
-4.3	-0.0456	0.7945	-0.9314	0.3278	0.4667
-4.2	-0.0479	0.8367	-0.9804	0.3427	0.494
-4.1	-0.0502	0.8816	-1.0322	0.3581	0.5235
-4	-0.0526	0.9293	-1.0871	0.374	0.5553
-3.9	-0.0549	0.9801	-1.1449	0.3904	0.5897
-3.8	-0.0573	1.0341	-1.2059	0.4071	0.627
-3.7	-0.0595	1.0916	-1.2701	0.424	0.6676
-3.6	-0.0616	1.1528	-1.3375	0.441	0.7118
-3.5	-0.0633	1.2179	-1.4079	0.4577	0.7602
-3.4	-0.0647	1.2872	-1.4812	0.4739	0.8133
-3.3	-0.0654	1.361	-1.5572	0.4891	0.8719
-3.2	-0.0653	1.4395	-1.6354	0.5029	0.9366
-3.1	-0.064	1.5232	-1.7151	0.5145	1.0087
-3	-0.0611	1.6124	-1.7956	0.5231	1.0893
-2.9	-0.056	1.7078	-1.8758	0.5278	1.18
-2.8	-0.0481	1.8097	-1.954	0.5272	1.2825
-2.7	-0.0365	1.9189	-2.0285	0.5198	1.3991
-2.6	-0.0202	2.036	-2.0967	0.5037	1.5323
-2.5	0.0021	2.1618	-2.1555	0.4768	1.685
-2.4	0.032	2.2969	-2.201	0.4366	1.8603
-2.3	0.0712	2.4421	-2.2284	0.3803	2.0618
-2.2	0.1222	2.5983	-2.2317	0.3052	2.2931
-2.1	0.1877	2.7665	-2.2035	0.2087	2.5578
-2	0.2712	2.9486	-2.1348	0.0889	2.8597
-1.9	0.3774	3.1469	-2.0148	-0.0549	3.2018
-1.8	0.5118	3.3652	-1.8299	-0.2212	3.5864
-1.7	0.6813	3.6081	-1.5643	-0.4061	4.0142
-1.6	0.8941	3.8809	-1.1986	-0.6018	4.4827

-1.5	1.1595	4.1889	-0.7104	-0.7963	4.9852
-1.4	1.4866	4.534	-0.0741	-0.9731	5.5071
-1.3	1.8835	4.912	0.7384	-1.1114	6.0234
-1.2	2.3541	5.3064	1.7559	-1.1877	6.4941
-1.1	2.8955	5.6813	3.0051	-1.179	6.8603
-1	3.4935	5.9736	4.5068	-1.0686	7.0422
-0.9	4.1186	6.0849	6.2709	-0.8551	6.94
-0.8	4.723	5.8772	8.2917	-0.5645	6.4417
-0.7	5.2395	5.1731	10.5456	-0.2656	5.4387
-0.6	5.5853	3.7651	12.9909	-0.0846	3.8497
-0.5	5.6699	1.4377	15.5719	-0.2116	1.6493
-0.4	5.4094	-1.9968	18.2249	-0.8907	-1.1061
-0.3	4.7468	-6.6417	20.8821	-2.3776	-4.2641
-0.2	3.675	-12.4433	23.4682	-4.8599	-7.5834
-0.1	2.2575	-19.1145	25.8868	-8.3492	-10.7653
0	0.637	-26.0918	28.0027	-12.5868	-13.505
0.1	-0.9803	-32.5735	29.6327	-17.0256	-15.5479
0.2	-2.3688	-37.6709	30.5644	-20.9356	-16.7353
0.3	-3.3456	-40.643	30.6062	-23.6163	-17.0267
0.4	-3.8225	-41.1206	29.653	-24.6232	-16.4974
0.5	-3.8255	-39.2086	27.7321	-23.8955	-15.3131
0.6	-3.4707	-35.4187	25.0067	-21.7291	-13.6896
0.7	-2.9147	-30.4791	21.7349	-18.6309	-11.8482
0.8	-2.3046	-25.121	18.2071	-15.1428	-9.9782
0.9	-1.7455	-19.9257	14.689	-11.7106	-8.2151
1	-1.2921	-15.2621	11.3857	-8.625	-6.6371
1.1	-0.9571	-11.3008	8.4296	-6.026	-5.2748
1.2	-0.7265	-8.0656	5.886	-3.9393	-4.1263
1.3	-0.5754	-5.4938	3.7675	-2.3218	-3.172
1.4	-0.4783	-3.4864	2.0517	-1.1006	-2.3858
1.5	-0.4143	-1.9389	0.6958	-0.1974	-1.7415
1.6	-0.3695	-0.7576	-0.351	0.458	-1.2156
1.7	-0.3353	0.1344	-1.1404	0.923	-0.7886
1.8	-0.3073	0.7983	-1.7201	1.2426	-0.4443
1.9	-0.2833	1.2819	-2.1318	1.4514	-0.1695
2	-0.2626	1.623	-2.411	1.576	0.047
2.1	-0.245	1.8518	-2.5868	1.637	0.2148
2.2	-0.23	1.993	-2.6829	1.6508	0.3422
2.3	-0.2172	2.0665	-2.7182	1.6302	0.4363
2.4	-0.2063	2.0889	-2.7079	1.5855	0.5034
2.5	-0.1966	2.0741	-2.664	1.525	0.5491
2.6	-0.1877	2.0328	-2.5959	1.4549	0.5779
2.7	-0.1792	1.9733	-2.511	1.3798	0.5935
2.8	-0.1709	1.9024	-2.415	1.3032	0.5992
2.9	-0.1625	1.8247	-2.3124	1.2274	0.5973
3	-0.1542	1.7437	-2.2064	1.1539	0.5898
3.1	-0.1459	1.662	-2.0996	1.0837	0.5783
3.2	-0.1376	1.5811	-1.9939	1.0173	0.5638
3.3	-0.1295	1.5021	-1.8905	0.9548	0.5473

3.4	-0.1216	1.4256	-1.7905	0.8962	0.5294
3.5	-0.114	1.3523	-1.6944	0.8416	0.5107
3.6	-0.1068	1.2823	-1.6025	0.7907	0.4916
3.7	-0.0999	1.2156	-1.5152	0.7433	0.4723
3.8	-0.0934	1.1523	-1.4325	0.6991	0.4532
3.9	-0.0873	1.0924	-1.3543	0.658	0.4344
4	-0.0816	1.0358	-1.2806	0.6198	0.416
4.1	-0.0763	0.9823	-1.2112	0.5842	0.3981
4.2	-0.0713	0.9319	-1.1459	0.5511	0.3808
4.3	-0.0667	0.8843	-1.0846	0.5202	0.3641
4.4	-0.0625	0.8396	-1.027	0.4915	0.3481
4.5	-0.0585	0.7973	-0.9729	0.4646	0.3327
4.6	-0.0549	0.7576	-0.9222	0.4396	0.318
4.7	-0.0515	0.7202	-0.8746	0.4162	0.304
4.8	-0.0483	0.6849	-0.8299	0.3943	0.2906
4.9	-0.0454	0.6517	-0.788	0.3739	0.2778
5	-0.0427	0.6204	-0.7486	0.3548	0.2656

1,2 Dithiin (C_2), 27

```
Charge =  0 Multiplicity = 1
S,0,0.5455023588,1.5428163613,-0.236423513
 C,0,0.0509335194,0.4372462179,-1.5389206118
 C,0,-0.0947849365,-0.885515972,-1.3592708099
 C,0,0.1009033955,-1.5839273207,-0.0949276076
 C,0,-0.0424398011,-1.0312654325,1.1204708295
 S,0,-0.5352357478,0.6605118055,1.362541758
 H,0,-0.0686859381,0.9055584649,-2.5095960286
 H,0,-0.3597897229,-1.4886110506,-2.2221169929
 H,0,0.3653776014,-2.6355378059,-0.1462243889
 H,0,0.0786192713,-1.603475268,2.0335673652
```

Sum of electronic and zero-point Energies= -951.194041
Sum of electronic and thermal Energies= -951.188295
Sum of electronic and thermal Enthalpies= -951.187350
Sum of electronic and thermal Free Energies= -951.223940

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.1313	1.2816	-0.8877	0.6488	0.6328
-4.9	0.1399	1.3456	-0.9259	0.6809	0.6647
-4.8	0.1491	1.4132	-0.9658	0.7148	0.6984
-4.7	0.1592	1.4851	-1.0075	0.7508	0.7343
-4.6	0.1701	1.5614	-1.051	0.7889	0.7725
-4.5	0.1821	1.6423	-1.0962	0.8293	0.813
-4.4	0.1951	1.7284	-1.1432	0.8722	0.8562
-4.3	0.2093	1.8196	-1.1918	0.9176	0.902
-4.2	0.2248	1.9164	-1.242	0.9657	0.9507
-4.1	0.2418	2.0192	-1.2937	1.0167	1.0025
-4	0.2604	2.1279	-1.3466	1.0705	1.0574
-3.9	0.2808	2.243	-1.4005	1.1273	1.1157
-3.8	0.3032	2.3647	-1.4551	1.1872	1.1775
-3.7	0.3277	2.493	-1.5098	1.2502	1.2428

-3.6	0.3546	2.6278	-1.564	1.3161	1.3117
-3.5	0.384	2.7691	-1.6171	1.3849	1.3842
-3.4	0.4161	2.9162	-1.668	1.4562	1.46
-3.3	0.451	3.0686	-1.7156	1.5296	1.539
-3.2	0.4888	3.2246	-1.7584	1.6042	1.6204
-3.1	0.5294	3.3827	-1.7945	1.679	1.7037
-3	0.5727	3.5398	-1.8218	1.7524	1.7874
-2.9	0.6183	3.6924	-1.8374	1.8223	1.8701
-2.8	0.6657	3.8351	-1.8382	1.8858	1.9493
-2.7	0.7138	3.9615	-1.8201	1.9393	2.0222
-2.6	0.7615	4.0626	-1.7782	1.9779	2.0847
-2.5	0.8071	4.1278	-1.7067	1.9958	2.132
-2.4	0.8485	4.1441	-1.5986	1.986	2.1581
-2.3	0.8833	4.0959	-1.4459	1.94	2.1559
-2.2	0.9089	3.9655	-1.2387	1.8485	2.117
-2.1	0.9224	3.7332	-0.9661	1.7011	2.0321
-2	0.921	3.3781	-0.6152	1.4867	1.8914
-1.9	0.9024	2.8789	-0.1717	1.1945	1.6844
-1.8	0.8651	2.2152	0.3801	0.814	1.4012
-1.7	0.8086	1.3687	1.0572	0.3361	1.0326
-1.6	0.734	0.325	1.877	-0.2464	0.5714
-1.5	0.644	-0.9247	2.8567	-0.9376	0.0129
-1.4	0.5433	-2.3818	4.0116	-1.7381	-0.6437
-1.3	0.4382	-4.0391	5.3536	-2.6444	-1.3947
-1.2	0.3364	-5.8791	6.8885	-3.6482	-2.2309
-1.1	0.2465	-7.8735	8.6131	-4.7362	-3.1373
-1	0.1765	-9.9832	10.5126	-5.8907	-4.0925
-0.9	0.1327	-12.16	12.558	-7.0896	-5.0704
-0.8	0.1186	-14.3485	14.7042	-8.3071	-6.0414
-0.7	0.1336	-16.49	16.8908	-9.5147	-6.9753
-0.6	0.173	-18.5242	19.0432	-10.681	-7.8432
-0.5	0.2285	-20.3913	21.0768	-11.7713	-8.62
-0.4	0.2901	-22.0323	22.9025	-12.7476	-9.2847
-0.3	0.3478	-23.3893	24.4328	-13.5689	-9.8204
-0.2	0.3939	-24.4077	25.5895	-14.1943	-10.2134
-0.1	0.4231	-25.0407	26.3102	-14.5873	-10.4534
0	0.4328	-25.2563	26.5547	-14.7228	-10.5335
0.1	0.4221	-25.0427	26.3091	-14.5913	-10.4514
0.2	0.392	-24.4113	25.5873	-14.2019	-10.2094
0.3	0.345	-23.3945	24.4296	-13.5798	-9.8147
0.4	0.2866	-22.0387	22.8984	-12.7611	-9.2776
0.5	0.2245	-20.3987	21.072	-11.7869	-8.6118
0.6	0.1686	-18.5322	19.0379	-10.6979	-7.8343
0.7	0.1289	-16.4984	16.8852	-9.5323	-6.9661
0.8	0.1138	-14.3571	14.6986	-8.3248	-6.0323
0.9	0.128	-12.1684	12.5524	-7.1069	-5.0615
1	0.172	-9.9914	10.5073	-5.9074	-4.084
1.1	0.2423	-7.8814	8.6082	-4.752	-3.1294
1.2	0.3325	-5.8867	6.884	-3.663	-2.2237

1.3	0.4345	-4.0462	5.3497	-2.6581	-1.3881
1.4	0.5399	-2.3885	4.0083	-1.7508	-0.6377
1.5	0.641	-0.9309	2.8539	-0.9492	0.0183
1.6	0.7313	0.3192	1.8748	-0.257	0.5762
1.7	0.8063	1.3633	1.0555	0.3264	1.0369
1.8	0.863	2.2103	0.3788	0.8053	1.405
1.9	0.9006	2.8745	-0.1727	1.1866	1.6879
2	0.9194	3.3741	-0.6159	1.4796	1.8945
2.1	0.921	3.7295	-0.9665	1.6946	2.0349
2.2	0.9077	3.9623	-1.239	1.8428	2.1195
2.3	0.8823	4.093	-1.446	1.9349	2.1581
2.4	0.8476	4.1414	-1.5986	1.9813	2.1601
2.5	0.8063	4.1255	-1.7065	1.9917	2.1338
2.6	0.7608	4.0605	-1.778	1.9742	2.0863
2.7	0.7132	3.9595	-1.8198	1.9359	2.0236
2.8	0.6652	3.8334	-1.8379	1.8828	1.9506
2.9	0.6179	3.6909	-1.8371	1.8196	1.8713
3	0.5723	3.5385	-1.8215	1.75	1.7885
3.1	0.5291	3.3814	-1.7942	1.6768	1.7046
3.2	0.4885	3.2235	-1.7581	1.6022	1.6213
3.3	0.4507	3.0675	-1.7153	1.5278	1.5397
3.4	0.4159	2.9153	-1.6677	1.4546	1.4607
3.5	0.3838	2.7682	-1.6168	1.3834	1.3848
3.6	0.3544	2.627	-1.5638	1.3147	1.3123
3.7	0.3276	2.4922	-1.5095	1.2489	1.2433
3.8	0.3031	2.364	-1.4548	1.186	1.178
3.9	0.2807	2.2424	-1.4003	1.1262	1.1162
4	0.2603	2.1274	-1.3464	1.0695	1.0579
4.1	0.2417	2.0186	-1.2935	1.0157	1.0029
4.2	0.2247	1.916	-1.2418	0.9649	0.9511
4.3	0.2092	1.8192	-1.1916	0.9168	0.9024
4.4	0.195	1.728	-1.143	0.8715	0.8565
4.5	0.182	1.642	-1.0961	0.8286	0.8134
4.6	0.1701	1.5611	-1.0509	0.7883	0.7728
4.7	0.1591	1.4847	-1.0074	0.7501	0.7346
4.8	0.1491	1.4129	-0.9657	0.7142	0.6987
4.9	0.1398	1.3452	-0.9258	0.6803	0.6649
5	0.1313	1.2814	-0.8876	0.6483	0.6331

1,4 Dithiin (C_{2v}), 28

```
Charge =  0 Multiplicity = 1
S,0,1.6664042165,0.,-0.2748427098
 C,0,0.6656936192,1.3649585755,0.2731973951
 C,0,-0.6656936192,1.3649585755,0.2731973951
 S,0,-1.6664042165,0.,-0.2748427098
 C,0,-0.6656936192,-1.3649585755,0.2731973951
 C,0,0.6656936192,-1.3649585755,0.2731973951
 H,0,1.229388788,2.2029458355,0.667353024
 H,0,-1.229388788,2.2029458355,0.667353024
 H,0,-1.229388788,-2.2029458355,0.667353024
 H,0,1.229388788,-2.2029458355,0.667353024
```

Sum of electronic and zero-point Energies= -951.189667

Sum of electronic and thermal Energies= -951.184004
Sum of electronic and thermal Enthalpies= -951.183060
Sum of electronic and thermal Free Energies= -951.218863

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.0117	1.4781	-1.443	0.9062	0.5719
-4.9	0.0135	1.5554	-1.5148	0.9569	0.5985
-4.8	0.0157	1.6379	-1.5908	1.0115	0.6264
-4.7	0.0181	1.7259	-1.6715	1.0702	0.6557
-4.6	0.0209	1.8199	-1.7571	1.1335	0.6864
-4.5	0.0241	1.9201	-1.8479	1.2017	0.7184
-4.4	0.0277	2.0272	-1.9442	1.2753	0.7519
-4.3	0.0318	2.1416	-2.0462	1.355	0.7866
-4.2	0.0365	2.2637	-2.1544	1.4411	0.8226
-4.1	0.0418	2.3943	-2.2688	1.5345	0.8598
-4	0.0479	2.5336	-2.39	1.6357	0.8979
-3.9	0.0547	2.6822	-2.518	1.7456	0.9366
-3.8	0.0624	2.8404	-2.6531	1.8648	0.9756
-3.7	0.071	3.0084	-2.7955	1.994	1.0144
-3.6	0.0804	3.1863	-2.9451	2.1342	1.0521
-3.5	0.0906	3.3738	-3.102	2.2858	1.088
-3.4	0.1013	3.5698	-3.2659	2.4493	1.1205
-3.3	0.1122	3.7733	-3.4365	2.625	1.1483
-3.2	0.1229	3.9816	-3.613	2.8126	1.169
-3.1	0.1324	4.1919	-3.7946	3.0116	1.1803
-3	0.1398	4.3992	-3.9798	3.2205	1.1787
-2.9	0.1437	4.5979	-4.1669	3.4374	1.1605
-2.8	0.1424	4.7805	-4.3532	3.6593	1.1212
-2.7	0.134	4.9377	-4.5356	3.8824	1.0553
-2.6	0.1164	5.059	-4.7099	4.1021	0.9569
-2.5	0.0872	5.1324	-4.8708	4.313	0.8194
-2.4	0.0445	5.1449	-5.0115	4.5094	0.6355
-2.3	-0.0138	5.0825	-5.124	4.6852	0.3973
-2.2	-0.0891	4.9311	-5.1985	4.8347	0.0964
-2.1	-0.1821	4.6766	-5.223	4.9525	-0.2759
-2	-0.2929	4.3055	-5.184	5.0345	-0.729
-1.9	-0.4205	3.8045	-5.0658	5.0774	-1.2729
-1.8	-0.5631	3.1618	-4.8511	5.0797	-1.9179
-1.7	-0.7184	2.3661	-4.5213	5.0408	-2.6747
-1.6	-0.8832	1.4076	-4.0572	4.9617	-3.5541
-1.5	-1.0542	0.2775	-3.44	4.8438	-4.5663
-1.4	-1.2282	-1.0314	-2.6532	4.6885	-5.7199
-1.3	-1.4027	-2.5244	-1.6837	4.4961	-7.0205
-1.2	-1.5763	-4.204	-0.5248	4.2643	-8.4683
-1.1	-1.7492	-6.0688	0.8213	3.9868	-10.0556
-1	-1.9238	-8.1117	2.3404	3.6516	-11.7633
-0.9	-2.1045	-10.317	4.0035	3.2404	-13.5574
-0.8	-2.2976	-12.6563	5.7635	2.7289	-15.3852
-0.7	-2.51	-15.0846	7.5546	2.0892	-17.1738

-0.6	-2.7478	-17.5361	9.2926	1.2942	-18.8303
-0.5	-3.0143	-19.9222	10.8793	0.3247	-20.2469
-0.4	-3.3085	-22.1357	12.2104	-0.8237	-21.312
-0.3	-3.6243	-24.0595	13.1865	-2.1345	-21.925
-0.2	-3.9512	-25.5807	13.7271	-3.5669	-22.0138
-0.1	-4.2754	-26.6079	13.7815	-5.0571	-21.5508
0	-4.5819	-27.0837	13.3379	-6.5237	-20.56
0.1	-4.8556	-26.9914	12.4245	-7.8759	-19.1155
0.2	-5.0823	-26.352	11.1052	-9.0237	-17.3283
0.3	-5.2486	-25.2159	9.47	-9.8892	-15.3267
0.4	-5.3431	-23.6516	7.6224	-10.4159	-13.2357
0.5	-5.3566	-21.7378	5.668	-10.5765	-11.1613
0.6	-5.2842	-19.5575	3.7048	-10.3755	-9.182
0.7	-5.1265	-17.196	1.8163	-9.8479	-7.3481
0.8	-4.8901	-14.7387	0.0685	-9.0526	-5.6861
0.9	-4.5872	-12.2694	-1.4924	-8.0634	-4.206
1	-4.2344	-9.8647	-2.8384	-6.9577	-2.907
1.1	-3.8501	-7.5915	-3.9587	-5.8084	-1.7831
1.2	-3.4529	-5.5023	-4.8563	-4.6773	-0.825
1.3	-3.0595	-3.6341	-5.5444	-3.6117	-0.0224
1.4	-2.6838	-2.0078	-6.0435	-2.6438	0.636
1.5	-2.3359	-0.6301	-6.3777	-1.7923	1.1622
1.6	-2.0224	0.5047	-6.572	-1.0646	1.5693
1.7	-1.7465	1.4118	-6.6512	-0.4592	1.871
1.8	-1.5083	2.1128	-6.6376	0.0314	2.0814
1.9	-1.306	2.6332	-6.5512	0.4185	2.2147
2	-1.1363	3.0005	-6.4093	0.7155	2.285
2.1	-0.995	3.2414	-6.2263	0.9363	2.3051
2.2	-0.8776	3.3811	-6.0139	1.0943	2.2868
2.3	-0.78	3.4419	-5.782	1.2016	2.2403
2.4	-0.6985	3.4428	-5.5382	1.2689	2.1739
2.5	-0.6296	3.3998	-5.2888	1.3052	2.0946
2.6	-0.571	3.3254	-5.0383	1.3179	2.0075
2.7	-0.5203	3.2295	-4.7905	1.3128	1.9167
2.8	-0.4762	3.1195	-4.5481	1.2947	1.8248
2.9	-0.4373	3.001	-4.3129	1.2671	1.7339
3	-0.4027	2.8783	-4.0865	1.2329	1.6454
3.1	-0.3718	2.7541	-3.8695	1.1941	1.56
3.2	-0.344	2.6306	-3.6626	1.1524	1.4782
3.3	-0.3189	2.5093	-3.466	1.1091	1.4002
3.4	-0.2961	2.3914	-3.2796	1.0651	1.3263
3.5	-0.2754	2.2773	-3.1034	1.021	1.2563
3.6	-0.2565	2.1676	-2.937	0.9774	1.1902
3.7	-0.2392	2.0625	-2.7802	0.9347	1.1278
3.8	-0.2234	1.9621	-2.6325	0.8931	1.069
3.9	-0.209	1.8666	-2.4935	0.8529	1.0137
4	-0.1957	1.7757	-2.3627	0.8141	0.9616
4.1	-0.1835	1.6894	-2.2398	0.7769	0.9125
4.2	-0.1722	1.6076	-2.1243	0.7412	0.8664

4.3	-0.1618	1.5302	-2.0157	0.7071	0.8231
4.4	-0.1523	1.4568	-1.9136	0.6746	0.7822
4.5	-0.1434	1.3874	-1.8177	0.6436	0.7438
4.6	-0.1352	1.3219	-1.7274	0.6142	0.7077
4.7	-0.1276	1.2598	-1.6426	0.5861	0.6737
4.8	-0.1205	1.2011	-1.5628	0.5595	0.6416
4.9	-0.114	1.1458	-1.4876	0.5343	0.6115
5	-0.1079	1.0933	-1.4169	0.5103	0.583

9b-boraphenalene (D_{3h}), 29

```
Charge =  0 Multiplicity = 1
C,0,-1.3017176095,0.7515470059,0.
 B,0,0.,-0.0000000015,0.
 C,0,0.0000000042,-1.5030940237,0.
 C,0,-1.2582692458,-2.1495866932,0.
 C,0,-2.4577640195,-1.4189907289,0.
 C,0,-2.4907313054,-0.0148998012,0.
 C,0,1.3017176054,0.7515470132,0.
 C,0,2.4907313055,-0.0148997873,0.
 C,0,2.4577640275,-1.4189907152,0.
 C,0,1.2582692578,-2.1495866862,0.
 C,0,-1.2324620597,2.164486476,0.
 C,0,-0.0000000079,2.8379814396,0.
 C,0,1.2324620476,2.1644864829,0.
 H,0,-1.3242455071,-3.2376115414,0.
 H,0,-3.3967934448,-1.9611396239,0.
 H,0,-3.4659765973,0.4719754991,0.
 H,0,3.4659765946,0.4719755185,0.
 H,0,3.3967934557,-1.9611396049,0.
 H,0,1.3242455251,-3.237611534,0.
 H,0,-2.1417310876,2.7656360184,0.
 H,0,-0.000000011,3.9222792243,0.
 H,0,2.1417310721,2.7656360303,0.
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Sum of electronic and zero-point Energies= -487.477145
Sum of electronic and thermal Energies= -487.468010
Sum of electronic and thermal Enthalpies= -487.467066
Sum of electronic and thermal Free Energies= -487.509348

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.5059	0.8102	0.7073	0.4286	0.3816
-4.9	0.5321	0.8408	0.7555	0.4457	0.3951
-4.8	0.5602	0.8728	0.8079	0.4637	0.4091
-4.7	0.5904	0.9064	0.8648	0.4827	0.4237
-4.6	0.6228	0.9414	0.927	0.5026	0.4388
-4.5	0.6577	0.9781	0.9948	0.5236	0.4545
-4.4	0.6952	1.0165	1.0692	0.5457	0.4708
-4.3	0.7358	1.0568	1.1507	0.569	0.4878
-4.2	0.7798	1.099	1.2403	0.5936	0.5054
-4.1	0.8274	1.1431	1.3392	0.6195	0.5236
-4	0.8793	1.1894	1.4485	0.6469	0.5425
-3.9	0.9358	1.2379	1.5697	0.6757	0.5622
-3.8	0.9977	1.2885	1.7045	0.706	0.5825
-3.7	1.0655	1.3415	1.8549	0.7379	0.6036
-3.6	1.1401	1.3969	2.0233	0.7715	0.6254
-3.5	1.2224	1.4545	2.2126	0.8066	0.6479
-3.4	1.3135	1.5144	2.4261	0.8433	0.6711
-3.3	1.4147	1.5763	2.6679	0.8813	0.695

-3.2	1.5275	1.6398	2.9427	0.9204	0.7194
-3.1	1.6536	1.7045	3.2563	0.9603	0.7442
-3	1.795	1.7695	3.6154	1.0003	0.7692
-2.9	1.954	1.8337	4.0282	1.0395	0.7942
-2.8	2.1333	1.8955	4.5043	1.0768	0.8187
-2.7	2.3359	1.9528	5.0548	1.1106	0.8422
-2.6	2.5652	2.0026	5.6931	1.1387	0.8639
-2.5	2.8252	2.0412	6.4343	1.1586	0.8826
-2.4	3.1201	2.0641	7.2961	1.167	0.8971
-2.3	3.4548	2.0658	8.2986	1.1601	0.9057
-2.2	3.8346	2.0395	9.4643	1.1333	0.9062
-2.1	4.2654	1.9778	10.8182	1.0817	0.8961
-2	4.7535	1.8727	12.3877	1.0001	0.8726
-1.9	5.3058	1.7156	14.2017	0.8831	0.8325
-1.8	5.9294	1.4978	16.2903	0.7254	0.7724
-1.7	6.6315	1.2114	18.683	0.5228	0.6886
-1.6	7.4188	0.8496	21.4069	0.272	0.5776
-1.5	8.2965	0.4069	24.4826	-0.0289	0.4358
-1.4	9.2672	-0.1189	27.9205	-0.379	0.2601
-1.3	10.3286	-0.7276	31.7134	-0.7752	0.0476
-1.2	11.472	-1.4141	35.83	-1.2105	-0.2036
-1.1	12.6793	-2.1684	40.2063	-1.6744	-0.494
-1	13.922	-2.9741	44.7402	-2.152	-0.8221
-0.9	15.1604	-3.8081	49.2894	-2.6248	-1.1833
-0.8	16.346	-4.6409	53.6788	-3.0715	-1.5694
-0.7	17.4263	-5.438	57.717	-3.4702	-1.9678
-0.6	18.3538	-6.1641	61.2256	-3.802	-2.3621
-0.5	19.0948	-6.7882	64.0725	-4.0546	-2.7336
-0.4	19.6377	-7.2893	66.2025	-4.2258	-3.0635
-0.3	19.9965	-7.6604	67.6498	-4.3251	-3.3353
-0.2	20.2054	-7.9079	68.5241	-4.3713	-3.5366
-0.1	20.3071	-8.0467	68.9681	-4.3868	-3.6599
0	20.3366	-8.0909	69.1007	-4.3896	-3.7013
0.1	20.3071	-8.0467	68.9681	-4.3868	-3.6599
0.2	20.2054	-7.9079	68.5241	-4.3713	-3.5366
0.3	19.9965	-7.6604	67.6498	-4.3251	-3.3353
0.4	19.6377	-7.2893	66.2025	-4.2258	-3.0635
0.5	19.0948	-6.7882	64.0725	-4.0546	-2.7336
0.6	18.3538	-6.1641	61.2256	-3.802	-2.3621
0.7	17.4263	-5.438	57.717	-3.4702	-1.9678
0.8	16.346	-4.6409	53.6788	-3.0715	-1.5694
0.9	15.1604	-3.8081	49.2894	-2.6248	-1.1833
1	13.922	-2.9741	44.7402	-2.152	-0.8221
1.1	12.6793	-2.1684	40.2063	-1.6744	-0.494
1.2	11.472	-1.4141	35.83	-1.2105	-0.2036
1.3	10.3286	-0.7276	31.7134	-0.7752	0.0476
1.4	9.2672	-0.1189	27.9205	-0.379	0.2601
1.5	8.2965	0.4069	24.4826	-0.0289	0.4358
1.6	7.4188	0.8496	21.4069	0.272	0.5776
1.7	6.6315	1.2114	18.683	0.5228	0.6886
1.8	5.9294	1.4978	16.2903	0.7254	0.7724
1.9	5.3058	1.7156	14.2017	0.8831	0.8325
2	4.7535	1.8727	12.3877	1.0001	0.8726
2.1	4.2654	1.9778	10.8182	1.0817	0.8961
2.2	3.8346	2.0395	9.4643	1.1333	0.9062
2.3	3.4548	2.0658	8.2986	1.1601	0.9057
2.4	3.1201	2.0641	7.2961	1.167	0.8971
2.5	2.8252	2.0412	6.4343	1.1586	0.8826

2.6	2.5652	2.0026	5.6931	1.1387	0.8639
2.7	2.3359	1.9528	5.0548	1.1106	0.8422
2.8	2.1333	1.8955	4.5043	1.0768	0.8187
2.9	1.954	1.8337	4.0282	1.0395	0.7942
3	1.795	1.7695	3.6154	1.0003	0.7692
3.1	1.6536	1.7045	3.2563	0.9603	0.7442
3.2	1.5275	1.6398	2.9427	0.9204	0.7194
3.3	1.4147	1.5763	2.6679	0.8813	0.695
3.4	1.3135	1.5144	2.4261	0.8433	0.6711
3.5	1.2224	1.4545	2.2126	0.8066	0.6479
3.6	1.1401	1.3969	2.0233	0.7715	0.6254
3.7	1.0655	1.3415	1.8549	0.7379	0.6036
3.8	0.9977	1.2885	1.7045	0.706	0.5825
3.9	0.9358	1.2379	1.5697	0.6757	0.5622
4	0.8793	1.1894	1.4485	0.6469	0.5425
4.1	0.8274	1.1431	1.3392	0.6195	0.5236
4.2	0.7798	1.099	1.2403	0.5936	0.5054
4.3	0.7358	1.0568	1.1507	0.569	0.4878
4.4	0.6952	1.0165	1.0692	0.5457	0.4708
4.5	0.6577	0.9781	0.9948	0.5236	0.4545
4.6	0.6228	0.9414	0.927	0.5026	0.4388
4.7	0.5904	0.9064	0.8648	0.4827	0.4237
4.8	0.5602	0.8728	0.8079	0.4637	0.4091
4.9	0.5321	0.8408	0.7555	0.4457	0.3951
5	0.5059	0.8102	0.7073	0.4286	0.3816

9b-azaphenalene (D_{3h}), 30

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Charge =  0 Multiplicity = 1
C,0,1.2238281779,-0.706577528,0.
 N,0,0.,0.,0.
 C,0,-1.2238281779,-0.706577528,0.
 C,0,-1.1988278465,-2.1160300443,0.
 C,0,0.,-2.8045629534,0.
 C,0,1.1988278465,-2.1160300443,0.
 C,0,0.,1.4131550559,0.
 C,0,-1.2331218502,2.096230392,0.
 C,0,-2.4288227641,1.4022814767,0.
 C,0,-2.4319496968,0.0197996523,0.
 C,0,2.4319496968,0.0197996523,0.
 C,0,2.4288227641,1.4022814767,0.
 C,0,1.2331218502,2.096230392,0.
 H,0,-2.1498943261,-2.6300641562,0.
 H,0,0.,-3.8890705683,0.
 H,0,2.1498943261,-2.6300641562,0.
 H,0,-1.2027552098,3.1768951799,0.
 H,0,-3.3680339092,1.9445352841,0.
 H,0,-3.3526495358,-0.5468310237,0.
 H,0,3.3526495358,-0.5468310237,0.
 H,0,3.3680339092,1.9445352841,0.
 H,0,1.2027552098,3.1768951799,0.
```

Sum of electronic and zero-point Energies= -517.377032
Sum of electronic and thermal Energies= -517.368137
Sum of electronic and thermal Enthalpies= -517.367193
Sum of electronic and thermal Free Energies= -517.409189

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	1.5441	1.087	3.5454	0.5378	0.5492
-4.9	1.6197	1.1312	3.7279	0.5599	0.5713
-4.8	1.7	1.1776	3.9224	0.583	0.5946

-4.7	1.7854	1.2263	4.13	0.6074	0.6189
-4.6	1.8764	1.2775	4.3517	0.633	0.6445
-4.5	1.9733	1.3312	4.5887	0.6599	0.6713
-4.4	2.0766	1.3877	4.8422	0.6883	0.6994
-4.3	2.1869	1.447	5.1137	0.7181	0.7289
-4.2	2.3047	1.5093	5.4048	0.7495	0.7598
-4.1	2.4307	1.5749	5.7172	0.7827	0.7922
-4	2.5655	1.6437	6.0529	0.8175	0.8262
-3.9	2.7099	1.716	6.4139	0.8542	0.8618
-3.8	2.8648	1.7919	6.8026	0.8929	0.899
-3.7	3.031	1.8713	7.2218	0.9335	0.9378
-3.6	3.2096	1.9546	7.6743	0.9762	0.9784
-3.5	3.4017	2.0415	8.1636	1.021	1.0205
-3.4	3.6084	2.1319	8.6933	1.0678	1.0641
-3.3	3.8311	2.2258	9.2675	1.1167	1.1091
-3.2	4.0712	2.3227	9.8911	1.1675	1.1552
-3.1	4.3304	2.422	10.5691	1.22	1.202
-3	4.6101	2.5229	11.3076	1.2738	1.2491
-2.9	4.9124	2.6241	12.113	1.3285	1.2956
-2.8	5.239	2.7242	12.9928	1.3835	1.3407
-2.7	5.592	2.8208	13.9552	1.4378	1.383
-2.6	5.9735	2.9114	15.0091	1.4904	1.421
-2.5	6.3856	2.9923	16.1646	1.5398	1.4525
-2.4	6.8306	3.0592	17.4326	1.5841	1.4751
-2.3	7.3107	3.1069	18.8252	1.6212	1.4857
-2.2	7.828	3.1288	20.3552	1.6483	1.4805
-2.1	8.3849	3.1177	22.0369	1.6622	1.4555
-2	8.9833	3.0644	23.8855	1.6589	1.4055
-1.9	9.6255	2.9591	25.9174	1.634	1.3251
-1.8	10.3134	2.7899	28.1503	1.5819	1.208
-1.7	11.0488	2.5439	30.6027	1.4967	1.0472
-1.6	11.8332	2.2061	33.2933	1.3711	0.835
-1.5	12.667	1.7605	36.2405	1.1973	0.5632
-1.4	13.5496	1.189	39.4597	0.9661	0.2229
-1.3	14.4782	0.473	42.9615	0.6678	-0.1948
-1.2	15.4471	-0.4062	46.7476	0.2919	-0.6981
-1.1	16.4471	-1.4658	50.807	-0.1722	-1.2936
-1	17.4643	-2.7183	55.1112	-0.7338	-1.9845
-0.9	18.4807	-4.1677	59.6097	-1.3993	-2.7684
-0.8	19.4741	-5.8044	64.2268	-2.1694	-3.635
-0.7	20.4203	-7.5987	68.8595	-3.0348	-4.5639
-0.6	21.2941	-9.4956	73.378	-3.9726	-5.523
-0.5	22.0725	-11.412	77.6295	-4.943	-6.469
-0.4	22.7353	-13.2388	81.4447	-5.8889	-7.3499
-0.3	23.2665	-14.8498	84.6493	-6.7395	-8.1103
-0.2	23.6542	-16.1165	87.079	-7.4189	-8.6976
-0.1	23.89	-16.9275	88.5976	-7.8587	-9.0688
0	23.9692	-17.2069	89.1144	-8.0111	-9.1958
0.1	23.89	-16.9275	88.5976	-7.8587	-9.0688
0.2	23.6542	-16.1165	87.079	-7.4189	-8.6976
0.3	23.2665	-14.8498	84.6493	-6.7395	-8.1103
0.4	22.7353	-13.2388	81.4447	-5.8889	-7.3499
0.5	22.0725	-11.412	77.6295	-4.943	-6.469
0.6	21.2941	-9.4956	73.378	-3.9726	-5.523
0.7	20.4203	-7.5987	68.8595	-3.0348	-4.5639
0.8	19.4741	-5.8044	64.2268	-2.1694	-3.635
0.9	18.4807	-4.1677	59.6097	-1.3993	-2.7684
1	17.4643	-2.7183	55.1112	-0.7338	-1.9845

1.1	16.4471	-1.4658	50.807	-0.1722	-1.2936
1.2	15.4471	-0.4062	46.7476	0.2919	-0.6981
1.3	14.4782	0.473	42.9615	0.6678	-0.1948
1.4	13.5496	1.189	39.4597	0.9661	0.2229
1.5	12.667	1.7605	36.2405	1.1973	0.5632
1.6	11.8332	2.2061	33.2933	1.3711	0.835
1.7	11.0488	2.5439	30.6027	1.4967	1.0472
1.8	10.3134	2.7899	28.1503	1.5819	1.208
1.9	9.6255	2.9591	25.9174	1.634	1.3251
2	8.9833	3.0644	23.8855	1.6589	1.4055
2.1	8.3849	3.1177	22.0369	1.6622	1.4555
2.2	7.828	3.1288	20.3552	1.6483	1.4805
2.3	7.3107	3.1069	18.8252	1.6212	1.4857
2.4	6.8306	3.0592	17.4326	1.5841	1.4751
2.5	6.3856	2.9923	16.1646	1.5398	1.4525
2.6	5.9735	2.9114	15.0091	1.4904	1.421
2.7	5.592	2.8208	13.9552	1.4378	1.383
2.8	5.239	2.7242	12.9928	1.3835	1.3407
2.9	4.9124	2.6241	12.113	1.3285	1.2956
3	4.6101	2.5229	11.3076	1.2738	1.2491
3.1	4.3304	2.422	10.5691	1.22	1.202
3.2	4.0712	2.3227	9.8911	1.1675	1.1552
3.3	3.8311	2.2258	9.2675	1.1167	1.1091
3.4	3.6084	2.1319	8.6933	1.0678	1.0641
3.5	3.4017	2.0415	8.1636	1.021	1.0205
3.6	3.2096	1.9546	7.6743	0.9762	0.9784
3.7	3.031	1.8713	7.2218	0.9335	0.9378
3.8	2.8648	1.7919	6.8026	0.8929	0.899
3.9	2.7099	1.716	6.4139	0.8542	0.8618
4	2.5655	1.6437	6.0529	0.8175	0.8262
4.1	2.4307	1.5749	5.7172	0.7827	0.7922
4.2	2.3047	1.5093	5.4048	0.7495	0.7598
4.3	2.1869	1.447	5.1137	0.7181	0.7289
4.4	2.0766	1.3877	4.8422	0.6883	0.6994
4.5	1.9733	1.3312	4.5887	0.6599	0.6713
4.6	1.8764	1.2775	4.3517	0.633	0.6445
4.7	1.7854	1.2263	4.13	0.6074	0.6189
4.8	1.7	1.1776	3.9224	0.583	0.5946
4.9	1.6197	1.1312	3.7279	0.5599	0.5713
5	1.5441	1.087	3.5454	0.5378	0.5492

c-C_8 (C_{2h}), 31

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Charge =  0 Multiplicity = 1
C,0,0.,0.6728991857,1.7132749139
 C,0,0.,1.4103566094,0.5436797132
 C,0,0.,1.715126265,-0.6735317364
 C,0,0.,0.5450408823,-1.4106421063
 C,0,0.,-0.6728991857,-1.7132749139
 C,0,0.,-1.4103566094,-0.5436797132
 C,0,0.,-1.715126265,0.6735317364
 C,0,0.,-0.5450408823,1.4106421063
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Sum of electronic and zero-point Energies= -304.436575
Sum of electronic and thermal Energies= -304.430409
Sum of electronic and thermal Enthalpies= -304.429465
Sum of electronic and thermal Free Energies= -304.465864

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)

-5	1.8256	0.7829	4.6939	0.3916	0.3913
-4.9	1.932	0.8168	4.9793	0.4085	0.4083
-4.8	2.0466	0.8523	5.2877	0.4263	0.426
-4.7	2.1702	0.8893	5.6213	0.4448	0.4445
-4.6	2.3036	0.9281	5.9828	0.4642	0.4639
-4.5	2.4478	0.9685	6.375	0.4844	0.4841
-4.4	2.6038	1.0105	6.801	0.5054	0.5051
-4.3	2.7729	1.0541	7.2645	0.5272	0.5269
-4.2	2.9563	1.0994	7.7695	0.5499	0.5495
-4.1	3.1555	1.1461	8.3203	0.5732	0.5729
-4	3.3721	1.1943	8.9221	0.5973	0.597
-3.9	3.608	1.2437	9.5805	0.622	0.6217
-3.8	3.8653	1.2939	10.3018	0.6471	0.6468
-3.7	4.1461	1.3449	11.0932	0.6726	0.6723
-3.6	4.453	1.3961	11.9628	0.6982	0.6979
-3.5	4.7889	1.4471	12.9195	0.7237	0.7234
-3.4	5.1569	1.4972	13.9736	0.7487	0.7485
-3.3	5.5606	1.5455	15.1363	0.7729	0.7726
-3.2	6.0039	1.5912	16.4205	0.7957	0.7955
-3.1	6.491	1.6328	17.8403	0.8165	0.8163
-3	7.0269	1.669	19.4117	0.8346	0.8344
-2.9	7.6167	1.6979	21.1523	0.849	0.8489
-2.8	8.2662	1.7171	23.0814	0.8586	0.8585
-2.7	8.9814	1.7238	25.2205	0.8619	0.8619
-2.6	9.7691	1.7147	27.5927	0.8573	0.8574
-2.5	10.636	1.6851	30.223	0.8425	0.8426
-2.4	11.5893	1.63	33.1379	0.8149	0.8151
-2.3	12.636	1.5425	36.3654	0.7711	0.7714
-2.2	13.7829	1.415	39.9336	0.7073	0.7077
-2.1	15.0361	1.2375	43.8709	0.6185	0.619
-2	16.4008	0.9986	48.204	0.4991	0.4995
-1.9	17.8804	0.6849	52.9563	0.3422	0.3427
-1.8	19.4757	0.281	58.1462	0.1403	0.1407
-1.7	21.1845	-0.2301	63.7838	-0.1152	-0.1149
-1.6	23.0001	-0.8671	69.8674	-0.4336	-0.4335
-1.5	24.9101	-1.6491	76.3795	-0.8244	-0.8247
-1.4	26.8957	-2.5952	83.2823	-1.2972	-1.298
-1.3	28.9299	-3.7229	90.5126	-1.8607	-1.8622
-1.2	30.9775	-5.0461	97.9788	-2.5218	-2.5243
-1.1	32.9949	-6.573	105.5578	-3.2847	-3.2883
-1	34.9315	-8.3025	113.097	-4.1487	-4.1538
-0.9	36.733	-10.2209	120.4198	-5.107	-5.1139
-0.8	38.3464	-12.2977	127.3368	-6.1444	-6.1533
-0.7	39.7266	-14.4826	133.6624	-7.2357	-7.2469
-0.6	40.8441	-16.7034	139.2355	-8.3449	-8.3585
-0.5	41.6905	-18.8672	143.9386	-9.4256	-9.4416
-0.4	42.2822	-20.865	147.7116	-10.4234	-10.4416
-0.3	42.6577	-22.5802	150.5532	-11.28	-11.3002
-0.2	42.8691	-23.9015	152.5087	-11.9399	-11.9616
-0.1	42.9694	-24.7357	153.6439	-12.3565	-12.3792
0	42.998	-25.021	154.0149	-12.499	-12.522
0.1	42.9694	-24.7357	153.6439	-12.3565	-12.3792
0.2	42.8691	-23.9015	152.5087	-11.9399	-11.9616
0.3	42.6577	-22.5802	150.5532	-11.28	-11.3002
0.4	42.2822	-20.865	147.7116	-10.4234	-10.4416
0.5	41.6905	-18.8672	143.9386	-9.4256	-9.4416
0.6	40.8441	-16.7034	139.2355	-8.3449	-8.3585
0.7	39.7266	-14.4826	133.6624	-7.2357	-7.2469

0.8	38.3464	-12.2977	127.3368	-6.1444	-6.1533
0.9	36.733	-10.2209	120.4198	-5.107	-5.1139
1	34.9315	-8.3025	113.097	-4.1487	-4.1538
1.1	32.9949	-6.573	105.5578	-3.2847	-3.2883
1.2	30.9775	-5.0461	97.9788	-2.5218	-2.5243
1.3	28.9299	-3.7229	90.5126	-1.8607	-1.8622
1.4	26.8957	-2.5952	83.2823	-1.2972	-1.298
1.5	24.9101	-1.6491	76.3795	-0.8244	-0.8247
1.6	23.0001	-0.8671	69.8674	-0.4336	-0.4335
1.7	21.1845	-0.2301	63.7838	-0.1152	-0.1149
1.8	19.4757	0.281	58.1462	0.1403	0.1407
1.9	17.8804	0.6849	52.9563	0.3422	0.3427
2	16.4008	0.9986	48.204	0.4991	0.4995
2.1	15.0361	1.2375	43.8709	0.6185	0.619
2.2	13.7829	1.415	39.9336	0.7073	0.7077
2.3	12.636	1.5425	36.3654	0.7711	0.7714
2.4	11.5893	1.63	33.1379	0.8149	0.8151
2.5	10.636	1.6851	30.223	0.8425	0.8426
2.6	9.7691	1.7147	27.5927	0.8573	0.8574
2.7	8.9814	1.7238	25.2205	0.8619	0.8619
2.8	8.2662	1.7171	23.0814	0.8586	0.8585
2.9	7.6167	1.6979	21.1523	0.849	0.8489
3	7.0269	1.669	19.4117	0.8346	0.8344
3.1	6.491	1.6328	17.8403	0.8165	0.8163
3.2	6.0039	1.5912	16.4205	0.7957	0.7955
3.3	5.5606	1.5455	15.1363	0.7729	0.7726
3.4	5.1569	1.4972	13.9736	0.7487	0.7485
3.5	4.7889	1.4471	12.9195	0.7237	0.7234
3.6	4.453	1.3961	11.9628	0.6982	0.6979
3.7	4.1461	1.3449	11.0932	0.6726	0.6723
3.8	3.8653	1.2939	10.3018	0.6471	0.6468
3.9	3.608	1.2437	9.5805	0.622	0.6217
4	3.3721	1.1943	8.9221	0.5973	0.597
4.1	3.1555	1.1461	8.3203	0.5732	0.5729
4.2	2.9563	1.0994	7.7695	0.5499	0.5495
4.3	2.7729	1.0541	7.2645	0.5272	0.5269
4.4	2.6038	1.0105	6.801	0.5054	0.5051
4.5	2.4478	0.9685	6.375	0.4844	0.4841
4.6	2.3036	0.9281	5.9828	0.4642	0.4639
4.7	2.1702	0.8893	5.6213	0.4448	0.4445
4.8	2.0466	0.8523	5.2877	0.4263	0.426
4.9	1.932	0.8168	4.9793	0.4085	0.4083
5	1.8256	0.7829	4.6939	0.3916	0.3913

C_8 (O_h), 32

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Charge =  0 Multiplicity = 1
 C,0,-0.7366755299,0.7366755299,0.7366755299
 C,0,0.7366755299,-0.7366755299,-0.7366755299
 C,0,-0.7366755299,-0.7366755299,0.7366755299
 C,0,0.7366755299,0.7366755299,0.7366755299
 C,0,0.7366755299,-0.7366755299,0.7366755299
 C,0,0.7366755299,0.7366755299,-0.7366755299
 C,0,-0.7366755299,-0.7366755299,-0.7366755299
 C,0,-0.7366755299,0.7366755299,-0.7366755299
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Sum of electronic and zero-point Energies= -304.235270
Sum of electronic and thermal Energies= -304.230905
Sum of electronic and thermal Enthalpies= -304.229961
Sum of electronic and thermal Free Energies= -304.260163

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.03	-0.0852	0.1754	-0.0426	-0.0426
-4.9	0.0328	-0.0934	0.1917	-0.0467	-0.0467
-4.8	0.0359	-0.1026	0.2102	-0.0513	-0.0513
-4.7	0.0393	-0.1132	0.231	-0.0566	-0.0566
-4.6	0.0431	-0.1254	0.2546	-0.0627	-0.0627
-4.5	0.0473	-0.1394	0.2815	-0.0697	-0.0697
-4.4	0.0521	-0.1556	0.3121	-0.0778	-0.0778
-4.3	0.0575	-0.1746	0.3471	-0.0873	-0.0873
-4.2	0.0637	-0.1964	0.3874	-0.0982	-0.0982
-4.1	0.0707	-0.222	0.4339	-0.111	-0.111
-4	0.0787	-0.2516	0.4878	-0.1258	-0.1258
-3.9	0.088	-0.2864	0.5505	-0.1432	-0.1432
-3.8	0.0989	-0.327	0.6237	-0.1635	-0.1635
-3.7	0.1117	-0.3746	0.7097	-0.1873	-0.1873
-3.6	0.1269	-0.4304	0.8111	-0.2152	-0.2152
-3.5	0.1451	-0.4956	0.9311	-0.2478	-0.2478
-3.4	0.1674	-0.5718	1.074	-0.2859	-0.2859
-3.3	0.1948	-0.6602	1.2447	-0.3301	-0.3301
-3.2	0.2292	-0.7622	1.4497	-0.3811	-0.3811
-3.1	0.2727	-0.8786	1.6966	-0.4393	-0.4393
-3	0.3286	-1.0096	1.9954	-0.5048	-0.5048
-2.9	0.4013	-1.1542	2.358	-0.5771	-0.5771
-2.8	0.4969	-1.3088	2.7994	-0.6544	-0.6544
-2.7	0.6236	-1.4672	3.3379	-0.7336	-0.7336
-2.6	0.7924	-1.6188	3.996	-0.8094	-0.8094
-2.5	1.018	-1.7466	4.8007	-0.8733	-0.8733
-2.4	1.3195	-1.8258	5.7843	-0.9129	-0.9129
-2.3	1.7215	-1.82	6.9846	-0.91	-0.91
-2.2	2.2544	-1.681	8.444	-0.8405	-0.8405
-2.1	2.9537	-1.3466	10.2077	-0.6733	-0.6733
-2	3.858	-0.7454	12.3195	-0.3727	-0.3727
-1.9	5.0025	0.193	14.8145	0.0965	0.0965
-1.8	6.4065	1.513	17.7067	0.7565	0.7565
-1.7	8.0547	3.1916	20.9726	1.5958	1.5958
-1.6	9.8706	5.0826	24.5294	2.5413	2.5413
-1.5	11.6887	6.8534	28.2128	3.4267	3.4267
-1.4	13.2367	7.9492	31.7609	3.9746	3.9746
-1.3	14.1458	7.6236	34.8137	3.8118	3.8118
-1.2	14.0114	5.0902	36.944	2.5451	2.5451
-1.1	12.5144	-0.1844	37.7278	-0.0922	-0.0922
-1	9.5843	-8.1004	36.8531	-4.0502	-4.0502
-0.9	5.5385	-17.6242	34.2396	-8.8121	-8.8121
-0.8	1.101	-26.8116	30.1146	-13.4058	-13.4058
-0.7	-2.7684	-33.3006	24.9952	-16.6503	-16.6503
-0.6	-5.1999	-35.1594	19.5597	-17.5797	-17.5797
-0.5	-5.7421	-31.6884	14.462	-15.8442	-15.8442

-0.4	-4.525	-23.7482	10.1733	-11.8741	-11.8741
-0.3	-2.1833	-13.4686	6.9185	-6.7343	-6.7343
-0.2	0.3913	-3.5396	4.7137	-1.7698	-1.7698
-0.1	2.3396	3.5562	3.4628	1.7781	1.7781
0	3.0603	6.1206	3.0603	3.0603	3.0603
0.1	2.3396	3.5562	3.4628	1.7781	1.7781
0.2	0.3913	-3.5396	4.7137	-1.7698	-1.7698
0.3	-2.1833	-13.4686	6.9185	-6.7343	-6.7343
0.4	-4.525	-23.7482	10.1733	-11.8741	-11.8741
0.5	-5.7421	-31.6884	14.462	-15.8442	-15.8442
0.6	-5.1999	-35.1594	19.5597	-17.5797	-17.5797
0.7	-2.7684	-33.3006	24.9952	-16.6503	-16.6503
0.8	1.101	-26.8116	30.1146	-13.4058	-13.4058
0.9	5.5385	-17.6242	34.2396	-8.8121	-8.8121
1	9.5843	-8.1004	36.8531	-4.0502	-4.0502
1.1	12.5144	-0.1844	37.7278	-0.0922	-0.0922
1.2	14.0114	5.0902	36.944	2.5451	2.5451
1.3	14.1458	7.6236	34.8137	3.8118	3.8118
1.4	13.2367	7.9492	31.7609	3.9746	3.9746
1.5	11.6887	6.8534	28.2128	3.4267	3.4267
1.6	9.8706	5.0826	24.5294	2.5413	2.5413
1.7	8.0547	3.1916	20.9726	1.5958	1.5958
1.8	6.4065	1.513	17.7067	0.7565	0.7565
1.9	5.0025	0.193	14.8145	0.0965	0.0965
2	3.858	-0.7454	12.3195	-0.3727	-0.3727
2.1	2.9537	-1.3466	10.2077	-0.6733	-0.6733
2.2	2.2544	-1.681	8.444	-0.8405	-0.8405
2.3	1.7215	-1.82	6.9846	-0.91	-0.91
2.4	1.3195	-1.8258	5.7843	-0.9129	-0.9129
2.5	1.018	-1.7466	4.8007	-0.8733	-0.8733
2.6	0.7924	-1.6188	3.996	-0.8094	-0.8094
2.7	0.6236	-1.4672	3.3379	-0.7336	-0.7336
2.8	0.4969	-1.3088	2.7994	-0.6544	-0.6544
2.9	0.4013	-1.1542	2.358	-0.5771	-0.5771
3	0.3286	-1.0096	1.9954	-0.5048	-0.5048
3.1	0.2727	-0.8786	1.6966	-0.4393	-0.4393
3.2	0.2292	-0.7622	1.4497	-0.3811	-0.3811
3.3	0.1948	-0.6602	1.2447	-0.3301	-0.3301
3.4	0.1674	-0.5718	1.074	-0.2859	-0.2859
3.5	0.1451	-0.4956	0.9311	-0.2478	-0.2478
3.6	0.1269	-0.4304	0.8111	-0.2152	-0.2152
3.7	0.1117	-0.3746	0.7097	-0.1873	-0.1873
3.8	0.0989	-0.327	0.6237	-0.1635	-0.1635
3.9	0.088	-0.2864	0.5505	-0.1432	-0.1432
4	0.0787	-0.2516	0.4878	-0.1258	-0.1258
4.1	0.0707	-0.222	0.4339	-0.111	-0.111
4.2	0.0637	-0.1964	0.3874	-0.0982	-0.0982
4.3	0.0575	-0.1746	0.3471	-0.0873	-0.0873
4.4	0.0521	-0.1556	0.3121	-0.0778	-0.0778

4.5	0.0473	-0.1394	0.2815	-0.0697	-0.0697
4.6	0.0431	-0.1254	0.2546	-0.0627	-0.0627
4.7	0.0393	-0.1132	0.231	-0.0566	-0.0566
4.8	0.0359	-0.1026	0.2102	-0.0513	-0.0513
4.9	0.0328	-0.0934	0.1917	-0.0467	-0.0467
5	0.03	-0.0852	0.1754	-0.0426	-0.0426

c-C_{12} (C_{2h}), 33

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Charge =  0 Multiplicity = 1
C,0,-0.4087412856,2.5508593966,0.
 C,0,-2.4093180569,0.9216227832,0.
 C,0,-2.0000567664,-1.6257138769,0.
 C,0,0.4087412856,-2.5508593966,0.
 C,0,2.4093180569,-0.9216227832,0.
 C,0,2.0000567664,1.6257138769,0.
 C,0,2.3518632357,0.3191453658,0.
 C,0,1.4538826593,-1.8793977388,0.
 C,0,-0.8981698564,-2.1984756266,0.
 C,0,-2.3518632357,-0.3191453658,0.
 C,0,-1.4538826593,1.8793977388,0.
 C,0,0.8981698564,2.1984756266,0.
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Sum of electronic and zero-point Energies= -456.844070
Sum of electronic and thermal Energies= -456.834191
Sum of electronic and thermal Enthalpies= -456.833247
Sum of electronic and thermal Free Energies= -456.878528

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	4.3532	0.8992	12.1604	0.4536	0.4456
-4.9	4.5741	0.9262	12.7961	0.4673	0.4589
-4.8	4.8092	0.9534	13.4741	0.4811	0.4723
-4.7	5.0594	0.9807	14.1975	0.4949	0.4858
-4.6	5.3259	1.0079	14.9698	0.5087	0.4992
-4.5	5.61	1.035	15.795	0.5224	0.5126
-4.4	5.9128	1.0615	16.677	0.5359	0.5256
-4.3	6.2359	1.0872	17.6203	0.5489	0.5383
-4.2	6.5806	1.112	18.6299	0.5615	0.5505
-4.1	6.9486	1.1352	19.7107	0.5733	0.5619
-4	7.3417	1.1567	20.8684	0.5842	0.5725
-3.9	7.7615	1.1757	22.1089	0.5939	0.5818
-3.8	8.2102	1.1918	23.4387	0.6021	0.5897
-3.7	8.6896	1.2043	24.8645	0.6085	0.5958
-3.6	9.202	1.2124	26.3937	0.6127	0.5997
-3.5	9.7497	1.2152	28.0339	0.6142	0.601
-3.4	10.335	1.2117	29.7933	0.6125	0.5992
-3.3	10.9603	1.2007	31.6803	0.607	0.5937
-3.2	11.6282	1.1809	33.7039	0.5971	0.5838
-3.1	12.3413	1.1508	35.873	0.5819	0.5689
-3	13.102	1.1089	38.1972	0.5608	0.5481
-2.9	13.9129	1.0532	40.6856	0.5326	0.5206
-2.8	14.7764	0.9818	43.3475	0.4965	0.4853
-2.7	15.6947	0.8923	46.1919	0.4512	0.4411
-2.6	16.6698	0.7825	49.227	0.3956	0.3869
-2.5	17.7033	0.6497	52.4603	0.3284	0.3213
-2.4	18.7964	0.4912	55.8979	0.2481	0.2431

-2.3	19.9495	0.3041	59.5443	0.1533	0.1508
-2.2	21.1623	0.0854	63.4016	0.0425	0.0429
-2.1	22.4338	-0.1679	67.4694	-0.0858	-0.0821
-2	23.7616	-0.4587	71.7437	-0.233	-0.2257
-1.9	25.1422	-0.79	76.2165	-0.4006	-0.3894
-1.8	26.5704	-1.1641	80.8751	-0.5898	-0.5743
-1.7	28.0396	-1.5831	85.7018	-0.8015	-0.7816
-1.6	29.5415	-2.0481	90.6726	-1.0362	-1.0119
-1.5	31.0659	-2.5597	95.7574	-1.2942	-1.2655
-1.4	32.6009	-3.1167	100.9195	-1.5747	-1.542
-1.3	34.1329	-3.7166	106.1152	-1.8764	-1.8402
-1.2	35.6466	-4.3548	111.2945	-2.197	-2.1578
-1.1	37.1257	-5.0245	116.4016	-2.5329	-2.4916
-1	38.5529	-5.7166	121.3751	-2.8796	-2.837
-0.9	39.9104	-6.4192	126.1503	-3.2311	-3.1881
-0.8	41.1805	-7.1184	130.6598	-3.5804	-3.538
-0.7	42.3461	-7.7977	134.836	-3.9194	-3.8783
-0.6	43.3911	-8.4394	138.6128	-4.2393	-4.2001
-0.5	44.3011	-9.0245	141.9278	-4.5307	-4.4938
-0.4	45.0633	-9.5346	144.7244	-4.7845	-4.7501
-0.3	45.6671	-9.9523	146.9536	-4.9922	-4.9601
-0.2	46.1043	-10.2626	148.5754	-5.1464	-5.1162
-0.1	46.369	-10.4536	149.5605	-5.2413	-5.2123
0	46.4576	-10.518	149.8909	-5.2733	-5.2447
0.1	46.369	-10.4536	149.5605	-5.2413	-5.2123
0.2	46.1043	-10.2626	148.5754	-5.1464	-5.1162
0.3	45.6671	-9.9523	146.9536	-4.9922	-4.9601
0.4	45.0633	-9.5346	144.7244	-4.7845	-4.7501
0.5	44.3011	-9.0245	141.9278	-4.5307	-4.4938
0.6	43.3911	-8.4394	138.6128	-4.2393	-4.2001
0.7	42.3461	-7.7977	134.836	-3.9194	-3.8783
0.8	41.1805	-7.1184	130.6598	-3.5804	-3.538
0.9	39.9104	-6.4192	126.1503	-3.2311	-3.1881
1	38.5529	-5.7166	121.3751	-2.8796	-2.837
1.1	37.1257	-5.0245	116.4016	-2.5329	-2.4916
1.2	35.6466	-4.3548	111.2945	-2.197	-2.1578
1.3	34.1329	-3.7166	106.1152	-1.8764	-1.8402
1.4	32.6009	-3.1167	100.9195	-1.5747	-1.542
1.5	31.0659	-2.5597	95.7574	-1.2942	-1.2655
1.6	29.5415	-2.0481	90.6726	-1.0362	-1.0119
1.7	28.0396	-1.5831	85.7018	-0.8015	-0.7816
1.8	26.5704	-1.1641	80.8751	-0.5898	-0.5743
1.9	25.1422	-0.79	76.2165	-0.4006	-0.3894
2	23.7616	-0.4587	71.7437	-0.233	-0.2257
2.1	22.4338	-0.1679	67.4694	-0.0858	-0.0821
2.2	21.1623	0.0854	63.4016	0.0425	0.0429
2.3	19.9495	0.3041	59.5443	0.1533	0.1508
2.4	18.7964	0.4912	55.8979	0.2481	0.2431
2.5	17.7033	0.6497	52.4603	0.3284	0.3213
2.6	16.6698	0.7825	49.227	0.3956	0.3869
2.7	15.6947	0.8923	46.1919	0.4512	0.4411
2.8	14.7764	0.9818	43.3475	0.4965	0.4853
2.9	13.9129	1.0532	40.6856	0.5326	0.5206
3	13.102	1.1089	38.1972	0.5608	0.5481
3.1	12.3413	1.1508	35.873	0.5819	0.5689
3.2	11.6282	1.1809	33.7039	0.5971	0.5838
3.3	10.9603	1.2007	31.6803	0.607	0.5937
3.4	10.335	1.2117	29.7933	0.6125	0.5992

3.5	9.7497	1.2152	28.0339	0.6142	0.601
3.6	9.202	1.2124	26.3937	0.6127	0.5997
3.7	8.6896	1.2043	24.8645	0.6085	0.5958
3.8	8.2102	1.1918	23.4387	0.6021	0.5897
3.9	7.7615	1.1757	22.1089	0.5939	0.5818
4	7.3417	1.1567	20.8684	0.5842	0.5725
4.1	6.9486	1.1352	19.7107	0.5733	0.5619
4.2	6.5806	1.112	18.6299	0.5615	0.5505
4.3	6.2359	1.0872	17.6203	0.5489	0.5383
4.4	5.9128	1.0615	16.677	0.5359	0.5256
4.5	5.61	1.035	15.795	0.5224	0.5126
4.6	5.3259	1.0079	14.9698	0.5087	0.4992
4.7	5.0594	0.9807	14.1975	0.4949	0.4858
4.8	4.8092	0.9534	13.4741	0.4811	0.4723
4.9	4.5741	0.9262	12.7961	0.4673	0.4589
5	4.3532	0.8992	12.1604	0.4536	0.4456

c-$C_{12}H_4$ (D_{2h}), 34

Charge = 0 Multiplicity = 1
C,0,-0.0569075436,2.7781075318,0.
C,0,-2.0757088694,1.177150432,0.
C,0,-2.0291281651,-1.1588163572,0.
C,0,0.0384358316,-2.7744056453,0.
C,0,2.0571507171,-1.1734639998,0.
C,0,2.0105858001,1.1625242008,0.
C,0,2.7685937718,-0.0486460089,0.
C,0,1.1645009168,-2.0645908099,0.
C,0,-1.1717519865,-2.0151412233,0.
C,0,-2.7872668371,0.0523967246,0.
C,0,-1.1827087652,2.0679286404,0.
C,0,1.1535224864,2.0191764718,0.
H,0,3.8533423459,-0.0337628435,0.
H,0,-0.0403761873,3.8628432446,0.
H,0,-3.8719927677,0.0374373123,0.
H,0,0.0215092523,-3.8591376704,0.

Sum of electronic and zero-point Energies= -459.369073
Sum of electronic and thermal Energies= -459.358768
Sum of electronic and thermal Enthalpies= -459.357824
Sum of electronic and thermal Free Energies= -459.404560

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	4.9974	0.9607	14.0315	0.5718	0.3889
-4.9	5.2526	0.9916	14.7661	0.5921	0.3995
-4.8	5.5241	1.0231	15.5492	0.613	0.4101
-4.7	5.8132	1.0551	16.3845	0.6346	0.4205
-4.6	6.1211	1.0875	17.2758	0.6567	0.4308
-4.5	6.4492	1.1201	18.2274	0.6794	0.4407
-4.4	6.799	1.1528	19.244	0.7026	0.4502
-4.3	7.172	1.1854	20.3305	0.7262	0.4592
-4.2	7.5699	1.2176	21.4922	0.7502	0.4674
-4.1	7.9946	1.2491	22.7347	0.7744	0.4747
-4	8.4479	1.2797	24.0641	0.7989	0.4808
-3.9	8.9319	1.3088	25.4868	0.8233	0.4855
-3.8	9.4486	1.3361	27.0098	0.8476	0.4885
-3.7	10.0004	1.3609	28.6403	0.8715	0.4894

-3.6	10.5896	1.3829	30.3858	0.8949	0.488
-3.5	11.2185	1.401	32.2545	0.9174	0.4836
-3.4	11.8897	1.4145	34.2546	0.9387	0.4758
-3.3	12.6057	1.4225	36.3947	0.9585	0.464
-3.2	13.3691	1.424	38.6834	0.9764	0.4476
-3.1	14.1824	1.4176	41.1296	0.9917	0.4259
-3	15.048	1.4021	43.742	1.0041	0.398
-2.9	15.9683	1.3759	46.529	1.0129	0.363
-2.8	16.9452	1.3373	49.4985	1.0173	0.32
-2.7	17.9807	1.2844	52.6576	1.0166	0.2678
-2.6	19.0759	1.2151	56.0125	1.0099	0.2052
-2.5	20.2317	1.1272	59.5678	0.9963	0.1309
-2.4	21.4481	1.0182	63.3261	0.9747	0.0435
-2.3	22.7245	0.8856	67.288	0.944	-0.0584
-2.2	24.0591	0.7264	71.4509	0.9029	-0.1765
-2.1	25.4489	0.5378	75.809	0.8502	-0.3124
-2	26.8897	0.3166	80.3526	0.7844	-0.4678
-1.9	28.3757	0.0598	85.0673	0.7041	-0.6443
-1.8	29.8994	-0.2357	89.934	0.6079	-0.8436
-1.7	31.4518	-0.5726	94.9282	0.4944	-1.067
-1.6	33.0221	-0.9534	100.0198	0.3623	-1.3157
-1.5	34.5978	-1.3796	105.1731	0.2107	-1.5903
-1.4	36.1649	-1.8519	110.3467	0.039	-1.8909
-1.3	37.7082	-2.3694	115.4941	-0.1528	-2.2166
-1.2	39.2116	-2.9296	120.5644	-0.364	-2.5656
-1.1	40.6585	-3.5275	125.503	-0.5928	-2.9347
-1	42.0325	-4.1556	130.2531	-0.8365	-3.3191
-0.9	43.318	-4.8033	134.7574	-1.0907	-3.7126
-0.8	44.5005	-5.4576	138.9592	-1.3502	-4.1074
-0.7	45.5674	-6.1023	142.8043	-1.6082	-4.4941
-0.6	46.5079	-6.7189	146.2426	-1.8569	-4.862
-0.5	47.3139	-7.2876	149.2293	-2.0878	-5.1998
-0.4	47.9792	-7.7881	151.7256	-2.2921	-5.496
-0.3	48.4995	-8.2012	153.6999	-2.4615	-5.7397
-0.2	48.8725	-8.5099	155.1274	-2.5885	-5.9214
-0.1	49.0967	-8.7008	155.9909	-2.6672	-6.0336
0	49.1715	-8.7653	156.2799	-2.6938	-6.0715
0.1	49.0967	-8.7008	155.9909	-2.6672	-6.0336
0.2	48.8725	-8.5099	155.1274	-2.5885	-5.9214
0.3	48.4995	-8.2012	153.6999	-2.4615	-5.7397
0.4	47.9792	-7.7881	151.7256	-2.2921	-5.496
0.5	47.3139	-7.2876	149.2293	-2.0878	-5.1998
0.6	46.5079	-6.7189	146.2426	-1.8569	-4.862
0.7	45.5674	-6.1023	142.8043	-1.6082	-4.4941
0.8	44.5005	-5.4576	138.9592	-1.3502	-4.1074
0.9	43.318	-4.8033	134.7574	-1.0907	-3.7126
1	42.0325	-4.1556	130.2531	-0.8365	-3.3191
1.1	40.6585	-3.5275	125.503	-0.5928	-2.9347
1.2	39.2116	-2.9296	120.5644	-0.364	-2.5656

1.3	37.7082	-2.3694	115.4941	-0.1528	-2.2166
1.4	36.1649	-1.8519	110.3467	0.039	-1.8909
1.5	34.5978	-1.3796	105.1731	0.2107	-1.5903
1.6	33.0221	-0.9534	100.0198	0.3623	-1.3157
1.7	31.4518	-0.5726	94.9282	0.4944	-1.067
1.8	29.8994	-0.2357	89.934	0.6079	-0.8436
1.9	28.3757	0.0598	85.0673	0.7041	-0.6443
2	26.8897	0.3166	80.3526	0.7844	-0.4678
2.1	25.4489	0.5378	75.809	0.8502	-0.3124
2.2	24.0591	0.7264	71.4509	0.9029	-0.1765
2.3	22.7245	0.8856	67.288	0.944	-0.0584
2.4	21.4481	1.0182	63.3261	0.9747	0.0435
2.5	20.2317	1.1272	59.5678	0.9963	0.1309
2.6	19.0759	1.2151	56.0125	1.0099	0.2052
2.7	17.9807	1.2844	52.6576	1.0166	0.2678
2.8	16.9452	1.3373	49.4985	1.0173	0.32
2.9	15.9683	1.3759	46.529	1.0129	0.363
3	15.048	1.4021	43.742	1.0041	0.398
3.1	14.1824	1.4176	41.1296	0.9917	0.4259
3.2	13.3691	1.424	38.6834	0.9764	0.4476
3.3	12.6057	1.4225	36.3947	0.9585	0.464
3.4	11.8897	1.4145	34.2546	0.9387	0.4758
3.5	11.2185	1.401	32.2545	0.9174	0.4836
3.6	10.5896	1.3829	30.3858	0.8949	0.488
3.7	10.0004	1.3609	28.6403	0.8715	0.4894
3.8	9.4486	1.3361	27.0098	0.8476	0.4885
3.9	8.9319	1.3088	25.4868	0.8233	0.4855
4	8.4479	1.2797	24.0641	0.7989	0.4808
4.1	7.9946	1.2491	22.7347	0.7744	0.4747
4.2	7.5699	1.2176	21.4922	0.7502	0.4674
4.3	7.172	1.1854	20.3305	0.7262	0.4592
4.4	6.799	1.1528	19.244	0.7026	0.4502
4.5	6.4492	1.1201	18.2274	0.6794	0.4407
4.6	6.1211	1.0875	17.2758	0.6567	0.4308
4.7	5.8132	1.0551	16.3845	0.6346	0.4205
4.8	5.5241	1.0231	15.5492	0.613	0.4101
4.9	5.2526	0.9916	14.7661	0.5921	0.3995
5	4.9974	0.9607	14.0315	0.5718	0.3889

[*c*-As_2Te_2]$^{2-}$ (C_{2v}), 35

```
Charge = -2 Multiplicity = 1
As,0,-1.2979546566,1.2898664267,0.5454261424
 Te,0,-1.2978130612,-1.3059822924,-0.2854261424
 Te,0,1.2978130612,1.3059822924,-0.2854261424
 As,0,1.2979546566,-1.2898664267,0.5454261424
```

Sum of electronic and zero-point Energies= -4487.948156
Sum of electronic and thermal Energies= -4487.941317
Sum of electronic and thermal Enthalpies= -4487.940373
Sum of electronic and thermal Free Energies= -4487.984138

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	1.1221	2.3845	0.9818	1.1967	1.1878
-4.9	1.1797	2.4958	1.0433	1.2525	1.2433
-4.8	1.2407	2.6124	1.1098	1.3111	1.3013
-4.7	1.3054	2.7344	1.1819	1.3724	1.362
-4.6	1.3741	2.8619	1.2602	1.4364	1.4255
-4.5	1.4469	2.9953	1.3453	1.5034	1.4919
-4.4	1.5241	3.1343	1.438	1.5732	1.5611
-4.3	1.606	3.279	1.5391	1.6459	1.6331
-4.2	1.6929	3.4292	1.6495	1.7214	1.7078
-4.1	1.7851	3.5848	1.7705	1.7996	1.7852
-4	1.8828	3.7453	1.9031	1.8802	1.8651
-3.9	1.9863	3.9101	2.0489	1.9631	1.947
-3.8	2.0959	4.0781	2.2095	2.0476	2.0305
-3.7	2.2117	4.2485	2.3867	2.1333	2.1152
-3.6	2.3341	4.4195	2.5829	2.2194	2.2001
-3.5	2.4632	4.589	2.8005	2.3048	2.2842
-3.4	2.5991	4.7549	3.0426	2.3885	2.3664
-3.3	2.7421	4.9138	3.3125	2.4687	2.4451
-3.2	2.8922	5.0623	3.6145	2.5439	2.5184
-3.1	3.0497	5.1958	3.9532	2.6116	2.5842
-3	3.2146	5.3094	4.3342	2.6696	2.6398
-2.9	3.3872	5.3972	4.7643	2.7148	2.6824
-2.8	3.5678	5.4523	5.2511	2.7439	2.7084
-2.7	3.757	5.4671	5.8038	2.753	2.7141
-2.6	3.9553	5.4329	6.433	2.7379	2.695
-2.5	4.1637	5.3395	7.1515	2.6935	2.646
-2.4	4.3833	5.176	7.9738	2.6145	2.5615
-2.3	4.6156	4.9298	8.917	2.4945	2.4353
-2.2	4.8624	4.5865	10.0006	2.3265	2.26
-2.1	5.1257	4.1302	11.2469	2.1025	2.0277
-2	5.4079	3.5429	12.6809	1.8136	1.7293
-1.9	5.7117	2.8049	14.3302	1.4501	1.3548
-1.8	6.0395	1.8942	16.2243	1.0009	0.8933
-1.7	6.3938	0.7872	18.3942	0.4542	0.333
-1.6	6.7764	-0.5413	20.8705	-0.2025	-0.3388
-1.5	7.1882	-2.1173	23.6818	-0.9823	-1.135
-1.4	7.6284	-3.9664	26.8516	-1.8982	-2.0682
-1.3	8.0942	-6.112	30.3947	-2.962	-3.15
-1.2	8.5799	-8.5728	34.3126	-4.1834	-4.3894
-1.1	9.0769	-11.3579	38.5885	-5.5672	-5.7907
-1	9.5736	-14.4615	43.1821	-7.111	-7.3505
-0.9	10.0563	-17.8557	48.0247	-8.8013	-9.0544
-0.8	10.5109	-21.4829	53.0157	-10.6098	-10.8731
-0.7	10.9243	-25.2489	58.0218	-12.4899	-12.759
-0.6	11.2869	-29.0186	62.8794	-14.3744	-14.6442
-0.5	11.5946	-32.6173	67.401	-16.1763	-16.441
-0.4	11.849	-35.8395	71.3865	-17.7929	-18.0466
-0.3	12.0573	-38.4655	74.6375	-19.1142	-19.3513
-0.2	12.2297	-40.2855	76.9747	-20.0349	-20.2506
-0.1	12.376	-41.1277	78.2556	-20.4686	-20.6591
0	12.5015	-40.8851	78.3896	-20.361	-20.5241
0.1	12.6047	-39.5352	77.3492	-19.7001	-19.8351
0.2	12.6754	-37.1483	75.1744	-18.5202	-18.6281
0.3	12.6963	-33.8806	71.9694	-16.8987	-16.9819
0.4	12.646	-29.955	67.8929	-14.9466	-15.0084
0.5	12.5036	-25.6316	63.1423	-12.7936	-12.838

0.6	12.2531	-21.1751	57.9345	-10.572	-10.6031
0.7	11.8874	-16.8251	52.4873	-8.4017	-8.4234
0.8	11.4092	-12.7747	47.0024	-6.3794	-6.3953
0.9	10.8312	-9.1587	41.6521	-4.5729	-4.5858
1	10.1736	-6.0519	36.5726	-3.02	-3.0319
1.1	9.4613	-3.4768	31.8608	-1.7323	-1.7445
1.2	8.7207	-1.4142	27.5762	-0.7005	-0.7137
1.3	7.9763	0.1827	23.7462	0.0986	0.0841
1.4	7.2494	1.3766	20.3716	0.6961	0.6805
1.5	6.5565	2.2351	17.4344	1.1257	1.1094
1.6	5.9093	2.8244	14.9036	1.4205	1.4039
1.7	5.3148	3.2039	12.7406	1.6101	1.5938
1.8	4.7763	3.4249	10.9041	1.7203	1.7046
1.9	4.2939	3.5294	9.3524	1.7721	1.7573
2	3.8656	3.5506	8.0461	1.782	1.7686
2.1	3.4877	3.5145	6.9488	1.7632	1.7513
2.2	3.156	3.4399	6.0281	1.7251	1.7148
2.3	2.8657	3.3413	5.2557	1.675	1.6663
2.4	2.6118	3.2285	4.6069	1.6178	1.6107
2.5	2.3898	3.1084	4.061	1.5569	1.5515
2.6	2.1954	2.9858	3.6003	1.4949	1.4909
2.7	2.0245	2.8635	3.2101	1.4331	1.4304
2.8	1.8738	2.7436	2.878	1.3725	1.3711
2.9	1.7403	2.6269	2.5939	1.3136	1.3133
3	1.6213	2.5144	2.3496	1.2569	1.2575
3.1	1.5148	2.4062	2.138	1.2024	1.2038
3.2	1.4189	2.3028	1.9538	1.1503	1.1525
3.3	1.3322	2.2041	1.7923	1.1007	1.1034
3.4	1.2534	2.1103	1.6499	1.0536	1.0567
3.5	1.1817	2.0214	1.5236	1.0089	1.0125
3.6	1.1161	1.9374	1.4109	0.9668	0.9706
3.7	1.056	1.8581	1.3098	0.927	0.9311
3.8	1.0009	1.7837	1.2188	0.8897	0.894
3.9	0.9502	1.714	1.1365	0.8548	0.8592
4	0.9035	1.6487	1.0619	0.8221	0.8266
4.1	0.8605	1.5876	0.9939	0.7915	0.7961
4.2	0.8208	1.5306	0.9319	0.763	0.7676
4.3	0.7841	1.4772	0.8752	0.7363	0.7409
4.4	0.7502	1.4274	0.8231	0.7114	0.716
4.5	0.7187	1.3807	0.7754	0.6881	0.6926
4.6	0.6894	1.3367	0.7315	0.6661	0.6706
4.7	0.6621	1.2953	0.691	0.6454	0.6499
4.8	0.6365	1.256	0.6536	0.6258	0.6302
4.9	0.6126	1.2185	0.6191	0.6071	0.6114
5	0.59	1.1827	0.5872	0.5892	0.5935

[*c*-As_2Te_2]$^{2-}$ (Singlet, TS) (C_{2h})

```
Charge = -2 Multiplicity = 1
As,0,-1.9332684135,0.0016575391,0.
 Te,0,0.0020469993,1.945413716,0.
 Te,0,-0.0020469993,-1.945413716,0.
 As,0,1.9332684135,-0.0016575391,0.
```

Sum of electronic and zero-point Energies= -4487.941808
Sum of electronic and thermal Energies= -4487.935855
Sum of electronic and thermal Enthalpies= -4487.934911
Sum of electronic and thermal Free Energies= -4487.976509

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.868	2.5298	0.0742	1.2698	1.26
-4.9	0.9542	2.767	0.0955	1.389	1.378
-4.8	1.0497	3.0298	0.1194	1.5211	1.5087
-4.7	1.1558	3.321	0.1463	1.6675	1.6535
-4.6	1.2735	3.644	0.1766	1.8298	1.8142
-4.5	1.4043	4.0021	0.2107	2.0098	1.9923
-4.4	1.5494	4.3993	0.249	2.2095	2.1898
-4.3	1.7107	4.84	0.2921	2.431	2.409
-4.2	1.8899	5.329	0.3407	2.6768	2.6522
-4.1	2.089	5.8716	0.3954	2.9496	2.922
-4	2.3103	6.4738	0.4572	3.2523	3.2215
-3.9	2.5564	7.1422	0.5269	3.5883	3.5539
-3.8	2.8299	7.8838	0.6058	3.9611	3.9227
-3.7	3.134	8.7069	0.6952	4.3749	4.332
-3.6	3.4721	9.6197	0.7965	4.8338	4.7859
-3.5	3.8479	10.6319	0.9118	5.3427	5.2892
-3.4	4.2656	11.7536	1.0431	5.9067	5.8469
-3.3	4.7295	12.9955	1.193	6.5311	6.4644
-3.2	5.2445	14.369	1.3645	7.2218	7.1472
-3.1	5.8156	15.8857	1.5612	7.9845	7.9012
-3	6.4483	17.5576	1.7874	8.8253	8.7323
-2.9	7.1481	19.3961	2.0481	9.75	9.6461
-2.8	7.9206	21.4126	2.3491	10.7643	10.6483
-2.7	8.7715	23.6168	2.6977	11.8732	11.7436
-2.6	9.7063	26.0169	3.1018	13.0808	12.9361
-2.5	10.73	28.6187	3.5714	14.3901	14.2286
-2.4	11.8472	31.4239	4.1177	15.802	15.6219
-2.3	13.0612	34.4298	4.7538	17.3152	17.1146
-2.2	14.3742	37.6276	5.495	18.9254	18.7022
-2.1	15.7865	41.0009	6.3587	20.6245	20.3764
-2	17.2961	44.5237	7.3645	22.3994	22.1243
-1.9	18.8979	48.1592	8.5346	24.2319	23.9273
-1.8	20.5834	51.8573	9.8929	26.0968	25.7605
-1.7	22.3398	55.5542	11.4652	27.9623	27.5919
-1.6	24.1496	59.1707	13.278	29.7886	29.3821
-1.5	25.99	62.6132	15.3569	31.5289	31.0843
-1.4	27.8335	65.7756	17.725	33.13	32.6456
-1.3	29.6479	68.5439	20.3999	34.5346	34.0093
-1.2	31.3977	70.8034	23.3898	35.6851	35.1183
-1.1	33.0459	72.4482	26.6895	36.5283	35.9199
-1	34.5567	73.3946	30.2756	37.022	36.3726
-0.9	35.8989	73.5949	34.1018	37.1419	36.453
-0.8	37.0488	73.051	38.0953	36.8887	36.1623
-0.7	37.9934	71.8252	42.1551	36.2931	35.5321
-0.6	38.7327	70.0453	46.1528	35.4187	34.6266
-0.5	39.2796	67.9007	49.938	34.36	33.5407
-0.4	39.6584	65.629	53.3463	33.2355	32.3935
-0.3	39.9014	63.4919	56.2124	32.1759	31.316
-0.2	40.043	61.744	58.3849	31.3084	30.4356
-0.1	40.1137	60.5996	59.7416	30.7401	29.8595
0	40.1348	60.2014	60.2031	30.5423	29.6591
0.1	40.1137	60.5996	59.7416	30.7401	29.8595
0.2	40.043	61.744	58.3849	31.3084	30.4356
0.3	39.9014	63.4919	56.2124	32.1759	31.316
0.4	39.6584	65.629	53.3463	33.2355	32.3935
0.5	39.2796	67.9007	49.938	34.36	33.5407

0.6	38.7327	70.0453	46.1528	35.4187	34.6266
0.7	37.9934	71.8252	42.1551	36.2931	35.5321
0.8	37.0488	73.051	38.0953	36.8887	36.1623
0.9	35.8989	73.5949	34.1018	37.1419	36.453
1	34.5567	73.3946	30.2756	37.022	36.3726
1.1	33.0459	72.4482	26.6895	36.5283	35.9199
1.2	31.3977	70.8034	23.3898	35.6851	35.1183
1.3	29.6479	68.5439	20.3999	34.5346	34.0093
1.4	27.8335	65.7756	17.725	33.13	32.6456
1.5	25.99	62.6132	15.3569	31.5289	31.0843
1.6	24.1496	59.1707	13.278	29.7886	29.3821
1.7	22.3398	55.5542	11.4652	27.9623	27.5919
1.8	20.5834	51.8573	9.8929	26.0968	25.7605
1.9	18.8979	48.1592	8.5346	24.2319	23.9273
2	17.2961	44.5237	7.3645	22.3994	22.1243
2.1	15.7865	41.0009	6.3587	20.6245	20.3764
2.2	14.3742	37.6276	5.495	18.9254	18.7022
2.3	13.0612	34.4298	4.7538	17.3152	17.1146
2.4	11.8472	31.4239	4.1177	15.802	15.6219
2.5	10.73	28.6187	3.5714	14.3901	14.2286
2.6	9.7063	26.0169	3.1018	13.0808	12.9361
2.7	8.7715	23.6168	2.6977	11.8732	11.7436
2.8	7.9206	21.4126	2.3491	10.7643	10.6483
2.9	7.1481	19.3961	2.0481	9.75	9.6461
3	6.4483	17.5576	1.7874	8.8253	8.7323
3.1	5.8156	15.8857	1.5612	7.9845	7.9012
3.2	5.2445	14.369	1.3645	7.2218	7.1472
3.3	4.7295	12.9955	1.193	6.5311	6.4644
3.4	4.2656	11.7536	1.0431	5.9067	5.8469
3.5	3.8479	10.6319	0.9118	5.3427	5.2892
3.6	3.4721	9.6197	0.7965	4.8338	4.7859
3.7	3.134	8.7069	0.6952	4.3749	4.332
3.8	2.8299	7.8838	0.6058	3.9611	3.9227
3.9	2.5564	7.1422	0.5269	3.5883	3.5539
4	2.3103	6.4738	0.4572	3.2523	3.2215
4.1	2.089	5.8716	0.3954	2.9496	2.922
4.2	1.8899	5.329	0.3407	2.6768	2.6522
4.3	1.7107	4.84	0.2921	2.431	2.409
4.4	1.5494	4.3993	0.249	2.2095	2.1898
4.5	1.4043	4.0021	0.2107	2.0098	1.9923
4.6	1.2735	3.644	0.1766	1.8298	1.8142
4.7	1.1558	3.321	0.1463	1.6675	1.6535
4.8	1.0497	3.0298	0.1194	1.5211	1.5087
4.9	0.9542	2.767	0.0955	1.389	1.378
5	0.868	2.5298	0.0742	1.2698	1.26

$[c\text{-}As_2Te_2]^{2-}$ (Triplet, TS) (C_{2h})

```
Charge = -2 Multiplicity = 3
As,0,-1.8354765967,0.0014888699,0.
 Te,0,0.0022213333,2.0054721625,0.
 Te,0,-0.0022213333,-2.0054721625,0.
 As,0,1.8354765967,-0.0014888699,0.
```

Sum of electronic and zero-point Energies= -4487.953494
Sum of electronic and thermal Energies= -4487.947220
Sum of electronic and thermal Enthalpies= -4487.946276
Sum of electronic and thermal Free Energies= -4487.990241

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.2266	1.483	-2.1629	0.7577	0.7253
-4.9	-0.2342	1.5565	-2.259	0.7955	0.761
-4.8	-0.2417	1.6349	-2.3602	0.8358	0.7991
-4.7	-0.2492	1.7191	-2.4667	0.8791	0.84
-4.6	-0.2566	1.8091	-2.5788	0.9253	0.8838
-4.5	-0.2637	1.9057	-2.6968	0.9749	0.9308
-4.4	-0.2706	2.0092	-2.821	1.0281	0.9811
-4.3	-0.2771	2.1204	-2.9516	1.0852	1.0352
-4.2	-0.2831	2.2396	-3.0888	1.1464	1.0932
-4.1	-0.2885	2.3675	-3.2331	1.212	1.1555
-4	-0.2932	2.5049	-3.3844	1.2825	1.2224
-3.9	-0.2969	2.6524	-3.543	1.3582	1.2942
-3.8	-0.2995	2.8107	-3.7091	1.4394	1.3713
-3.7	-0.3007	2.9804	-3.8826	1.5264	1.454
-3.6	-0.3004	3.1623	-4.0635	1.6197	1.5426
-3.5	-0.2982	3.357	-4.2515	1.7196	1.6374
-3.4	-0.2938	3.5648	-4.4462	1.8262	1.7386
-3.3	-0.287	3.786	-4.6471	1.9397	1.8463
-3.2	-0.2776	4.0205	-4.8533	2.0601	1.9604
-3.1	-0.2653	4.2677	-5.0635	2.1871	2.0806
-3	-0.2499	4.5264	-5.276	2.3202	2.2062
-2.9	-0.2313	4.7947	-5.4886	2.4584	2.3363
-2.8	-0.2096	5.0696	-5.6985	2.6003	2.4693
-2.7	-0.185	5.347	-5.9021	2.7438	2.6032
-2.6	-0.1579	5.6209	-6.0948	2.8861	2.7348
-2.5	-0.129	5.8841	-6.271	3.0235	2.8606
-2.4	-0.099	6.1266	-6.4237	3.1512	2.9754
-2.3	-0.0693	6.3365	-6.5445	3.2631	3.0734
-2.2	-0.0415	6.4988	-6.6233	3.3519	3.1469
-2.1	-0.0177	6.5951	-6.6481	3.4084	3.1867
-2	-0.0002	6.6039	-6.6047	3.4218	3.1821
-1.9	0.0077	6.4995	-6.4765	3.3793	3.1202
-1.8	0.0024	6.2523	-6.245	3.266	2.9863
-1.7	-0.0203	5.8284	-5.8893	3.0649	2.7635
-1.6	-0.0654	5.1906	-5.3867	2.7573	2.4333
-1.5	-0.1382	4.2994	-4.714	2.3233	1.9761
-1.4	-0.2446	3.1141	-3.8479	1.7423	1.3718
-1.3	-0.3903	1.5968	-2.7677	0.9952	0.6016
-1.2	-0.5805	-0.2841	-1.4575	0.0658	-0.3499
-1.1	-0.8192	-2.5481	0.0905	-1.0557	-1.4924
-1	-1.1082	-5.1965	1.8719	-2.3703	-2.8262
-0.9	-1.446	-8.2048	3.8669	-3.8659	-4.3389
-0.8	-1.827	-11.5171	6.0361	-5.5147	-6.0024
-0.7	-2.2405	-15.0406	8.319	-7.2704	-7.7702
-0.6	-2.6709	-18.6459	10.6333	-9.0682	-9.5777
-0.5	-3.0974	-22.17	12.8779	-10.8266	-11.3434
-0.4	-3.4959	-25.4268	14.939	-12.4524	-12.9744
-0.3	-3.841	-28.222	16.699	-13.8483	-14.3737
-0.2	-4.1082	-30.373	18.0484	-14.9227	-15.4503
-0.1	-4.2774	-31.7297	18.8974	-15.6005	-16.1292
0	-4.3354	-32.1934	19.1872	-15.8322	-16.3612
0.1	-4.2774	-31.7297	18.8974	-15.6005	-16.1292
0.2	-4.1082	-30.373	18.0484	-14.9227	-15.4503
0.3	-3.841	-28.222	16.699	-13.8483	-14.3737
0.4	-3.4959	-25.4268	14.939	-12.4524	-12.9744
0.5	-3.0974	-22.17	12.8779	-10.8266	-11.3434

0.6	-2.6709	-18.6459	10.6333	-9.0682	-9.5777
0.7	-2.2405	-15.0406	8.319	-7.2704	-7.7702
0.8	-1.827	-11.5171	6.0361	-5.5147	-6.0024
0.9	-1.446	-8.2048	3.8669	-3.8659	-4.3389
1	-1.1082	-5.1965	1.8719	-2.3703	-2.8262
1.1	-0.8192	-2.5481	0.0905	-1.0557	-1.4924
1.2	-0.5805	-0.2841	-1.4575	0.0658	-0.3499
1.3	-0.3903	1.5968	-2.7677	0.9952	0.6016
1.4	-0.2446	3.1141	-3.8479	1.7423	1.3718
1.5	-0.1382	4.2994	-4.714	2.3233	1.9761
1.6	-0.0654	5.1906	-5.3867	2.7573	2.4333
1.7	-0.0203	5.8284	-5.8893	3.0649	2.7635
1.8	0.0024	6.2523	-6.245	3.266	2.9863
1.9	0.0077	6.4995	-6.4765	3.3793	3.1202
2	-0.0002	6.6039	-6.6047	3.4218	3.1821
2.1	-0.0177	6.5951	-6.6481	3.4084	3.1867
2.2	-0.0415	6.4988	-6.6233	3.3519	3.1469
2.3	-0.0693	6.3365	-6.5445	3.2631	3.0734
2.4	-0.099	6.1266	-6.4237	3.1512	2.9754
2.5	-0.129	5.8841	-6.271	3.0235	2.8606
2.6	-0.1579	5.6209	-6.0948	2.8861	2.7348
2.7	-0.185	5.347	-5.9021	2.7438	2.6032
2.8	-0.2096	5.0696	-5.6985	2.6003	2.4693
2.9	-0.2313	4.7947	-5.4886	2.4584	2.3363
3	-0.2499	4.5264	-5.276	2.3202	2.2062
3.1	-0.2653	4.2677	-5.0635	2.1871	2.0806
3.2	-0.2776	4.0205	-4.8533	2.0601	1.9604
3.3	-0.287	3.786	-4.6471	1.9397	1.8463
3.4	-0.2938	3.5648	-4.4462	1.8262	1.7386
3.5	-0.2982	3.357	-4.2515	1.7196	1.6374
3.6	-0.3004	3.1623	-4.0635	1.6197	1.5426
3.7	-0.3007	2.9804	-3.8826	1.5264	1.454
3.8	-0.2995	2.8107	-3.7091	1.4394	1.3713
3.9	-0.2969	2.6524	-3.543	1.3582	1.2942
4	-0.2932	2.5049	-3.3844	1.2825	1.2224
4.1	-0.2885	2.3675	-3.2331	1.212	1.1555
4.2	-0.2831	2.2396	-3.0888	1.1464	1.0932
4.3	-0.2771	2.1204	-2.9516	1.0852	1.0352
4.4	-0.2706	2.0092	-2.821	1.0281	0.9811
4.5	-0.2637	1.9057	-2.6968	0.9749	0.9308
4.6	-0.2566	1.8091	-2.5788	0.9253	0.8838
4.7	-0.2492	1.7191	-2.4667	0.8791	0.84
4.8	-0.2417	1.6349	-2.3602	0.8358	0.7991
4.9	-0.2342	1.5565	-2.259	0.7955	0.761
5	-0.2266	1.483	-2.1629	0.7577	0.7253

[*c*-As_2Te_2]$^{2-}$ (Singlet, exp.) (C_{2h})

```
Charge = -2 Multiplicity = 1
As    -1.0387     1.2520      0.0000
Te    -1.6408     -1.4897     0.0000
Te    1.6408      1.4897      -0.0000
As    1.0387      -1.2520     -0.0000
```

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.6507	3.0858	-1.1337	1.9398	1.146
-4.9	0.6987	3.2706	-1.1746	2.0546	1.216

-4.8	0.7512	3.4703	-1.2169	2.1785	1.2918
-4.7	0.8086	3.6864	-1.2607	2.3123	1.3741
-4.6	0.8714	3.9201	-1.306	2.4568	1.4633
-4.5	0.9401	4.1731	-1.3527	2.6129	1.5602
-4.4	1.0154	4.4472	-1.4009	2.7818	1.6654
-4.3	1.0979	4.7442	-1.4506	2.9645	1.7797
-4.2	1.1882	5.0661	-1.5015	3.1622	1.9039
-4.1	1.2871	5.415	-1.5538	3.3762	2.0388
-4	1.3954	5.7934	-1.6071	3.6079	2.1855
-3.9	1.514	6.2034	-1.6614	3.8585	2.3449
-3.8	1.6438	6.6478	-1.7164	4.1297	2.5181
-3.7	1.7859	7.1294	-1.7718	4.4231	2.7063
-3.6	1.9412	7.6506	-1.8271	4.7401	2.9105
-3.5	2.1108	8.2144	-1.8819	5.0823	3.1321
-3.4	2.2959	8.8234	-1.9356	5.4513	3.3721
-3.3	2.4976	9.4802	-1.9873	5.8486	3.6316
-3.2	2.717	10.1869	-2.036	6.2754	3.9115
-3.1	2.9549	10.9453	-2.0806	6.7327	4.2126
-3	3.2124	11.7565	-2.1194	7.2214	4.5351
-2.9	3.49	12.6207	-2.1506	7.7418	4.8789
-2.8	3.7884	13.5371	-2.1719	8.2937	5.2434
-2.7	4.1076	14.5034	-2.1805	8.8763	5.6271
-2.6	4.4475	15.5157	-2.1732	9.4882	6.0275
-2.5	4.8074	16.568	-2.1458	10.127	6.441
-2.4	5.1862	17.652	-2.0935	10.7894	6.8626
-2.3	5.582	18.7567	-2.0107	11.4711	7.2856
-2.2	5.9923	19.8675	-1.8907	12.1663	7.7012
-2.1	6.4138	20.967	-1.7258	12.8685	8.0985
-2	6.8422	22.0337	-1.507	13.5698	8.4639
-1.9	7.2727	23.0422	-1.2242	14.2613	8.7809
-1.8	7.6993	23.9638	-0.866	14.9337	9.0301
-1.7	8.1156	24.7667	-0.42	15.5777	9.189
-1.6	8.5149	25.4176	0.127	16.1849	9.2327
-1.5	8.8907	25.8833	0.7888	16.7491	9.1342
-1.4	9.2374	26.1337	1.5785	17.2676	8.8661
-1.3	9.5511	26.1451	2.5082	17.7425	8.4026
-1.2	9.8301	25.9037	3.5867	18.1817	7.722
-1.1	10.0758	25.4091	4.8183	18.5989	6.8102
-1	10.2926	24.678	6.1997	19.0131	5.6649
-0.9	10.4874	23.7442	7.7181	19.4456	4.2986
-0.8	10.6689	22.6588	9.3479	19.9162	2.7426
-0.7	10.8451	21.486	11.0492	20.4375	1.0485
-0.6	11.0213	20.2976	12.7664	21.0099	-0.7123
-0.5	11.1985	19.166	14.4294	21.6171	-2.4511
-0.4	11.3712	18.1563	15.9573	22.2247	-4.0684
-0.3	11.5287	17.322	17.2641	22.7838	-5.4618
-0.2	11.6567	16.7022	18.268	23.2385	-6.5363
-0.1	11.7408	16.3215	18.9008	23.5363	-7.2148
0	11.7701	16.1933	19.117	23.6401	-7.4468
0.1	11.7408	16.3215	18.9008	23.5363	-7.2148
0.2	11.6567	16.7022	18.268	23.2385	-6.5363
0.3	11.5287	17.322	17.2641	22.7838	-5.4618
0.4	11.3712	18.1563	15.9573	22.2247	-4.0684
0.5	11.1985	19.166	14.4294	21.6171	-2.4511
0.6	11.0213	20.2976	12.7664	21.0099	-0.7123
0.7	10.8451	21.486	11.0492	20.4375	1.0485
0.8	10.6689	22.6588	9.3479	19.9162	2.7426
0.9	10.4874	23.7442	7.7181	19.4456	4.2986

1	10.2926	24.678	6.1997	19.0131	5.6649
1.1	10.0758	25.4091	4.8183	18.5989	6.8102
1.2	9.8301	25.9037	3.5867	18.1817	7.722
1.3	9.5511	26.1451	2.5082	17.7425	8.4026
1.4	9.2374	26.1337	1.5785	17.2676	8.8661
1.5	8.8907	25.8833	0.7888	16.7491	9.1342
1.6	8.5149	25.4176	0.127	16.1849	9.2327
1.7	8.1156	24.7667	-0.42	15.5777	9.189
1.8	7.6993	23.9638	-0.866	14.9337	9.0301
1.9	7.2727	23.0422	-1.2242	14.2613	8.7809
2	6.8422	22.0337	-1.507	13.5698	8.4639
2.1	6.4138	20.967	-1.7258	12.8685	8.0985
2.2	5.9923	19.8675	-1.8907	12.1663	7.7012
2.3	5.582	18.7567	-2.0107	11.4711	7.2856
2.4	5.1862	17.652	-2.0935	10.7894	6.8626
2.5	4.8074	16.568	-2.1458	10.127	6.441
2.6	4.4475	15.5157	-2.1732	9.4882	6.0275
2.7	4.1076	14.5034	-2.1805	8.8763	5.6271
2.8	3.7884	13.5371	-2.1719	8.2937	5.2434
2.9	3.49	12.6207	-2.1506	7.7418	4.8789
3	3.2124	11.7565	-2.1194	7.2214	4.5351
3.1	2.9549	10.9453	-2.0806	6.7327	4.2126
3.2	2.717	10.1869	-2.036	6.2754	3.9115
3.3	2.4976	9.4802	-1.9873	5.8486	3.6316
3.4	2.2959	8.8234	-1.9356	5.4513	3.3721
3.5	2.1108	8.2144	-1.8819	5.0823	3.1321
3.6	1.9412	7.6506	-1.8271	4.7401	2.9105
3.7	1.7859	7.1294	-1.7718	4.4231	2.7063
3.8	1.6438	6.6478	-1.7164	4.1297	2.5181
3.9	1.514	6.2034	-1.6614	3.8585	2.3449
4	1.3954	5.7934	-1.6071	3.6079	2.1855
4.1	1.2871	5.415	-1.5538	3.3762	2.0388
4.2	1.1882	5.0661	-1.5015	3.1622	1.9039
4.3	1.0979	4.7442	-1.4506	2.9645	1.7797
4.4	1.0154	4.4472	-1.4009	2.7818	1.6654
4.5	0.9401	4.1731	-1.3527	2.6129	1.5602
4.6	0.8714	3.9201	-1.306	2.4568	1.4633
4.7	0.8086	3.6864	-1.2607	2.3123	1.3741
4.8	0.7512	3.4703	-1.2169	2.1785	1.2918
4.9	0.6987	3.2706	-1.1746	2.0546	1.216
5	0.6507	3.0858	-1.1337	1.9398	1.146

$[c\text{-}P_4]^{2-}$ (D_{4h}), 36

```
Charge = -2 Multiplicity = 1
 P,0,-0.8481414019,-0.0003744273,0.0045810185
 P,0,0.6981682741,-1.5509770139,-0.003840006
 P,0,2.2482637418,-0.0061172384,0.0042888464
 P,0,0.703809386,1.5453686797,0.011470141
```

Sum of electronic and zero-point Energies= -1365.470327
Sum of electronic and thermal Energies= -1365.465423
Sum of electronic and thermal Enthalpies= -1365.464479
Sum of electronic and thermal Free Energies= -1365.499833

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.0696	0.5394	-0.7481	0.2697	0.2697
-4.9	-0.08	0.5508	-0.791	0.2754	0.2754

-4.8	-0.0916	0.562	-0.837	0.281	0.281
-4.7	-0.1044	0.5728	-0.8861	0.2864	0.2864
-4.6	-0.1185	0.5832	-0.9388	0.2916	0.2916
-4.5	-0.1339	0.5934	-0.9953	0.2967	0.2967
-4.4	-0.1508	0.6034	-1.0557	0.3017	0.3017
-4.3	-0.169	0.6136	-1.1205	0.3068	0.3068
-4.2	-0.1886	0.624	-1.1899	0.312	0.312
-4.1	-0.2097	0.635	-1.2641	0.3175	0.3175
-4	-0.2321	0.6472	-1.3435	0.3236	0.3236
-3.9	-0.2557	0.6612	-1.4283	0.3306	0.3306
-3.8	-0.2803	0.6778	-1.5188	0.3389	0.3389
-3.7	-0.3058	0.6976	-1.6152	0.3488	0.3488
-3.6	-0.3318	0.722	-1.7174	0.361	0.361
-3.5	-0.3579	0.7518	-1.8257	0.3759	0.3759
-3.4	-0.3837	0.7886	-1.9397	0.3943	0.3943
-3.3	-0.4086	0.8334	-2.0591	0.4167	0.4167
-3.2	-0.4318	0.8878	-2.1833	0.4439	0.4439
-3.1	-0.4527	0.9532	-2.3112	0.4766	0.4766
-3	-0.4702	1.0306	-2.4413	0.5153	0.5153
-2.9	-0.4834	1.1212	-2.5714	0.5606	0.5606
-2.8	-0.491	1.2256	-2.6985	0.6128	0.6128
-2.7	-0.4915	1.3438	-2.8183	0.6719	0.6719
-2.6	-0.4836	1.4748	-2.9255	0.7374	0.7374
-2.5	-0.4652	1.6168	-3.0124	0.8084	0.8084
-2.4	-0.4343	1.7666	-3.0695	0.8833	0.8833
-2.3	-0.3884	1.9188	-3.084	0.9594	0.9594
-2.2	-0.3245	2.0658	-3.0392	1.0329	1.0329
-2.1	-0.2391	2.1964	-2.9137	1.0982	1.0982
-2	-0.1281	2.2958	-2.6802	1.1479	1.1479
-1.9	0.0133	2.344	-2.3042	1.172	1.172
-1.8	0.1907	2.3144	-1.7424	1.1572	1.1572
-1.7	0.4104	2.173	-0.942	1.0865	1.0865
-1.6	0.6791	1.8772	0.1602	0.9386	0.9386
-1.5	1.0041	1.3744	1.6378	0.6872	0.6872
-1.4	1.3921	0.603	3.5732	0.3015	0.3015
-1.3	1.849	-0.5072	6.0541	-0.2536	-0.2536
-1.2	2.3789	-2.03	9.1669	-1.015	-1.015
-1.1	2.9829	-4.0382	12.9871	-2.0191	-2.0191
-1	3.6576	-6.5928	17.5657	-3.2964	-3.2964
-0.9	4.3942	-9.7292	22.9119	-4.8646	-4.8646
-0.8	5.1775	-13.4416	28.9739	-6.7208	-6.7208
-0.7	5.9851	-17.6648	35.6202	-8.8324	-8.8324
-0.6	6.7886	-22.26	42.6259	-11.13	-11.13
-0.5	7.5545	-27.0064	49.6699	-13.5032	-13.5032
-0.4	8.2468	-31.6082	56.3485	-15.8041	-15.8041
-0.3	8.8298	-35.7184	62.2079	-17.8592	-17.8592
-0.2	9.2719	-38.9804	66.7961	-19.4902	-19.4902
-0.1	9.5478	-41.0818	69.7253	-20.5409	-20.5409
0	9.6417	-41.8078	70.7327	-20.9039	-20.9039
0.1	9.5478	-41.0818	69.7253	-20.5409	-20.5409
0.2	9.2719	-38.9804	66.7961	-19.4902	-19.4902
0.3	8.8298	-35.7184	62.2079	-17.8592	-17.8592
0.4	8.2468	-31.6082	56.3485	-15.8041	-15.8041
0.5	7.5545	-27.0064	49.6699	-13.5032	-13.5032
0.6	6.7886	-22.26	42.6259	-11.13	-11.13
0.7	5.9851	-17.6648	35.6202	-8.8324	-8.8324
0.8	5.1775	-13.4416	28.9739	-6.7208	-6.7208
0.9	4.3942	-9.7292	22.9119	-4.8646	-4.8646

1	3.6576	-6.5928	17.5657	-3.2964	-3.2964
1.1	2.9829	-4.0382	12.9871	-2.0191	-2.0191
1.2	2.3789	-2.03	9.1669	-1.015	-1.015
1.3	1.849	-0.5072	6.0541	-0.2536	-0.2536
1.4	1.3921	0.603	3.5732	0.3015	0.3015
1.5	1.0041	1.3744	1.6378	0.6872	0.6872
1.6	0.6791	1.8772	0.1602	0.9386	0.9386
1.7	0.4104	2.173	-0.942	1.0865	1.0865
1.8	0.1907	2.3144	-1.7424	1.1572	1.1572
1.9	0.0133	2.344	-2.3042	1.172	1.172
2	-0.1281	2.2958	-2.6802	1.1479	1.1479
2.1	-0.2391	2.1964	-2.9137	1.0982	1.0982
2.2	-0.3245	2.0658	-3.0392	1.0329	1.0329
2.3	-0.3884	1.9188	-3.084	0.9594	0.9594
2.4	-0.4343	1.7666	-3.0695	0.8833	0.8833
2.5	-0.4652	1.6168	-3.0124	0.8084	0.8084
2.6	-0.4836	1.4748	-2.9255	0.7374	0.7374
2.7	-0.4915	1.3438	-2.8183	0.6719	0.6719
2.8	-0.491	1.2256	-2.6985	0.6128	0.6128
2.9	-0.4834	1.1212	-2.5714	0.5606	0.5606
3	-0.4702	1.0306	-2.4413	0.5153	0.5153
3.1	-0.4527	0.9532	-2.3112	0.4766	0.4766
3.2	-0.4318	0.8878	-2.1833	0.4439	0.4439
3.3	-0.4086	0.8334	-2.0591	0.4167	0.4167
3.4	-0.3837	0.7886	-1.9397	0.3943	0.3943
3.5	-0.3579	0.7518	-1.8257	0.3759	0.3759
3.6	-0.3318	0.722	-1.7174	0.361	0.361
3.7	-0.3058	0.6976	-1.6152	0.3488	0.3488
3.8	-0.2803	0.6778	-1.5188	0.3389	0.3389
3.9	-0.2557	0.6612	-1.4283	0.3306	0.3306
4	-0.2321	0.6472	-1.3435	0.3236	0.3236
4.1	-0.2097	0.635	-1.2641	0.3175	0.3175
4.2	-0.1886	0.624	-1.1899	0.312	0.312
4.3	-0.169	0.6136	-1.1205	0.3068	0.3068
4.4	-0.1508	0.6034	-1.0557	0.3017	0.3017
4.5	-0.1339	0.5934	-0.9953	0.2967	0.2967
4.6	-0.1185	0.5832	-0.9388	0.2916	0.2916
4.7	-0.1044	0.5728	-0.8861	0.2864	0.2864
4.8	-0.0916	0.562	-0.837	0.281	0.281
4.9	-0.08	0.5508	-0.791	0.2754	0.2754
5	-0.0696	0.5394	-0.7481	0.2697	0.2697

$Na^{+}[c\text{-}P_4]^{2-}$ (C_{4v})

```
Charge = -1 Multiplicity = 1
P,0,0.,-1.5555955624,0.3470176161
 P,0,1.5555955624,0.,0.3470176161
 P,0,0.,1.5555955624,0.3470176161
 P,0,-1.5555955624,0.,0.3470176161
 Na,0,0.,0.,-1.9648821743
```

Sum of electronic and zero-point Energies= -1527.902558
Sum of electronic and thermal Energies= -1527.895989
Sum of electronic and thermal Enthalpies= -1527.895045
Sum of electronic and thermal Free Energies= -1527.932926

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.0615	1.0862	-0.9017	0.5431	0.5431

-4.9	0.0563	1.1224	-0.9534	0.5612	0.5612
-4.8	0.0501	1.1592	-1.0088	0.5796	0.5796
-4.7	0.0428	1.1964	-1.0682	0.5982	0.5982
-4.6	0.0341	1.234	-1.1319	0.617	0.617
-4.5	0.0239	1.2718	-1.2001	0.6359	0.6359
-4.4	0.0121	1.3098	-1.2733	0.6549	0.6549
-4.3	-0.0013	1.3476	-1.3516	0.6738	0.6738
-4.2	-0.0167	1.3854	-1.4355	0.6927	0.6927
-4.1	-0.0339	1.4232	-1.525	0.7116	0.7116
-4	-0.0531	1.4612	-1.6206	0.7306	0.7306
-3.9	-0.0743	1.4994	-1.7223	0.7497	0.7497
-3.8	-0.0971	1.5386	-1.8301	0.7693	0.7693
-3.7	-0.1216	1.5792	-1.9439	0.7896	0.7896
-3.6	-0.1471	1.622	-2.0633	0.811	0.811
-3.5	-0.1732	1.6682	-2.1878	0.8341	0.8341
-3.4	-0.1991	1.719	-2.3162	0.8595	0.8595
-3.3	-0.2237	1.7758	-2.4469	0.8879	0.8879
-3.2	-0.2458	1.8402	-2.5777	0.9201	0.9201
-3.1	-0.2638	1.9136	-2.7052	0.9568	0.9568
-3	-0.2757	1.9978	-2.825	0.9989	0.9989
-2.9	-0.2791	2.0938	-2.931	1.0469	1.0469
-2.8	-0.271	2.2022	-3.0151	1.1011	1.1011
-2.7	-0.2478	2.3228	-3.0663	1.1614	1.1614
-2.6	-0.2053	2.4544	-3.0705	1.2272	1.2272
-2.5	-0.1383	2.594	-3.0088	1.297	1.297
-2.4	-0.0403	2.7364	-2.8573	1.3682	1.3682
-2.3	0.0963	2.874	-2.585	1.437	1.437
-2.2	0.2807	2.9952	-2.1531	1.4976	1.4976
-2.1	0.5235	3.0838	-1.5132	1.5419	1.5419
-2	0.8371	3.118	-0.6069	1.559	1.559
-1.9	1.235	3.0696	0.6356	1.5348	1.5348
-1.8	1.7319	2.9018	2.2938	1.4509	1.4509
-1.7	2.3418	2.5702	4.4553	1.2851	1.2851
-1.6	3.0774	2.0214	7.2108	1.0107	1.0107
-1.5	3.9473	1.1962	10.6459	0.5981	0.5981
-1.4	4.9538	0.0318	14.8297	0.0159	0.0159
-1.3	6.0896	-1.5302	19.799	-0.7651	-0.7651
-1.2	7.3354	-3.5332	25.5393	-1.7666	-1.7666
-1.1	8.6576	-5.9914	31.9642	-2.9957	-2.9957
-1	10.0086	-8.8718	38.8977	-4.4359	-4.4359
-0.9	11.3284	-12.078	46.0633	-6.039	-6.039
-0.8	12.5496	-15.4384	53.0871	-7.7192	-7.7192
-0.7	13.6042	-18.7078	59.5203	-9.3539	-9.3539
-0.6	14.4318	-21.586	64.8813	-10.793	-10.793
-0.5	14.987	-23.7546	68.7155	-11.8773	-11.8773
-0.4	15.2449	-24.927	70.6618	-12.4635	-12.4635
-0.3	15.2026	-24.902	70.5098	-12.451	-12.451
-0.2	14.8781	-23.6014	68.2358	-11.8007	-11.8007
-0.1	14.3062	-21.086	64.0046	-10.543	-10.543

0	13.5331	-17.5396	58.1388	-8.7698	-8.7698
0.1	12.6113	-13.2288	51.0629	-6.6144	-6.6144
0.2	11.5947	-8.4518	43.2361	-4.2259	-4.2259
0.3	10.534	-3.4874	35.0894	-1.7437	-1.7437
0.4	9.4726	1.4422	26.9755	0.7211	0.7211
0.5	8.4429	6.1902	19.1385	3.0951	3.0951
0.6	7.4617	10.687	11.6981	5.3435	5.3435
0.7	6.5241	14.9268	4.6455	7.4634	7.4634
0.8	5.5936	18.9408	-2.1599	9.4704	9.4704
0.9	4.5812	22.7456	-9.0019	11.3728	11.3728
1	3.3009	26.239	-16.3362	13.1195	13.1195
1.1	1.3798	28.9868	-24.8475	14.4934	14.4934
1.2	-1.9044	29.8264	-35.5395	14.9132	14.9132
1.3	-7.9039	26.1486	-49.8603	13.0743	13.0743
1.4	-19.1305	12.424	-69.8155	6.212	6.212
1.5	-40.1229	-22.5296	-97.8393	-11.2648	-11.2648
1.6	-77.494	-96.623	-135.859	-48.3115	-48.3115
1.7	-136.563	-226.087	-183.601	-113.044	-113.044
1.8	-214.078	-397.889	-244.346	-198.944	-198.944
1.9	-373.46	-699.351	-421.029	-349.676	-349.676
2	-221.804	-217.55	-447.86	-108.775	-108.775
2.1	-142.044	-176.806	-249.324	-88.4032	-88.4032
2.2	-128.911	-200.505	-186.227	-100.252	-100.252
2.3	-87.4523	-124.161	-138.196	-62.0804	-62.0804
2.4	-52.1504	-56.568	-99.8832	-28.284	-28.284
2.5	-29.5269	-16.878	-71.7027	-8.439	-8.439
2.6	-16.4894	2.4642	-51.9322	1.2321	1.2321
2.7	-9.2488	10.5198	-38.2662	5.2599	5.2599
2.8	-5.2947	12.9072	-28.7912	6.4536	6.4536
2.9	-3.1485	12.6984	-22.144	6.3492	6.3492
3	-1.9787	11.4662	-17.4023	5.7331	5.7331
3.1	-1.3359	9.9468	-13.9545	4.9734	4.9734
3.2	-0.9808	8.4552	-11.3976	4.2276	4.2276
3.3	-0.784	7.1122	-9.4643	3.5561	3.5561
3.4	-0.6743	5.9522	-7.9753	2.9761	2.9761
3.5	-0.612	4.9722	-6.8083	2.4861	2.4861
3.6	-0.5753	4.1528	-5.8786	2.0764	2.0764
3.7	-0.5522	3.4704	-5.1269	1.7352	1.7352
3.8	-0.5364	2.9014	-4.5106	1.4507	1.4507
3.9	-0.5244	2.4258	-3.9991	1.2129	1.2129
4	-0.5143	2.0268	-3.5698	1.0134	1.0134
4.1	-0.5049	1.691	-3.2059	0.8455	0.8455
4.2	-0.4956	1.4078	-2.8946	0.7039	0.7039
4.3	-0.4859	1.1684	-2.6261	0.5842	0.5842
4.4	-0.4756	0.9662	-2.3929	0.4831	0.4831
4.5	-0.4644	0.7956	-2.1889	0.3978	0.3978
4.6	-0.4525	0.652	-2.0095	0.326	0.326
4.7	-0.4398	0.5312	-1.8507	0.2656	0.2656
4.8	-0.4264	0.4302	-1.7094	0.2151	0.2151

4.9	-0.4125	0.3456	-1.5832	0.1728	0.1728
5	-0.3982	0.2754	-1.4699	0.1377	0.1377

$[Na_2]^{2+}[c\text{-}P_4]^{2-}$ (D_{4h})

```
Charge =  0 Multiplicity = 1
P,0,0.,1.5616127032,0.
 P,0,1.5616127032,0.,0.
 P,0,0.,-1.5616127032,0.
 P,0,-1.5616127032,0.,0.
 Na,0,0.,0.,2.376693168
 Na,0,0.,0.,-2.376693168
```

Sum of electronic and zero-point Energies= -1690.195010
Sum of electronic and thermal Energies= -1690.186475
Sum of electronic and thermal Enthalpies= -1690.185531
Sum of electronic and thermal Free Energies= -1690.227539

NICS-scan

Distance	NICSiso	NICS(in)	NICSzz(out)	NICSxx(in)	NICSyy(in)
-5	-0.1625	1.441	-1.9286	0.7205	0.7205
-4.9	-0.1708	1.5918	-2.1043	0.7959	0.7959
-4.8	-0.1796	1.7662	-2.3048	0.8831	0.8831
-4.7	-0.1889	1.9686	-2.5351	0.9843	0.9843
-4.6	-0.1991	2.2042	-2.8015	1.1021	1.1021
-4.5	-0.2109	2.4794	-3.1121	1.2397	1.2397
-4.4	-0.2249	2.8024	-3.4771	1.4012	1.4012
-4.3	-0.2422	3.1836	-3.9102	1.5918	1.5918
-4.2	-0.2643	3.6364	-4.4293	1.8182	1.8182
-4.1	-0.2937	4.1776	-5.0586	2.0888	2.0888
-4	-0.3343	4.8282	-5.8311	2.4141	2.4141
-3.9	-0.3931	5.6134	-6.7927	2.8067	2.8067
-3.8	-0.4826	6.56	-8.0079	3.28	3.28
-3.7	-0.625	7.6936	-9.5687	3.8468	3.8468
-3.6	-0.8604	9.0276	-11.6089	4.5138	4.5138
-3.5	-1.2606	10.5434	-14.3251	5.2717	5.2717
-3.4	-1.9571	12.1406	-18.012	6.0703	6.0703
-3.3	-3.1985	13.5198	-23.1152	6.7599	6.7599
-3.2	-5.4603	13.9304	-30.3113	6.9652	6.9652
-3.1	-9.6391	11.7028	-40.6199	5.8514	5.8514
-3	-17.3642	3.447	-55.5397	1.7235	1.7235
-2.9	-31.5002	-17.3604	-77.14	-8.6802	-8.6802
-2.8	-56.5049	-61.7304	-107.784	-30.8652	-30.8652
-2.7	-96.3141	-139.986	-148.956	-69.9932	-69.9932
-2.6	-145.86	-237.444	-200.136	-118.722	-118.722
-2.5	-183.069	-273.249	-275.958	-136.624	-136.624
-2.4	-445.459	-786.824	-549.553	-393.412	-393.412
-2.3	-325.297	-617.912	-357.979	-308.956	-308.956
-2.2	-197.159	-361.388	-230.089	-180.694	-180.694
-2.1	-122.49	-194.508	-172.963	-97.2539	-97.2539
-2	-69.1177	-80.5094	-126.844	-40.2547	-40.2547
-1.9	-36.6797	-18.9096	-91.1297	-9.4548	-9.4548
-1.8	-18.8187	8.838	-65.2941	4.419	4.419

-1.7	-9.2626	19.2898	-47.0776	9.6449	9.6449
-1.6	-4.0463	21.9386	-34.0776	10.9693	10.9693
-1.5	-1.0258	21.3372	-24.4145	10.6686	10.6686
-1.4	0.9369	19.5628	-16.7521	9.7814	9.7814
-1.3	2.4336	17.4652	-10.1643	8.7326	8.7326
-1.2	3.7615	15.2974	-4.0131	7.6487	7.6487
-1.1	5.0645	13.0558	2.1376	6.5279	6.5279
-1	6.4068	10.6462	8.5741	5.3231	5.3231
-0.9	7.8073	7.9636	15.4584	3.9818	3.9818
-0.8	9.2557	4.9316	22.8355	2.4658	2.4658
-0.7	10.7211	1.5314	30.632	0.7657	0.7657
-0.6	12.158	-2.179	38.6529	-1.0895	-1.0895
-0.5	13.5113	-6.0532	46.5871	-3.0266	-3.0266
-0.4	14.7222	-9.8598	54.0265	-4.9299	-4.9299
-0.3	15.7337	-13.3032	60.5043	-6.6516	-6.6516
-0.2	16.4956	-16.0646	65.5515	-8.0323	-8.0323
-0.1	16.9691	-17.8564	68.7638	-8.9282	-8.9282
0	17.1297	-18.4778	69.867	-9.2389	-9.2389
0.1	16.9691	-17.8564	68.7638	-8.9282	-8.9282
0.2	16.4956	-16.0646	65.5515	-8.0323	-8.0323
0.3	15.7337	-13.3032	60.5043	-6.6516	-6.6516
0.4	14.7222	-9.8598	54.0265	-4.9299	-4.9299
0.5	13.5113	-6.0532	46.5871	-3.0266	-3.0266
0.6	12.158	-2.179	38.6529	-1.0895	-1.0895
0.7	10.7211	1.5314	30.632	0.7657	0.7657
0.8	9.2557	4.9316	22.8355	2.4658	2.4658
0.9	7.8073	7.9636	15.4584	3.9818	3.9818
1	6.4068	10.6462	8.5741	5.3231	5.3231
1.1	5.0645	13.0558	2.1376	6.5279	6.5279
1.2	3.7615	15.2974	-4.0131	7.6487	7.6487
1.3	2.4336	17.4652	-10.1643	8.7326	8.7326
1.4	0.9369	19.5628	-16.7521	9.7814	9.7814
1.5	-1.0258	21.3372	-24.4145	10.6686	10.6686
1.6	-4.0463	21.9386	-34.0776	10.9693	10.9693
1.7	-9.2626	19.2898	-47.0776	9.6449	9.6449
1.8	-18.8187	8.838	-65.2941	4.419	4.419
1.9	-36.6797	-18.9096	-91.1297	-9.4548	-9.4548
2	-69.1177	-80.5094	-126.844	-40.2547	-40.2547
2.1	-122.49	-194.508	-172.963	-97.2539	-97.2539
2.2	-197.159	-361.388	-230.089	-180.694	-180.694
2.3	-325.297	-617.912	-357.979	-308.956	-308.956
2.4	-445.459	-786.824	-549.553	-393.412	-393.412
2.5	-183.069	-273.249	-275.958	-136.624	-136.624
2.6	-145.86	-237.444	-200.136	-118.722	-118.722
2.7	-96.3141	-139.986	-148.956	-69.9932	-69.9932
2.8	-56.5049	-61.7304	-107.784	-30.8652	-30.8652
2.9	-31.5002	-17.3604	-77.14	-8.6802	-8.6802
3	-17.3642	3.447	-55.5397	1.7235	1.7235
3.1	-9.6391	11.7028	-40.6199	5.8514	5.8514

3.2	-5.4603	13.9304	-30.3113	6.9652	6.9652
3.3	-3.1985	13.5198	-23.1152	6.7599	6.7599
3.4	-1.9571	12.1406	-18.012	6.0703	6.0703
3.5	-1.2606	10.5434	-14.3251	5.2717	5.2717
3.6	-0.8604	9.0276	-11.6089	4.5138	4.5138
3.7	-0.625	7.6936	-9.5687	3.8468	3.8468
3.8	-0.4826	6.56	-8.0079	3.28	3.28
3.9	-0.3931	5.6134	-6.7927	2.8067	2.8067
4	-0.3343	4.8282	-5.8311	2.4141	2.4141
4.1	-0.2937	4.1776	-5.0586	2.0888	2.0888
4.2	-0.2643	3.6364	-4.4293	1.8182	1.8182
4.3	-0.2422	3.1836	-3.9102	1.5918	1.5918
4.4	-0.2249	2.8024	-3.4771	1.4012	1.4012
4.5	-0.2109	2.4794	-3.1121	1.2397	1.2397
4.6	-0.1991	2.2042	-2.8015	1.1021	1.1021
4.7	-0.1889	1.9686	-2.5351	0.9843	0.9843
4.8	-0.1796	1.7662	-2.3048	0.8831	0.8831
4.9	-0.1708	1.5918	-2.1043	0.7959	0.7959
5	-0.1625	1.441	-1.9286	0.7205	0.7205

$[c\text{-As}_4]^{2-}$ (D_{4h}), 37

```
Charge = -2 Multiplicity = 1
 As,0,-1.7112602412,0.,0.
 As,0,0.,-1.7112602412,0.
 As,0,1.7112602412,0.,0.
 As,0,0.,1.7112602412,0.
```

Sum of electronic and zero-point Energies= -8943.566551
Sum of electronic and thermal Energies= -8943.560427
Sum of electronic and thermal Enthalpies= -8943.559483
Sum of electronic and thermal Free Energies= -8943.598508

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.0037	1.2346	-1.2233	0.6173	0.6173
-4.9	0.0034	1.2968	-1.2865	0.6484	0.6484
-4.8	0.0034	1.3638	-1.3536	0.6819	0.6819
-4.7	0.0037	1.436	-1.4248	0.718	0.718
-4.6	0.0045	1.5138	-1.5004	0.7569	0.7569
-4.5	0.0058	1.5978	-1.5804	0.7989	0.7989
-4.4	0.0076	1.6882	-1.6653	0.8441	0.8441
-4.3	0.0101	1.7856	-1.7552	0.8928	0.8928
-4.2	0.0134	1.8904	-1.8503	0.9452	0.9452
-4.1	0.0175	2.0034	-1.9509	1.0017	1.0017
-4	0.0226	2.1248	-2.057	1.0624	1.0624
-3.9	0.0288	2.2552	-2.1689	1.1276	1.1276
-3.8	0.0362	2.395	-2.2864	1.1975	1.1975
-3.7	0.045	2.5444	-2.4095	1.2722	1.2722

-3.6	0.0553	2.7038	-2.538	1.3519	1.3519
-3.5	0.0673	2.8734	-2.6714	1.4367	1.4367
-3.4	0.0813	3.0528	-2.809	1.5264	1.5264
-3.3	0.0973	3.2418	-2.9498	1.6209	1.6209
-3.2	0.1158	3.4396	-3.0923	1.7198	1.7198
-3.1	0.1369	3.645	-3.2344	1.8225	1.8225
-3	0.161	3.8564	-3.3733	1.9282	1.9282
-2.9	0.1887	4.0714	-3.5053	2.0357	2.0357
-2.8	0.2204	4.2866	-3.6255	2.1433	2.1433
-2.7	0.2569	4.4982	-3.7276	2.2491	2.2491
-2.6	0.2992	4.7006	-3.8031	2.3503	2.3503
-2.5	0.3485	4.887	-3.8414	2.4435	2.4435
-2.4	0.4066	5.0488	-3.829	2.5244	2.5244
-2.3	0.4754	5.175	-3.7488	2.5875	2.5875
-2.2	0.5576	5.2518	-3.5791	2.6259	2.6259
-2.1	0.6563	5.262	-3.2931	2.631	2.631
-2	0.7753	5.1838	-2.8578	2.5919	2.5919
-1.9	0.919	4.9898	-2.2329	2.4949	2.4949
-1.8	1.0921	4.6466	-1.3703	2.3233	2.3233
-1.7	1.2999	4.1132	-0.2134	2.0566	2.0566
-1.6	1.5478	3.3408	1.3025	1.6704	1.6704
-1.5	1.8405	2.2724	3.2493	1.1362	1.1362
-1.4	2.1825	0.845	5.7025	0.4225	0.4225
-1.3	2.5764	-1.008	8.7372	-0.504	-0.504
-1.2	3.023	-3.3508	12.4198	-1.6754	-1.6754
-1.1	3.5202	-6.2374	16.7981	-3.1187	-3.1187
-1	4.0628	-9.6998	21.8883	-4.8499	-4.8499
-0.9	4.6417	-13.7352	27.6604	-6.8676	-6.8676
-0.8	5.2439	-18.2918	34.0237	-9.1459	-9.1459
-0.7	5.8528	-23.2572	40.8157	-11.6286	-11.6286
-0.6	6.4483	-28.452	47.797	-14.226	-14.226
-0.5	7.008	-33.632	54.6561	-16.816	-16.816
-0.4	7.5085	-38.5018	61.0273	-19.2509	-19.2509
-0.3	7.9268	-42.7408	66.521	-21.3704	-21.3704
-0.2	8.2422	-46.0382	70.765	-23.0191	-23.0191
-0.1	8.4386	-48.1334	73.4492	-24.0667	-24.0667
0	8.5052	-48.8522	74.368	-24.4261	-24.4261
0.1	8.4386	-48.1334	73.4492	-24.0667	-24.0667
0.2	8.2422	-46.0382	70.765	-23.0191	-23.0191
0.3	7.9268	-42.7408	66.521	-21.3704	-21.3704
0.4	7.5085	-38.5018	61.0273	-19.2509	-19.2509
0.5	7.008	-33.632	54.6561	-16.816	-16.816
0.6	6.4483	-28.452	47.797	-14.226	-14.226
0.7	5.8528	-23.2572	40.8157	-11.6286	-11.6286
0.8	5.2439	-18.2918	34.0237	-9.1459	-9.1459
0.9	4.6417	-13.7352	27.6604	-6.8676	-6.8676
1	4.0628	-9.6998	21.8883	-4.8499	-4.8499
1.1	3.5202	-6.2374	16.7981	-3.1187	-3.1187
1.2	3.023	-3.3508	12.4198	-1.6754	-1.6754

1.3	2.5764	-1.008	8.7372	-0.504	-0.504
1.4	2.1825	0.845	5.7025	0.4225	0.4225
1.5	1.8405	2.2724	3.2493	1.1362	1.1362
1.6	1.5478	3.3408	1.3025	1.6704	1.6704
1.7	1.2999	4.1132	-0.2134	2.0566	2.0566
1.8	1.0921	4.6466	-1.3703	2.3233	2.3233
1.9	0.919	4.9898	-2.2329	2.4949	2.4949
2	0.7753	5.1838	-2.8578	2.5919	2.5919
2.1	0.6563	5.262	-3.2931	2.631	2.631
2.2	0.5576	5.2518	-3.5791	2.6259	2.6259
2.3	0.4754	5.175	-3.7488	2.5875	2.5875
2.4	0.4066	5.0488	-3.829	2.5244	2.5244
2.5	0.3485	4.887	-3.8414	2.4435	2.4435
2.6	0.2992	4.7006	-3.8031	2.3503	2.3503
2.7	0.2569	4.4982	-3.7276	2.2491	2.2491
2.8	0.2204	4.2866	-3.6255	2.1433	2.1433
2.9	0.1887	4.0714	-3.5053	2.0357	2.0357
3	0.161	3.8564	-3.3733	1.9282	1.9282
3.1	0.1369	3.645	-3.2344	1.8225	1.8225
3.2	0.1158	3.4396	-3.0923	1.7198	1.7198
3.3	0.0973	3.2418	-2.9498	1.6209	1.6209
3.4	0.0813	3.0528	-2.809	1.5264	1.5264
3.5	0.0673	2.8734	-2.6714	1.4367	1.4367
3.6	0.0553	2.7038	-2.538	1.3519	1.3519
3.7	0.045	2.5444	-2.4095	1.2722	1.2722
3.8	0.0362	2.395	-2.2864	1.1975	1.1975
3.9	0.0288	2.2552	-2.1689	1.1276	1.1276
4	0.0226	2.1248	-2.057	1.0624	1.0624
4.1	0.0175	2.0034	-1.9509	1.0017	1.0017
4.2	0.0134	1.8904	-1.8503	0.9452	0.9452
4.3	0.0101	1.7856	-1.7552	0.8928	0.8928
4.4	0.0076	1.6882	-1.6653	0.8441	0.8441
4.5	0.0058	1.5978	-1.5804	0.7989	0.7989
4.6	0.0045	1.5138	-1.5004	0.7569	0.7569
4.7	0.0037	1.436	-1.4248	0.718	0.718
4.8	0.0034	1.3638	-1.3536	0.6819	0.6819
4.9	0.0034	1.2968	-1.2865	0.6484	0.6484
5	0.0037	1.2346	-1.2233	0.6173	0.6173

$[c\text{-}Sb_4]^{2-}$ (D_{4h}), 38

```
Charge = -2 Multiplicity = 1
Sb,0,0.,2.0029801337,0.
 Sb,0,2.0029801337,0.,0.
 Sb,0,0.,-2.0029801337,0.
 Sb,0,-2.0029801337,0.,0.
```

Sum of electronic and zero-point Energies= -25261.338983
Sum of electronic and thermal Energies= -25261.332195
Sum of electronic and thermal Enthalpies= -25261.331251
Sum of electronic and thermal Free Energies= -25261.374239

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	-0.1092	2.1024	-2.43	1.0512	1.0512
-4.9	-0.1203	2.1838	-2.5448	1.0919	1.0919
-4.8	-0.1326	2.2678	-2.6656	1.1339	1.1339
-4.7	-0.1462	2.3542	-2.7927	1.1771	1.1771
-4.6	-0.1611	2.4432	-2.9265	1.2216	1.2216
-4.5	-0.1775	2.5344	-3.067	1.2672	1.2672
-4.4	-0.1956	2.6274	-3.2143	1.3137	1.3137
-4.3	-0.2154	2.7224	-3.3687	1.3612	1.3612
-4.2	-0.2371	2.8186	-3.53	1.4093	1.4093
-4.1	-0.2607	2.916	-3.6981	1.458	1.458
-4	-0.2863	3.0138	-3.8728	1.5069	1.5069
-3.9	-0.314	3.1116	-4.0536	1.5558	1.5558
-3.8	-0.3437	3.2086	-4.2399	1.6043	1.6043
-3.7	-0.3755	3.3042	-4.4307	1.6521	1.6521
-3.6	-0.4092	3.397	-4.6246	1.6985	1.6985
-3.5	-0.4446	3.4862	-4.8198	1.7431	1.7431
-3.4	-0.4814	3.5698	-5.014	1.7849	1.7849
-3.3	-0.5193	3.6462	-5.2042	1.8231	1.8231
-3.2	-0.5578	3.7128	-5.3863	1.8564	1.8564
-3.1	-0.5962	3.7668	-5.5555	1.8834	1.8834
-3	-0.6337	3.8046	-5.7056	1.9023	1.9023
-2.9	-0.6692	3.8212	-5.8289	1.9106	1.9106
-2.8	-0.7016	3.811	-5.9158	1.9055	1.9055
-2.7	-0.7295	3.7662	-5.9547	1.8831	1.8831
-2.6	-0.7512	3.678	-5.9314	1.839	1.839
-2.5	-0.7648	3.5346	-5.8289	1.7673	1.7673
-2.4	-0.7684	3.3218	-5.627	1.6609	1.6609
-2.3	-0.7598	3.0222	-5.3015	1.5111	1.5111
-2.2	-0.7366	2.615	-4.8246	1.3075	1.3075
-2.1	-0.6964	2.0748	-4.1641	1.0374	1.0374
-2	-0.637	1.3728	-3.2837	0.6864	0.6864
-1.9	-0.5561	0.4748	-2.1431	0.2374	0.2374
-1.8	-0.4517	-0.6562	-0.6987	-0.3281	-0.3281
-1.7	-0.3222	-2.0616	1.0949	-1.0308	-1.0308
-1.6	-0.1666	-3.7832	3.2835	-1.8916	-1.8916
-1.5	0.0156	-5.863	5.9099	-2.9315	-2.9315
-1.4	0.2239	-8.3388	9.0106	-4.1694	-4.1694
-1.3	0.4571	-11.2396	12.6109	-5.6198	-5.6198
-1.2	0.7126	-14.5816	16.7193	-7.2908	-7.2908
-1.1	0.9869	-18.3604	21.3213	-9.1802	-9.1802
-1	1.2753	-22.547	26.3729	-11.2735	-11.2735
-0.9	1.5718	-27.0804	31.7957	-13.5402	-13.5402
-0.8	1.8694	-31.8646	37.4728	-15.9323	-15.9323
-0.7	2.1604	-36.7668	43.248	-18.3834	-18.3834
-0.6	2.4363	-41.6208	48.9298	-20.8104	-20.8104
-0.5	2.6886	-46.233	54.2987	-23.1165	-23.1165
-0.4	2.9087	-50.3952	59.1213	-25.1976	-25.1976
-0.3	3.0891	-53.8994	63.1667	-26.9497	-26.9497

-0.2	3.2231	-56.557	66.2264	-28.2785	-28.2785
-0.1	3.3056	-58.2172	68.1341	-29.1086	-29.1086
0	3.3335	-58.782	68.7823	-29.391	-29.391
0.1	3.3056	-58.2172	68.1341	-29.1086	-29.1086
0.2	3.2231	-56.557	66.2264	-28.2785	-28.2785
0.3	3.0891	-53.8994	63.1667	-26.9497	-26.9497
0.4	2.9087	-50.3952	59.1213	-25.1976	-25.1976
0.5	2.6886	-46.233	54.2987	-23.1165	-23.1165
0.6	2.4363	-41.6208	48.9298	-20.8104	-20.8104
0.7	2.1604	-36.7668	43.248	-18.3834	-18.3834
0.8	1.8694	-31.8646	37.4728	-15.9323	-15.9323
0.9	1.5718	-27.0804	31.7957	-13.5402	-13.5402
1	1.2753	-22.547	26.3729	-11.2735	-11.2735
1.1	0.9869	-18.3604	21.3213	-9.1802	-9.1802
1.2	0.7126	-14.5816	16.7193	-7.2908	-7.2908
1.3	0.4571	-11.2396	12.6109	-5.6198	-5.6198
1.4	0.2239	-8.3388	9.0106	-4.1694	-4.1694
1.5	0.0156	-5.863	5.9099	-2.9315	-2.9315
1.6	-0.1666	-3.7832	3.2835	-1.8916	-1.8916
1.7	-0.3222	-2.0616	1.0949	-1.0308	-1.0308
1.8	-0.4517	-0.6562	-0.6987	-0.3281	-0.3281
1.9	-0.5561	0.4748	-2.1431	0.2374	0.2374
2	-0.637	1.3728	-3.2837	0.6864	0.6864
2.1	-0.6964	2.0748	-4.1641	1.0374	1.0374
2.2	-0.7366	2.615	-4.8246	1.3075	1.3075
2.3	-0.7598	3.0222	-5.3015	1.5111	1.5111
2.4	-0.7684	3.3218	-5.627	1.6609	1.6609
2.5	-0.7648	3.5346	-5.8289	1.7673	1.7673
2.6	-0.7512	3.678	-5.9314	1.839	1.839
2.7	-0.7295	3.7662	-5.9547	1.8831	1.8831
2.8	-0.7016	3.811	-5.9158	1.9055	1.9055
2.9	-0.6692	3.8212	-5.8289	1.9106	1.9106
3	-0.6337	3.8046	-5.7056	1.9023	1.9023
3.1	-0.5962	3.7668	-5.5555	1.8834	1.8834
3.2	-0.5578	3.7128	-5.3863	1.8564	1.8564
3.3	-0.5193	3.6462	-5.2042	1.8231	1.8231
3.4	-0.4814	3.5698	-5.014	1.7849	1.7849
3.5	-0.4446	3.4862	-4.8198	1.7431	1.7431
3.6	-0.4092	3.397	-4.6246	1.6985	1.6985
3.7	-0.3755	3.3042	-4.4307	1.6521	1.6521
3.8	-0.3437	3.2086	-4.2399	1.6043	1.6043
3.9	-0.314	3.1116	-4.0536	1.5558	1.5558
4	-0.2863	3.0138	-3.8728	1.5069	1.5069
4.1	-0.2607	2.916	-3.6981	1.458	1.458
4.2	-0.2371	2.8186	-3.53	1.4093	1.4093
4.3	-0.2154	2.7224	-3.3687	1.3612	1.3612
4.4	-0.1956	2.6274	-3.2143	1.3137	1.3137
4.5	-0.1775	2.5344	-3.067	1.2672	1.2672
4.6	-0.1611	2.4432	-2.9265	1.2216	1.2216

4.7	-0.1462	2.3542	-2.7927	1.1771	1.1771
4.8	-0.1326	2.2678	-2.6656	1.1339	1.1339
4.9	-0.1203	2.1838	-2.5448	1.0919	1.0919
5	-0.1092	2.1024	-2.43	1.0512	1.0512

$[c\text{-}Bi_4]^{2-}$ (D_{4h}), 39

```
Charge = -2 Multiplicity = 1
 Bi,0,0.,2.1094566252,0.
 Bi,0,2.1094566252,0.,0.
 Bi,0,0.,-2.1094566252,0.
 Bi,0,-2.1094566252,0.,0.
```

Sum of electronic and zero-point Energies= -21.697483
Sum of electronic and thermal Energies= -21.690221
Sum of electronic and thermal Enthalpies= -21.689277
Sum of electronic and thermal Free Energies= -21.736036

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.0663	1.5044	-1.3057	0.7522	0.7522
-4.9	0.0664	1.5622	-1.3628	0.7811	0.7811
-4.8	0.0663	1.6214	-1.4223	0.8107	0.8107
-4.7	0.0659	1.6818	-1.4842	0.8409	0.8409
-4.6	0.065	1.7436	-1.5484	0.8718	0.8718
-4.5	0.0637	1.806	-1.6148	0.903	0.903
-4.4	0.0618	1.8686	-1.6831	0.9343	0.9343
-4.3	0.0593	1.9312	-1.7532	0.9656	0.9656
-4.2	0.0561	1.993	-1.8246	0.9965	0.9965
-4.1	0.0521	2.053	-1.8968	1.0265	1.0265
-4	0.0471	2.1104	-1.9691	1.0552	1.0552
-3.9	0.0411	2.1642	-2.0407	1.0821	1.0821
-3.8	0.0341	2.2126	-2.1104	1.1063	1.1063
-3.7	0.0258	2.2542	-2.1768	1.1271	1.1271
-3.6	0.0163	2.287	-2.2382	1.1435	1.1435
-3.5	0.0056	2.309	-2.2922	1.1545	1.1545
-3.4	-0.0063	2.3172	-2.3363	1.1586	1.1586
-3.3	-0.0193	2.3092	-2.367	1.1546	1.1546
-3.2	-0.033	2.2812	-2.3802	1.1406	1.1406
-3.1	-0.047	2.23	-2.371	1.115	1.115
-3	-0.0607	2.1514	-2.3334	1.0757	1.0757
-2.9	-0.0732	2.0406	-2.2603	1.0203	1.0203
-2.8	-0.0833	1.8932	-2.143	0.9466	0.9466
-2.7	-0.0893	1.7036	-1.9714	0.8518	0.8518
-2.6	-0.0892	1.4658	-1.7334	0.7329	0.7329
-2.5	-0.0803	1.1738	-1.4148	0.5869	0.5869
-2.4	-0.0596	0.8206	-0.9994	0.4103	0.4103
-2.3	-0.0231	0.3988	-0.4681	0.1994	0.1994
-2.2	0.0336	-0.1	0.2008	-0.05	-0.05
-2.1	0.1155	-0.685	1.0314	-0.3425	-0.3425
-2	0.2282	-1.366	2.0507	-0.683	-0.683
-1.9	0.3778	-2.1542	3.2877	-1.0771	-1.0771

-1.8	0.5705	-3.0614	4.773	-1.5307	-1.5307
-1.7	0.8123	-4.1002	6.5373	-2.0501	-2.0501
-1.6	1.1088	-5.284	8.6102	-2.642	-2.642
-1.5	1.4642	-6.625	11.0175	-3.3125	-3.3125
-1.4	1.8813	-8.1342	13.7782	-4.0671	-4.0671
-1.3	2.3606	-9.8194	16.9014	-4.9097	-4.9097
-1.2	2.8998	-11.6826	20.382	-5.8413	-5.8413
-1.1	3.4929	-13.7182	24.1969	-6.8591	-6.8591
-1	4.1305	-15.9096	28.301	-7.9548	-7.9548
-0.9	4.7993	-18.227	32.6249	-9.1135	-9.1135
-0.8	5.4825	-20.626	37.0735	-10.313	-10.313
-0.7	6.1603	-23.0462	41.5271	-11.5231	-11.5231
-0.6	6.8109	-25.4124	45.845	-12.7062	-12.7062
-0.5	7.4114	-27.6384	49.8726	-13.8192	-13.8192
-0.4	7.9395	-29.6314	53.4498	-14.8157	-14.8157
-0.3	8.3745	-31.2994	56.4228	-15.6497	-15.6497
-0.2	8.6988	-32.559	58.6554	-16.2795	-16.2795
-0.1	8.899	-33.3436	60.0406	-16.6718	-16.6718
0	8.9667	-33.61	60.5102	-16.805	-16.805
0.1	8.899	-33.3436	60.0406	-16.6718	-16.6718
0.2	8.6988	-32.559	58.6554	-16.2795	-16.2795
0.3	8.3745	-31.2994	56.4228	-15.6497	-15.6497
0.4	7.9395	-29.6314	53.4498	-14.8157	-14.8157
0.5	7.4114	-27.6384	49.8726	-13.8192	-13.8192
0.6	6.8109	-25.4124	45.845	-12.7062	-12.7062
0.7	6.1603	-23.0462	41.5271	-11.5231	-11.5231
0.8	5.4825	-20.626	37.0735	-10.313	-10.313
0.9	4.7993	-18.227	32.6249	-9.1135	-9.1135
1	4.1305	-15.9096	28.301	-7.9548	-7.9548
1.1	3.4929	-13.7182	24.1969	-6.8591	-6.8591
1.2	2.8998	-11.6826	20.382	-5.8413	-5.8413
1.3	2.3606	-9.8194	16.9014	-4.9097	-4.9097
1.4	1.8813	-8.1342	13.7782	-4.0671	-4.0671
1.5	1.4642	-6.625	11.0175	-3.3125	-3.3125
1.6	1.1088	-5.284	8.6102	-2.642	-2.642
1.7	0.8123	-4.1002	6.5373	-2.0501	-2.0501
1.8	0.5705	-3.0614	4.773	-1.5307	-1.5307
1.9	0.3778	-2.1542	3.2877	-1.0771	-1.0771
2	0.2282	-1.366	2.0507	-0.683	-0.683
2.1	0.1155	-0.685	1.0314	-0.3425	-0.3425
2.2	0.0336	-0.1	0.2008	-0.05	-0.05
2.3	-0.0231	0.3988	-0.4681	0.1994	0.1994
2.4	-0.0596	0.8206	-0.9994	0.4103	0.4103
2.5	-0.0803	1.1738	-1.4148	0.5869	0.5869
2.6	-0.0892	1.4658	-1.7334	0.7329	0.7329
2.7	-0.0893	1.7036	-1.9714	0.8518	0.8518
2.8	-0.0833	1.8932	-2.143	0.9466	0.9466
2.9	-0.0732	2.0406	-2.2603	1.0203	1.0203
3	-0.0607	2.1514	-2.3334	1.0757	1.0757

3.1	-0.047	2.23	-2.371	1.115	1.115
3.2	-0.033	2.2812	-2.3802	1.1406	1.1406
3.3	-0.0193	2.3092	-2.367	1.1546	1.1546
3.4	-0.0063	2.3172	-2.3363	1.1586	1.1586
3.5	0.0056	2.309	-2.2922	1.1545	1.1545
3.6	0.0163	2.287	-2.2382	1.1435	1.1435
3.7	0.0258	2.2542	-2.1768	1.1271	1.1271
3.8	0.0341	2.2126	-2.1104	1.1063	1.1063
3.9	0.0411	2.1642	-2.0407	1.0821	1.0821
4	0.0471	2.1104	-1.9691	1.0552	1.0552
4.1	0.0521	2.053	-1.8968	1.0265	1.0265
4.2	0.0561	1.993	-1.8246	0.9965	0.9965
4.3	0.0593	1.9312	-1.7532	0.9656	0.9656
4.4	0.0618	1.8686	-1.6831	0.9343	0.9343
4.5	0.0637	1.806	-1.6148	0.903	0.903
4.6	0.065	1.7436	-1.5484	0.8718	0.8718
4.7	0.0659	1.6818	-1.4842	0.8409	0.8409
4.8	0.0663	1.6214	-1.4223	0.8107	0.8107
4.9	0.0664	1.5622	-1.3628	0.7811	0.7811
5	0.0663	1.5044	-1.3057	0.7522	0.7522

[*c*-P_4]$^-$ (Doublet) (D_{2h}), 40

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Charge = -1 Multiplicity = 2
 P,0,1.0584630151,-1.1246808054,0.
 P,0,1.0584630151,1.1246808054,0.
 P,0,-1.0584630151,1.1246808054,0.
 P,0,-1.0584630151,-1.1246808054,0.
```

Sum of electronic and zero-point Energies= -1365.549246
Sum of electronic and thermal Energies= -1365.544118
Sum of electronic and thermal Enthalpies= -1365.543174
Sum of electronic and thermal Free Energies= -1365.578546

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.7017	0.3374	1.7678	0.1702	0.1672
-4.9	0.7436	0.343	1.8876	0.1731	0.1699
-4.8	0.7888	0.3478	2.0185	0.1756	0.1722
-4.7	0.8378	0.3516	2.1618	0.1777	0.1739
-4.6	0.891	0.3543	2.3189	0.1792	0.1751
-4.5	0.9489	0.3555	2.4914	0.18	0.1755
-4.4	1.0121	0.3551	2.6813	0.18	0.1751
-4.3	1.0812	0.3529	2.8906	0.1792	0.1737
-4.2	1.1569	0.3488	3.1219	0.1774	0.1714
-4.1	1.2401	0.3424	3.3779	0.1746	0.1678
-4	1.3318	0.3337	3.6617	0.1707	0.163
-3.9	1.4331	0.3223	3.9769	0.1655	0.1568
-3.8	1.5453	0.3082	4.3277	0.1591	0.1491
-3.7	1.6699	0.2911	4.7185	0.1513	0.1398
-3.6	1.8085	0.2708	5.1548	0.1421	0.1287

-3.5	1.9632	0.2472	5.6424	0.1314	0.1158
-3.4	2.1361	0.2202	6.1881	0.1193	0.1009
-3.3	2.3297	0.1895	6.7997	0.1056	0.0839
-3.2	2.5469	0.155	7.4858	0.0904	0.0646
-3.1	2.791	0.1166	8.2565	0.0737	0.0429
-3	3.0657	0.0737	9.1232	0.0553	0.0184
-2.9	3.3751	0.0262	10.0991	0.0352	-0.009
-2.8	3.7242	-0.0265	11.1991	0.0132	-0.0397
-2.7	4.1184	-0.0855	12.4406	-0.011	-0.0745
-2.6	4.5639	-0.1518	13.8436	-0.038	-0.1138
-2.5	5.0679	-0.2273	15.4311	-0.0684	-0.1589
-2.4	5.6384	-0.3145	17.2295	-0.1034	-0.2111
-2.3	6.2841	-0.4168	19.2691	-0.1445	-0.2723
-2.2	7.015	-0.5391	21.5842	-0.1941	-0.345
-2.1	7.8417	-0.6879	24.2128	-0.2551	-0.4328
-2	8.7751	-0.8717	27.1971	-0.3318	-0.5399
-1.9	9.8265	-1.1023	30.5819	-0.4299	-0.6724
-1.8	11.0062	-1.3944	34.413	-0.5568	-0.8376
-1.7	12.3227	-1.7671	38.735	-0.7221	-1.045
-1.6	13.7813	-2.2436	43.5874	-0.9377	-1.3059
-1.5	15.3823	-2.8523	48.9993	-1.2184	-1.6339
-1.4	17.1193	-3.6255	54.9835	-1.581	-2.0445
-1.3	18.9767	-4.599	61.5292	-2.0447	-2.5543
-1.2	20.9288	-5.8089	68.5953	-2.629	-3.1799
-1.1	22.9385	-7.2886	76.1039	-3.3526	-3.936
-1	24.9581	-9.0625	83.9367	-4.2298	-4.8327
-0.9	26.9316	-11.1397	91.9345	-5.2673	-5.8724
-0.8	28.799	-13.5055	99.9024	-6.4594	-7.0461
-0.7	30.5022	-16.1126	107.6193	-7.7834	-8.3292
-0.6	31.9922	-18.8757	114.8523	-9.1962	-9.6795
-0.5	33.2352	-21.6687	121.3745	-10.6327	-11.036
-0.4	34.2173	-24.3296	126.9814	-12.008	-12.3216
-0.3	34.9436	-26.6737	131.5044	-13.2242	-13.4495
-0.2	35.4341	-28.5151	134.8173	-14.1825	-14.3326
-0.1	35.7142	-29.6933	136.836	-14.7968	-14.8965
0	35.805	-30.0989	137.5139	-15.0085	-15.0904
0.1	35.7142	-29.6933	136.836	-14.7968	-14.8965
0.2	35.4341	-28.5151	134.8173	-14.1825	-14.3326
0.3	34.9436	-26.6737	131.5044	-13.2242	-13.4495
0.4	34.2173	-24.3296	126.9814	-12.008	-12.3216
0.5	33.2352	-21.6687	121.3745	-10.6327	-11.036
0.6	31.9922	-18.8757	114.8523	-9.1962	-9.6795
0.7	30.5022	-16.1126	107.6193	-7.7834	-8.3292
0.8	28.799	-13.5055	99.9024	-6.4594	-7.0461
0.9	26.9316	-11.1397	91.9345	-5.2673	-5.8724
1	24.9581	-9.0625	83.9367	-4.2298	-4.8327
1.1	22.9385	-7.2886	76.1039	-3.3526	-3.936
1.2	20.9288	-5.8089	68.5953	-2.629	-3.1799
1.3	18.9767	-4.599	61.5292	-2.0447	-2.5543

1.4	17.1193	-3.6255	54.9835	-1.581	-2.0445
1.5	15.3823	-2.8523	48.9993	-1.2184	-1.6339
1.6	13.7813	-2.2436	43.5874	-0.9377	-1.3059
1.7	12.3227	-1.7671	38.735	-0.7221	-1.045
1.8	11.0062	-1.3944	34.413	-0.5568	-0.8376
1.9	9.8265	-1.1023	30.5819	-0.4299	-0.6724
2	8.7751	-0.8717	27.1971	-0.3318	-0.5399
2.1	7.8417	-0.6879	24.2128	-0.2551	-0.4328
2.2	7.015	-0.5391	21.5842	-0.1941	-0.345
2.3	6.2841	-0.4168	19.2691	-0.1445	-0.2723
2.4	5.6384	-0.3145	17.2295	-0.1034	-0.2111
2.5	5.0679	-0.2273	15.4311	-0.0684	-0.1589
2.6	4.5639	-0.1518	13.8436	-0.038	-0.1138
2.7	4.1184	-0.0855	12.4406	-0.011	-0.0745
2.8	3.7242	-0.0265	11.1991	0.0132	-0.0397
2.9	3.3751	0.0262	10.0991	0.0352	-0.009
3	3.0657	0.0737	9.1232	0.0553	0.0184
3.1	2.791	0.1166	8.2565	0.0737	0.0429
3.2	2.5469	0.155	7.4858	0.0904	0.0646
3.3	2.3297	0.1895	6.7997	0.1056	0.0839
3.4	2.1361	0.2202	6.1881	0.1193	0.1009
3.5	1.9632	0.2472	5.6424	0.1314	0.1158
3.6	1.8085	0.2708	5.1548	0.1421	0.1287
3.7	1.6699	0.2911	4.7185	0.1513	0.1398
3.8	1.5453	0.3082	4.3277	0.1591	0.1491
3.9	1.4331	0.3223	3.9769	0.1655	0.1568
4	1.3318	0.3337	3.6617	0.1707	0.163
4.1	1.2401	0.3424	3.3779	0.1746	0.1678
4.2	1.1569	0.3488	3.1219	0.1774	0.1714
4.3	1.0812	0.3529	2.8906	0.1792	0.1737
4.4	1.0121	0.3551	2.6813	0.18	0.1751
4.5	0.9489	0.3555	2.4914	0.18	0.1755
4.6	0.891	0.3543	2.3189	0.1792	0.1751
4.7	0.8378	0.3516	2.1618	0.1777	0.1739
4.8	0.7888	0.3478	2.0185	0.1756	0.1722
4.9	0.7436	0.343	1.8876	0.1731	0.1699
5	0.7017	0.3374	1.7678	0.1702	0.1672

[*c*-As$_4$]$^-$ (Doublet) (D_{2h}), 41

```
Charge = -1 Multiplicity = 2
 As,0,1.2374628605,1.1724304291,0.
 As,0,1.2374628605,-1.1724304291,0.
 As,0,-1.2374628605,-1.1724304291,0.
 As,0,-1.2374628605,1.1724304291,0.
```

Sum of electronic and zero-point Energies= -8943.639579
Sum of electronic and thermal Energies= -8943.633360
Sum of electronic and thermal Enthalpies= -8943.632416
Sum of electronic and thermal Free Energies= -8943.673330

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	0.9671	0.9328	1.9685	0.5211	0.4117
-4.9	1.0275	0.9747	2.1078	0.5467	0.428
-4.8	1.0931	1.0189	2.2602	0.574	0.4449
-4.7	1.1643	1.0655	2.4273	0.6031	0.4624
-4.6	1.2417	1.1145	2.6108	0.6342	0.4803
-4.5	1.3262	1.166	2.8126	0.6673	0.4987
-4.4	1.4184	1.2203	3.0351	0.7028	0.5175
-4.3	1.5193	1.2772	3.2807	0.7407	0.5365
-4.2	1.6298	1.337	3.5524	0.7814	0.5556
-4.1	1.7511	1.3996	3.8536	0.825	0.5746
-4	1.8844	1.4653	4.1879	0.8719	0.5934
-3.9	2.0312	1.5339	4.5599	0.9224	0.6115
-3.8	2.1932	1.6053	4.9743	0.9767	0.6286
-3.7	2.3721	1.6794	5.4368	1.0353	0.6441
-3.6	2.57	1.7559	5.954	1.0985	0.6574
-3.5	2.7892	1.8345	6.5331	1.1668	0.6677
-3.4	3.0323	1.9144	7.1824	1.2405	0.6739
-3.3	3.3021	1.9949	7.9114	1.3202	0.6747
-3.2	3.6019	2.075	8.7308	1.4063	0.6687
-3.1	3.9352	2.1531	9.6526	1.4992	0.6539
-3	4.3059	2.2274	10.6903	1.5993	0.6281
-2.9	4.7183	2.2955	11.8594	1.7069	0.5886
-2.8	5.1772	2.3546	13.1768	1.8222	0.5324
-2.7	5.6876	2.4012	14.6617	1.9453	0.4559
-2.6	6.2554	2.4307	16.3354	2.0757	0.355
-2.5	6.8865	2.438	18.2215	2.213	0.225
-2.4	7.5875	2.4163	20.3461	2.3558	0.0605
-2.3	8.3651	2.3577	22.7376	2.502	-0.1443
-2.2	9.2263	2.2522	25.4268	2.6485	-0.3963
-2.1	10.1779	2.0874	28.4462	2.7903	-0.7029
-2	11.2259	1.8481	31.8296	2.9204	-1.0723
-1.9	12.3753	1.5151	35.6107	3.0288	-1.5137
-1.8	13.6289	1.0653	39.8215	3.1018	-2.0365
-1.7	14.9867	0.4704	44.4895	3.1209	-2.6505
-1.6	16.4441	-0.3027	49.635	3.0625	-3.3652
-1.5	17.9916	-1.2921	55.2667	2.8966	-4.1887
-1.4	19.6128	-2.5388	61.3773	2.588	-5.1268
-1.3	21.2847	-4.085	67.939	2.0963	-6.1813
-1.2	22.9765	-5.9691	74.8987	1.3793	-7.3484
-1.1	24.6517	-8.2201	82.1752	0.3971	-8.6172
-1	26.269	-10.85	89.6571	-0.8817	-9.9683
-0.9	27.7862	-13.8455	97.2042	-2.472	-11.3735
-0.8	29.1638	-17.1597	104.6512	-4.3633	-12.7964
-0.7	30.3696	-20.7065	111.8153	-6.5124	-14.1941
-0.6	31.3824	-24.3583	118.5054	-8.8378	-15.5205
-0.5	32.1946	-27.949	124.5329	-11.2198	-16.7292
-0.4	32.8128	-31.2849	129.7232	-13.5071	-17.7778
-0.3	33.2546	-34.1607	133.9243	-15.5306	-18.6301

-0.2	33.5442	-36.3813	137.014	-17.1231	-19.2582
-0.1	33.7061	-37.7853	138.9034	-18.1428	-19.6425
0	33.7578	-38.2657	139.5391	-18.4939	-19.7718
0.1	33.7061	-37.7853	138.9034	-18.1428	-19.6425
0.2	33.5442	-36.3813	137.014	-17.1231	-19.2582
0.3	33.2546	-34.1607	133.9243	-15.5306	-18.6301
0.4	32.8128	-31.2849	129.7232	-13.5071	-17.7778
0.5	32.1946	-27.949	124.5329	-11.2198	-16.7292
0.6	31.3824	-24.3583	118.5054	-8.8378	-15.5205
0.7	30.3696	-20.7065	111.8153	-6.5124	-14.1941
0.8	29.1638	-17.1597	104.6512	-4.3633	-12.7964
0.9	27.7862	-13.8455	97.2042	-2.472	-11.3735
1	26.269	-10.85	89.6571	-0.8817	-9.9683
1.1	24.6517	-8.2201	82.1752	0.3971	-8.6172
1.2	22.9765	-5.9691	74.8987	1.3793	-7.3484
1.3	21.2847	-4.085	67.939	2.0963	-6.1813
1.4	19.6128	-2.5388	61.3773	2.588	-5.1268
1.5	17.9916	-1.2921	55.2667	2.8966	-4.1887
1.6	16.4441	-0.3027	49.635	3.0625	-3.3652
1.7	14.9867	0.4704	44.4895	3.1209	-2.6505
1.8	13.6289	1.0653	39.8215	3.1018	-2.0365
1.9	12.3753	1.5151	35.6107	3.0288	-1.5137
2	11.2259	1.8481	31.8296	2.9204	-1.0723
2.1	10.1779	2.0874	28.4462	2.7903	-0.7029
2.2	9.2263	2.2522	25.4268	2.6485	-0.3963
2.3	8.3651	2.3577	22.7376	2.502	-0.1443
2.4	7.5875	2.4163	20.3461	2.3558	0.0605
2.5	6.8865	2.438	18.2215	2.213	0.225
2.6	6.2554	2.4307	16.3354	2.0757	0.355
2.7	5.6876	2.4012	14.6617	1.9453	0.4559
2.8	5.1772	2.3546	13.1768	1.8222	0.5324
2.9	4.7183	2.2955	11.8594	1.7069	0.5886
3	4.3059	2.2274	10.6903	1.5993	0.6281
3.1	3.9352	2.1531	9.6526	1.4992	0.6539
3.2	3.6019	2.075	8.7308	1.4063	0.6687
3.3	3.3021	1.9949	7.9114	1.3202	0.6747
3.4	3.0323	1.9144	7.1824	1.2405	0.6739
3.5	2.7892	1.8345	6.5331	1.1668	0.6677
3.6	2.57	1.7559	5.954	1.0985	0.6574
3.7	2.3721	1.6794	5.4368	1.0353	0.6441
3.8	2.1932	1.6053	4.9743	0.9767	0.6286
3.9	2.0312	1.5339	4.5599	0.9224	0.6115
4	1.8844	1.4653	4.1879	0.8719	0.5934
4.1	1.7511	1.3996	3.8536	0.825	0.5746
4.2	1.6298	1.337	3.5524	0.7814	0.5556
4.3	1.5193	1.2772	3.2807	0.7407	0.5365
4.4	1.4184	1.2203	3.0351	0.7028	0.5175
4.5	1.3262	1.166	2.8126	0.6673	0.4987
4.6	1.2417	1.1145	2.6108	0.6342	0.4803

4.7	1.1643	1.0655	2.4273	0.6031	0.4624
4.8	1.0931	1.0189	2.2602	0.574	0.4449
4.9	1.0275	0.9747	2.1078	0.5467	0.428
5	0.9671	0.9328	1.9685	0.5211	0.4117

[*c*-Sb$_4$]$^-$ (Doublet) (D_{2h}), 42

```
Charge = -1 Multiplicity = 2
 Sb,0,1.4421345028,1.378870719,0.
 Sb,0,1.4421345028,-1.378870719,0.
 Sb,0,-1.4421345028,-1.378870719,0.
 Sb,0,-1.4421345028,1.378870719,0.
```

Sum of electronic and zero-point Energies= -25261.402298
Sum of electronic and thermal Energies= -25261.395418
Sum of electronic and thermal Enthalpies= -25261.394474
Sum of electronic and thermal Free Energies= -25261.439599

NICS-scan

Distance (Å)	$NICS_{iso}$	NICS(in)	$NICS_{zz}$(out)	$NICS_{xx}$(in)	$NICS_{yy}$(in)
-5	1.3595	1.7651	2.3134	0.9634	0.8017
-4.9	1.4444	1.838	2.495	1.0055	0.8325
-4.8	1.5362	1.9139	2.6949	1.0498	0.8641
-4.7	1.6359	1.9925	2.9151	1.0961	0.8964
-4.6	1.744	2.074	3.1581	1.1447	0.9293
-4.5	1.8616	2.1583	3.4267	1.1956	0.9627
-4.4	1.9897	2.2451	3.7239	1.2489	0.9962
-4.3	2.1292	2.3344	4.0533	1.3047	1.0297
-4.2	2.2816	2.4258	4.4189	1.3631	1.0627
-4.1	2.4481	2.5191	4.8251	1.4241	1.095
-4	2.6303	2.6138	5.2771	1.4879	1.1259
-3.9	2.83	2.7094	5.7806	1.5546	1.1548
-3.8	3.0491	2.8052	6.342	1.6241	1.1811
-3.7	3.2897	2.9004	6.9688	1.6966	1.2038
-3.6	3.5543	2.9939	7.6691	1.7721	1.2218
-3.5	3.8456	3.0843	8.4524	1.8505	1.2338
-3.4	4.1664	3.1702	9.329	1.9318	1.2384
-3.3	4.5201	3.2497	10.3106	2.0159	1.2338
-3.2	4.9102	3.3201	11.4104	2.1024	1.2177
-3.1	5.3405	3.3787	12.6429	2.191	1.1877
-3	5.8152	3.4215	14.0241	2.2809	1.1406
-2.9	6.3386	3.4441	15.5717	2.3711	1.073
-2.8	6.9151	3.4408	17.3046	2.4603	0.9805
-2.7	7.5493	3.4045	19.2435	2.5462	0.8583
-2.6	8.2456	3.3267	21.41	2.6261	0.7006
-2.5	9.0079	3.1972	23.8264	2.6963	0.5009
-2.4	9.8396	3.0033	26.5154	2.7515	0.2518
-2.3	10.743	2.73	29.499	2.785	-0.055
-2.2	11.7192	2.3599	32.7979	2.7884	-0.4285
-2.1	12.7674	1.8724	36.4297	2.7507	-0.8783
-2	13.8842	1.2444	40.4081	2.6585	-1.4141
-1.9	15.0637	0.4503	44.7409	2.4957	-2.0454

-1.8	16.2967	-0.5379	49.428	2.2433	-2.7812
-1.7	17.5705	-1.7486	54.4603	1.88	-3.6286
-1.6	18.8689	-3.2104	59.817	1.382	-4.5924
-1.5	20.1719	-4.9492	65.4648	0.725	-5.6742
-1.4	21.4568	-6.9863	71.3568	-0.1149	-6.8714
-1.3	22.6988	-9.335	77.4314	-1.1588	-8.1762
-1.2	23.8722	-11.997	83.6136	-2.4217	-9.5753
-1.1	24.9521	-14.9594	89.8157	-3.9102	-11.0492
-1	25.9164	-18.1906	95.9397	-5.618	-12.5726
-0.9	26.7478	-21.6376	101.8811	-7.5229	-14.1147
-0.8	27.436	-25.2245	107.5326	-9.5842	-15.6403
-0.7	27.9787	-28.8527	112.7888	-11.7417	-17.111
-0.6	28.3824	-32.4031	117.5505	-13.9159	-18.4872
-0.5	28.6622	-35.7423	121.7288	-16.0122	-19.7301
-0.4	28.8395	-38.7292	125.2476	-17.9262	-20.803
-0.3	28.9398	-41.2261	128.0454	-19.5525	-21.6736
-0.2	28.9887	-43.1096	130.0758	-20.7942	-22.3154
-0.1	29.0082	-44.2819	131.3065	-21.5733	-22.7086
0	29.0129	-44.68	131.7188	-21.8389	-22.8411
0.1	29.0082	-44.2819	131.3065	-21.5733	-22.7086
0.2	28.9887	-43.1096	130.0758	-20.7942	-22.3154
0.3	28.9398	-41.2261	128.0454	-19.5525	-21.6736
0.4	28.8395	-38.7292	125.2476	-17.9262	-20.803
0.5	28.6622	-35.7423	121.7288	-16.0122	-19.7301
0.6	28.3824	-32.4031	117.5505	-13.9159	-18.4872
0.7	27.9787	-28.8527	112.7888	-11.7417	-17.111
0.8	27.436	-25.2245	107.5326	-9.5842	-15.6403
0.9	26.7478	-21.6376	101.8811	-7.5229	-14.1147
1	25.9164	-18.1906	95.9397	-5.618	-12.5726
1.1	24.9521	-14.9594	89.8157	-3.9102	-11.0492
1.2	23.8722	-11.997	83.6136	-2.4217	-9.5753
1.3	22.6988	-9.335	77.4314	-1.1588	-8.1762
1.4	21.4568	-6.9863	71.3568	-0.1149	-6.8714
1.5	20.1719	-4.9492	65.4648	0.725	-5.6742
1.6	18.8689	-3.2104	59.817	1.382	-4.5924
1.7	17.5705	-1.7486	54.4603	1.88	-3.6286
1.8	16.2967	-0.5379	49.428	2.2433	-2.7812
1.9	15.0637	0.4503	44.7409	2.4957	-2.0454
2	13.8842	1.2444	40.4081	2.6585	-1.4141
2.1	12.7674	1.8724	36.4297	2.7507	-0.8783
2.2	11.7192	2.3599	32.7979	2.7884	-0.4285
2.3	10.743	2.73	29.499	2.785	-0.055
2.4	9.8396	3.0033	26.5154	2.7515	0.2518
2.5	9.0079	3.1972	23.8264	2.6963	0.5009
2.6	8.2456	3.3267	21.41	2.6261	0.7006
2.7	7.5493	3.4045	19.2435	2.5462	0.8583
2.8	6.9151	3.4408	17.3046	2.4603	0.9805
2.9	6.3386	3.4441	15.5717	2.3711	1.073
3	5.8152	3.4215	14.0241	2.2809	1.1406

3.1	5.3405	3.3787	12.6429	2.191	1.1877
3.2	4.9102	3.3201	11.4104	2.1024	1.2177
3.3	4.5201	3.2497	10.3106	2.0159	1.2338
3.4	4.1664	3.1702	9.329	1.9318	1.2384
3.5	3.8456	3.0843	8.4524	1.8505	1.2338
3.6	3.5543	2.9939	7.6691	1.7721	1.2218
3.7	3.2897	2.9004	6.9688	1.6966	1.2038
3.8	3.0491	2.8052	6.342	1.6241	1.1811
3.9	2.83	2.7094	5.7806	1.5546	1.1548
4	2.6303	2.6138	5.2771	1.4879	1.1259
4.1	2.4481	2.5191	4.8251	1.4241	1.095
4.2	2.2816	2.4258	4.4189	1.3631	1.0627
4.3	2.1292	2.3344	4.0533	1.3047	1.0297
4.4	1.9897	2.2451	3.7239	1.2489	0.9962
4.5	1.8616	2.1583	3.4267	1.1956	0.9627
4.6	1.744	2.074	3.1581	1.1447	0.9293
4.7	1.6359	1.9925	2.9151	1.0961	0.8964
4.8	1.5362	1.9139	2.6949	1.0498	0.8641
4.9	1.4444	1.838	2.495	1.0055	0.8325
5	1.3595	1.7651	2.3134	0.9634	0.8017

[*c*-Bi$_4$]$^-$ (Doublet) (D_{2h}), 43

```
Charge = -1 Multiplicity = 2
 Bi,0,-0.0457376057,2.0949004616,0.
 Bi,0,2.0949004616,-0.0457376057,0.
 Bi,0,0.0457376057,-2.0949004616,0.
 Bi,0,-2.0949004616,0.0457376057,0.
```

Sum of electronic and zero-point Energies= -21.781601
Sum of electronic and thermal Energies= -21.774440
Sum of electronic and thermal Enthalpies= -21.773496
Sum of electronic and thermal Free Energies= -21.821337

NICS-scan

Distance (Å)	NICS$_{iso}$	NICS(in)	NICS$_{zz}$(out)	NICS$_{xx}$(in)	NICS$_{yy}$(in)
-5	1.4092	1.124	3.1036	0.6119	0.5121
-4.9	1.4994	1.1712	3.3271	0.639	0.5322
-4.8	1.5973	1.2201	3.5717	0.6673	0.5528
-4.7	1.7035	1.2707	3.8399	0.6969	0.5738
-4.6	1.8191	1.3229	4.1344	0.7278	0.5951
-4.5	1.9449	1.3766	4.4581	0.7601	0.6165
-4.4	2.082	1.4314	4.8147	0.7936	0.6378
-4.3	2.2317	1.4871	5.2079	0.8285	0.6586
-4.2	2.3952	1.5434	5.6422	0.8646	0.6788
-4.1	2.574	1.5995	6.1224	0.9019	0.6976
-4	2.7697	1.6549	6.6541	0.9402	0.7147
-3.9	2.984	1.7087	7.2434	0.9795	0.7292
-3.8	3.2189	1.7596	7.8971	1.0194	0.7402
-3.7	3.4765	1.8067	8.6227	1.0598	0.7469
-3.6	3.7589	1.8481	9.4287	1.1003	0.7478

-3.5	4.0687	1.8821	10.3242	1.1405	0.7416
-3.4	4.4085	1.9065	11.319	1.18	0.7265
-3.3	4.781	1.9188	12.4242	1.2181	0.7007
-3.2	5.1891	1.9162	13.6512	1.2542	0.662
-3.1	5.636	1.8955	15.0126	1.2875	0.608
-3	6.1249	1.8533	16.5216	1.3171	0.5362
-2.9	6.6592	1.7857	18.1918	1.3419	0.4438
-2.8	7.2422	1.6889	20.0377	1.3608	0.3281
-2.7	7.8775	1.5585	22.0739	1.3724	0.1861
-2.6	8.5684	1.39	24.3151	1.375	0.015
-2.5	9.3182	1.179	26.7756	1.3668	-0.1878
-2.4	10.1299	0.9208	29.4688	1.3456	-0.4248
-2.3	11.0058	0.6107	32.4068	1.3086	-0.6979
-2.2	11.9477	0.2439	35.5993	1.2526	-1.0087
-2.1	12.9561	-0.1841	39.0525	1.1737	-1.3578
-2	14.0302	-0.6777	42.7684	1.0672	-1.7449
-1.9	15.167	-1.2415	46.7426	0.9271	-2.1686
-1.8	16.3614	-1.8792	50.9635	0.7468	-2.626
-1.7	17.6053	-2.5943	55.4102	0.5183	-3.1126
-1.6	18.8873	-3.3897	60.0516	0.2325	-3.6222
-1.5	20.1928	-4.2671	64.8453	-0.1202	-4.1469
-1.4	21.5036	-5.2264	69.7371	-0.5496	-4.6768
-1.3	22.7987	-6.2658	74.6618	-1.0647	-5.2011
-1.2	24.055	-7.3802	79.5451	-1.6726	-5.7076
-1.1	25.2484	-8.561	84.3061	-2.3768	-6.1842
-1	26.3558	-9.7948	88.8622	-3.1754	-6.6194
-0.9	27.3567	-11.0632	93.1334	-4.0595	-7.0037
-0.8	28.2353	-12.3422	97.048	-5.012	-7.3302
-0.7	28.9818	-13.6019	100.5473	-6.0063	-7.5956
-0.6	29.5938	-14.8077	103.589	-7.0071	-7.8006
-0.5	30.0758	-15.9213	106.1486	-7.9714	-7.9499
-0.4	30.4384	-16.9031	108.2184	-8.8517	-8.0514
-0.3	30.6965	-17.7147	109.8041	-9.5997	-8.115
-0.2	30.8659	-18.3219	110.9195	-10.1709	-8.151
-0.1	30.9609	-18.6978	111.5806	-10.5293	-8.1685
0	30.9914	-18.8251	111.7994	-10.6515	-8.1736
0.1	30.9609	-18.6978	111.5806	-10.5293	-8.1685
0.2	30.8659	-18.3219	110.9195	-10.1709	-8.151
0.3	30.6965	-17.7147	109.8041	-9.5997	-8.115
0.4	30.4384	-16.9031	108.2184	-8.8517	-8.0514
0.5	30.0758	-15.9213	106.1486	-7.9714	-7.9499
0.6	29.5938	-14.8077	103.589	-7.0071	-7.8006
0.7	28.9818	-13.6019	100.5473	-6.0063	-7.5956
0.8	28.2353	-12.3422	97.048	-5.012	-7.3302
0.9	27.3567	-11.0632	93.1334	-4.0595	-7.0037
1	26.3558	-9.7948	88.8622	-3.1754	-6.6194
1.1	25.2484	-8.561	84.3061	-2.3768	-6.1842
1.2	24.055	-7.3802	79.5451	-1.6726	-5.7076
1.3	22.7987	-6.2658	74.6618	-1.0647	-5.2011

1.4	21.5036	-5.2264	69.7371	-0.5496	-4.6768
1.5	20.1928	-4.2671	64.8453	-0.1202	-4.1469
1.6	18.8873	-3.3897	60.0516	0.2325	-3.6222
1.7	17.6053	-2.5943	55.4102	0.5183	-3.1126
1.8	16.3614	-1.8792	50.9635	0.7468	-2.626
1.9	15.167	-1.2415	46.7426	0.9271	-2.1686
2	14.0302	-0.6777	42.7684	1.0672	-1.7449
2.1	12.9561	-0.1841	39.0525	1.1737	-1.3578
2.2	11.9477	0.2439	35.5993	1.2526	-1.0087
2.3	11.0058	0.6107	32.4068	1.3086	-0.6979
2.4	10.1299	0.9208	29.4688	1.3456	-0.4248
2.5	9.3182	1.179	26.7756	1.3668	-0.1878
2.6	8.5684	1.39	24.3151	1.375	0.015
2.7	7.8775	1.5585	22.0739	1.3724	0.1861
2.8	7.2422	1.6889	20.0377	1.3608	0.3281
2.9	6.6592	1.7857	18.1918	1.3419	0.4438
3	6.1249	1.8533	16.5216	1.3171	0.5362
3.1	5.636	1.8955	15.0126	1.2875	0.608
3.2	5.1891	1.9162	13.6512	1.2542	0.662
3.3	4.781	1.9188	12.4242	1.2181	0.7007
3.4	4.4085	1.9065	11.319	1.18	0.7265
3.5	4.0687	1.8821	10.3242	1.1405	0.7416
3.6	3.7589	1.8481	9.4287	1.1003	0.7478
3.7	3.4765	1.8067	8.6227	1.0598	0.7469
3.8	3.2189	1.7596	7.8971	1.0194	0.7402
3.9	2.984	1.7087	7.2434	0.9795	0.7292
4	2.7697	1.6549	6.6541	0.9402	0.7147
4.1	2.574	1.5995	6.1224	0.9019	0.6976
4.2	2.3952	1.5434	5.6422	0.8646	0.6788
4.3	2.2317	1.4871	5.2079	0.8285	0.6586
4.4	2.082	1.4314	4.8147	0.7936	0.6378
4.5	1.9449	1.3766	4.4581	0.7601	0.6165
4.6	1.8191	1.3229	4.1344	0.7278	0.5951
4.7	1.7035	1.2707	3.8399	0.6969	0.5738
4.8	1.5973	1.2201	3.5717	0.6673	0.5528
4.9	1.4994	1.1712	3.3271	0.639	0.5322
5	1.4092	1.124	3.1036	0.6119	0.5121

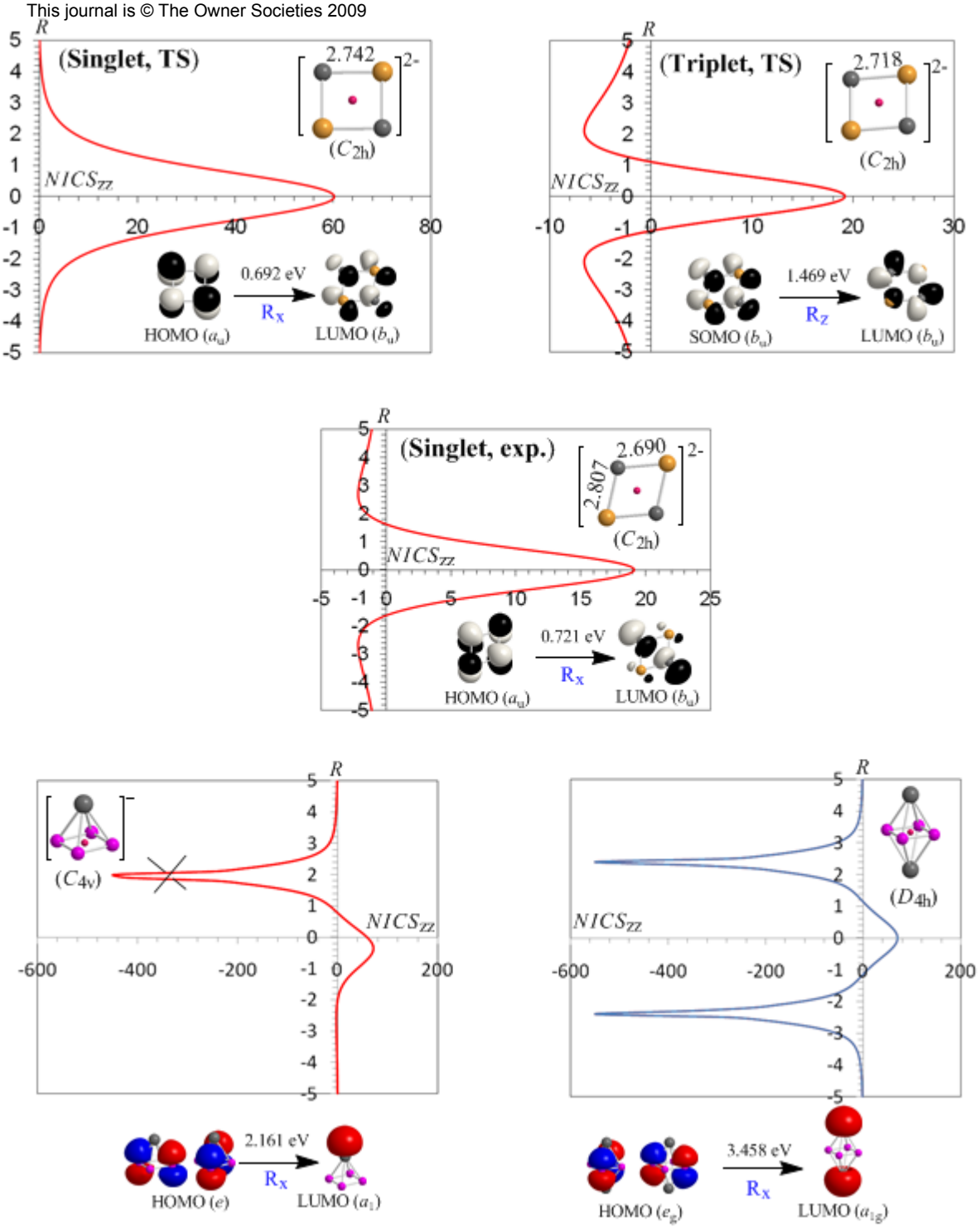

Figure S1. $NICS_{zz}$-scan profiles ($NICS_{zz}$ in ppm, R in Å) of the $[c\text{-}As_2Te_2]^{2-}$ (Singlet, TS) (C_{2h}), $[c\text{-}As_2Te_2]^{2-}$ (Triplet, TS) (C_{2h}), $[c\text{-}As_2Te_2]^{2-}$ (Singlet, exp.) (C_{2h}), $Na^+[c\text{-}P_4]^{2-}$ (C_{4v}), $[Na_2]^{2+}[c\text{-}P_4]^{2-}$ (D_{4h}), and $[c\text{-}P_4]^-$ (Doublet) (D_{2h}) along with the 3-D molecular orbital pictures of HOMO → LUMO transitions computed at the B3LYP/6-311+G**(P,As,Na)∪RSC-SDD(Te)level.

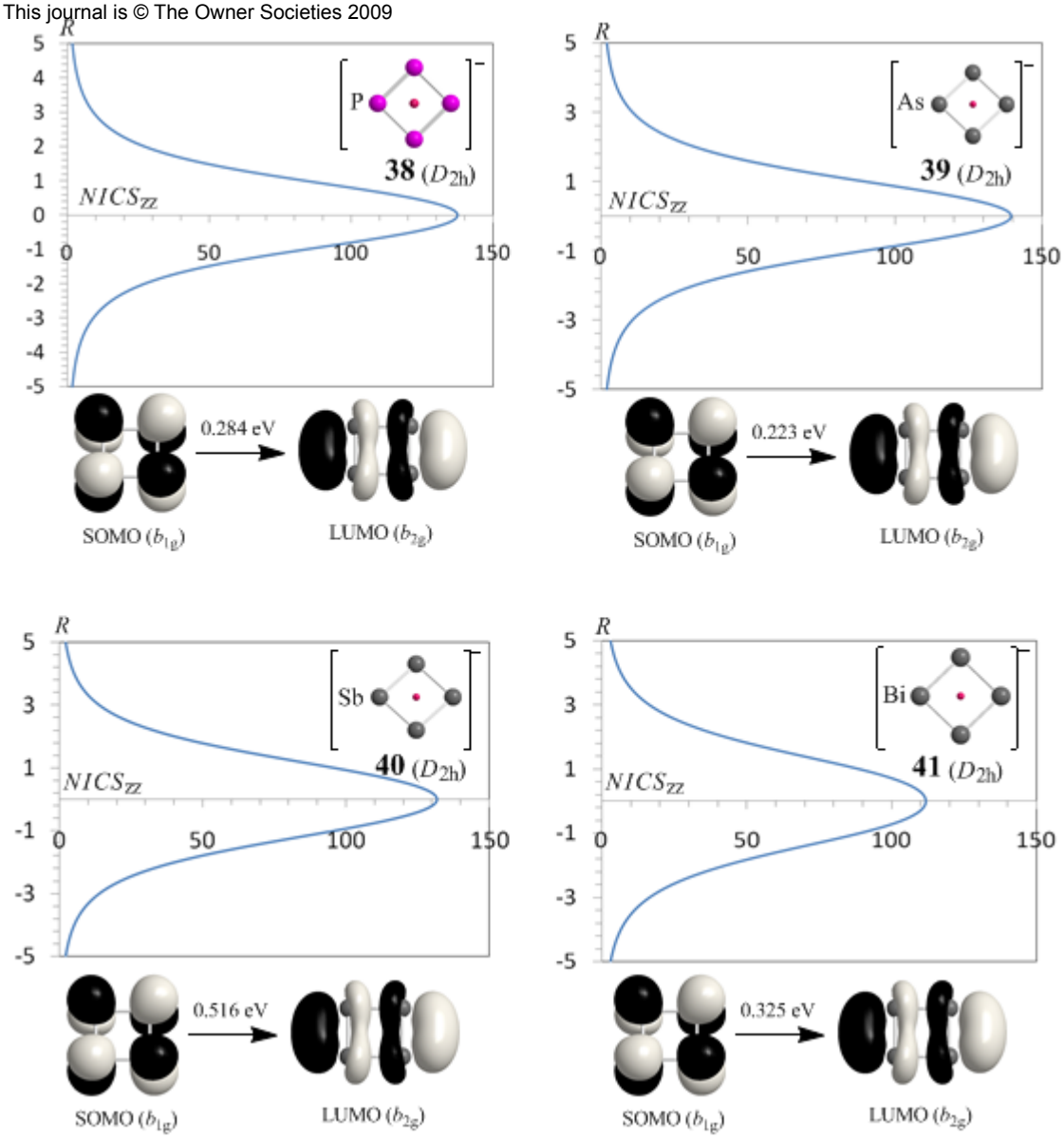

Fig. S2. $NICS_{ZZ}$-scan profiles ($NICS_{ZZ}$ in ppm, *R* in Å) of representative antiaromatic cyclic conjugated hydrocarbons along with the 3-D molecular orbital pictures of HOMO → LUMO transitions computed at the B3LYP/6-311+G**(P,As) ∪ RSC-SDD(Sb,Bi) level for Sb and Bi clusters.

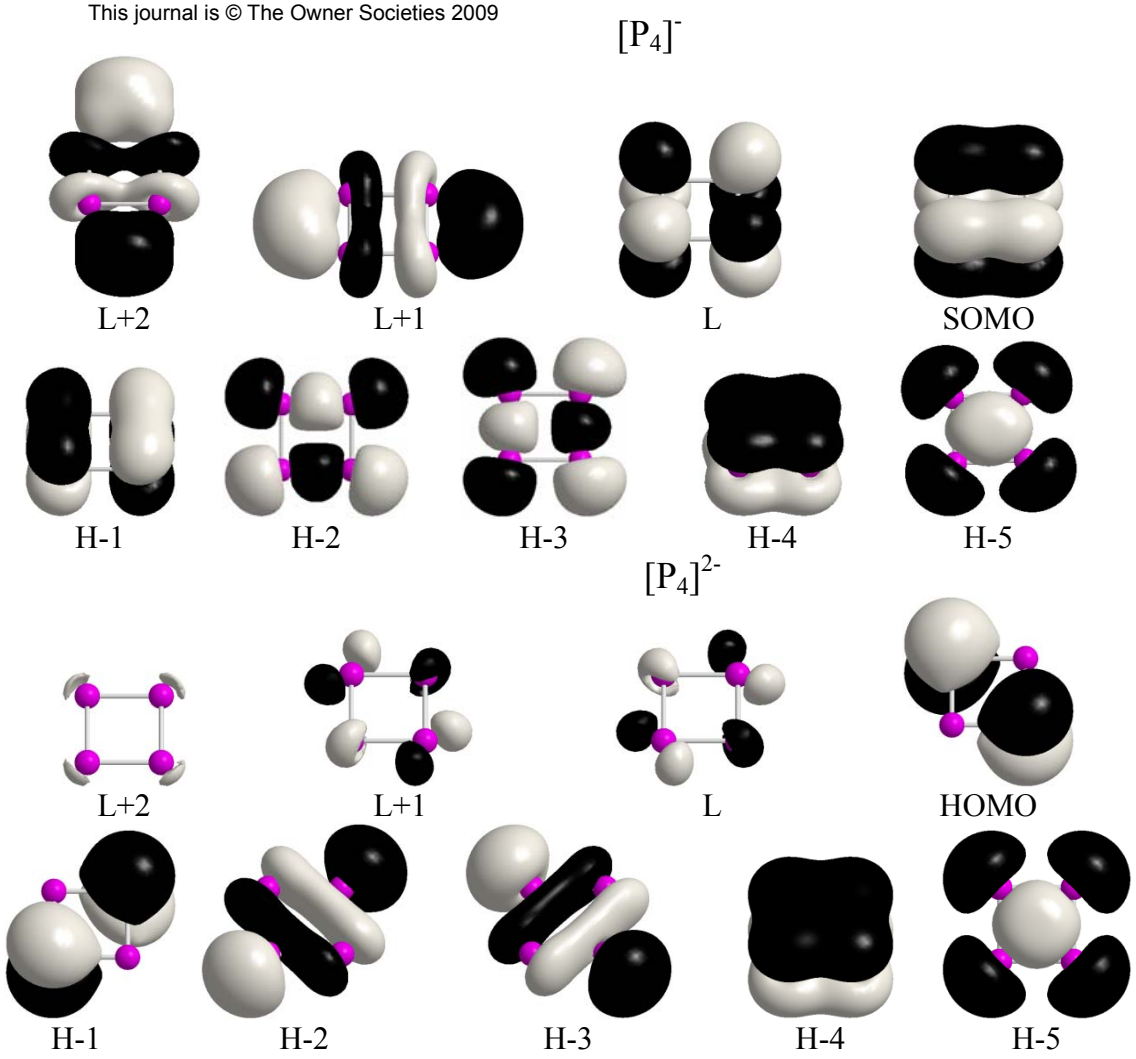

Fig. S3. 3-D molecular orbital patterns in the $[c\text{-}P_4]^{2-}$ and $[c\text{-}P_4]^{-}$ clusters.