

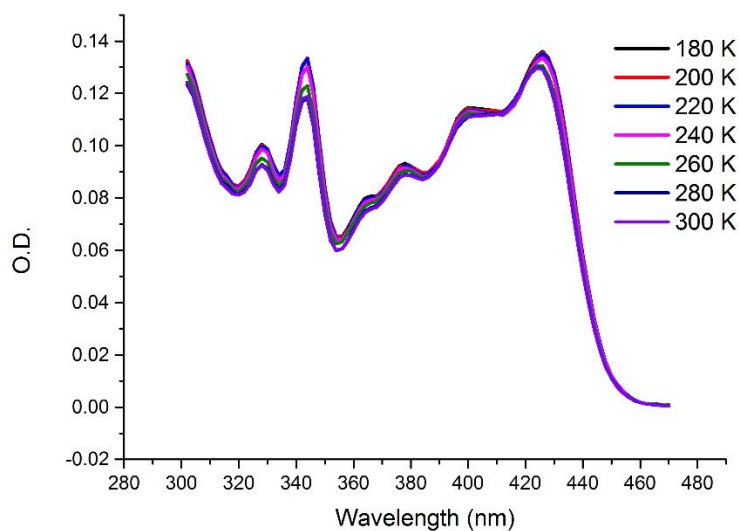
## Supporting Information

# Insights into the Luminescence Thermochromism of a Triarylboron Derivative: the Role of Intramolecular Group Interaction

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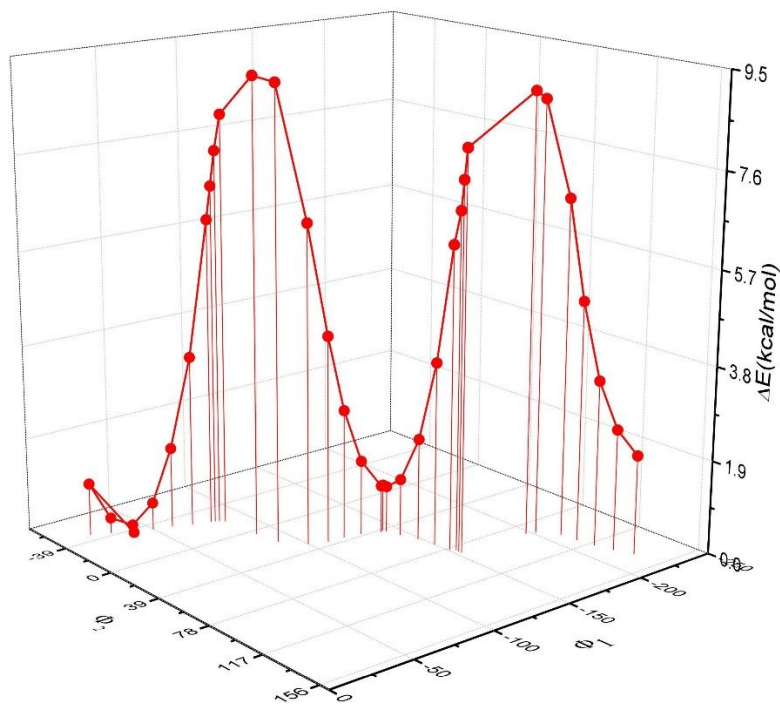
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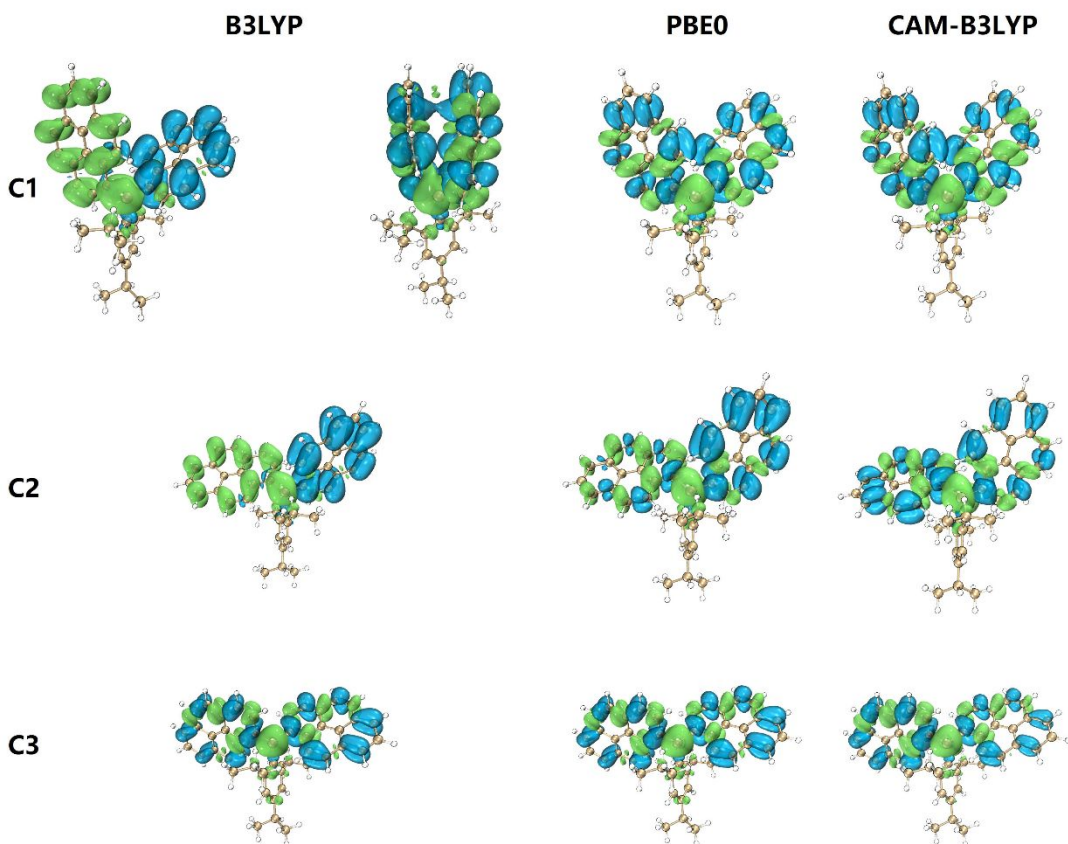
**Figure S1** The temperature-dependent absorption spectra of DPTB in THF

**Table S1** The decay lifetime of DPTB luminescence in THF

Wavelength (nm)	$\tau_1$ (ns, Fixed)	$\tau_2$ (ns, Fitted)	$B\tau_2/B\tau_1$	$\chi^2$
440	2.91	9.49	1.000	1.011
460	2.91	9.40	1.597	1.018
480	2.91	9.45	2.390	1.080
500	2.91	9.53	3.463	1.045
520	2.91	9.52	4.264	1.078
540	2.91	9.51	5.711	1.148
560	2.91	9.40	11.47	0.959



**Figure S2** The relaxed potential energy curves of GS for the three conformers calculated as functions of the two pyrenyl-related dihedral angles at 300 K



**Figure S3.** The electron density differences ( $\Delta\rho$ ) between the ES and the GS calculated by three (TD)DFT approaches. (density enhancement (green), density decrement (blue))

The Sr, D, H, t indexes were proposed by Tian Lu who is the author of MultiWfn. These indexes are used for charge transfer analysis.<sup>S1</sup> As listed in Table S2, the high Sr values are shown in all calculated ES structures. The inadequate separation of hole and electron suggests that all ES have a considerable LE component. The large H indexes demonstrate the wide distribution of hole and electron in all calculated structures. The C1(1) and C2(B3LYP) may be assigned to CT state due to the large D and positive t values, while all others are more like LE state. However, it's hard to believe that the CT from one to another same subunit can actually make a difference in an isolated molecule. The small ES dipole moments also suggest there are no typical CT states (Table 3). Therefore, the above indexes, especially D&t, are likely to not be applicable in this work.

**Table S2.** The calculated Sr, D, H and t indexes of the three ES conformers.

		Sr (a.u.)	D (Å)	H (Å)	t (Å)
C1	B3LYP (1)	0.540	3.935	3.698	1.363
	B3LYP (2)	0.766	0.719	3.574	-1.740
	PBE0	0.506	0.938	4.051	-1.493

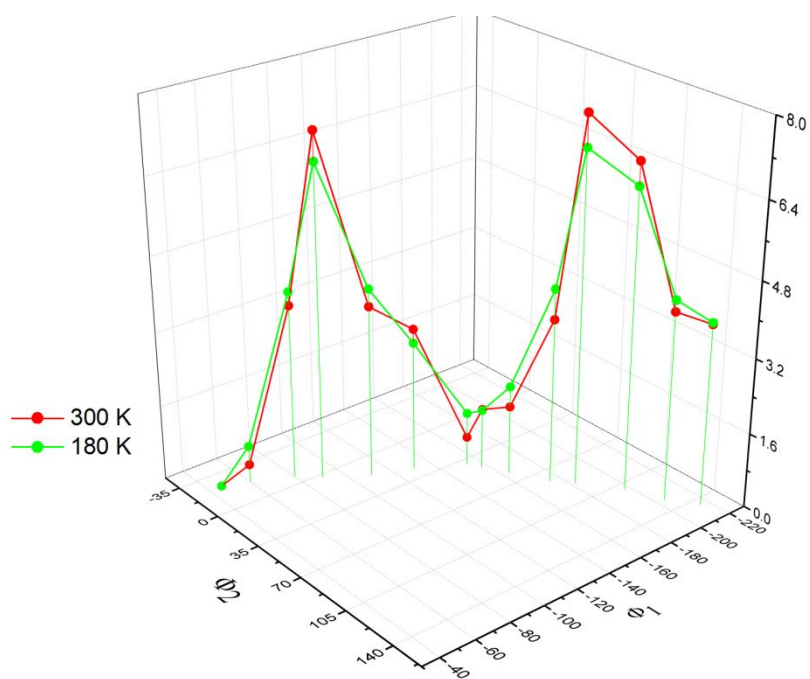
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	CAM-B3LYP	0.781	0.711	3.866	-1.548
	B3LYP	0.557	4.488	3.958	1.348
C2	PBE0	0.733	1.925	4.425	-1.709
	CAM-B3LYP	0.796	0.386	4.361	-1.990
	B3LYP	0.747	0.349	4.813	-3.583
C3	PBE0	0.755	0.151	4.816	-2.432
	CAM-B3LYP	0.800	0.372	4.589	-3.647

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S1. Tian, Lu., Multiwfn Manual, version 3.6(dev), Section 3.21.1, available at

<http://sobereva.com/multiwfn> (accessed Aug 30, 2018).



**Figure S4.** The relaxed potential energy curves of  $S_1$  state for the three conformers calculated as functions of the two pyrenyl-related dihedral angles at 300 K (red) and 180 K (green).

**Table S3** The calculated vertical transition wavelength (nm) of three ES conformers in rigid media

	B3LYP			PBE0			CAM-B3LYP		
	C1	C2	C3	C1	C2	C3	C1	C2	C3
$\lambda_{(\text{STEOM})}$									
-DLPNO-	446	423	417	449	423	417	447	424	416
CCSD)									

## The Cartesian coordinates:

GS C1 structure (B3LYP)

C	0.17661000	-1.35107800	-0.37766800
C	-1.07069400	-1.78591800	0.15883300
C	-1.71051200	-1.11960800	1.26313300
H	-1.21839100	-0.25696800	1.70844800
C	-2.90654800	-1.54197500	1.76618100
H	-3.36652700	-1.01287600	2.60454000
C	-3.58826400	-2.68106300	1.22039500
C	-4.82692000	-3.12744700	1.71723300
H	-5.29236500	-2.58669700	2.54492800
C	-5.45586900	-4.24353100	1.16461500
H	-6.41808000	-4.57605900	1.56085100
C	-4.86325100	-4.93940700	0.10885400
C	-3.62478800	-4.53057600	-0.41721600
C	-2.98824500	-5.22855000	-1.50152900
H	-3.49056400	-6.10329500	-1.92207500
C	-1.78587000	-4.81665100	-1.99691400
H	-1.31016000	-5.35763300	-2.81859300
C	-1.11038800	-3.66798800	-1.45779400
C	0.13646100	-3.24079500	-1.94596200
H	0.61194500	-3.79953700	-2.75588800
C	0.76364400	-2.12608600	-1.39966500
H	1.73905900	-1.82620100	-1.78851800
C	-1.71708000	-2.94360000	-0.38258200
C	-2.97365600	-3.38452200	0.13939800
C	2.52076300	-0.11779200	0.08790000
C	3.18475300	-0.82435200	1.11151400
C	4.58571300	-0.86720600	1.12453400
H	5.10397200	-1.41234400	1.91833500
C	5.34920800	-0.22684600	0.14214700
C	6.86779400	-0.28834000	0.17446000
C	7.43333300	-0.99769200	-1.06518000
H	8.52945600	-1.09012500	-0.99750000
H	7.20153100	-0.43615500	-1.98484300
H	7.00917200	-2.00812900	-1.17310300
C	2.38209300	-1.54154600	2.19149900
H	1.33103500	-1.22111300	2.08924000

C	2.82122700	-1.15724400	3.61061900
H	2.78315100	-0.06649100	3.75816000
H	3.85072800	-1.48894500	3.81960200
H	2.16377700	-1.62737100	4.35932100
C	2.40791000	-3.06264300	1.98399200
H	2.02578500	-3.32813900	0.98690300
H	1.78698700	-3.57294400	2.73810700
H	3.43563400	-3.45195800	2.06976500
B	0.94509100	-0.05784500	0.05510800
C	0.25963200	1.29101900	0.45689000
C	-0.92075200	1.82335500	-0.13941000
C	-1.55348400	1.21127500	-1.27864600
H	-1.10825300	0.31361100	-1.70382500
C	-2.68560700	1.72707700	-1.83917900
H	-3.14202300	1.23731900	-2.70298300
C	-3.30340900	2.91476300	-1.32158300
C	-4.47678800	3.45749100	-1.87749300
H	-4.94024300	2.95674700	-2.73109000
C	-5.04447900	4.61775200	-1.35010800
H	-5.95664900	5.02510900	-1.79217000
C	-4.45409200	5.26272900	-0.26128700
C	-3.27933600	4.75755600	0.32385300
C	-2.64637500	5.40124700	1.44328000
H	-3.09977000	6.31167200	1.84319500
C	-1.50650300	4.89561700	1.99626100
H	-1.03272000	5.39602000	2.84431600
C	-0.89583600	3.69899800	1.48480100
C	0.28763300	3.17467800	2.03246400
H	0.76370800	3.69281200	2.86864500
C	0.85305500	2.01554400	1.51155600
H	1.78139300	1.63967800	1.94689600
C	-1.50158100	3.02678900	0.37568700
C	-2.69178700	3.56561800	-0.20645200
C	3.27811900	0.53466100	-0.90960000
C	4.67527500	0.47065400	-0.87018700
H	5.25533000	0.97557100	-1.64656000
H	7.14613400	-0.88884100	1.05728500
C	7.48878500	1.10591400	0.34813000
H	8.58571300	1.03853600	0.43061000
H	7.10577800	1.60172100	1.25365400
H	7.25769500	1.75406000	-0.51289200

C	2.57429100	1.30890900	-2.01896900
H	1.49980500	1.06381300	-1.96268200
C	3.04426700	0.89736500	-3.42038200
H	2.93696200	-0.18789000	-3.57421100
H	4.10201500	1.15724500	-3.58537900
H	2.45273000	1.41333300	-4.19345100
C	2.70000700	2.82384600	-1.80299300
H	2.29914800	3.11395800	-0.82026800
H	2.14742700	3.37900000	-2.57828900
H	3.75566100	3.13834100	-1.84643100
H	-5.35960600	-5.81306200	-0.32066800
H	-4.90257700	6.17103900	0.14850800



GS C1 structure (PBE0)

C	0.16647800	-1.35532200	-0.37494400
C	-1.07823700	-1.79129000	0.15604500
C	-1.72435200	-1.12083900	1.24953200
H	-1.23754900	-0.24977500	1.68829500
C	-2.91709400	-1.54599700	1.74981900
H	-3.38431800	-1.01325600	2.58196300
C	-3.58638300	-2.69173300	1.21087900
C	-4.82070800	-3.14131900	1.70572600
H	-5.29263800	-2.59717600	2.52770900
C	-5.43863000	-4.26297900	1.16059900
H	-6.39997300	-4.59910500	1.55590800
C	-4.83888600	-4.96070600	0.11463200
C	-3.60448500	-4.54783500	-0.40828600
C	-2.96179300	-5.24808400	-1.48307200
H	-3.45694000	-6.12914900	-1.89922900
C	-1.76333600	-4.83277600	-1.97623700
H	-1.28132600	-5.37637600	-2.79263200
C	-1.09932600	-3.67862100	-1.44333200
C	0.14392100	-3.24916900	-1.92892500
H	0.62587500	-3.81083400	-2.73313200
C	0.76161400	-2.13052000	-1.38734000
H	1.73925900	-1.82761700	-1.77106900
C	-1.71265400	-2.95312400	-0.37856800
C	-2.96528500	-3.39715800	0.14078500
C	2.50935600	-0.11926700	0.08808700
C	3.17003900	-0.81217400	1.11817800
C	4.56797400	-0.85558000	1.13129000
H	5.08696400	-1.39136200	1.93223200
C	5.32987300	-0.22894500	0.14304300
C	6.84298700	-0.29094600	0.17529100
C	7.40271000	-1.01834200	-1.04695600
H	8.49824000	-1.11033800	-0.98015900
H	7.17026200	-0.47289500	-1.97568000
H	6.97874600	-2.02987100	-1.13759800
C	2.36668100	-1.51024600	2.20169500
H	1.31427000	-1.19333700	2.08190200
C	2.79269100	-1.09853200	3.60902800
H	2.74678700	-0.00634400	3.73858200
H	3.82309600	-1.41915500	3.82909800

H	2.13558400	-1.55969500	4.36258900
C	2.39904600	-3.02715000	2.02288000
H	2.02331400	-3.31355500	1.02918600
H	1.77662900	-3.52588200	2.78249300
H	3.42713400	-3.41141500	2.12131800
B	0.93297300	-0.05820000	0.05513000
C	0.25216200	1.29559200	0.45429200
C	-0.92478700	1.83106100	-0.13651700
C	-1.56605800	1.21612200	-1.26494900
H	-1.12917200	0.30930200	-1.68349800
C	-2.69377900	1.73657600	-1.82270000
H	-3.15924700	1.24415700	-2.68026000
C	-3.29559400	2.93162100	-1.31195600
C	-4.46325600	3.47955100	-1.86596100
H	-4.93482000	2.97657800	-2.71398000
C	-5.01653000	4.64607600	-1.34608900
H	-5.92669600	5.05875400	-1.78735000
C	-4.41693500	5.29158100	-0.26701400
C	-3.24744500	4.78043800	0.31491600
C	-2.60611200	5.42525700	1.42463500
H	-3.04943800	6.34281200	1.81985100
C	-1.47143800	4.91428000	1.97547400
H	-0.98962200	5.41638700	2.81810700
C	-0.87582700	3.71127400	1.47044900
C	0.30273200	3.18254600	2.01574500
H	0.78685100	3.70233400	2.84640100
C	0.85563200	2.01879300	1.49955100
H	1.78534500	1.63789900	1.93007100
C	-1.49032400	3.03924700	0.37179800
C	-2.67529200	3.58317500	-0.20776300
C	3.26368500	0.51930200	-0.91553600
C	4.65778600	0.45505700	-0.87566600
H	5.23847100	0.95053100	-1.65939300
H	7.11847800	-0.87794300	1.06812600
C	7.46123600	1.09866700	0.32658100
H	8.55754500	1.03251100	0.40906300
H	7.08022000	1.60906500	1.22403700
H	7.23063600	1.73385900	-0.54370900
C	2.55904500	1.27552700	-2.02855000
H	1.48202000	1.03762100	-1.95325900
C	3.01037900	0.83425300	-3.41886400

H	2.88985000	-0.25160700	-3.55364600
H	4.06955900	1.07852300	-3.59633300
H	2.41998900	1.34272800	-4.19680300
C	2.69699800	2.78564300	-1.84274500
H	2.30606600	3.09834000	-0.86294500
H	2.14323200	3.33031300	-2.62365400
H	3.75399300	3.09199900	-1.90004900
H	-5.32748700	-5.84100400	-0.31059000
H	-4.85492900	6.20708000	0.13851300

GS C1 structure (CAM-B3LYP)

C	0.15462800	-1.34912900	-0.39087900
C	-1.07936100	-1.79370700	0.14927900
C	-1.71168300	-1.14318600	1.27036800
H	-1.22082200	-0.28227900	1.71995200
C	-2.89027800	-1.57707500	1.77929900
H	-3.34412800	-1.06258000	2.62923700
C	-3.57183100	-2.71516500	1.22719200
C	-4.79536700	-3.17231800	1.73346700
H	-5.25234600	-2.64508000	2.57383600
C	-5.42298500	-4.28096700	1.17705500
H	-6.37710300	-4.62489500	1.58128500
C	-4.84135200	-4.95569800	0.10787000
C	-3.61850500	-4.53224800	-0.42532500
C	-2.99225300	-5.21251500	-1.52912600
H	-3.49625000	-6.08365300	-1.95365000
C	-1.80762100	-4.78970600	-2.03129400
H	-1.33893400	-5.31465600	-2.86650700
C	-1.13067000	-3.64307500	-1.48395500
C	0.10077400	-3.20637500	-1.98209200
H	0.56769100	-3.75072900	-2.80584300
C	0.72909600	-2.10055100	-1.42891400
H	1.69860900	-1.79340400	-1.82581100
C	-1.72296200	-2.94083200	-0.39698000
C	-2.97082500	-3.39638800	0.13535300
C	2.50349800	-0.12616500	0.08645700
C	3.16290700	-0.83820900	1.10212200
C	4.55897700	-0.88442900	1.11568000
H	5.07456800	-1.43607300	1.90620600
C	5.32233900	-0.24250200	0.14225400
C	6.83756100	-0.30759200	0.17580600
C	7.40118600	-1.00700600	-1.06356400
H	8.49586800	-1.10125200	-0.99543800
H	7.17177900	-0.43949000	-1.97891700
H	6.97708800	-2.01536600	-1.17932800
C	2.36532500	-1.55957800	2.17912900
H	1.31192500	-1.25145900	2.07537500
C	2.79704000	-1.16867200	3.59343800
H	2.74630100	-0.07950400	3.74090600
H	3.82901300	-1.48784600	3.80386500

H	2.14494500	-1.64481100	4.34122400
C	2.40805000	-3.07601600	1.97884300
H	2.03379700	-3.35182200	0.98250300
H	1.79003700	-3.58876900	2.73184900
H	3.43817000	-3.45426700	2.07124700
B	0.92829200	-0.06086400	0.05361300
C	0.24618300	1.28831700	0.46668400
C	-0.91814900	1.83593400	-0.13029900
C	-1.54917600	1.24065800	-1.28240900
H	-1.11229800	0.34098900	-1.71136400
C	-2.66114100	1.77258700	-1.84533100
H	-3.11590300	1.29770000	-2.71753100
C	-3.26929700	2.96477900	-1.32246500
C	-4.42438000	3.52346900	-1.88457100
H	-4.88403700	3.03626600	-2.74735700
C	-4.98160200	4.68169500	-1.35485100
H	-5.88306100	5.10478400	-1.80249100
C	-4.39615100	5.30570600	-0.25733000
C	-3.24005700	4.78078600	0.33162500
C	-2.61121800	5.40668600	1.46571200
H	-3.05853600	6.31832300	1.86816500
C	-1.49218500	4.88503300	2.02242400
H	-1.02086300	5.36931000	2.88039600
C	-0.89004100	3.68421400	1.50465100
C	0.27442900	3.14450200	2.05967700
H	0.74612300	3.64768800	2.90658100
C	0.83217400	1.98873200	1.53347600
H	1.75207400	1.60059200	1.97501200
C	-1.48729600	3.03406100	0.38837800
C	-2.66518300	3.59353600	-0.20124400
C	3.26128900	0.52806400	-0.90275900
C	4.65317200	0.46017600	-0.86225100
H	5.23484400	0.96860400	-1.63491700
H	7.11188500	-0.91437600	1.05408400
C	7.45927800	1.07902800	0.35936900
H	8.55473700	1.00856200	0.44208700
H	7.07801900	1.56950000	1.26716200
H	7.23100300	1.73330300	-0.49644400
C	2.56784000	1.30977600	-2.00959700
H	1.49074700	1.08151900	-1.95366600
C	3.03014900	0.89106700	-3.40611000

H	2.90627300	-0.19116100	-3.56122400
H	4.09076000	1.13420800	-3.57085400
H	2.44753200	1.41544700	-4.17855100
C	2.71624400	2.81818500	-1.79923800
H	2.32301100	3.11935800	-0.81772100
H	2.17083100	3.37815800	-2.57436500
H	3.77511400	3.11712200	-1.84667900
H	-5.33687300	-5.82654300	-0.32702000
H	-4.83648100	6.21556700	0.15650100

GS C2 structure (B3LYP)

C	-0.54799700	-0.98191400	0.57024500
C	-1.79038400	-1.36088000	-0.02247900
C	-2.45384100	-0.55784700	-1.01699600
H	-1.99282800	0.37648600	-1.32374000
C	-3.64162700	-0.93125700	-1.57538700
H	-4.11712400	-0.29405700	-2.32530900
C	-4.29533800	-2.15265000	-1.20176400
C	-5.52387200	-2.55168800	-1.75978600
H	-6.00190600	-1.90946900	-2.50354700
C	-6.12715000	-3.74871900	-1.37247200
H	-7.08165800	-4.04375400	-1.81432000
C	-5.51829400	-4.57234600	-0.42365700
C	-4.28930700	-4.21354600	0.15867200
C	-3.63927100	-5.04252600	1.13672100
H	-4.12263300	-5.97813400	1.42885300
C	-2.44734100	-4.67692500	1.69043300
H	-1.96104400	-5.31548800	2.43186200
C	-1.79761300	-3.45029100	1.31912600
C	-0.56560000	-3.06523700	1.87677000
H	-0.08693600	-3.71583900	2.61280300
C	0.03766500	-1.87398300	1.49692300
H	0.99334500	-1.60315000	1.94964000
C	-2.41552400	-2.59639600	0.35172200
C	-3.66324200	-2.98674600	-0.22943300
C	-0.62222600	1.73377400	0.08805600
C	-0.42192400	2.40940800	-1.13751700
C	-1.10530900	3.60454400	-1.39102300
H	-0.95572800	4.12278200	-2.34212700
C	-1.98809800	4.15883400	-0.45690700
C	-2.72346800	5.45522200	-0.75448100
C	-4.24456800	5.24520600	-0.80028200
H	-4.76059100	6.17891000	-1.07683400
H	-4.63162400	4.92742700	0.18156400
H	-4.51698700	4.47125400	-1.53465600
C	0.51263400	1.82743800	-2.19368000
H	0.77005600	0.80230200	-1.87918400
C	1.82726800	2.61616900	-2.27408100
H	2.32911900	2.64480600	-1.29584800
H	1.64000000	3.65495000	-2.59195600

H	2.51606000	2.15670000	-3.00133400
C	-0.15298600	1.70320000	-3.57154200
H	-1.08765600	1.12380100	-3.51423200
H	0.52088700	1.19447000	-4.27918200
H	-0.39393700	2.69049500	-3.99627300
B	0.16522800	0.39724500	0.37521500
C	1.71362100	0.53552300	0.60128100
C	2.69858300	-0.33674300	0.05731100
C	2.36318700	-1.41454600	-0.83862000
H	1.31625400	-1.57565900	-1.09308700
C	3.31628100	-2.23018900	-1.37506400
H	3.02938500	-3.03870000	-2.05212100
C	4.70921500	-2.05355700	-1.07340600
C	5.70759900	-2.88776100	-1.60912600
H	5.41634700	-3.70308200	-2.27593300
C	7.05194600	-2.68105400	-1.29703600
H	7.81462000	-3.33883900	-1.72028300
C	7.42957600	-1.63833800	-0.44870100
C	6.46581800	-0.77781800	0.10707600
C	6.82380200	0.30822800	0.97927500
H	7.88061100	0.45994900	1.21267400
C	5.87393300	1.13548100	1.50279600
H	6.15902100	1.96086100	2.15981100
C	4.47895300	0.95219200	1.20722400
C	3.48950700	1.80950100	1.71871000
H	3.78605700	2.64242700	2.36114300
C	2.15016400	1.61319600	1.39780400
H	1.40692800	2.31363400	1.78520000
C	4.08433200	-0.12564400	0.35302600
C	5.08422900	-0.98431300	-0.20264300
C	-1.50933400	2.28400700	1.04096400
C	-2.17487700	3.48221300	0.75477500
H	-2.85890600	3.90041700	1.49731100
H	-2.40241700	5.78359000	-1.75773400
C	-2.34492200	6.56387000	0.23910900
H	-2.83829200	7.51274000	-0.02689600
H	-1.25698000	6.73344300	0.25006000
H	-2.65451300	6.30217100	1.26402700
C	-1.75163500	1.59394700	2.37902700
H	-1.04994800	0.74813600	2.44944200
C	-3.16953800	1.00919400	2.45886600



H	-3.35616700	0.31141900	1.62951000
H	-3.92844700	1.80703100	2.40691500
H	-3.31593900	0.46515700	3.40607300
C	-1.45617100	2.51522100	3.57124000
H	-0.43091100	2.91463200	3.52209000
H	-1.56390300	1.96630900	4.52055400
H	-2.14842100	3.37172700	3.60302300
H	-5.99416100	-5.50876600	-0.12246700
H	8.48371300	-1.48005000	-0.20797700

GS C2 structure (PBE0)

C	-0.54766700	-0.98113000	0.56466700
C	-1.78864300	-1.36406400	-0.01815000
C	-2.46095200	-0.56132100	-1.00163500
H	-2.00619400	0.38049900	-1.30218400
C	-3.64638900	-0.93952000	-1.55425700
H	-4.13151600	-0.30161400	-2.29756900
C	-4.28602800	-2.16574000	-1.18400800
C	-5.51100200	-2.57023400	-1.73704100
H	-5.99729000	-1.92792400	-2.47558600
C	-6.10183000	-3.77071800	-1.35347700
H	-7.05606300	-4.07114700	-1.79228800
C	-5.48372500	-4.59171200	-0.41338200
C	-4.25804200	-4.22632000	0.16317800
C	-3.59958300	-5.05279100	1.13291000
H	-4.07458900	-5.99329700	1.42352400
C	-2.41097200	-4.68127400	1.68197200
H	-1.91689700	-5.31908800	2.41905200
C	-1.77394300	-3.45110600	1.31275900
C	-0.54516600	-3.06063400	1.86533800
H	-0.05892200	-3.70990900	2.59771800
C	0.04778000	-1.86738200	1.48520500
H	1.00555700	-1.59030400	1.93226600
C	-2.40067900	-2.60121600	0.35402100
C	-3.64524900	-2.99711400	-0.22152100
C	-0.62995800	1.73920400	0.08386800
C	-0.43700000	2.40930600	-1.14181500
C	-1.11973600	3.60189000	-1.39288100
H	-0.97663400	4.11825900	-2.34707300
C	-1.99375400	4.15763500	-0.45588300
C	-2.72916800	5.44819700	-0.75086800
C	-4.24234300	5.23536000	-0.78996500
H	-4.76175000	6.16682600	-1.06501200
H	-4.62500200	4.91816900	0.19340100
H	-4.51706800	4.46065400	-1.52175300
C	0.48762200	1.82384600	-2.19602000
H	0.75002200	0.80148100	-1.86900100
C	1.79240000	2.61243000	-2.29238700
H	2.30379900	2.64925400	-1.31920500
H	1.59956500	3.64833300	-2.61499500

H	2.47590900	2.15139700	-3.02268300
C	-0.18557000	1.68492000	-3.56037400
H	-1.11606900	1.10076400	-3.49347400
H	0.48511300	1.17584800	-4.26976300
H	-0.43554100	2.66746200	-3.99023600
B	0.15993000	0.40204400	0.36590000
C	1.70960600	0.54219300	0.58844300
C	2.69280600	-0.32948000	0.05037900
C	2.35800300	-1.40671300	-0.84080300
H	1.30949300	-1.56769600	-1.09490400
C	3.30955400	-2.22204300	-1.37259700
H	3.02361500	-3.03245800	-2.04792500
C	4.69866800	-2.04391400	-1.06954200
C	5.69490000	-2.87782700	-1.60050600
H	5.40412300	-3.69491600	-2.26559500
C	7.03552500	-2.67101500	-1.28772700
H	7.79879700	-3.33001000	-1.70800000
C	7.41084500	-1.62854800	-0.44365400
C	6.44823400	-0.76893900	0.10650100
C	6.80497900	0.31662600	0.97434800
H	7.86154900	0.46893800	1.20897800
C	5.85673200	1.14347000	1.49309400
H	6.14101500	1.97058700	2.14843500
C	4.46554000	0.95927300	1.19607300
C	3.47852400	1.81691300	1.70241000
H	3.77457700	2.65199200	2.34245100
C	2.14254100	1.62043900	1.38006500
H	1.39704000	2.32274100	1.76238000
C	4.07350700	-0.11739400	0.34663600
C	5.07163000	-0.97572300	-0.20393000
C	-1.50727500	2.29001600	1.04036700
C	-2.17194300	3.48569900	0.75639600
H	-2.85102500	3.90656600	1.50380400
H	-2.41146000	5.77289300	-1.75645700
C	-2.34782400	6.55310200	0.23390400
H	-2.84324400	7.50054600	-0.03051900
H	-1.26080400	6.72472300	0.23928900
H	-2.65165700	6.29390100	1.26079300
C	-1.73743900	1.60368800	2.37567600
H	-1.03797000	0.75263700	2.43243500
C	-3.15064100	1.02995900	2.47077300

H	-3.35155800	0.33274800	1.64406200
H	-3.90576700	1.83143500	2.42731700
H	-3.28998300	0.48733900	3.41907700
C	-1.42302900	2.51843700	3.55830500
H	-0.39588800	2.91025600	3.50047700
H	-1.52597400	1.97186000	4.50870100
H	-2.10793100	3.38025000	3.59648300
H	-5.95074800	-5.53327300	-0.11380200
H	8.46463200	-1.46932700	-0.20132600

GS C2 structure (CAM-B3LYP)

C	-0.55963100	-0.96906900	0.59266500
C	-1.78439100	-1.36759100	-0.00569900
C	-2.44701700	-0.58239300	-1.01812300
H	-1.99481100	0.35495200	-1.32807700
C	-3.61322300	-0.97582200	-1.58512700
H	-4.08816000	-0.35436600	-2.34768500
C	-4.25519600	-2.20412600	-1.20752200
C	-5.46393200	-2.62286000	-1.77782900
H	-5.93868400	-1.99545400	-2.53547800
C	-6.05493300	-3.81934600	-1.38777800
H	-6.99784700	-4.13271100	-1.84021000
C	-5.45062400	-4.61979900	-0.42344500
C	-4.24150600	-4.23723400	0.16933100
C	-3.59498400	-5.04677800	1.16844700
H	-4.07108400	-5.98459600	1.46330600
C	-2.42523400	-4.66111300	1.73188900
H	-1.94086000	-5.28230500	2.48831200
C	-1.78552200	-3.42855300	1.35445700
C	-0.57334300	-3.02473100	1.92429200
H	-0.09808000	-3.65945400	2.67531200
C	0.02087700	-1.83569400	1.53700300
H	0.96819200	-1.55063500	1.99781000
C	-2.39578700	-2.59937400	0.37299000
C	-3.63013100	-3.01358800	-0.22204800
C	-0.63001600	1.74718700	0.08544900
C	-0.43921600	2.40598400	-1.14461200
C	-1.11540300	3.59857000	-1.40304400
H	-0.97158900	4.10543400	-2.36070900
C	-1.98160200	4.16674600	-0.46995000
C	-2.71078800	5.46146500	-0.77390600
C	-4.22798200	5.26043800	-0.80329600
H	-4.74064300	6.19319700	-1.08429600
H	-4.60749500	4.95561900	0.18444500
H	-4.51255900	4.48175000	-1.52627800
C	0.48136700	1.81478200	-2.20388700
H	0.74684100	0.79470000	-1.88293200
C	1.78740300	2.60465000	-2.31224100
H	2.30368300	2.64943900	-1.34303100
H	1.59234900	3.63730000	-2.64146900

H	2.46698500	2.13865500	-3.04218400
C	-0.19890900	1.67506400	-3.56747000
H	-1.12943400	1.09268100	-3.49558100
H	0.46787100	1.16314000	-4.27761900
H	-0.44852000	2.65637800	-3.99812200
B	0.15349300	0.40975900	0.38054900
C	1.70429700	0.54168000	0.60237000
C	2.68049100	-0.32841100	0.05759800
C	2.33894600	-1.40523500	-0.84083000
H	1.29126200	-1.56393700	-1.09257000
C	3.28184300	-2.21624000	-1.37838600
H	2.99227200	-3.02201300	-2.05659700
C	4.67746500	-2.04449400	-1.07896000
C	5.66568100	-2.87763400	-1.61826100
H	5.36941500	-3.68890800	-2.28695800
C	7.00678300	-2.67835900	-1.30971700
H	7.76591000	-3.33675000	-1.73671600
C	7.38733700	-1.64366100	-0.46081500
C	6.43074800	-0.78706400	0.09675800
C	6.79535800	0.29500900	0.97410100
H	7.85295700	0.44015100	1.20541000
C	5.85631200	1.11774900	1.49916500
H	6.14373500	1.93877600	2.15961900
C	4.45824800	0.94075300	1.20424100
C	3.47983200	1.79628300	1.72067000
H	3.78092800	2.62430200	2.36627300
C	2.14287800	1.60812600	1.40222300
H	1.40496000	2.31078100	1.79478600
C	4.05966600	-0.12519800	0.35072900
C	5.05591700	-0.98617000	-0.21001600
C	-1.49975700	2.31219800	1.03815700
C	-2.15846300	3.50715900	0.74633600
H	-2.83189400	3.93737800	1.49141400
H	-2.39687600	5.77571200	-1.78261700
C	-2.31831400	6.57484700	0.20032400
H	-2.80871600	7.52224000	-0.07121700
H	-1.23072700	6.73968400	0.19971700
H	-2.61955300	6.32683200	1.23002200
C	-1.73513400	1.64367800	2.38528100
H	-1.03767700	0.79651300	2.46534000
C	-3.15053300	1.06924800	2.48290900

H	-3.34802900	0.36051100	1.66639000
H	-3.90500800	1.86937800	2.42460100
H	-3.29311900	0.54063900	3.43795900
C	-1.43100600	2.57771200	3.55863600
H	-0.40624900	2.97413300	3.49993300
H	-1.53455900	2.04251200	4.51475800
H	-2.12051200	3.43521100	3.58329400
H	-5.91718100	-5.55901500	-0.11819900
H	8.44180900	-1.48939600	-0.22123900

GS C3 structure (B3LYP)

C	1.35001100	-1.33270300	0.18179000
C	2.64277700	-0.88464400	-0.22378300
C	2.83819000	0.30046300	-1.01848400
H	1.96642400	0.87333100	-1.32089100
C	4.07905200	0.72507200	-1.39453800
H	4.18811000	1.63131700	-1.99569600
C	5.26311300	0.00695600	-1.01807200
C	6.55259600	0.43300500	-1.38633000
H	6.66065300	1.34498200	-1.97858400
C	7.67992900	-0.29426500	-1.00300500
H	8.67423100	0.05081300	-1.29578900
C	7.54549000	-1.46082900	-0.24764400
C	6.27581200	-1.92466700	0.14074000
C	6.10735000	-3.12247400	0.91792900
H	6.99932400	-3.68313200	1.20838800
C	4.86741500	-3.55471700	1.28687300
H	4.75074900	-4.46721700	1.87664400
C	3.68346100	-2.82979900	0.91487200
C	2.39929200	-3.26597800	1.28309300
H	2.29508000	-4.18294700	1.86841800
C	1.27405200	-2.54080200	0.91031500
H	0.29240700	-2.90299600	1.22207500
C	3.81043900	-1.63152200	0.14383400
C	5.11303100	-1.18478000	-0.24458700
C	0.00736600	1.05489600	0.08160100
C	0.44929100	1.72212500	1.25049600
C	0.43026900	3.12208400	1.30067700
H	0.76678000	3.63223300	2.20733200
C	-0.01325600	3.89605800	0.22490300
C	-0.02244600	5.41312400	0.30490900
C	0.91795900	6.03982800	-0.73567600
H	0.94919200	7.13583600	-0.62490300
H	0.58106400	5.81682900	-1.76113600
H	1.94354900	5.65382200	-0.62770300
C	0.91305900	0.95429000	2.48504000
H	0.75545500	-0.11683400	2.29301800
C	0.08549700	1.30527600	3.73142600
H	-0.98948300	1.13948600	3.55970800
H	0.22043600	2.35840300	4.02500300



H	0.39265700	0.68052700	4.58552900
C	2.41451100	1.15015300	2.74150900
H	3.00793900	0.85902400	1.86313900
H	2.74635500	0.54109100	3.59790300
H	2.64229800	2.20427600	2.96956200
B	0.01614500	-0.52258000	0.00182900
C	-1.30764000	-1.32784600	-0.25729300
C	-2.60548400	-0.94066000	0.19265100
C	-2.81612100	0.16097000	1.09630300
H	-1.95237100	0.71774000	1.44783300
C	-4.06175800	0.52747500	1.51519200
H	-4.18236400	1.37122400	2.19936500
C	-5.23591600	-0.17171200	1.07728200
C	-6.53009800	0.19564500	1.48961200
H	-6.64977200	1.04552500	2.16601800
C	-7.64744000	-0.51120000	1.04396900
H	-8.64561100	-0.21244800	1.37236500
C	-7.49811300	-1.59840900	0.18073200
C	-6.22321400	-2.00173100	-0.25521500
C	-6.03958600	-3.11752600	-1.14314900
H	-6.92382100	-3.66335100	-1.48158200
C	-4.79486300	-3.49166600	-1.55677000
H	-4.66661600	-4.34199700	-2.23100000
C	-3.62086600	-2.78549500	-1.12241600
C	-2.33186100	-3.16320000	-1.53563500
H	-2.21604800	-4.01826900	-2.20626600
C	-1.21644400	-2.45885100	-1.09903500
H	-0.23070600	-2.77401200	-1.44690700
C	-3.76297800	-1.66819900	-0.24037500
C	-5.07057100	-1.28214100	0.19371500
C	-0.44483800	1.83207500	-1.01594400
C	-0.44677900	3.22773300	-0.92659600
H	-0.79265500	3.81324900	-1.78179400
H	0.35820300	5.68461900	1.30428000
C	-1.44562100	5.97783900	0.18093400
H	-1.44373700	7.07315400	0.30231100
H	-2.11164300	5.54815500	0.94531500
H	-1.87860200	5.75180700	-0.80711500
C	-0.89905100	1.18462600	-2.32124900
H	-0.72253400	0.10231300	-2.23921500
C	-0.08215600	1.67508500	-3.52686400

H	0.99638500	1.51403900	-3.37391400
H	-0.23815000	2.74964100	-3.71259500
H	-0.37995000	1.13400200	-4.43935900
C	-2.40449300	1.37953400	-2.55367700
H	-2.98946800	0.99018900	-1.70835400
H	-2.72935000	0.85573000	-3.46722500
H	-2.65046200	2.44750100	-2.67201100
H	8.43098900	-2.02708600	0.05132100
H	-8.37587200	-2.14863700	-0.16700600

GS C3 structure (PBE0)

C	1.34856900	-1.31931100	0.18614000
C	2.64067100	-0.87821600	-0.21436800
C	2.84123200	0.30705900	-1.00102700
H	1.96954300	0.88796500	-1.29554300
C	4.08163400	0.72382800	-1.37635600
H	4.19653400	1.63271000	-1.97265200
C	5.25773600	-0.00430400	-1.00608900
C	6.54620600	0.41303300	-1.37448600
H	6.65952100	1.32669300	-1.96343700
C	7.66618500	-0.32208100	-0.99695900
H	8.66246300	0.01677200	-1.29030600
C	7.52474100	-1.48749000	-0.24738600
C	6.25532300	-1.94169500	0.14034800
C	6.08076000	-3.13814100	0.91221400
H	6.96927200	-3.70617900	1.19939900
C	4.84136900	-3.56171300	1.28127900
H	4.71930400	-4.47524500	1.86854400
C	3.66515800	-2.82838100	0.91376800
C	2.38182300	-3.25640000	1.28169800
H	2.27205700	-4.17421000	1.86487900
C	1.26346000	-2.52490800	0.91091300
H	0.27792700	-2.88161600	1.21997800
C	3.79932000	-1.63234500	0.14862300
C	5.10120000	-1.19427600	-0.23932400
C	0.00713800	1.07378500	0.08116800
C	0.44405600	1.73975400	1.24855900
C	0.42196600	3.13680000	1.29747100
H	0.75481900	3.64864500	2.20570400
C	-0.01839800	3.90770400	0.22200800
C	-0.03126500	5.41932500	0.30077900
C	0.90729500	6.04329100	-0.73176800
H	0.93587300	7.13884600	-0.62263100
H	0.57518600	5.81920900	-1.75816800
H	1.93311900	5.66068800	-0.62025200
C	0.90501000	0.97461700	2.47832000
H	0.75440600	-0.09779400	2.27718300
C	0.07321300	1.31535100	3.71525900
H	-0.99981800	1.14211000	3.54154300
H	0.19920100	2.36883900	4.01067000

H	0.38171100	0.69287900	4.56967500
C	2.39674200	1.17836100	2.73996400
H	2.99684200	0.89123600	1.86445400
H	2.72859100	0.57173200	3.59725900
H	2.61775000	2.23328400	2.96943200
B	0.01686100	-0.50458600	0.00310300
C	-1.30417800	-1.31564100	-0.25779600
C	-2.60162800	-0.93509300	0.18555400
C	-2.81846100	0.16885300	1.07919500
H	-1.95541900	0.73547200	1.42301200
C	-4.06387900	0.52753300	1.49561400
H	-4.19118500	1.37543300	2.17361700
C	-5.22926600	-0.18373400	1.06394000
C	-6.52264500	0.17481200	1.47459200
H	-6.64841300	1.02779700	2.14621300
C	-7.63185400	-0.54191200	1.03507400
H	-8.63218200	-0.24953900	1.36265700
C	-7.47452900	-1.62993600	0.17981000
C	-6.19965800	-2.02365800	-0.25352300
C	-6.00889300	-3.14005100	-1.13387400
H	-6.88900400	-3.69486400	-1.46881800
C	-4.76450600	-3.50537200	-1.54588900
H	-4.63005200	-4.35806700	-2.21607900
C	-3.59904200	-2.78878300	-1.11637200
C	-2.31065800	-3.15817500	-1.52765600
H	-2.18849500	-4.01529100	-2.19470400
C	-1.20283600	-2.44586400	-1.09345900
H	-0.21299000	-2.75563100	-1.43741400
C	-3.74933900	-1.67179100	-0.24245900
C	-5.05645400	-1.29447900	0.18935700
C	-0.44186100	1.84651700	-1.01650100
C	-0.44570700	3.23928600	-0.92827400
H	-0.79007400	3.82380600	-1.78640900
H	0.34606000	5.68942600	1.30186200
C	-1.44900100	5.97621400	0.17385200
H	-1.45130900	7.07098200	0.29394000
H	-2.11587400	5.54609800	0.93635200
H	-1.87926300	5.74859600	-0.81462100
C	-0.88984000	1.19750600	-2.31611000
H	-0.71700000	0.11354800	-2.22284400
C	-0.06823000	1.67698500	-3.51318100

H	1.00876100	1.51148000	-3.35728700
H	-0.21789300	2.75154300	-3.70283000
H	-0.36474600	1.13572700	-4.42517900
C	-2.38600000	1.39572400	-2.55547500
H	-2.97777500	1.00971800	-1.71298700
H	-2.70776000	0.87207800	-3.46943500
H	-2.62862400	2.46377400	-2.67704400
H	8.40642300	-2.06167800	0.04827900
H	-8.34786400	-2.18956500	-0.16454200

GS C3 structure (CAM-B3LYP)

C	1.34641600	-1.29536900	0.21187000
C	2.63900100	-0.87493400	-0.19700600
C	2.85308000	0.30189100	-1.00317000
H	1.99087700	0.88921100	-1.30438200
C	4.09092200	0.69547900	-1.38857400
H	4.21526000	1.59367900	-1.99777100
C	5.26425800	-0.04384500	-1.01323400
C	6.55233700	0.35239800	-1.39455400
H	6.67315200	1.25517500	-1.99742000
C	7.66449500	-0.38934400	-1.01255200
H	8.66269900	-0.06766800	-1.31612600
C	7.51203400	-1.53986300	-0.24509800
C	6.24147300	-1.97029400	0.15492500
C	6.05562100	-3.15635800	0.94924700
H	6.93919200	-3.72896700	1.23995800
C	4.81905100	-3.55710800	1.32928200
H	4.68725300	-4.45877600	1.93129700
C	3.64516300	-2.81333000	0.95451800
C	2.36274200	-3.22109300	1.33476500
H	2.24531700	-4.12788300	1.93215400
C	1.25142100	-2.48549400	0.95547000
H	0.26516500	-2.83105900	1.27037000
C	3.78835900	-1.63427100	0.17210100
C	5.09746100	-1.21675200	-0.22971400
C	0.00431600	1.09797400	0.08765200
C	0.39431100	1.76384700	1.26821300
C	0.37346500	3.15931100	1.31519200
H	0.67318000	3.67062600	2.23351100
C	-0.02442400	3.92845000	0.22521600
C	-0.03944600	5.44254600	0.30298800
C	0.93350500	6.06882600	-0.69908400
H	0.95739900	7.16377300	-0.58830000
H	0.63567800	5.84493400	-1.73529000
H	1.95496800	5.68731600	-0.55385200
C	0.81262800	0.99957900	2.51787200
H	0.63581800	-0.06962400	2.33404000
C	-0.02626500	1.37905700	3.74151400
H	-1.10136700	1.24192700	3.55302200
H	0.13220300	2.42828000	4.03287100

H	0.24802800	0.75190700	4.60332600
C	2.30734700	1.16627700	2.80248300
H	2.91401000	0.85082500	1.94261800
H	2.60798900	0.56413800	3.67363600
H	2.55124200	2.21797600	3.01973200
B	0.01678100	-0.48053700	0.01097400
C	-1.29976600	-1.29372100	-0.26841600
C	-2.59917200	-0.93497100	0.17635100
C	-2.83261600	0.15690200	1.08956000
H	-1.98009600	0.72665100	1.44680200
C	-4.07683900	0.49281500	1.50760000
H	-4.21585900	1.32750300	2.19847100
C	-5.23791300	-0.22647000	1.06196300
C	-6.53239700	0.11158200	1.47622400
H	-6.66807100	0.95177200	2.16085800
C	-7.63222100	-0.60886400	1.02426000
H	-8.63563600	-0.33318000	1.35471300
C	-7.46086600	-1.67969100	0.15252800
C	-6.18333400	-2.05027700	-0.28361500
C	-5.97795900	-3.15354300	-1.18521000
H	-6.85190400	-3.71082100	-1.52979300
C	-4.73494800	-3.49674100	-1.59906400
H	-4.58839000	-4.33574000	-2.28273100
C	-3.57343200	-2.77241500	-1.15422800
C	-2.28448300	-3.12154000	-1.56919900
H	-2.15212700	-3.96607000	-2.24903600
C	-1.18541400	-2.40661800	-1.12094600
H	-0.19368800	-2.70473200	-1.46575200
C	-3.73595400	-1.67462300	-0.26465600
C	-5.05181600	-1.31783800	0.17215700
C	-0.40005100	1.86952100	-1.02487400
C	-0.40800000	3.26044200	-0.93781500
H	-0.72037900	3.84384600	-1.80697000
H	0.30335400	5.71409900	1.31466000
C	-1.45334000	6.00196500	0.12710800
H	-1.45828000	7.09625100	0.24652600
H	-2.14598700	5.57325200	0.86634100
H	-1.84910200	5.77399100	-0.87485500
C	-0.80401400	1.22073500	-2.34288500
H	-0.60590500	0.14244900	-2.26298400
C	0.02623400	1.73341200	-3.52306600

H	1.10398600	1.60020300	-3.34739500
H	-0.15325500	2.80261300	-3.71152400
H	-0.23616600	1.18759300	-4.44201700
C	-2.30192200	1.38462900	-2.61169600
H	-2.90152900	0.97609000	-1.78681900
H	-2.59163200	0.86366500	-3.53717000
H	-2.56628300	2.44748100	-2.72658500
H	8.38739700	-2.12034600	0.05460500
H	-8.32671100	-2.24331200	-0.20202600



ES C1(1) structure (B3LYP)

C	-0.34625500	1.13050200	-0.57656200
C	0.83279100	1.64838800	0.07750000
C	1.42546400	0.97895600	1.18326600
H	0.95366500	0.07339400	1.55889600
C	2.58311000	1.44310200	1.77887500
H	3.01818400	0.90040800	2.62052800
C	3.22468700	2.62300900	1.31386100
C	4.41935000	3.11312200	1.90052000
H	4.86436900	2.56104500	2.73117600
C	5.01957700	4.27938800	1.42879100
H	5.93921600	4.64362000	1.89009200
C	4.44724900	4.98463400	0.36966200
C	3.25365600	4.53453600	-0.24885600
C	2.65156800	5.24090700	-1.33029400
H	3.12442300	6.15646800	-1.69169300
C	1.48859000	4.78012200	-1.91375900
H	1.03279400	5.33216300	-2.73851400
C	0.86324400	3.58794300	-1.46083600
C	-0.33997100	3.09776900	-2.04226500
H	-0.79779500	3.66516500	-2.85624800
C	-0.92074400	1.92274300	-1.59873800
H	-1.84293200	1.57868100	-2.06954700
C	1.44323900	2.85534200	-0.38202700
C	2.63640100	3.33802500	0.22701700
C	-2.60631600	-0.14320300	0.04333000
C	-3.14325900	0.40984700	1.22720700
C	-4.53263900	0.49576300	1.39246400
H	-4.94376900	0.92330100	2.31135200
C	-5.41886000	0.04660300	0.40784600
C	-6.92252300	0.14502700	0.60844100
C	-7.57993800	1.04879000	-0.44543600
H	-8.65904500	1.15900100	-0.24989200
H	-7.46536800	0.62749200	-1.45751200
H	-7.12667100	2.05240400	-0.44672700
C	-2.21190700	0.93382500	2.31306000
H	-1.20832200	0.54291700	2.08224900
C	-2.57058100	0.42525700	3.71461200
H	-2.61969700	-0.67463400	3.73595000
H	-3.54420100	0.81362800	4.05419600

H	-1.81418200	0.74868500	4.44790800
C	-2.12609600	2.46702600	2.27540400
H	-1.81938900	2.82059200	1.27933200
H	-1.39522900	2.84046000	3.01141200
H	-3.10453100	2.91950900	2.50696900
B	-1.03162800	-0.23643200	-0.17711100
C	-0.27515000	-1.53283000	0.03822400
C	1.07124100	-1.80839900	-0.43867100
C	1.68693800	-1.04109200	-1.46587300
H	1.09520600	-0.28161700	-1.97598900
C	2.99656200	-1.23610000	-1.84997300
H	3.43605600	-0.61583100	-2.63544900
C	3.79701400	-2.25139400	-1.25009200
C	5.15301600	-2.46210800	-1.60332200
H	5.61329700	-1.80990000	-2.34971700
C	5.88754300	-3.48904300	-1.01250100
H	6.93316300	-3.63789200	-1.29493000
C	5.30133400	-4.33620600	-0.07003500
C	3.94935300	-4.16914700	0.31401200
C	3.31181500	-5.02755900	1.26085700
H	3.89190800	-5.84020000	1.70527600
C	1.98734700	-4.84730400	1.60190800
H	1.50937700	-5.52452700	2.31532800
C	1.21389900	-3.79384600	1.04963800
C	-0.16432200	-3.60287200	1.37489800
H	-0.64399100	-4.31108900	2.05622500
C	-0.86808900	-2.53083700	0.87665000
H	-1.90713000	-2.38835200	1.18409500
C	1.82380500	-2.89504500	0.11329100
C	3.18688000	-3.10376200	-0.27274800
C	-3.49492300	-0.59219100	-0.96285900
C	-4.87793300	-0.49691900	-0.76500500
H	-5.55398500	-0.85768400	-1.54420400
H	-7.08498100	0.61207200	1.59500000
C	-7.58250300	-1.24191500	0.63890500
H	-8.66191900	-1.15881100	0.84591800
H	-7.13148200	-1.87932900	1.41531900
H	-7.46612700	-1.75806400	-0.32801300
C	-2.95544800	-1.21239400	-2.24759900
H	-1.87833200	-0.97817200	-2.29162500
C	-3.60151500	-0.63396200	-3.51324300

H	-3.52202900	0.46458400	-3.54004300
H	-4.67060600	-0.89174300	-3.58072700
H	-3.11035600	-1.03411700	-4.41474600
C	-3.07580300	-2.74325900	-2.20952800
H	-2.54446800	-3.15620600	-1.33941600
H	-2.64833300	-3.19552300	-3.11954200
H	-4.13267100	-3.05024700	-2.14117700
H	4.91666300	5.90066200	0.00422600
H	5.88196100	-5.14559000	0.37973400

ES C1(2) structure (B3LYP)

C	-0.51290000	1.23962100	0.20942900
C	0.80466900	1.16046300	0.79837300
C	1.18738500	0.08695700	1.64586900
H	0.42240200	-0.59823800	2.00763700
C	2.50935500	-0.13243800	1.98947600
H	2.77636600	-0.99032600	2.61038600
C	3.54148200	0.71097400	1.50051400
C	4.91401200	0.43761800	1.72784000
H	5.19005800	-0.44189700	2.31263700
C	5.89495700	1.27260500	1.19666400
H	6.94990500	1.04058500	1.35769000
C	5.54242300	2.39751700	0.45013500
C	4.18172200	2.73133800	0.22515500
C	3.78455500	3.89104600	-0.50788600
H	4.55851600	4.56351400	-0.88539700
C	2.45241000	4.16491000	-0.74256900
H	2.16864300	5.06020200	-1.30159100
C	1.42929200	3.27962400	-0.30389800
C	0.05026300	3.47500300	-0.61239000
H	-0.24542400	4.39021200	-1.13212100
C	-0.88486400	2.48409800	-0.36111400
H	-1.91198500	2.61202300	-0.71407700
C	1.79941200	2.11716300	0.43902800
C	3.17087000	1.86576900	0.74020100
C	-2.94973600	-0.01146200	0.08364300
C	-3.59598900	0.06703100	1.33716200
C	-4.99636000	0.10322000	1.39924500
H	-5.49403000	0.16582900	2.37111700
C	-5.78506600	0.06132800	0.24492000
C	-7.30211100	0.10230700	0.33524600
C	-7.87787200	1.35232900	-0.34727200
H	-8.97192300	1.39934400	-0.22194300
H	-7.66515000	1.34762000	-1.42877400
H	-7.44367700	2.27162800	0.07576200
C	-2.77441400	0.13668700	2.61884300
H	-1.74159700	-0.13825200	2.34983400
C	-3.23694900	-0.86215000	3.68672000
H	-3.25588200	-1.88887900	3.28843400
H	-4.24746800	-0.62614500	4.05713600

H	-2.55677900	-0.84329200	4.55354500
C	-2.73053200	1.57063200	3.16641600
H	-2.32873000	2.26442400	2.41227500
H	-2.09319100	1.63205900	4.06385100
H	-3.74062400	1.91635100	3.44180900
B	-1.37123800	-0.04671400	-0.00907300
C	-0.57776400	-1.34729200	-0.29338100
C	0.71475500	-1.27684500	-0.93244600
C	1.05257200	-0.22659500	-1.82463800
H	0.25892400	0.41172000	-2.21116800
C	2.36617000	0.02999500	-2.17787100
H	2.60202800	0.86975100	-2.83549200
C	3.42878400	-0.74633800	-1.64611100
C	4.79183400	-0.41571700	-1.86256500
H	5.03605400	0.45024700	-2.48126000
C	5.79875600	-1.16628200	-1.26573900
H	6.84395100	-0.88437200	-1.41103200
C	5.48872700	-2.27118400	-0.46656900
C	4.14448700	-2.67116200	-0.26176500
C	3.78751200	-3.81295600	0.52107400
H	4.58568700	-4.42666800	0.94575000
C	2.46618700	-4.14000700	0.74773100
H	2.21646900	-5.01797500	1.34921800
C	1.40931700	-3.32421800	0.25712700
C	0.03661500	-3.54586600	0.58629300
H	-0.22929400	-4.44737700	1.14478200
C	-0.92116100	-2.58121500	0.32370400
H	-1.93586300	-2.70942100	0.71200300
C	1.73971700	-2.18732100	-0.54251000
C	3.10228800	-1.88638300	-0.84121500
C	-3.73915300	-0.05241900	-1.09016900
C	-5.13517000	-0.01745000	-0.99430800
H	-5.73429300	-0.05206600	-1.90753000
H	-7.55866600	0.16068300	1.40694000
C	-7.93999500	-1.17821400	-0.22426000
H	-9.03457400	-1.15982700	-0.09619600
H	-7.54921700	-2.07238300	0.28592400
H	-7.73146600	-1.28818600	-1.30098100
C	-3.07089500	-0.16137400	-2.45596000
H	-2.00794300	0.09400800	-2.31177800
C	-3.63216900	0.82605100	-3.48625000

H	-3.59376600	1.86013900	-3.10893000
H	-4.67993300	0.60011800	-3.74158600
H	-3.05045000	0.78014700	-4.42096600
C	-3.11999600	-1.60600000	-2.97445400
H	-2.64497700	-2.29428500	-2.25900200
H	-2.59570700	-1.69824200	-3.93987400
H	-4.16276300	-1.93333100	-3.12003100
H	6.31872800	3.04885600	0.04118100
H	6.28925300	-2.85513600	-0.00563500

ES C1 structure (PBE0)

C	0.35670300	-1.36247600	-0.18959700
C	-0.95209600	-1.65795200	0.34347900
C	-1.52331800	-0.89365900	1.39474000
H	-0.91349600	-0.12470800	1.87040000
C	-2.81388400	-1.10115200	1.82695600
H	-3.22962400	-0.48338700	2.62669000
C	-3.62163600	-2.12235200	1.25726300
C	-4.95680100	-2.34406500	1.66403400
H	-5.39252900	-1.69420700	2.42691800
C	-5.70535900	-3.37509000	1.10671500
H	-6.73671900	-3.53324600	1.43011600
C	-5.14746100	-4.21348000	0.14462500
C	-3.81688800	-4.03295100	-0.29220800
C	-3.21555400	-4.88287700	-1.26515700
H	-3.80556600	-5.70066000	-1.68583800
C	-1.91394100	-4.68754100	-1.66432600
H	-1.46053900	-5.35623900	-2.40062200
C	-1.13416200	-3.62517000	-1.14118500
C	0.21779200	-3.41170500	-1.52760200
H	0.67546900	-4.10519100	-2.23827600
C	0.93113600	-2.33302500	-1.05130500
H	1.95535400	-2.17199100	-1.39859000
C	-1.71056000	-2.74614600	-0.17732000
C	-3.04683200	-2.96758800	0.26238100
C	2.70584200	-0.06071900	0.09518700
C	3.39646100	-0.55030600	1.22124100
C	4.79600200	-0.56329400	1.22707300
H	5.33099200	-0.94676800	2.10193500
C	5.53943200	-0.09820500	0.14124700
C	7.05390500	-0.12124900	0.16964100
C	7.62472400	-1.03037100	-0.91844900
H	8.72264900	-1.08543100	-0.84828400
H	7.37352300	-0.65382700	-1.92307000
H	7.22422100	-2.05201900	-0.83437000
C	2.62708800	-1.08061800	2.41795900
H	1.57079700	-0.79748000	2.26182300
C	3.07270700	-0.45329900	3.73639900
H	3.01304300	0.64529000	3.69626000
H	4.11112600	-0.72354400	3.98609900

H	2.43517200	-0.79921000	4.56519700
C	2.68087200	-2.60666900	2.47276400
H	2.29319300	-3.04636300	1.54137300
H	2.07909900	-2.99359500	3.31065300
H	3.71628800	-2.95956500	2.60830600
B	1.11644200	-0.03968400	0.06769200
C	0.38756800	1.30785100	0.29757200
C	-0.88051600	1.65036500	-0.30094200
C	-1.42524900	0.90528600	-1.37973900
H	-0.82191000	0.11165100	-1.82183100
C	-2.68294900	1.16089000	-1.87828300
H	-3.08014300	0.55709800	-2.69784100
C	-3.47917700	2.21374800	-1.35195300
C	-4.78150000	2.48583900	-1.82862400
H	-5.20100300	1.85172000	-2.61348600
C	-5.51836100	3.54590700	-1.31164300
H	-6.52419700	3.74314100	-1.68921800
C	-4.98013000	4.36348700	-0.32094200
C	-3.68250500	4.13240100	0.18582200
C	-3.10201500	4.95956200	1.19038400
H	-3.68205500	5.79934100	1.58044900
C	-1.83188600	4.71498700	1.65801500
H	-1.39309700	5.36625500	2.41834100
C	-1.06661600	3.62331000	1.17515000
C	0.25352000	3.35882000	1.63265300
H	0.69831500	4.03423100	2.36841800
C	0.95082500	2.25471700	1.19145500
H	1.94912000	2.05618200	1.59074900
C	-1.62385500	2.76649100	0.18085100
C	-2.92560200	3.03794100	-0.32811000
C	3.44776600	0.41104600	-1.00854000
C	4.84421300	0.38753400	-0.97063800
H	5.40828600	0.75793200	-1.83217100
H	7.34748500	-0.54444500	1.14570000
C	7.64178500	1.28682200	0.08111400
H	8.73992500	1.25989000	0.16333400
H	7.25371900	1.93167400	0.88412200
H	7.39146500	1.76253200	-0.88078500
C	2.73080200	0.96057100	-2.22909800
H	1.66385700	0.70065400	-2.10954900
C	3.20616700	0.32555200	-3.53329400



H	3.12038100	-0.77143600	-3.49744100
H	4.25825000	0.57261000	-3.74744100
H	2.60492800	0.68714500	-4.38226100
C	2.82065400	2.48512800	-2.27818500
H	2.41235200	2.93209200	-1.35913700
H	2.25608100	2.88716100	-3.13464300
H	3.86782000	2.81453100	-2.37813700
H	-5.73722700	-5.02883100	-0.28186800
H	-5.55968300	5.20166700	0.07404500

ES C1 structure (CAM-B3LYP)

C	0.36503000	-1.35158100	-0.17751100
C	-0.94227600	-1.64532600	0.36055000
C	-1.51605900	-0.87382900	1.40640900
H	-0.90917400	-0.10530900	1.88185900
C	-2.80552800	-1.07410400	1.83205000
H	-3.22283300	-0.45105500	2.62594000
C	-3.61596100	-2.09688900	1.26473100
C	-4.95166600	-2.31002600	1.66534800
H	-5.38896900	-1.65347700	2.42067300
C	-5.70032900	-3.34100700	1.11250200
H	-6.73341500	-3.49298500	1.43103700
C	-5.14011300	-4.18738300	0.16068400
C	-3.80933900	-4.01428400	-0.26859100
C	-3.20353700	-4.87453500	-1.23299700
H	-3.79381000	-5.69330700	-1.64971800
C	-1.90389700	-4.68663500	-1.62540800
H	-1.44829700	-5.36077600	-2.35421400
C	-1.12345700	-3.62114100	-1.10623100
C	0.23130900	-3.41458700	-1.49072900
H	0.68926100	-4.11688500	-2.19123400
C	0.94197400	-2.33568300	-1.02561400
H	1.96645100	-2.18229400	-1.37110000
C	-1.69959800	-2.73536100	-0.15386800
C	-3.04014800	-2.94952000	0.28106800
C	2.70853000	-0.04696700	0.09471000
C	3.39450400	-0.49433100	1.23898200
C	4.79225300	-0.50951200	1.25133700
H	5.32150000	-0.86114000	2.14121400
C	5.54044000	-0.08815000	0.15436700
C	7.05698500	-0.11363000	0.19023700
C	7.63257900	-1.06409100	-0.86254700
H	8.72942800	-1.11849800	-0.78420600
H	7.38741600	-0.72373300	-1.88074600
H	7.22974700	-2.08079500	-0.74348100
C	2.62592600	-0.98483900	2.45734800
H	1.57255400	-0.70006200	2.30830400
C	3.08680800	-0.32671700	3.75838000
H	3.04050200	0.77049500	3.68859400
H	4.12169700	-0.60330700	4.01186800

H	2.44791500	-0.64162400	4.59769500
C	2.66934300	-2.51153500	2.55649800
H	2.27357100	-2.97589600	1.64151700
H	2.07025200	-2.86902600	3.40853700
H	3.70256600	-2.86707700	2.69613500
B	1.11694200	-0.02580100	0.05929400
C	0.38893000	1.31864100	0.26321500
C	-0.88476200	1.64533700	-0.33317900
C	-1.43022100	0.88815700	-1.40444300
H	-0.82233800	0.10400800	-1.85231800
C	-2.69349800	1.12116900	-1.88792500
H	-3.09022100	0.50855900	-2.70029300
C	-3.50224700	2.16493000	-1.35750300
C	-4.81229100	2.41229800	-1.81847900
H	-5.23157100	1.76675800	-2.59324900
C	-5.55838900	3.46279100	-1.29995400
H	-6.57148400	3.64140500	-1.66541000
C	-5.02050300	4.29484000	-0.32295400
C	-3.71580100	4.08736600	0.16674500
C	-3.13282600	4.93180300	1.15886800
H	-3.72044400	5.76528600	1.54937300
C	-1.85770500	4.71071700	1.60987800
H	-1.41870500	5.37301100	2.35945100
C	-1.08186400	3.62552600	1.12559500
C	0.24821400	3.38451000	1.57112900
H	0.69154100	4.07499100	2.29246500
C	0.95157900	2.28773500	1.13771800
H	1.95509000	2.10824600	1.52914100
C	-1.63656100	2.75455800	0.14720200
C	-2.95002300	3.00291400	-0.34809000
C	3.45713700	0.38062300	-1.02072500
C	4.85142600	0.35574900	-0.97561400
H	5.41919900	0.69271700	-1.84648700
H	7.34665700	-0.50022800	1.18111400
C	7.65121400	1.29002900	0.05055400
H	8.74832300	1.26215300	0.13856900
H	7.26234300	1.96581800	0.82658300
H	7.40645200	1.72904600	-0.92927200
C	2.75433600	0.89207500	-2.27001000
H	1.68866900	0.63352100	-2.16794900
C	3.25513400	0.22517300	-3.55163500

H	3.17953800	-0.87070700	-3.48687000
H	4.30640700	0.47708500	-3.75937400
H	2.66115300	0.55694000	-4.41700800
C	2.84045800	2.41738100	-2.36280400
H	2.41725800	2.89031200	-1.46467000
H	2.28837200	2.79153100	-3.23909100
H	3.88758200	2.74647600	-2.45622200
H	-5.73012200	-5.00319400	-0.26296000
H	-5.60782000	5.12606400	0.07357900

ES C2 structure (B3LYP)

C	-0.60977000	-1.08712500	0.41479000
C	-1.96271200	-1.31922100	-0.07806400
C	-2.63757200	-0.38666000	-0.91646500
H	-2.11455300	0.51768800	-1.21556100
C	-3.92793200	-0.58449500	-1.35722100
H	-4.40690800	0.16288800	-1.99524100
C	-4.66113200	-1.75275100	-1.00185500
C	-5.99434500	-1.97553400	-1.42829700
H	-6.48645800	-1.21753700	-2.04277800
C	-6.66606000	-3.14222300	-1.07139900
H	-7.69477600	-3.29928700	-1.40668700
C	-6.03857700	-4.11705600	-0.29175000
C	-4.70887100	-3.94215800	0.15639900
C	-4.03638000	-4.92458900	0.94565700
H	-4.57174900	-5.83918800	1.21266000
C	-2.73588900	-4.72895600	1.35928000
H	-2.23020900	-5.49350500	1.95589800
C	-2.02087000	-3.54855800	1.03200300
C	-0.67036700	-3.33972300	1.44163800
H	-0.17161400	-4.12164300	2.02117000
C	-0.01071600	-2.17453400	1.13697000
H	1.01024900	-2.05147500	1.50446800
C	-2.66131300	-2.52752100	0.25284500
C	-4.00642400	-2.73907200	-0.19499900
C	-0.49993300	1.65969500	0.04491500
C	-0.22074200	2.33304300	-1.16781200
C	-0.76153600	3.60220900	-1.40881000
H	-0.54631800	4.11309300	-2.35166700
C	-1.58307800	4.23988700	-0.47306600
C	-2.17298400	5.61114800	-0.75783400
C	-3.70655700	5.55955100	-0.83662400
H	-4.11964300	6.54605700	-1.10318300
H	-4.14346000	5.26363000	0.13104800
H	-4.04083500	4.83094600	-1.59152200
C	0.65727200	1.67129400	-2.22246700
H	0.78255100	0.62113900	-1.91375500
C	2.05464800	2.30619100	-2.26991500
H	2.53387400	2.28317800	-1.27960400
H	1.99539500	3.35939800	-2.59058300

H	2.70752800	1.77122800	-2.97894000
C	0.00496300	1.64401000	-3.61104600
H	-0.99019500	1.17421300	-3.57222200
H	0.62621500	1.07126700	-4.31853400
H	-0.11589000	2.65802700	-4.02457200
B	0.13752100	0.23062000	0.34103500
C	1.68387800	0.32751000	0.69145000
C	2.70762900	-0.47169700	0.06308100
C	2.39352300	-1.41535900	-0.95423400
H	1.35482100	-1.52180800	-1.26274100
C	3.36802600	-2.19633600	-1.54898300
H	3.09328600	-2.91270200	-2.32586300
C	4.73249400	-2.07965600	-1.17034700
C	5.75002700	-2.87129400	-1.76346100
H	5.47328300	-3.59769800	-2.53059300
C	7.08135800	-2.72806600	-1.37801400
H	7.85260900	-3.34418400	-1.84341400
C	7.43249500	-1.79699800	-0.39953600
C	6.45189400	-0.98288100	0.22149500
C	6.79002800	-0.02366500	1.21895500
H	7.83551500	0.08549400	1.51470500
C	5.81524200	0.76050800	1.80347700
H	6.08651400	1.49667600	2.56310300
C	4.45065700	0.63085200	1.43289900
C	3.43004100	1.43663300	2.01275000
H	3.71062900	2.17486300	2.76787200
C	2.10738200	1.29416000	1.63453100
H	1.35612300	1.94059500	2.08976600
C	4.07873200	-0.32517500	0.44145300
C	5.08527000	-1.12661900	-0.16723300
C	-1.31987400	2.30457500	1.00504600
C	-1.84947600	3.57078000	0.72850800
H	-2.49236600	4.05024000	1.47125800
H	-1.79932500	5.92247300	-1.74841600
C	-1.70480100	6.65810600	0.26396500
H	-2.09275900	7.65727400	0.00723400
H	-0.60562500	6.71503500	0.29969500
H	-2.06140300	6.41206900	1.27741400
C	-1.66165600	1.63270400	2.33081900
H	-1.06302000	0.71008600	2.39041300
C	-3.13961800	1.21495200	2.38353800

H	-3.39557100	0.56193800	1.53743500
H	-3.80006400	2.09726000	2.34492100
H	-3.35877000	0.67147300	3.31724200
C	-1.29211100	2.50236700	3.54130300
H	-0.23031500	2.79530600	3.52038900
H	-1.47534500	1.95661700	4.48099600
H	-1.89036800	3.42721100	3.57417200
H	-6.57129600	-5.03172700	-0.01950300
H	8.47706600	-1.68323000	-0.10167300

ES C2 structure (PBE0)

C	0.44266800	-1.07186300	-0.31346600
C	1.76780300	-1.40967100	0.16693300
C	2.49199100	-0.55337700	1.03933700
H	2.01891000	0.36863900	1.37298100
C	3.76583800	-0.84600000	1.46758600
H	4.28924600	-0.15707900	2.13546400
C	4.42282000	-2.03846000	1.06051900
C	5.73745400	-2.35674500	1.47204500
H	6.27470700	-1.65483600	2.11474800
C	6.33692700	-3.54322900	1.06795600
H	7.35418100	-3.77546300	1.39280500
C	5.65075700	-4.44302400	0.25425400
C	4.33691300	-4.17020000	-0.18017000
C	3.60854300	-5.07677600	-1.00369600
H	4.08742000	-6.01039600	-1.30912600
C	2.32511000	-4.78781800	-1.40400800
H	1.77344500	-5.49543400	-2.02891500
C	1.68703300	-3.58111600	-1.02656000
C	0.35606200	-3.27285800	-1.42152000
H	-0.19190500	-3.99726200	-2.03028800
C	-0.22773700	-2.08124300	-1.07071300
H	-1.23660700	-1.87097500	-1.43358600
C	2.38778700	-2.63951800	-0.21215900
C	3.71240700	-2.94765900	0.22035000
C	0.63625500	1.66955900	-0.02707700
C	0.42520000	2.46090200	1.12421500
C	1.12462000	3.66012400	1.28852200
H	0.96066100	4.26430900	2.18671200
C	2.04006200	4.11244100	0.33708200
C	2.79145000	5.41216600	0.53529000
C	4.29820300	5.17864900	0.64492600
H	4.82804900	6.12268700	0.84841500
H	4.70496200	4.76278300	-0.29084700
H	4.53364100	4.47167200	1.45482500
C	-0.53497300	2.00205300	2.20779800
H	-0.84559200	0.97738800	1.93893200
C	-1.79513400	2.86440900	2.24789100
H	-2.30196300	2.86892700	1.27124700
H	-1.55084000	3.90770500	2.50625900



H	-2.50582200	2.48845300	3.00108800
C	0.13100500	1.91798300	3.58015300
H	1.02563300	1.27705400	3.55209700
H	-0.56487900	1.49786600	4.32338100
H	0.44096200	2.91092300	3.94265700
B	-0.18826600	0.32425400	-0.22996100
C	-1.71877700	0.54350600	-0.50721600
C	-2.77102300	-0.26476400	0.05054700
C	-2.50463400	-1.25289800	1.03523300
H	-1.48123100	-1.36240400	1.39672000
C	-3.49939600	-2.06421100	1.53795000
H	-3.26085000	-2.81999200	2.28984500
C	-4.84407700	-1.92656200	1.10451600
C	-5.88192900	-2.75066700	1.59866200
H	-5.63792400	-3.52827600	2.32639200
C	-7.19266900	-2.57651600	1.16934300
H	-7.98313200	-3.22093300	1.55929600
C	-7.50392600	-1.57994800	0.24769700
C	-6.50157100	-0.73111600	-0.27261900
C	-6.79695300	0.30022300	-1.20772900
H	-7.83046900	0.43590600	-1.53456300
C	-5.80240000	1.12004100	-1.68993800
H	-6.04314600	1.91566900	-2.39907300
C	-4.45464600	0.95584400	-1.28223100
C	-3.41437100	1.80212400	-1.75119700
H	-3.66616600	2.60652100	-2.44718200
C	-2.10783700	1.60914200	-1.35412500
H	-1.33065700	2.27509800	-1.73613100
C	-4.12387400	-0.07604900	-0.35848400
C	-5.15429700	-0.90926500	0.15617000
C	1.56099300	2.12165200	-0.99808400
C	2.24327800	3.32455700	-0.79941600
H	2.95784000	3.65964300	-1.55781200
H	2.44838400	5.83533500	1.49507100
C	2.46501100	6.42662200	-0.56039300
H	2.97252400	7.38567600	-0.37085900
H	1.38256400	6.61712300	-0.61736300
H	2.79410500	6.06522000	-1.54788300
C	1.82974600	1.32630900	-2.26358000
H	1.18958800	0.43034900	-2.21855300
C	3.27891700	0.84641500	-2.33823100

H	3.54843800	0.26141600	-1.44667400
H	3.97920500	1.69450300	-2.41206400
H	3.43271900	0.20995100	-3.22412300
C	1.43764100	2.10610200	-3.51832200
H	0.38141900	2.41497800	-3.48561300
H	1.58290700	1.49158800	-4.42094800
H	2.04777200	3.01657700	-3.63380500
H	6.12606500	-5.37703700	-0.05616700
H	-8.53646300	-1.44074300	-0.08180400

ES C2 structure (CAM-B3LYP)

C	0.36147900	-1.07297200	-0.26072700
C	1.67564000	-1.43542700	0.24699800
C	2.37086300	-0.61763400	1.16846700
H	1.88796900	0.28097300	1.54168500
C	3.64374800	-0.92146700	1.60456400
H	4.14849000	-0.26039600	2.31208000
C	4.31364600	-2.08373300	1.15168500
C	5.62795900	-2.40975600	1.56826100
H	6.14843400	-1.73334500	2.24967500
C	6.24420500	-3.56868800	1.12050800
H	7.25766200	-3.80724200	1.44878800
C	5.57670100	-4.43371900	0.25782200
C	4.26479800	-4.15233400	-0.18399600
C	3.55888200	-5.02544300	-1.05447600
H	4.04796100	-5.94020200	-1.39540800
C	2.27564000	-4.72890700	-1.45891000
H	1.73927800	-5.41307300	-2.12016400
C	1.62863500	-3.54815400	-1.03780500
C	0.29275400	-3.23020700	-1.43752300
H	-0.24162900	-3.93543700	-2.07818300
C	-0.29954200	-2.05844100	-1.05486700
H	-1.30166500	-1.83495500	-1.42266300
C	2.30851400	-2.64143500	-0.17521300
C	3.62610500	-2.95776300	0.26223700
C	0.66515200	1.64269300	-0.03374600
C	0.49273600	2.50023500	1.07539700
C	1.27322600	3.65185300	1.19791500
H	1.13708300	4.30610600	2.06347200
C	2.23324800	3.99507600	0.24896500
C	3.07195300	5.24883200	0.40506000
C	4.55700400	4.91549500	0.56989100
H	5.14741700	5.82877200	0.74146400
H	4.95542800	4.42447200	-0.33166800
H	4.72032300	4.23693200	1.42022300
C	-0.50671500	2.17439000	2.17752800
H	-0.91770300	1.17739500	1.96157800
C	-1.68124400	3.15476200	2.18552400
H	-2.19450300	3.16267200	1.21347200
H	-1.33923600	4.18030900	2.39669900

H	-2.41598300	2.87954200	2.95806300
C	0.15580800	2.09136400	3.55516800
H	0.98768600	1.37087800	3.55789400
H	-0.57284500	1.76931000	4.31490200
H	0.55657400	3.06578200	3.87357100
B	-0.24075500	0.34504300	-0.18774900
C	-1.75803600	0.59496600	-0.43440000
C	-2.81907100	-0.21343300	0.08576700
C	-2.58121500	-1.23841400	1.05388800
H	-1.56856800	-1.36363100	1.43584500
C	-3.58195200	-2.04449900	1.51585200
H	-3.36529900	-2.82244900	2.25124600
C	-4.92968100	-1.88024700	1.07070800
C	-5.97688600	-2.70190800	1.52622700
H	-5.75195600	-3.50454200	2.23201700
C	-7.27933200	-2.49686600	1.08879300
H	-8.08163400	-3.14344800	1.44967200
C	-7.56958700	-1.46824300	0.19727300
C	-6.55553700	-0.62163500	-0.28064800
C	-6.82621400	0.45221100	-1.18902900
H	-7.85542000	0.61009400	-1.51863100
C	-5.82589800	1.26759400	-1.63017300
H	-6.04636000	2.08958500	-2.31490200
C	-4.47441800	1.07429400	-1.21529100
C	-3.42765600	1.92027900	-1.64633600
H	-3.66303400	2.75179200	-2.31472500
C	-2.12903300	1.69479500	-1.24762500
H	-1.34220900	2.36153500	-1.60524700
C	-4.16508700	0.00805700	-0.32625700
C	-5.21592600	-0.83119000	0.15354600
C	1.64188600	1.98328300	-0.99821700
C	2.40151000	3.14274300	-0.84248700
H	3.14858900	3.39191900	-1.60036900
H	2.73712200	5.74446400	1.33099800
C	2.85024700	6.22840400	-0.74994200
H	3.41971900	7.15700300	-0.59052500
H	1.78688100	6.49160400	-0.85012200
H	3.18014200	5.79548700	-1.70719600
C	1.87830000	1.12433400	-2.23180700
H	1.23280400	0.23965900	-2.14146700
C	3.32147800	0.62368700	-2.32367300

H	3.61343100	0.08354500	-1.41166200
H	4.03011600	1.45470000	-2.46526000
H	3.43966300	-0.06116900	-3.17757400
C	1.45993900	1.85450300	-3.51086100
H	0.40516700	2.16424800	-3.46470300
H	1.58487500	1.20485200	-4.39102400
H	2.06774800	2.75869900	-3.67224400
H	6.06340200	-5.34897200	-0.08643900
H	-8.59629900	-1.30669500	-0.13865400

ES C3 structure (B3LYP)

C	1.37727000	-1.46792800	0.09143500
C	2.66191100	-0.93206000	-0.31751900
C	2.76866700	0.25255700	-1.10085700
H	1.85724000	0.74885900	-1.42207900
C	3.98676100	0.79441200	-1.45468300
H	4.02373300	1.70594100	-2.05592700
C	5.20888500	0.18671800	-1.05013700
C	6.47384300	0.73435900	-1.37995500
H	6.51390600	1.66414100	-1.95228600
C	7.64923200	0.09896600	-0.98378500
H	8.61663300	0.53410100	-1.24454500
C	7.59886800	-1.09244500	-0.25824200
C	6.35917700	-1.67939200	0.09346800
C	6.28137100	-2.90140400	0.82579200
H	7.20825000	-3.39692500	1.12370900
C	5.05942700	-3.45294500	1.14958400
H	5.01197400	-4.39293900	1.70509800
C	3.84291700	-2.82224100	0.77676800
C	2.57212500	-3.37951600	1.09490200
H	2.53610700	-4.32926600	1.63494700
C	1.40425000	-2.72596500	0.75967500
H	0.45519700	-3.16440000	1.07369600
C	3.87933700	-1.59084700	0.05025700
C	5.14514300	-1.02909000	-0.30019200
C	0.00752100	0.89624000	0.07662700
C	0.60545500	1.59409000	1.16041600
C	0.57017300	2.99473900	1.20039200
H	1.02541100	3.51893800	2.04572000
C	-0.03923400	3.75266900	0.19751400
C	-0.06252100	5.27027100	0.26540700
C	0.70524100	5.90190100	-0.90582700
H	0.73115800	6.99979600	-0.81207200
H	0.22834300	5.65983200	-1.86963400
H	1.74299300	5.53547100	-0.94369000
C	1.25073600	0.86521500	2.33536000
H	1.20832600	-0.21079700	2.11872600
C	0.46509300	1.08851500	3.63773600
H	-0.58515600	0.77485700	3.52994700
H	0.46913200	2.15038700	3.93313200

H	0.90789200	0.50900200	4.46431600
C	2.73051300	1.23580400	2.51149300
H	3.29603000	1.06619800	1.58399600
H	3.18995000	0.62815400	3.30802600
H	2.85014000	2.29531500	2.79143200
B	0.02864800	-0.69325400	0.01047400
C	-1.29946500	-1.49239900	-0.13812600
C	-2.59869700	-1.02216100	0.30449100
C	-2.73775800	0.08919900	1.18407600
H	-1.84011700	0.57586500	1.55505800
C	-3.97023000	0.57284500	1.57094000
H	-4.03196900	1.42970200	2.24602900
C	-5.17544900	-0.02489000	1.10551500
C	-6.45473400	0.46525000	1.46885800
H	-6.51970200	1.34228200	2.11713000
C	-7.61264100	-0.15992100	1.00995500
H	-8.59141900	0.23046200	1.29776600
C	-7.53036500	-1.28438200	0.18698500
C	-6.27528800	-1.81248000	-0.20154700
C	-6.16466900	-2.96634500	-1.03343700
H	-7.07800400	-3.45455600	-1.38109200
C	-4.92831600	-3.46260700	-1.39030600
H	-4.85565300	-4.35144300	-2.02209300
C	-3.72900100	-2.83966100	-0.95420900
C	-2.44368100	-3.34114500	-1.30529300
H	-2.38247100	-4.24196700	-1.92152300
C	-1.29334300	-2.69179200	-0.90735000
H	-0.33261100	-3.08158000	-1.24884200
C	-3.79834500	-1.67443200	-0.12784400
C	-5.07898600	-1.17159300	0.25669700
C	-0.61377200	1.66555500	-0.94718700
C	-0.62523500	3.06253300	-0.86993200
H	-1.09983800	3.63250200	-1.67287100
H	0.45497800	5.55852800	1.19649600
C	-1.49759100	5.81249800	0.34524500
H	-1.49765600	6.90940500	0.45308200
H	-2.03734300	5.38249300	1.20337800
H	-2.06639300	5.56598000	-0.56609200
C	-1.23425800	1.01751700	-2.18176600
H	-1.16207600	-0.07112000	-2.05467700
C	-0.45058700	1.37060200	-3.45633100

H	0.60750200	1.07758500	-3.36963600
H	-0.48281500	2.45320100	-3.66087200
H	-0.87457000	0.85119600	-4.33130800
C	-2.72325300	1.35939400	-2.33586400
H	-3.28680900	1.09757800	-1.42896500
H	-3.16201400	0.80683300	-3.18256300
H	-2.87260000	2.43455100	-2.52825000
H	8.52290800	-1.58930800	0.04710700
H	-8.44081200	-1.77381600	-0.16733500



ES C3 structure (PBE0)

C	1.37191700	-1.45529600	0.09803000
C	2.65664200	-0.92710500	-0.30540500
C	2.76848100	0.25871500	-1.07987700
H	1.85596500	0.76319300	-1.39197700
C	3.98660000	0.79238400	-1.43370200
H	4.02898600	1.70733900	-2.02969800
C	5.20201100	0.17309700	-1.03731600
C	6.46644400	0.71124200	-1.36845700
H	6.51152400	1.64381500	-1.93623000
C	7.63545400	0.06608800	-0.98104700
H	8.60539000	0.49467700	-1.24320300
C	7.57785700	-1.12573200	-0.26313900
C	6.33784700	-1.70239400	0.08896200
C	6.25396000	-2.92460900	0.81401700
H	7.17814900	-3.42885500	1.10618900
C	5.03194900	-3.46673200	1.13877100
H	4.97887100	-4.40909000	1.69002500
C	3.82239200	-2.82565600	0.77348500
C	2.55139000	-3.37379100	1.09225500
H	2.50961300	-4.32529700	1.62906600
C	1.39013300	-2.71245400	0.76188200
H	0.43701400	-3.14465900	1.07542200
C	3.86605500	-1.59497500	0.05489700
C	5.13162500	-1.04244600	-0.29591600
C	0.00679900	0.91449100	0.07998400
C	0.59923900	1.60910100	1.16429400
C	0.56695100	3.00703600	1.20271400
H	1.01877400	3.53114100	2.05122400
C	-0.03235700	3.76412100	0.19716200
C	-0.05053000	5.27650100	0.26201100
C	0.72805000	5.89828200	-0.89726500
H	0.75771400	6.99566900	-0.80679100
H	0.26026200	5.65616100	-1.86511600
H	1.76425300	5.52838400	-0.92442600
C	1.23396700	0.87979600	2.33670200
H	1.19076100	-0.19629200	2.10889400
C	0.44233600	1.09714100	3.62726600
H	-0.60695500	0.78409400	3.51336200
H	0.44445300	2.15787900	3.92593900

H	0.87913000	0.51609000	4.45505100
C	2.70504300	1.24827200	2.52337700
H	3.27950600	1.07677900	1.60131600
H	3.15759300	0.64299500	3.32477200
H	2.82321800	2.30797500	2.80215200
B	0.02627800	-0.67588900	0.01453000
C	-1.29921100	-1.47824400	-0.13722400
C	-2.59870900	-1.01283400	0.29573400
C	-2.74338600	0.10206700	1.16423200
H	-1.84498900	0.59730500	1.52788500
C	-3.97600600	0.57969000	1.54687000
H	-4.04371300	1.44147600	2.21537900
C	-5.17405600	-0.02931800	1.08687500
C	-6.45284200	0.45361400	1.44681900
H	-6.52320100	1.33494900	2.08899500
C	-7.60397200	-0.18116600	0.99424300
H	-8.58532500	0.20435800	1.27981800
C	-7.51408600	-1.30816000	0.18121900
C	-6.25869400	-1.82834600	-0.20287300
C	-6.14162800	-2.98465500	-1.02493300
H	-7.05198100	-3.48147200	-1.36868200
C	-4.90521300	-3.47374400	-1.37811000
H	-4.82656700	-4.36648000	-2.00388700
C	-3.71320500	-2.84066000	-0.94722600
C	-2.42772300	-3.33532500	-1.29429400
H	-2.36051200	-4.23937700	-1.90539800
C	-1.28424500	-2.67851100	-0.89949000
H	-0.31935500	-3.06380100	-1.23727200
C	-3.79007500	-1.67390100	-0.13134800
C	-5.07055100	-1.17794500	0.24891500
C	-0.60567200	1.68149700	-0.94605300
C	-0.61256300	3.07577500	-0.87087700
H	-1.08107700	3.64612300	-1.67890100
H	0.45995800	5.56156400	1.19801100
C	-1.47737700	5.82052000	0.32816600
H	-1.47517800	6.91695600	0.43365400
H	-2.02660000	5.39497200	1.18170400
H	-2.03929200	5.57481600	-0.58722800
C	-1.21970800	1.03342500	-2.17623700
H	-1.15151300	-0.05623100	-2.03597600
C	-0.43021400	1.37363600	-3.44133100

H	0.62568600	1.07604000	-3.34962200
H	-0.45585600	2.45513200	-3.65148500
H	-0.85187300	0.85307100	-4.31588400
C	-2.69860400	1.38053200	-2.33970000
H	-3.27083000	1.12147100	-1.43700500
H	-3.13417700	0.83105800	-3.18923500
H	-2.84200900	2.45609900	-2.53293400
H	8.49893600	-1.63194000	0.03648400
H	-8.42121100	-1.80679400	-0.16941500

ES C3 structure (CAM-B3LYP)

C	1.42099700	-1.40364900	0.23680200
C	2.67425200	-0.88075800	-0.23073200
C	2.75238900	0.29241100	-1.04724600
H	1.82972200	0.79279900	-1.32486100
C	3.94020900	0.80296800	-1.47890900
H	3.95562200	1.70055400	-2.10117500
C	5.18285300	0.18623100	-1.13474500
C	6.42065300	0.70355100	-1.55500600
H	6.43669600	1.61386000	-2.15837500
C	7.60747100	0.06845600	-1.21112900
H	8.56157900	0.48225600	-1.54361100
C	7.58703800	-1.09387800	-0.44665100
C	6.37246900	-1.64573800	-0.00763100
C	6.32439600	-2.84414200	0.77508200
H	7.26397500	-3.33701200	1.03408700
C	5.13327000	-3.36317400	1.18742200
H	5.10646600	-4.27975600	1.78103800
C	3.89645300	-2.73129300	0.86062300
C	2.65568300	-3.26042600	1.27544000
H	2.64382100	-4.18307000	1.86041100
C	1.47780700	-2.61895600	0.96712400
H	0.54396000	-3.04230600	1.34063600
C	3.90056900	-1.53508800	0.09090900
C	5.15031600	-0.99842800	-0.34972900
C	-0.03025500	0.91769200	0.15704800
C	0.51078500	1.65528500	1.23598600
C	0.45324400	3.05107700	1.22982500
H	0.86997400	3.60862000	2.07315700
C	-0.12437800	3.76440900	0.18386400
C	-0.16541200	5.27991500	0.19802800
C	0.63462100	5.87687700	-0.96253000
H	0.64634400	6.97630300	-0.90620200
H	0.19500400	5.59710200	-1.93265300
H	1.67575700	5.52190500	-0.95174800
C	1.12523700	0.97705600	2.45395600
H	1.06329100	-0.10724900	2.29567700
C	0.33885900	1.28687000	3.73149900
H	-0.71888700	0.99996000	3.63246200
H	0.37238700	2.35956400	3.97701900

H	0.75797100	0.73614000	4.58779000
C	2.60597900	1.32619800	2.62308700
H	3.17877800	1.08167600	1.71794500
H	3.04300100	0.76695400	3.46483100
H	2.74317100	2.39929200	2.82952000
B	0.04447200	-0.67333300	0.13239500
C	-1.24425300	-1.51941600	-0.00225600
C	-2.57480600	-1.06075500	0.37418100
C	-2.76597600	0.04945500	1.22719800
H	-1.89564700	0.54191000	1.65100000
C	-4.02219900	0.53449000	1.53187100
H	-4.12561600	1.40029700	2.18916100
C	-5.18700600	-0.07271600	1.00554100
C	-6.48700600	0.41788000	1.28272900
H	-6.59334200	1.30553100	1.90998100
C	-7.60794600	-0.21864700	0.76887900
H	-8.60342600	0.17095600	0.98989300
C	-7.47149000	-1.35445300	-0.02256100
C	-6.19473100	-1.88301900	-0.32552900
C	-6.03133600	-3.04809400	-1.11898900
H	-6.91823700	-3.55003500	-1.51078600
C	-4.77313500	-3.54597200	-1.38685900
H	-4.66029400	-4.45032800	-1.98876900
C	-3.61488000	-2.90796300	-0.89860200
C	-2.30215700	-3.41622600	-1.15357200
H	-2.20330300	-4.33639400	-1.73404700
C	-1.18752900	-2.75175600	-0.71529800
H	-0.20733600	-3.14578900	-0.98703600
C	-3.73770800	-1.72830100	-0.11102600
C	-5.03648100	-1.22855700	0.18801200
C	-0.62996000	1.64047300	-0.90544000
C	-0.66359100	3.03399000	-0.87454800
H	-1.12145900	3.57006100	-1.70960300
H	0.31526200	5.60429600	1.13549400
C	-1.60247000	5.80700400	0.20796100
H	-1.61656800	6.90565600	0.27732800
H	-2.16881300	5.40258200	1.05993700
H	-2.13553100	5.52402700	-0.71312300
C	-1.21521800	0.94650800	-2.12887700
H	-1.14415900	-0.13606400	-1.95855900
C	-0.40699500	1.25328500	-3.39367500

H	0.64776200	0.96334200	-3.27821100
H	-0.43482700	2.32732100	-3.63539600
H	-0.81401900	0.70533900	-4.25756700
C	-2.69544100	1.27858300	-2.33287400
H	-3.28297900	1.05704800	-1.43116700
H	-3.11235700	0.68977700	-3.16447900
H	-2.84032300	2.34282500	-2.57605600
H	8.52173400	-1.59179600	-0.17917700
H	-8.35666700	-1.85705300	-0.41866400

ES C1 structure (RI-CC2)

C	0.4677660	-0.9879051	-0.2909686
C	-0.8390589	-1.0973493	0.3359358
C	-1.2038591	-0.2852076	1.4397949
H	-0.4335854	0.3250704	1.9222655
C	-2.5114411	-0.2606386	1.9308494
H	-2.7643344	0.3905487	2.7754378
C	-3.5342539	-1.0190841	1.3090206
C	-4.8918614	-0.9401754	1.7211369
H	-5.1530293	-0.2793469	2.5542481
C	-5.8653431	-1.7698978	1.1326697
H	-6.9018034	-1.7174114	1.4798430
C	-5.5250552	-2.6313692	0.0937534
C	-4.1802482	-2.7254900	-0.3742867
C	-3.7929171	-3.6392692	-1.3914904
H	-4.5584415	-4.2629741	-1.8654367
C	-2.4676346	-3.7210176	-1.8109864
H	-2.1863409	-4.4422866	-2.5865777
C	-1.4577023	-2.9241406	-1.2181303
C	-0.0913062	-2.9713110	-1.6284526
H	0.2069202	-3.7292660	-2.3628526
C	0.8476152	-2.0655796	-1.1441606
H	1.8712263	-2.0811169	-1.5380079
C	-1.8358971	-1.9589981	-0.2249801
C	-3.1681834	-1.9400069	0.2707691
C	2.9217525	0.1919674	0.0107983
C	3.5111228	-0.4704979	1.1213309
C	4.9110958	-0.5488191	1.2291563
H	5.3649454	-1.0603008	2.0866191
C	5.7575522	0.0213952	0.2649508
C	7.2618546	-0.0675279	0.3982322
C	7.8786003	-0.8530291	-0.7609636
H	8.9657022	-0.9693840	-0.6241384
H	7.7119717	-0.3318651	-1.7166327
H	7.4295629	-1.8543209	-0.8397078
C	2.6425225	-1.0850707	2.2019884
H	1.5990295	-0.8191840	1.9605187
C	2.9524598	-0.5042650	3.5821958
H	2.8623644	0.5929998	3.5720078
H	3.9758726	-0.7568763	3.9021641

H	2.2564217	-0.9026784	4.3383397
C	2.7394368	-2.6108719	2.1927802
H	2.4568924	-3.0079399	1.2057635
H	2.0693013	-3.0534896	2.9480372
H	3.7680025	-2.9397330	2.4135912
B	1.3576356	0.2896638	-0.1228503
C	0.5443732	1.6007601	-0.0429171
C	-0.7333725	1.5988716	-0.7093778
C	-0.9542654	0.7882268	-1.8497710
H	-0.0926092	0.4646995	-2.4416536
C	-2.2438380	0.3941229	-2.2199785
H	-2.3929310	-0.2616818	-3.0857214
C	-3.3562543	0.7520611	-1.4238673
C	-4.6618345	0.2314490	-1.6687832
H	-4.8068758	-0.4649281	-2.5015582
C	-5.7243065	0.5825635	-0.8420265
H	-6.7179484	0.1646324	-1.0275169
C	-5.5346229	1.4570450	0.2438869
C	-4.2627482	2.0383823	0.5011380
C	-4.0411367	2.9601320	1.5652166
H	-4.8865875	3.2504110	2.1989197
C	-2.7666703	3.4449868	1.8403707
H	-2.6182867	4.1388768	2.6757570
C	-1.6449680	3.0514334	1.0666268
C	-0.2961437	3.3531427	1.4440484
H	-0.1267609	4.0847019	2.2431917
C	0.7729452	2.6450370	0.9060703
H	1.7759501	2.7635772	1.3353224
C	-1.8590062	2.1421399	-0.0207053
C	-3.1717969	1.7164193	-0.3682212
C	3.7741939	0.7634885	-0.9745853
C	5.1689691	0.6783511	-0.8308588
H	5.8153119	1.1272021	-1.5933546
H	7.4721635	-0.6211529	1.3309205
C	7.8933542	1.3202334	0.5255751
H	8.9807204	1.2452408	0.6869156
H	7.4548675	1.8754742	1.3680641
H	7.7275507	1.9091541	-0.3900374
C	3.1843037	1.4807163	-2.1741825
H	2.1035125	1.2530788	-2.1778185
C	3.7659979	0.9825734	-3.4973525



H	3.6629628	-0.1099757	-3.5860371
H	4.8359227	1.2290060	-3.5853066
H	3.2472972	1.4502380	-4.3497462
C	3.3299536	2.9960686	-2.0286790
H	2.8392136	3.3419280	-1.1065704
H	2.8717216	3.5224011	-2.8821794
H	4.3941105	3.2798408	-1.9802585
H	-6.2894689	-3.2621281	-0.3731145
H	-6.3822769	1.7310725	0.8823085