

On couplings and excimers: Lessons from studies of singlet fission in covalently linked dimers. *Supplementary Material.*

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Definition of structural parameters

Distance d is the length of the line segment perpendicular to the two tetracenes' long molecular axes. When the two tetracenes are parallel to each other (in D_{2h} symmetry), the rotation of one tetracene along its symmetry axis, which is perpendicular to the two tetracene's planes, gives angle α . Angle β equals to twice the average of four carbon-carbon-carbon angles. Angle γ is defined in Fig. S1, which shows the deformation of the xanthene bridge.

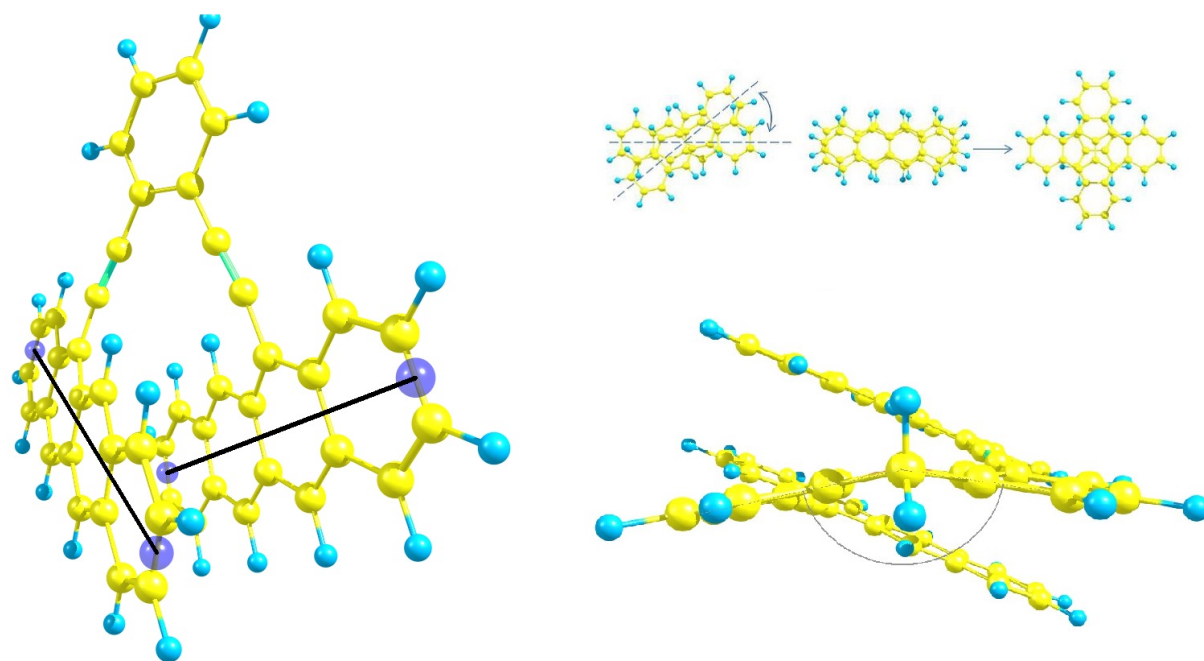


FIG. S1: Left: Distance d defined as the length of the line segment perpendicular to the two tetracenes' long molecular axes (black lines). Right top: Definition of angle α . Right bottom: Definition of angle γ .

Model BET-B structures

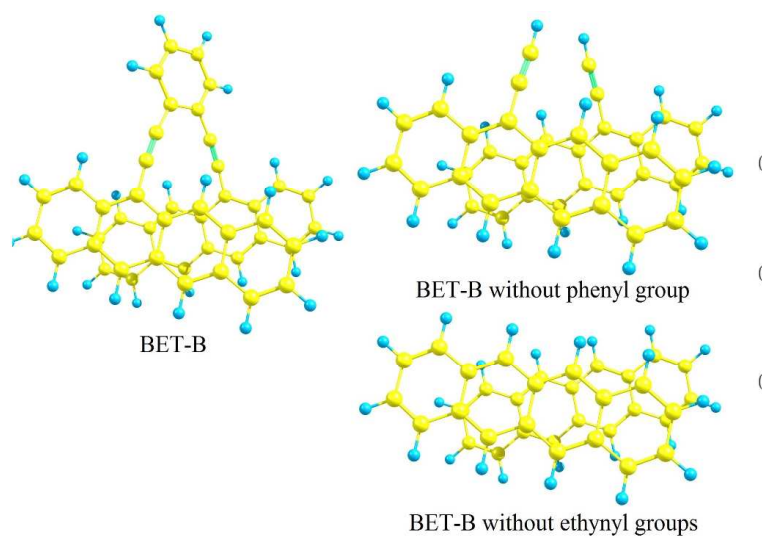


FIG. S2: Model BET-B structures used in calculations of couplings.

Tables

TABLE S1: Raw^a excitation energies and logarithmic relative rates of BET-B and BET-X dimers. All energies are in eV.

System	T ₁	¹ ME	⁵ ME	S ₁	S ₁ '	$\log \left[\frac{r_1}{r_1(Tc)} \right]$	$\log \left[\frac{r_{1'}}{r_1(Tc)} \right]$
Tc	1.772	3.682	3.703	3.886	4.026	0.00	0.66
BET-B(cry)	1.645	3.183	3.335	3.748	4.061	1.90	4.40
BET-B(i)	1.729	3.416	3.514	3.701	4.024	0.41	2.50
BET-B(S ₁)	1.180	2.456	2.685	2.617	3.388	0.21	5.33
BET-B(⁵ ME)	0.866	1.749	1.782	2.993	3.393		
BET-X(cry1)	1.577	3.248	3.317	3.400	3.953	0.13	3.52
BET-X(cry2)	1.708	3.465	3.508	3.701	4.057	0.31	2.82
BET-X(i)	1.740	3.201	3.513	3.781	4.007	2.05	4.45
BET-X(S ₁)	1.256	2.343	2.817	3.013	3.770	3.28	9.15
BET-X(⁵ ME)	0.885	1.741	1.801	3.125	3.341		

To obtain the corrected values, subtract 0.2 eV from triplets' excitation energy, 1.0 eV from singlets' excitation energy, and 0.4 eV from the multi-exciton states[?].

TABLE S2: Ground-state energy differences (eV) relative to the fully optimized structure of BET-B.

Method	BET-B(i)	BET-B(cry)	BET-B(S ₁)	BET-B(⁵ ME)
ω B97X-D	0.00	0.213	0.507	0.818
RASCI-2SF	0.00	-0.393	0.943	0.736

TABLE S3: Ground-state energy differences (eV) relative to the fully optimized structure of BET-X.

Method	BET-X(i)	BET-X(cry1)	BET-X(cry2)	BET-X(S ₁)	BET-X(⁵ ME)
ω B97X-D	0.00	0.540	0.472	0.352	0.828
RASCI-2SF	0.00	0.702	0.415	0.472	1.365

TABLE S4: Fragments molecular orbitals (FMOs) overlaps versus couplings.

System	$ \langle H_A H_B \rangle $	$ \langle L_A L_B \rangle $	$ \gamma^{1ME-S_1} ^2$
Tc	0.006	0.018	0.084
Tc-BET-B(cry)	0.007	0.003	0.044
Tc-BET-B(S ₁)	0.023	0.063	0.195
Tc-BET-B(33)	0.010	0.010	0.087
Tc-BET-B(23)	0.028	0.017	0.046
Tc-BET-B(22)	0.023	0.015	0.015

Relevant Cartesian geometries

Cartesian geometry of BET-B(cry)

C	-0.690709915	-0.099949854	6.599778821
H	-1.229148720	-0.176562151	7.545806471
C	-1.377347491	-0.215830649	5.401408844
H	-2.453807014	-0.392772823	5.394624030
C	-0.699887477	-0.126344164	4.177714820
C	-1.395684323	-0.320630403	2.942413843
C	-1.957131136	-0.524994658	1.898224859
C	-2.577619492	-0.724344596	0.625994878
C	-3.946440766	-0.427937713	0.454666937
C	-4.761176923	0.068210230	1.520881980
H	-4.303809365	0.216047516	2.500048706
C	-6.082452529	0.349037402	1.323704037
H	-6.687171063	0.727399564	2.149890995
C	-6.687371186	0.139592955	0.049231055
H	-7.749309696	0.355874021	-0.081904189
C	-5.942838535	-0.314841124	-0.994693984
H	-6.395119003	-0.461937306	-1.977903834
C	-4.547163878	-0.603578761	-0.842095044
C	-3.768350888	-1.031414968	-1.913981083
H	-4.224276833	-1.130954566	-2.901721765
C	-2.392878417	-1.298571550	-1.769955142
C	-1.593539924	-1.666682655	-2.872308181
H	-2.051938250	-1.729042546	-3.861827455
C	-0.234056335	-1.925738788	-2.731711239
C	0.599207988	-2.261872646	-3.850419278
H	0.146316931	-2.316218960	-4.842616467
C	1.931823821	-2.484781349	-3.683708334
H	2.559511937	-2.727304478	-4.543556148
C	2.525498272	-2.410046855	-2.388792355
H	3.596725490	-2.589213126	-2.277969248
C	1.767133194	-2.114067378	-1.296199320
H	2.216845564	-2.052521870	-0.303370415
C	0.365435518	-1.846230465	-1.424794260
C	-0.415880513	-1.482364479	-0.331409222
H	0.045907578	-1.406896946	0.654576501
C	-1.782950930	-1.180700541	-0.469632163
C	0.690709915	0.099949854	6.599778821
H	1.229148720	0.176562151	7.545806471
C	1.377347491	0.215830649	5.401408844
H	2.453807014	0.392772823	5.394624030
C	0.699887477	0.126344164	4.177714820
C	1.395684323	0.320630403	2.942413843
C	1.957131136	0.524994658	1.898224859
C	2.577619492	0.724344596	0.625994878

C	3.946440766	0.427937713	0.454666937
C	4.761176923	-0.068210230	1.520881980
H	4.303809365	-0.216047516	2.500048706
C	6.082452529	-0.349037402	1.323704037
H	6.687171063	-0.727399564	2.149890995
C	6.687371186	-0.139592955	0.049231055
H	7.749309696	-0.355874021	-0.081904189
C	5.942838535	0.314841124	-0.994693984
H	6.395119003	0.461937306	-1.977903834
C	4.547163878	0.603578761	-0.842095044
C	3.768350888	1.031414968	-1.913981083
H	4.224276833	1.130954566	-2.901721765
C	2.392878417	1.298571550	-1.769955142
C	1.593539924	1.666682655	-2.872308181
H	2.051938250	1.729042546	-3.861827455
C	0.234056335	1.925738788	-2.731711239
C	-0.599207988	2.261872646	-3.850419278
H	-0.146316931	2.316218960	-4.842616467
C	-1.931823821	2.484781349	-3.683708334
H	-2.559511937	2.727304478	-4.543556148
C	-2.525498272	2.410046855	-2.388792355
H	-3.596725490	2.589213126	-2.277969248
C	-1.767133194	2.114067378	-1.296199320
H	-2.216845564	2.052521870	-0.303370415
C	-0.365435518	1.846230465	-1.424794260
C	0.415880513	1.482364479	-0.331409222
H	-0.045907578	1.406896946	0.654576501
C	1.782950930	1.180700541	-0.469632163

Nuclear Repulsion Energy = 5166.0046643259 hartrees

Cartesian geometry of BET-B(ex)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39421200
H	0.94995631	0.00000000	1.93051789
C	-1.18905332	-0.00995523	2.14416960
C	-1.17187484	0.00265979	3.56285751
H	-0.20871122	0.01900030	4.07697451
C	-2.34359210	-0.02946027	4.28395505
H	-2.31352741	-0.02640448	5.37433237
C	-3.58734119	-0.08716747	3.61088610
H	-4.51091044	-0.11807352	4.19204232
C	-3.64020705	-0.11881727	2.23605513
H	-4.60110954	-0.16042932	1.71774630
C	-2.44848725	-0.06034529	1.45825887
C	-2.45630089	-0.07235954	0.05846724
H	-3.41029323	-0.09248279	-0.47481068
C	-1.26554414	0.01352422	-0.69828656
C	-1.27571787	0.05481273	-2.09461321

H	-2.23127496	0.06184598	-2.62418664
C	-0.08655654	0.11770141	-2.84836391
C	-0.11078419	0.16731516	-4.26928560
H	-1.07789563	0.19802089	-4.77638673
C	1.05252954	0.17231450	-5.00131800
H	1.01232454	0.21480563	-6.09116621
C	2.30292747	0.12347449	-4.33986560
H	3.22431966	0.12797028	-4.92487471
C	2.36267583	0.06732797	-2.96692656
H	3.32359742	0.02301732	-2.45142097
C	1.17951121	0.06526965	-2.18403049
C	1.21302277	-0.04843372	-0.76188217
C	2.40520494	-0.33054021	-0.07597928
C	3.33741131	-0.68622890	0.63766412
C	4.37279597	-1.06319558	1.52338666
C	5.71163503	-0.69876128	1.26358733
H	5.93130579	-0.14628092	0.34916671
C	6.71525904	-1.00254524	2.16428551
H	7.74405474	-0.70736474	1.95224220
C	6.41348169	-1.68463988	3.35531137
H	7.20856541	-1.92025641	4.06445666
C	5.11356626	-2.07068757	3.62639452
H	4.87998215	-2.62568856	4.53576091
C	4.07223678	-1.79232290	2.71487344
C	2.75610275	-2.26273713	2.93239947
C	1.60706587	-2.68612655	3.00724507
C	0.25608342	-3.05017484	2.86430828
C	-0.61876218	-3.18244384	3.98354655
C	-0.14769897	-3.13446370	5.32108295
H	0.92476866	-3.02898658	5.49520249
C	-1.01900470	-3.22438925	6.38247770
H	-0.63411168	-3.19308691	7.40345890
C	-2.41047124	-3.35532459	6.15983505
H	-3.09203203	-3.42464369	7.00937547
C	-2.89771885	-3.39530799	4.87493110
H	-3.97050152	-3.48613137	4.69075626
C	-2.02630840	-3.31446188	3.75472407
C	-2.52722567	-3.29993097	2.43805862
H	-3.60677712	-3.35699155	2.28133932
C	-1.68429436	-3.23198549	1.32738225
C	-2.18495244	-3.19019877	0.00596305
H	-3.26702949	-3.21078641	-0.14621956
C	-1.33928348	-3.19130387	-1.10890629
C	-1.82647632	-3.16683549	-2.44654576
H	-2.90611480	-3.15842399	-2.61398736
C	-0.95895890	-3.18739435	-3.51537486
H	-1.35063925	-3.17946422	-4.53417446

C	0.43963998	-3.19576934	-3.30606690
H	1.11588314	-3.18276247	-4.16183562
C	0.94471854	-3.19492888	-2.02472738
H	2.02280343	-3.17458629	-1.85172601
C	0.08079936	-3.19771544	-0.90007920
C	0.58166498	-3.17446001	0.41295102
H	1.66179416	-3.15762233	0.56090998
C	-0.25451505	-3.16148735	1.52941895

Nuclear Repulsion Energy = 5351.3083054653 hartrees

Cartesian geometry of BET-B(33)

C	-0.566536473	-0.407085294	6.665878679
H	-1.010825256	-0.726095099	7.610116433
C	-1.132907682	-0.816303063	5.462714571
H	-2.012787799	-1.460337911	5.455165064
C	-0.574959863	-0.416788527	4.241538999
C	-1.131318800	-0.828620157	2.989554318
C	-1.497145637	-1.092538029	1.859500235
C	-1.821508706	-1.296076161	0.483426856
C	-3.139936884	-1.141302929	0.030322885
C	-4.227931175	-0.872983189	0.926523440
H	-4.013585757	-0.805831281	1.994187317
C	-5.497165674	-0.708550202	0.457143162
H	-6.313100602	-0.511396946	1.155171619
C	-5.776662641	-0.795132383	-0.943699910
H	-6.800168397	-0.661704169	-1.298304261
C	-4.770867460	-1.038664425	-1.828845536
H	-4.971785365	-1.096670000	-2.900679416
C	-3.418226505	-1.215789217	-1.380833133
C	-2.380457046	-1.425781359	-2.277624534
H	-2.595780650	-1.449361425	-3.348742115
C	-1.051705493	-1.601671293	-1.844245316
C	0.002280966	-1.795277131	-2.760856378
H	-0.226252797	-1.809833708	-3.829656553
C	1.314030756	-1.959957883	-2.337262363
C	2.404864285	-2.126891920	-3.257581111
H	2.188675542	-2.127793982	-4.328600861
C	3.680632314	-2.283622862	-2.805553111
H	4.500638897	-2.401852190	-3.516476731
C	3.961817974	-2.290635632	-1.401075274
H	4.991128484	-2.409880078	-1.059884350
C	2.957922853	-2.128042383	-0.495523425
H	3.169176326	-2.110914101	0.575578996
C	1.599274760	-1.952344124	-0.925402130
C	0.568828666	-1.747586625	-0.015228847
H	0.797995719	-1.709723265	1.050648082
C	-0.759879900	-1.560502848	-0.435959279
C	0.566536473	0.407085294	6.665878679

H	1.010825256	0.726095099	7.610116433
C	1.132907682	0.816303063	5.462714571
H	2.012787799	1.460337911	5.455165064
C	0.574959863	0.416788527	4.241538999
C	1.131318800	0.828620157	2.989554318
C	1.497145637	1.092538029	1.859500235
C	1.821508706	1.296076161	0.483426856
C	3.139936884	1.141302929	0.030322885
C	4.227931175	0.872983189	0.926523440
H	4.013585757	0.805831281	1.994187317
C	5.497165674	0.708550202	0.457143162
H	6.313100602	0.511396946	1.155171619
C	5.776662641	0.795132383	-0.943699910
H	6.800168397	0.661704169	-1.298304261
C	4.770867460	1.038664425	-1.828845536
H	4.971785365	1.096670000	-2.900679416
C	3.418226505	1.215789217	-1.380833133
C	2.380457046	1.425781359	-2.277624534
H	2.595780650	1.449361425	-3.348742115
C	1.051705493	1.601671293	-1.844245316
C	-0.002280966	1.795277131	-2.760856378
H	0.226252797	1.809833708	-3.829656553
C	-1.314030756	1.959957883	-2.337262363
C	-2.404864285	2.126891920	-3.257581111
H	-2.188675542	2.127793982	-4.328600861
C	-3.680632314	2.283622862	-2.805553111
H	-4.500638897	2.401852190	-3.516476731
C	-3.961817974	2.290635632	-1.401075274
H	-4.991128484	2.409880078	-1.059884350
C	-2.957922853	2.128042383	-0.495523425
H	-3.169176326	2.110914101	0.575578996
C	-1.599274760	1.952344124	-0.925402130
C	-0.568828666	1.747586625	-0.015228847
H	-0.797995719	1.709723265	1.050648082
C	0.759879900	1.560502848	-0.435959279

Nuclear Repulsion Energy = 5322.8347461950 hartrees

Cartesian geometry of BET-B(23)

C	-0.029222575	0.597403568	1.814111790
C	0.863206358	-0.413250233	1.413478071
C	0.376422166	-1.729853538	1.148910748
C	-0.068173347	-2.813278463	0.818137625
C	-0.704830169	-3.999552281	0.334481938
C	-0.170716665	-5.272891263	0.570980758
H	0.761136714	-5.359074652	1.130800943
C	-0.815007866	-6.409189062	0.092620031
H	-0.387443748	-7.395402007	0.280100519
C	-2.009698562	-6.289745480	-0.618458363

H	-2.514115828	-7.181697340	-0.993204520
C	-2.552015334	-5.033101371	-0.868715533
H	-3.481365660	-4.931758602	-1.430071705
C	-1.911412813	-3.877648384	-0.404956857
C	-2.414720371	-2.566336037	-0.673897013
C	-2.682284405	-1.388427317	-0.818471258
C	-2.854734169	0.026951506	-0.893563296
C	-4.086022399	0.615916320	-0.570298343
C	-1.413052026	0.337421464	2.084869399
H	-1.780760302	-0.685435820	1.994494759
C	-2.262199990	1.347341953	2.429699304
H	-3.314069853	1.127260805	2.620905157
C	-1.796205499	2.695589154	2.526538972
H	-2.498540529	3.489922722	2.784991146
C	-0.488556736	2.986324630	2.282279594
H	-0.117658089	4.011475678	2.347875021
C	-5.242935264	-0.167447257	-0.244773733
H	-5.156825211	-1.254911520	-0.269475947
C	-6.422577431	0.430110620	0.086597073
H	-7.293243972	-0.183697750	0.324130350
C	-6.534911517	1.856825078	0.121396194
H	-7.488446890	2.315489715	0.388747056
C	-5.459089552	2.636995608	-0.176555898
H	-5.534754444	3.726504960	-0.151985398
C	0.442978035	1.953430257	1.924092008
C	1.772466567	2.245495792	1.650562771
H	2.119886825	3.279774907	1.712501065
C	2.686360703	1.245025451	1.271091917
C	4.026893275	1.551466215	0.961789143
H	4.362288393	2.588587004	1.041455337
C	4.916344992	0.576895010	0.531628510
C	6.275856747	0.881185911	0.179502400
H	6.618854717	1.914988415	0.264758747
C	7.119011453	-0.094433756	-0.259789561
H	8.147480079	0.151524991	-0.530093793
C	6.668639387	-1.450771860	-0.371645277
H	7.361654139	-2.216915156	-0.724194226
C	5.389284704	-1.783647957	-0.043126891
H	5.040456365	-2.815546988	-0.124914294
C	4.461601895	-0.786246215	0.414173171
C	3.144551546	-1.099372289	0.726538931
H	2.798526967	-2.130706457	0.633835430
C	2.231783860	-0.114629840	1.149136725
C	-4.194345916	2.051668660	-0.527112205
C	-3.080403950	2.835190102	-0.797587646
H	-3.163156798	3.923811750	-0.741805664
C	-1.835503938	2.265176300	-1.128120527

C	-0.697620620	3.064063341	-1.364616525
H	-0.791857957	4.150808106	-1.293120176
C	0.535131639	2.503215096	-1.669464485
C	1.713738264	3.298229814	-1.879696358
H	1.631812232	4.385190907	-1.802659133
C	2.908510185	2.711909895	-2.171038956
H	3.795828345	3.329056086	-2.324508264
C	3.017078785	1.287260114	-2.278529785
H	3.986329235	0.837664933	-2.500902863
C	1.925278252	0.497231553	-2.085418727
H	2.002871866	-0.590110169	-2.148561000
C	0.646237677	1.070330146	-1.769939929
C	-0.468151460	0.275248008	-1.533359715
H	-0.368893543	-0.810080820	-1.580378278
C	-1.716316089	0.833133756	-1.201600237

Nuclear Repulsion Energy = 5208.7183437902 hartrees

Cartesian geometry of BET-B(22)

C	0.799973997	1.538892376	-0.905415580
C	1.770420339	1.211278352	0.056167009
C	1.401359886	1.101536381	1.431330711
C	1.058422018	0.896950282	2.580301507
C	0.533582923	0.468895044	3.840319178
C	1.043826649	0.927257794	5.060472994
H	1.854477535	1.657011801	5.052320753
C	0.519780321	0.465585226	6.263872415
H	0.925280200	0.834299189	7.207224597
C	-0.519780321	-0.465585226	6.263872415
H	-0.925280200	-0.834299189	7.207224597
C	-1.043826649	-0.927257794	5.060472994
H	-1.854477535	-1.657011801	5.052320753
C	-0.533582923	-0.468895044	3.840319178
C	-1.058422018	-0.896950282	2.580301507
C	-1.401359886	-1.101536381	1.431330711
C	-1.770420339	-1.211278352	0.056167009
C	-0.799973997	-1.538892376	-0.905415580
C	-0.557793586	1.841863403	-0.554744498
H	-0.842671566	1.829417762	0.497817390
C	-1.487236261	2.109266573	-1.515182582
H	-2.520450147	2.310668664	-1.226541134
C	-1.128443649	2.108632044	-2.899795103
H	-1.890444184	2.324733799	-3.650648722
C	0.149791710	1.832169236	-3.277311434
H	0.437604391	1.824110633	-4.330651379
C	0.557793586	-1.841863403	-0.554744498
H	0.842671566	-1.829417762	0.497817390
C	1.487236261	-2.109266573	-1.515182582
H	2.520450147	-2.310668664	-1.226541134

C	1.128443649	-2.108632044	-2.899795103
H	1.890444184	-2.324733799	-3.650648722
C	-0.149791710	-1.832169236	-3.277311434
H	-0.437604391	-1.824110633	-4.330651379
C	1.159876509	1.533134839	-2.300408053
C	2.456052196	1.212224786	-2.678188152
H	2.720091585	1.200845938	-3.738667974
C	3.441768700	0.872309601	-1.730974511
C	4.745722583	0.501175308	-2.120027237
H	5.003099715	0.504825386	-3.182369926
C	5.704158801	0.122191643	-1.189117749
C	7.031365411	-0.276246920	-1.571006168
H	7.295208804	-0.272181951	-2.630974093
C	7.945162016	-0.652215155	-0.633373948
H	8.946803115	-0.959696971	-0.939352369
C	7.601230627	-0.655942936	0.758031926
H	8.350231378	-0.955365500	1.493300935
C	6.355238716	-0.284767841	1.164081748
H	6.085787719	-0.286165846	2.222401602
C	5.357990734	0.116827722	0.210783600
C	4.078256905	0.490303699	0.603853594
H	3.814404312	0.481940175	1.662968026
C	3.099523733	0.870557041	-0.333140952
C	-1.159876509	-1.533134839	-2.300408053
C	-2.456052196	-1.212224786	-2.678188152
H	-2.720091585	-1.200845938	-3.738667974
C	-3.441768700	-0.872309601	-1.730974511
C	-4.745722583	-0.501175308	-2.120027237
H	-5.003099715	-0.504825386	-3.182369926
C	-5.704158801	-0.122191643	-1.189117749
C	-7.031365411	0.276246920	-1.571006168
H	-7.295208804	0.272181951	-2.630974093
C	-7.945162016	0.652215155	-0.633373948
H	-8.946803115	0.959696971	-0.939352369
C	-7.601230627	0.655942936	0.758031926
H	-8.350231378	0.955365500	1.493300935
C	-6.355238716	0.284767841	1.164081748
H	-6.085787719	0.286165846	2.222401602
C	-5.357990734	-0.116827722	0.210783600
C	-4.078256905	-0.490303699	0.603853594
H	-3.814404312	-0.481940175	1.662968026
C	-3.099523733	-0.870557041	-0.333140952

Nuclear Repulsion Energy = 5019.9500110160 hartrees

Cartesian geometry of BET-B(5ME)

C	-1.22670	-0.68522	2.97997
C	-1.65181	-1.01466	1.88112
C	-2.07541	-1.33080	0.57925

C	-3.50028	-1.32055	0.25606
C	-4.47927	-1.15091	1.23859
H	-4.16653	-1.05328	2.27964
C	-5.83448	-1.11012	0.90368
H	-6.58274	-0.97628	1.68649
C	-6.22591	-1.23202	-0.42719
H	-7.28218	-1.19754	-0.69950
C	-5.26142	-1.39964	-1.42018
H	-5.56715	-1.48104	-2.46576
C	-3.89754	-1.45112	-1.10330
C	-2.89694	-1.59251	-2.12388
H	-3.22229	-1.63943	-3.16526
C	-1.52552	-1.65473	-1.82833
C	-0.56178	-1.76197	-2.82998
H	-0.89060	-1.78031	-3.87202
C	0.83713	-1.82091	-2.54168
C	1.81501	-1.87421	-3.55296
H	1.49228	-1.87618	-4.59665
C	3.16365	-1.92197	-3.23196
H	3.91209	-1.96035	-4.02578
C	3.57096	-1.92472	-1.89061
H	4.63155	-1.95004	-1.63607
C	2.62226	-1.86775	-0.87950
H	2.94152	-1.84457	0.16470
C	1.25239	-1.80688	-1.18210
C	0.25825	-1.68308	-0.15351
H	0.59679	-1.63785	0.88343
C	-1.08828	-1.57354	-0.43895
C	1.23042	0.71482	2.97838
C	1.66035	1.02559	1.87603
C	2.08330	1.32556	0.56989
C	3.50745	1.31076	0.24449
C	4.48768	1.14642	1.22673
H	4.17619	1.05537	2.26875
C	5.84237	1.10267	0.89018
H	6.59162	0.97313	1.67277
C	6.23211	1.21634	-0.44193
H	7.28799	1.17993	-0.71548
C	5.26637	1.37841	-1.43465
H	5.57083	1.45388	-2.48104
C	3.90298	1.43262	-1.11620
C	2.90108	1.56916	-2.13620
H	3.22519	1.61110	-3.17819
C	1.53018	1.63346	-1.83917
C	0.56517	1.73617	-2.84022
H	0.89286	1.75028	-3.88268
C	-0.83348	1.79641	-2.55059

C	-1.81262	1.84527	-3.56083
H	-1.49126	1.84359	-4.60495
C	-3.16095	1.89357	-3.23828
H	-3.91039	1.92824	-4.03133
C	-3.56660	1.90114	-1.89650
H	-4.62688	1.92630	-1.64062
C	-2.61655	1.84919	-0.88632
H	-2.93447	1.82928	0.15837
C	-1.24708	1.78819	-1.19047
C	-0.25160	1.67075	-0.16245
H	-0.58914	1.63099	0.87495
C	1.09474	1.56016	-0.44874
C	-0.64992	-0.24491	6.64464
H	-1.14969	-0.47045	7.58801
C	-1.26294	-0.57818	5.44158
H	-2.23863	-1.06512	5.43359
C	-0.63612	-0.29839	4.21896
C	0.60618	0.36357	6.64542
H	1.09192	0.61539	7.58942
C	1.23628	0.66553	5.44277
H	2.21188	1.15269	5.43584
C	0.62614	0.35531	4.21920

Nuclear Repulsion Energy = 5250.9802742415 hartrees

Cartesian geometry of BET-X(cry1)

C	0.296282163	1.521254509	2.123231926
H	1.085970013	0.773468066	2.021624828
C	0.584921433	2.751086201	2.602875928
H	1.605658098	2.995811359	2.901812886
C	-0.434886574	3.753630095	2.713626882
H	-0.183898677	4.744613903	3.093309386
C	-1.698993153	3.454760688	2.305278454
H	-2.484924848	4.212065808	2.373029092
C	-2.049283962	2.181304426	1.824328460
C	-3.361037184	1.871655045	1.473257558
H	-4.130777521	2.643667869	1.559463401
C	-3.733088331	0.584344483	1.047382104
C	-5.053484354	0.251704600	0.759696301
H	-5.817470674	1.030776528	0.843011885
C	-5.449778851	-1.035189233	0.390041999
C	-6.790683375	-1.372093635	0.113059242
H	-7.553585924	-0.594125078	0.196820070
C	-7.131299798	-2.630756789	-0.255620722
H	-8.173345656	-2.873377593	-0.473887991
C	-6.149139417	-3.645959222	-0.360560328
H	-6.447861217	-4.650760471	-0.664871744
C	-4.838802446	-3.372740922	-0.081983958
H	-4.079234033	-4.153999607	-0.164069944

C	-4.428150675	-2.062566493	0.297717995
C	-3.114596856	-1.737321666	0.561684593
H	-2.349166576	-2.510936729	0.469334426
C	-2.712182180	-0.449440490	0.944766183
C	-1.368804302	-0.107328439	1.262607256
C	-1.013696427	1.158306195	1.715931281
C	-0.354890453	-1.132546547	1.144141221
C	0.460494253	-2.022109443	1.075828874
C	1.353311796	-3.144321314	1.126981765
C	0.914865920	-4.359576637	1.667449765
H	-0.116213061	-4.401385951	2.023928189
C	1.737033901	-5.473912235	1.780955776
C	3.052076057	-5.326964852	1.328757465
H	3.744804371	-6.169588185	1.411126313
C	3.539676215	-4.148059860	0.773029125
C	4.998047932	-4.065132128	0.340037832
H	5.216740422	-4.846899886	-0.404273368
H	5.658587455	-4.243469944	1.203447697
C	5.286111298	-2.692206030	-0.252121245
C	6.574676422	-2.393060323	-0.732103338
H	7.325957162	-3.187285106	-0.699025355
C	6.926174045	-1.141108947	-1.227287743
C	5.946058702	-0.161785697	-1.241279689
H	6.170471410	0.834507114	-1.626849374
C	4.652362737	-0.406767902	-0.789677137
C	3.651258019	0.609997694	-0.841533446
C	2.787957030	1.447693590	-0.899293562
C	1.680988166	2.345560437	-0.961241109
C	1.823728423	3.666722034	-0.531263956
C	3.062146020	4.195793797	-0.053635659
H	3.941877057	3.550250268	-0.077622245
C	3.150414613	5.464377318	0.438106213
H	4.106788490	5.839236707	0.807265204
C	2.003150271	6.310291413	0.474330873
H	2.082991694	7.323550283	0.871109446
C	0.813552337	5.849230899	0.009958091
H	-0.071675182	6.490009420	0.034618544
C	0.664322842	4.526826666	-0.495866608
C	-0.568633859	4.028255990	-0.898060009
H	-1.447105832	4.676364235	-0.841575082
C	-0.723302561	2.716092317	-1.346670645
C	-1.970596105	2.206986001	-1.741481238
H	-2.837558258	2.872165401	-1.697911802
C	-2.146904934	0.899686320	-2.136416289
C	-3.426001627	0.360192224	-2.487030412
H	-4.298011325	1.016273668	-2.443384792
C	-3.556386746	-0.944240952	-2.822140114

H	-4.544203746	-1.346752255	-3.056672340
C	-2.429593796	-1.802446643	-2.879571390
H	-2.561688732	-2.846313587	-3.169388916
C	-1.205757375	-1.331068378	-2.573088195
H	-0.334552069	-1.990277712	-2.604062160
C	-1.002988406	0.018585004	-2.179638891
C	0.249057668	0.514764014	-1.818422152
H	1.108045101	-0.157821485	-1.825428276
C	0.424075544	1.842387704	-1.395578729
C	4.346914435	-1.680834820	-0.291554322
C	2.684946786	-3.055928002	0.675018378
O	3.045676250	-1.837243894	0.158015677
H	1.375877756	-6.408341763	2.206714108
H	7.932246625	-0.939606514	-1.593481432

Nuclear Repulsion Energy = 6781.4165228152 hartrees

Cartesian geometry of BET-X(cry2)

C	-0.630295369	-4.224902340	0.530065638
H	-1.640220216	-3.822602117	0.621632235
C	-0.441106078	-5.526960607	0.214504842
H	-1.300967900	-6.181767940	0.062285427
C	0.883603284	-6.062569086	0.069222082
H	1.010021553	-7.116906880	-0.183296214
C	1.953361327	-5.255640123	0.238058862
H	2.967405733	-5.651756884	0.136571666
C	1.809481107	-3.879913414	0.581924685
C	2.899020803	-3.054799013	0.809752613
H	3.906735383	-3.473343417	0.726291594
C	2.763318802	-1.720230027	1.212503208
C	3.861910225	-0.917334689	1.548964158
H	4.863868461	-1.352905713	1.488060874
C	3.728844906	0.386322122	1.988949864
C	4.834914730	1.199228024	2.391013716
H	5.836233094	0.761582592	2.364499346
C	4.665192430	2.483309811	2.790571268
H	5.525660169	3.087808147	3.082811290
C	3.359050084	3.069295991	2.810779268
H	3.242426518	4.110335432	3.114549442
C	2.277816411	2.328690711	2.460779857
H	1.276845335	2.765470149	2.476750365
C	2.401290031	0.966682470	2.053263592
C	1.307445771	0.181414221	1.723604064
H	0.306320751	0.614091642	1.774710223
C	1.431965207	-1.159258397	1.327765557
C	0.307664049	-1.990990516	1.096543674
C	0.469121625	-3.336906407	0.734160043
C	-1.006706042	-1.475529937	1.356748508
C	-2.094888794	-1.065430342	1.677777579

C	-3.381976133	-0.603762442	2.127026306
C	-3.883329627	-0.986573575	3.369569411
H	-3.270378384	-1.642095942	3.989871835
C	-5.124777806	-0.545263327	3.825079867
C	-5.855642971	0.288076008	2.980025025
H	-6.834556963	0.648998347	3.309306014
C	-5.407098283	0.692276036	1.723207091
C	-6.267297687	1.593144440	0.829232413
H	-6.495081220	2.532766934	1.357229817
H	-7.227701457	1.097148373	0.615005040
C	-5.534934567	1.904035716	-0.473659229
C	-6.088466364	2.729327378	-1.453269534
H	-7.092632088	3.124360627	-1.271082416
C	-5.436029549	3.080827957	-2.633782684
C	-4.142808230	2.578194119	-2.825465449
H	-3.578304057	2.832448680	-3.724278055
C	-3.546315350	1.749971191	-1.880935805
C	-2.218838070	1.237516343	-2.038423932
C	-1.112467218	0.762834374	-2.044581749
C	0.194116248	0.175845070	-2.055571968
C	1.318048002	0.971064230	-1.714271800
C	1.203052804	2.317593191	-1.340536369
H	0.205602159	2.760589800	-1.307201939
C	2.299993813	3.091248442	-0.999777401
C	2.185763411	4.451380842	-0.595621998
H	1.185372899	4.887184459	-0.543010501
C	3.280127950	5.198215891	-0.293890052
H	3.166751173	6.238860099	0.015451269
C	4.587297193	4.629357958	-0.368674440
H	5.456747519	5.241622579	-0.123804117
C	4.741271361	3.328325345	-0.740327609
H	5.740230879	2.887186772	-0.782931254
C	3.625214024	2.504934458	-1.064244495
C	3.748204240	1.173742754	-1.434187969
H	4.745104159	0.724944090	-1.461803893
C	2.639829569	0.371670729	-1.743421224
C	2.753779730	-0.993304840	-2.055454256
H	3.748489557	-1.447310131	-2.047075393
C	1.655352851	-1.778365418	-2.353794956
C	1.770120818	-3.175638098	-2.624702339
H	2.765314308	-3.623480323	-2.573801863
C	0.692489194	-3.929866931	-2.940190266
H	0.800893349	-4.998410395	-3.133847405
C	-0.606333744	-3.334980101	-3.003599944
H	-1.469392298	-3.954638999	-3.252279327
C	-0.775855005	-2.013187622	-2.724494851
H	-1.771301372	-1.569051345	-2.742594467

C	0.334445614	-1.182820938	-2.378003248
C	-4.260401745	1.406773961	-0.729172433
C	-4.157067315	0.235073519	1.317526404
O	-3.588155664	0.550713336	0.113996048
H	-5.914298117	3.726930331	-3.368253047
H	-5.512773632	-0.846636358	4.796883487

Nuclear Repulsion Energy = 6806.3476678542 hartrees

Cartesian geometry of BET-X(ex)

O	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.35844300
C	1.17380366	0.00000000	-0.68403027
C	2.41351721	-0.14543268	-0.06607768
C	1.17019355	-0.01342676	2.11437370
C	1.05117595	0.08778022	3.50114111
H	1.95715957	0.08921315	4.11177392
C	3.54363771	-0.22096824	-0.88180458
H	4.52529901	-0.34046262	-0.41773025
C	-0.19804808	0.18077971	4.11690058
H	-0.26092761	0.26961667	5.20195963
C	-1.35714326	0.13295164	3.35264078
H	-2.33962364	0.16145606	3.82412657
C	3.44157920	-0.14906909	-2.27211683
H	4.33980635	-0.22034466	-2.88655977
C	2.20354498	0.05449180	-2.86916746
H	2.11452555	0.16470140	-3.95026748
C	1.04755228	0.16685159	-2.08048180
C	-1.28040901	0.01666387	1.95447121
C	-2.42089905	-0.12959899	1.12593281
C	-3.35124696	-0.32766174	0.35601351
C	-4.38979041	-0.47042271	-0.57628969
C	-0.22294576	0.52277335	-2.60118803
C	-1.32100307	0.94434987	-2.93500460
C	-2.61084694	1.39912923	-3.25623480
C	-3.18225171	1.06484360	-4.51994141
C	-2.44268725	0.39329749	-5.52572914
H	-1.40254295	0.13252731	-5.32571797
C	-3.02437606	0.05200656	-6.72556582
H	-2.43269791	-0.46062069	-7.48507691
C	-4.38559918	0.34539963	-6.96737403
H	-4.84604576	0.06456736	-7.91609243
C	-5.13295578	0.98730033	-6.00599432
H	-6.18605235	1.21633365	-6.18773459
C	-4.55487307	1.38639787	-4.77042351
C	-5.30506394	2.04246126	-3.78100952
H	-6.34744713	2.29664024	-3.98850196
C	-4.72332784	2.49302898	-2.57416800
C	-5.45959079	3.21957354	-1.63358312

H	-6.49085422	3.49383080	-1.86737354
C	-4.91391330	3.58973919	-0.39315705
C	-5.67100896	4.28518208	0.59046865
H	-6.69274034	4.58475129	0.34675429
C	-5.13702867	4.55909547	1.82633526
H	-5.73501370	5.08159476	2.57531932
C	-3.81447445	4.15175515	2.14103030
H	-3.40116298	4.36426893	3.12865323
C	-3.04839073	3.49811596	1.20741345
H	-2.03228132	3.17704739	1.44878797
C	-3.56917600	3.19971579	-0.08381729
C	-2.80987472	2.50822843	-1.04483773
H	-1.78539035	2.22053611	-0.80301022
C	-3.35286636	2.14013290	-2.27895093
C	-5.65541206	0.13695966	-0.30998002
C	-5.95640804	0.74282543	0.93519499
H	-5.19661455	0.73771035	1.71763594
C	-7.16908277	1.35792604	1.15300186
H	-7.38150510	1.81815067	2.11865333
C	-8.13740938	1.40797446	0.12506666
H	-9.09275704	1.90579241	0.30122191
C	-7.87476478	0.82945831	-1.09610596
H	-8.62342582	0.85749295	-1.89174247
C	-6.64482918	0.16205161	-1.34521238
C	-6.36193000	-0.42540830	-2.58885194
H	-7.12950539	-0.41210114	-3.36656151
C	-5.16691104	-1.14134778	-2.82816747
C	-4.93302562	-1.78944949	-4.04442745
H	-5.71742317	-1.78836838	-4.80456716
C	-3.71463160	-2.43298707	-4.31795252
C	-3.45369604	-3.06146123	-5.56747862
H	-4.24647157	-3.07707087	-6.31873408
C	-2.23002935	-3.62814738	-5.82983922
H	-2.03722079	-4.10222498	-6.79382724
C	-1.20272682	-3.59414539	-4.85133735
H	-0.23263683	-4.04191538	-5.07554019
C	-1.42489099	-3.00600892	-3.63061006
H	-0.63313171	-2.97162905	-2.87879706
C	-2.68134069	-2.41082064	-3.32370315
C	-2.92519778	-1.78825099	-2.08627517
H	-2.13480704	-1.77387719	-1.33394357
C	-4.13700402	-1.14935481	-1.81445258
C	2.51144676	-0.18251001	1.44058490
H	3.20264735	0.60538963	1.78204022
H	2.95494087	-1.14104700	1.76004271

Nuclear Repulsion Energy = 7029.2156969879 hartrees

Cartesian geometry of BET-X(i)

C	-1.382044784	2.103307020	5.893793145
C	-2.045546404	3.057211106	5.129898170
C	-2.048076623	2.951174908	3.742471456
C	-1.375614556	1.899225442	3.109691533
H	-1.394385231	2.168453290	6.984313383
H	-2.574997323	3.875723527	5.618713305
H	-2.585947617	3.671337124	3.126152284
C	-1.424192606	1.722247446	1.693139474
C	-0.677974311	0.967718103	3.905898876
O	0.000000000	0.000000000	3.219289205
C	0.000000000	0.000000000	6.134701091
C	-0.695301027	1.042298329	5.296520338
H	-0.733740468	-0.489709340	6.796379601
H	0.733740468	0.489709340	6.796379601
C	0.677974311	-0.967718103	3.905898876
C	0.695301027	-1.042298329	5.296520338
C	1.382044784	-2.103307020	5.893793145
C	2.045546404	-3.057211106	5.129898170
C	2.048076623	-2.951174908	3.742471456
C	1.375614556	-1.899225442	3.109691533
H	1.394385231	-2.168453290	6.984313383
H	2.574997323	-3.875723527	5.618713305
H	2.585947617	-3.671337124	3.126152284
C	1.424192606	-1.722247446	1.693139474
C	1.495043601	-1.497418628	0.500523507
C	-1.495043601	1.497418628	0.500523507
C	1.711639919	-0.353958385	-3.583456188
C	1.576245253	-1.128667904	-0.875623821
H	1.755810819	-0.048685917	-4.632031184
C	1.768601390	0.642189207	-2.588285029
C	1.684128703	0.255896562	-1.205094110
C	1.687618518	1.259007859	-0.219647207
C	1.883643586	2.008433992	-2.915677054
H	1.587051104	0.966852556	0.826325385
H	1.945773867	2.301704933	-3.966495007
C	1.901241013	2.991507909	-1.935201759
C	1.783371398	2.604016062	-0.552842628
C	1.743614638	3.630692036	0.450034845
C	1.840497547	4.945945820	0.105971357
C	1.983693077	5.330480270	-1.266282982
C	2.009786412	4.388139197	-2.249980377
H	1.634847033	3.324728809	1.492738054
H	1.807513222	5.718544748	0.876504935
H	2.067992130	6.388529935	-1.521864914
H	2.099480109	4.684067990	-3.297567349
C	1.592469770	-1.699178315	-3.262882386
C	1.537477911	-2.105596142	-1.881943423

C	1.418000850	-3.502362311	-1.584243849
C	1.343773019	-4.428310947	-2.581496185
C	1.378290800	-4.025844351	-3.953386251
C	1.499711368	-2.708938698	-4.280567855
H	1.364606429	-3.813359606	-0.540110730
H	1.238690755	-5.485022809	-2.331578004
H	1.309774297	-4.783501837	-4.736309197
H	1.533644224	-2.388942181	-5.324420236
C	-1.711639919	0.353958385	-3.583456188
C	-1.576245253	1.128667904	-0.875623821
H	-1.755810819	0.048685917	-4.632031184
C	-1.768601390	-0.642189207	-2.588285029
C	-1.684128703	-0.255896562	-1.205094110
C	-1.687618518	-1.259007859	-0.219647207
C	-1.883643586	-2.008433992	-2.915677054
H	-1.587051104	-0.966852556	0.826325385
H	-1.945773867	-2.301704933	-3.966495007
C	-1.901241013	-2.991507909	-1.935201759
C	-1.783371398	-2.604016062	-0.552842628
C	-1.743614638	-3.630692036	0.450034845
C	-1.840497547	-4.945945820	0.105971357
C	-1.983693077	-5.330480270	-1.266282982
C	-2.009786412	-4.388139197	-2.249980377
H	-1.634847033	-3.324728809	1.492738054
H	-1.807513222	-5.718544748	0.876504935
H	-2.067992130	-6.388529935	-1.521864914
H	-2.099480109	-4.684067990	-3.297567349
C	-1.592469770	1.699178315	-3.262882386
C	-1.537477911	2.105596142	-1.881943423
C	-1.418000850	3.502362311	-1.584243849
C	-1.343773019	4.428310947	-2.581496185
C	-1.378290800	4.025844351	-3.953386251
C	-1.499711368	2.708938698	-4.280567855
H	-1.364606429	3.813359606	-0.540110730
H	-1.238690755	5.485022809	-2.331578004
H	-1.309774297	4.783501837	-4.736309197
H	-1.533644224	2.388942181	-5.324420236

Nuclear Repulsion Energy = 6970.6561820734 hartrees

Cartesian geometry of BET-X(5ME)

C	-1.29168	1.85432	1.73568
C	-1.47083	1.64507	0.54300
C	-1.72831	0.58642	-3.54934
C	-1.63452	1.30887	-0.80488
H	-1.73958	0.31147	-4.60656
C	-1.72517	-0.43873	-2.58386
C	-1.68115	-0.08619	-1.17091
C	-1.65686	-1.09194	-0.22768

C	-1.74195	-1.78445	-2.94219
H	-1.59548	-0.83200	0.83056
H	-1.75442	-2.05751	-4.00017
C	-1.72333	-2.83048	-1.96894
C	-1.67343	-2.47904	-0.59310
C	-1.61919	-3.49600	0.37656
C	-1.62446	-4.83033	0.00021
C	-1.68509	-5.17863	-1.35798
C	-1.73214	-4.19201	-2.32907
H	-1.56796	-3.21352	1.43036
H	-1.57954	-5.61067	0.76215
H	-1.68638	-6.22879	-1.65549
H	-1.75888	-4.46517	-3.38611
C	-1.72336	1.97779	-3.19398
C	-1.69856	2.35527	-1.82238
C	-1.70797	3.70953	-1.48709
C	-1.73294	4.69478	-2.47711
C	-1.73956	4.33043	-3.82009
C	-1.73438	2.98098	-4.17314
H	-1.68091	3.99916	-0.43556
H	-1.73270	5.74612	-2.18610
H	-1.75086	5.09644	-4.59761
H	-1.74326	2.68538	-5.22480
C	1.33138	-1.78377	1.73574
C	1.50967	-1.56106	0.54656
C	1.75355	-0.59226	-3.57285
C	1.66730	-1.24711	-0.81112
H	1.76394	-0.34455	-4.63678
C	1.75090	0.45477	-2.63260
C	1.70811	0.13615	-1.21085
C	1.68441	1.16579	-0.29267
C	1.76783	1.79169	-3.02343
H	1.62736	0.93159	0.77164
H	1.78054	2.03730	-4.08808
C	1.74885	2.86150	-2.07561
C	1.69894	2.54429	-0.69127
C	1.64399	3.58441	0.25271
C	1.65005	4.90956	-0.15697
C	1.71191	5.22362	-1.52275
C	1.75799	4.21305	-2.46970
H	1.59139	3.33037	1.31365
H	1.60557	5.70775	0.58630
H	1.71392	6.26596	-1.84646
H	1.78584	4.45843	-3.53348
C	1.74855	-1.97455	-3.18364
C	1.72810	-2.31803	-1.80292
C	1.73512	-3.66426	-1.43505

C	1.75391	-4.67226	-2.40201
C	1.75651	-4.34092	-3.75344
C	1.75360	-3.00025	-4.13893
H	1.70929	-3.92832	-0.37689
H	1.75144	-5.71624	-2.08559
H	1.76214	-5.12449	-4.51332
H	1.75913	-2.73077	-5.19760
C	-1.09566	2.18759	5.93373
C	-1.46213	3.29869	5.17708
C	-1.51244	3.20667	3.79106
C	-1.16041	2.01282	3.14145
H	-1.09536	2.24291	7.02471
H	-1.73591	4.23195	5.67050
H	-1.83732	4.05305	3.18516
C	-0.72295	0.92814	3.93011
O	-0.30177	-0.18089	3.24871
C	-0.43692	-0.26191	6.11634
C	-0.73511	0.98492	5.32202
H	-1.38968	-0.72403	6.43173
H	0.10156	-0.00507	7.04152
C	0.40849	-1.13640	3.92342
C	0.36861	-1.24933	5.31156
C	1.07660	-2.29071	5.91579
C	1.80806	-3.19915	5.15508
C	1.86840	-3.05486	3.77386
C	1.19068	-2.00441	3.13560
H	1.05153	-2.38071	7.00414
H	2.34519	-4.01367	5.64253
H	2.47017	-3.72960	3.16505

Nuclear Repulsion Energy = 6956.8386428163 hartrees