Supporting Information for

Generation of an Extremely Bent Pyrene System Using Kinetic Stabilization

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1. ^1H and ^{13}C NMR Spectra	S2–S50
2. Calculated structures of 2a-e , 3a-e and 13a-e	S51–S57
3. Computational Details and Cartesian Co-ordinates for Calculated Structures of 2a-e , 3a-e , 13a-e and 7a-e	S58–S100

1. ^1H and ^{13}C NMR Spectra

S-4

11a

11a

11b

11c

11d

11e

12a

12a

12d

12d

13a

13b

13b

13c

13e

13e

15a

15c

Table S1. Chemical shifts (δ ppm) of the protons on **11a-e**.

Compound	H _A	H _B	H _C	H _D	H _E	H _F
11a	6.94	6.66 (br)	4.43 (de)	2.49 (2.92) ^b $\Delta\delta=0.43$	-	-
11b	6.97	7.08 ^a	4.36 (de)	2.05 (2.62) $\Delta\delta=0.57$	1.21 (1.96) $\Delta\delta=0.75$	-
11c	7.00	6.87	4.43	1.73 (2.62) $\Delta\delta=0.89$	0.79 (1.59) $\Delta\delta=0.80$	-
11d	7.02 *	6.90	4.35 (de)	2.05 (2.62) $\Delta\delta=0.57$	0.88 (1.59) $\Delta\delta=0.71$	0.22 (1.29) $\Delta\delta=1.07$
11e	7.09 *	6.96	4.43	2.12 (2.62) $\Delta\delta=0.50$	0.96 (1.59) $\Delta\delta=0.63$	0.27 (1.29) $\Delta\delta=1.02$

Notes: “br” denotes a broad signal; “de” denotes a virtually degenerate AB system; (a) denotes that the chemical shifts were determined by a low cut of the ¹H, ¹H-COSY spectrum (for overlapping signals); (b) numbers in brackets are calculated values for the corresponding protons in the analogous 1,*n*-diphenylalkanes.

Table S2. Chemical shifts (δ ppm) of the protons on **12a-e**.

Compound	H _A	H _B	H _C	H _D	H _E	H _F
12a	-	-	4.22, 4.16 (AB)	2.46 (2.92) ^a $\Delta\delta=0.46$	-	-
12b	7.15	7.06	4.39 (s)	1.86 (2.62) $\Delta\delta=0.76$	1.21 (1.96) $\Delta\delta=0.75$	-
12c	7.01	6.96	4.26 (s)	1.70 (2.62) $\Delta\delta=0.92$	0.81 (1.59) $\Delta\delta=0.78$	-
12d	-	-	4.26, 4.25 (AB)	2.05 (2.62) $\Delta\delta=0.57$	0.88 (1.59) $\Delta\delta=0.72$	0.28 (1.29) $\Delta\delta=1.01$
12e	-	-	4.28, 4.26 (AB)	2.10 (2.62) $\Delta\delta=0.52$	0.97 (1.59) $\Delta\delta=0.62$	0.33 (1.29) $\Delta\delta=0.96$

Note: “AB” denotes an AB system; (a) numbers in brackets are calculated values for the corresponding protons in the analogous 1,*n*-diphenylalkanes.

2. Calculated Structures of 2a-e, 3a-e and 13a-e

Figure S1. Calculated Structure of **2a**.

Figure S2. Calculated Structure of **2b**.

Figure S3. Calculated Structure of **2c**.

Figure S4. Calculated Structure of **2d**.

Figure S5. Calculated Structure of **2e**.

Figure S6. Calculated Structure of **3a**.

Figure S7. Calculated Structure of **3b**.

Figure S8. Calculated Structure of **3c**.

Figure S9. Calculated Structure of **3d**.

Figure S10. Calculated Structure of **3e**.

Figure S11. Calculated Structure of **13a**.

Figure S12. Calculated Structure of **13b**.

Figure S13. Calculated Structure of **13c**.

Figure S14. Calculated Structure of **13d**.

Figure S15. Calculated Structure of **13e**.

3. Computational Details and Cartesian Co-ordinates for Calculated Structures of 2a-e, 3a-e, 13a-e and 7a-e

DFT Calculations of Pyrenophanes 7a-e

The molecular structures of pyrenophanes **2a-e**, **3a-e**, **4**, **7a-e**, and compounds **13a-e** were first constructed and pre-optimized at the AM1 level using Spartan'10 software package (Wavefun, Inc.). The structures were then optimized by DFT calculations at the B3LYP/6-31G(d) level of theory using Gaussian'09 software package. Visualization of molecular structures and frontier molecular orbitals was done by CYLview and GaussView 5.0 software packages. The optimized Cartesian coordinates and total energies of the compounds are provided below.

Compound **2a**: E(RB3LYP) = -850.33990530 a.u.

C	-0.42765300	0.57309100	-1.60678100
C	-1.71358600	2.27415800	0.16156200
C	0.15703300	1.84380100	-1.33396700
C	-1.81715500	0.37565600	-1.35137300
C	-2.45167800	1.26240600	-0.47238600
C	-0.51256500	2.68497800	-0.43099100
H	-3.43589400	0.99632100	-0.09011700
H	0.02820300	3.53298500	-0.01456000
C	0.42765300	-0.57309100	-1.60678100
C	1.71358600	-2.27415800	0.16156200
C	1.81715500	-0.37565600	-1.35137300
C	-0.15703300	-1.84380100	-1.33396700
C	0.51256500	-2.68497800	-0.43099100
C	2.45167800	-1.26240600	-0.47238600
H	-0.02820300	-3.53298500	-0.01456000
H	3.43589400	-0.99632100	-0.09011700
C	-1.56691300	-2.01765800	-1.61746100
H	-1.97947100	-3.02285600	-1.66010000
C	-2.38062600	-0.92925600	-1.63320200
H	-3.46084500	-1.04051400	-1.68901300
C	2.38062600	0.92925600	-1.63320200
H	3.46084500	1.04051400	-1.68901300
C	1.56691300	2.01765800	-1.61746100
H	1.97947100	3.02285600	-1.66010000
C	1.95956400	-2.53885500	1.63417600
C	-1.95956400	2.53885500	1.63417600
C	1.56691300	-1.25609400	2.46062600
H	2.21547400	-0.44445500	2.10770200
H	1.84992000	-1.43364900	3.50708700
C	0.08531200	-0.77329100	2.40205800
H	-0.39754100	-1.15762200	1.49680900
H	-0.46924500	-1.20536100	3.24692800

C	-0.08531200	0.77329100	2.40205800
H	0.39754100	1.15762200	1.49680900
H	0.46924500	1.20536100	3.24692800
C	-1.56691300	1.25609400	2.46062600
H	-1.84992000	1.43364900	3.50708700
H	-2.21547400	0.44445500	2.10770200
H	-1.37672700	3.40367400	1.97553200
H	-3.01537000	2.75473900	1.84616500
H	1.37672700	-3.40367400	1.97553200
H	3.01537000	-2.75473900	1.84616500

Compound **2b**: E(RB3LYP) = -889.68153441 a.u.

C	0.11710700	-0.01882300	3.05894400
H	0.15376700	2.13938700	3.01165700
C	0.56518300	1.22489600	2.58739600
C	1.50001800	-1.14519600	1.40007000
C	1.30238100	1.31019400	1.40021600
C	0.74527600	-1.17540700	2.58422800
C	1.61190500	0.09803400	0.71312500
C	1.44183200	2.55614900	0.67985300
H	0.46868300	-2.14288400	2.99951000
C	1.44183200	2.55614900	-0.67985300
H	1.40688300	3.49060800	1.23486300
H	1.40688300	3.49060800	-1.23486300
C	1.30238100	1.31019400	-1.40021600
C	0.56518300	1.22489600	-2.58739600
C	1.61190500	0.09803400	-0.71312500
C	0.11710700	-0.01882300	-3.05894400
H	0.15376700	2.13938700	-3.01165700
C	0.74527600	-1.17540700	-2.58422800
H	0.46868300	-2.14288400	-2.99951000
C	1.50001800	-1.14519600	-1.40007000
C	1.82683800	-2.35346200	0.68058300
H	1.93145200	-3.28336400	1.23457100
C	1.82683800	-2.35346200	-0.68058300
H	1.93145200	-3.28336400	-1.23457100
C	-1.25574700	-0.11381700	-3.69210300
C	-1.25574700	-0.11381700	3.69210300
C	-2.34131900	0.23193500	-2.61005600
H	-3.32646100	0.17467400	-3.09155100
H	-2.19770400	1.28681200	-2.34392100
C	-2.33995900	-0.62045400	-1.30279500
H	-1.39851300	-1.17436000	-1.22563800
H	-3.13059900	-1.38115000	-1.36097700

C	-2.34131900	0.23193500	2.61005600
H	-2.19770400	1.28681200	2.34392100
H	-3.32646100	0.17467400	3.09155100
C	-2.33995900	-0.62045400	1.30279500
H	-3.13059900	-1.38115000	1.36097700
H	-1.39851300	-1.17436000	1.22563800
C	-2.50821500	0.20221300	0.00000000
H	-3.48583000	0.70739100	0.00000000
H	-1.75230100	0.99960900	0.00000000
H	-1.42525700	-1.12264000	4.08881700
H	-1.37963600	0.58847900	4.52723600
H	-1.37963600	0.58847900	-4.52723600
H	-1.42525700	-1.12264000	-4.08881700

Compound **2c**: E(RB3LYP) = -929.01832661 a.u.

C	-0.00034900	0.71197600	-1.60489300
C	-0.00002800	3.21576800	-0.36185700
C	1.23274300	1.41158000	-1.43874800
C	-1.23295400	1.40752700	-1.43699000
C	-1.20359800	2.66560500	-0.81736200
C	1.20488700	2.67120600	-0.82553600
H	-2.14544300	3.12756800	-0.52707100
H	2.14788800	3.13547500	-0.54161100
C	0.00034900	-0.71197600	-1.60489300
C	0.00002800	-3.21576800	-0.36185700
C	1.23295400	-1.40752700	-1.43699000
C	-1.23274300	-1.41158000	-1.43874800
C	-1.20488700	-2.67120600	-0.82553600
C	1.20359800	-2.66560500	-0.81736200
H	-2.14788800	-3.13547500	-0.54161100
H	2.14544300	-3.12756800	-0.52707100
C	-2.46232300	-0.68268600	-1.63074600
H	-3.39835700	-1.23552200	-1.65811600
C	-2.46232300	0.67838500	-1.62754400
H	-3.39854200	1.23108300	-1.65225400
C	2.46232300	-0.67838500	-1.62754400
H	3.39854200	-1.23108300	-1.65225400
C	2.46232300	0.68268600	-1.63074600
H	3.39835700	1.23552200	-1.65811600
C	-0.00249500	-4.10130100	0.86322000
C	0.00249500	4.10130100	0.86322000
C	-0.39345500	-3.25676300	2.12444400
H	-1.45613500	-2.99878400	2.03039100
C	0.41725100	0.64969900	2.36077900

H	1.05367700	0.65196900	1.46614900
C	-0.42409100	1.95073400	2.37921700
H	1.10223200	0.65168200	3.22224700
C	0.42409100	-1.95073400	2.37921700
H	1.21786000	-1.85835400	1.62895700
H	0.93682200	-2.02602400	3.34734000
C	-0.41725100	-0.64969900	2.36077900
H	-1.05367700	-0.65196900	1.46614900
H	-1.10223200	-0.65168200	3.22224700
H	-0.93682200	2.02602400	3.34734000
H	-1.21786000	1.85835400	1.62895700
C	0.39345500	3.25676300	2.12444400
H	1.45613500	2.99878400	2.03039100
H	0.32263600	3.91915600	2.99687000
H	-0.32263600	-3.91915600	2.99687000
H	-0.71820600	-4.92924600	0.77345700
H	0.98948400	-4.54665700	1.00973400
H	0.71820600	4.92924600	0.77345700
H	-0.98948400	4.54665700	1.00973400

Compound **2d**: E(RB3LYP) = -968.35170567 a.u.

C	1.58272200	0.13305300	0.71181300
C	0.57544600	0.02790300	3.32813200
C	1.58774500	-1.10645000	1.41976900
C	1.31610700	1.34540900	1.41269900
C	0.82148100	1.26361000	2.72161400
C	1.09076900	-1.13052100	2.73087100
H	0.48929400	2.17552900	3.21392800
H	0.96268600	-2.09167800	3.22590900
C	1.58272200	0.13305300	-0.71181300
C	0.57544600	0.02790300	-3.32813200
C	1.58774500	-1.10645000	-1.41976900
C	1.31610700	1.34540900	-1.41269900
C	0.82148100	1.26361000	-2.72161400
C	1.09076900	-1.13052100	-2.73087100
H	0.48929400	2.17552900	-3.21392800
H	0.96268600	-2.09167800	-3.22590900
C	1.34148400	2.58486300	-0.68059900
H	1.26268500	3.51780500	-1.23371200
C	1.34148400	2.58486300	0.68059900
H	1.26268500	3.51780500	1.23371200
C	1.87774400	-2.30988500	-0.68086800
H	2.00185400	-3.23969200	-1.23105500
C	1.87774400	-2.30988500	0.68086800

H	2.00185400	-3.23969200	1.23105500
C	-0.45864500	-0.06640100	-4.42533300
C	-0.45864500	-0.06640100	4.42533300
C	-2.38480900	0.26491500	-2.61691200
H	-3.45887000	0.45177100	-2.75122600
C	-2.17502200	-0.47914100	-1.27911100
H	-2.77329800	-1.40299800	-1.29791500
H	-1.13118500	-0.80209300	-1.21251500
C	-2.38480900	0.26491500	2.61691200
H	-3.45887000	0.45177100	2.75122600
C	-1.84931500	-0.50506300	3.86054300
H	-1.91374200	1.25517300	2.56198700
C	-2.51343400	0.31520900	0.00000000
H	-3.57637700	0.60055800	0.00000000
H	-1.94098500	1.25410700	0.00000000
C	-2.17502200	-0.47914100	1.27911100
H	-2.77329800	-1.40299800	1.29791500
H	-1.13118500	-0.80209300	1.21251500
H	-1.79948400	-1.57502000	3.61783200
H	-1.91374200	1.25517300	-2.56198700
C	-1.84931500	-0.50506300	-3.86054300
H	-2.56855100	-0.41825100	-4.68528100
H	-1.79948400	-1.57502000	-3.61783200
H	-2.56855100	-0.41825100	4.68528100
H	-0.16258900	-0.78565500	5.20030300
H	-0.56404500	0.90839800	4.91807600
H	-0.56404500	0.90839800	-4.91807600
H	-0.16258900	-0.78565500	-5.20030300

Compound **2e**: E(RB3LYP) = -1007.67786298 a.u.

C	-0.13547300	0.69863500	-1.56175100
C	-0.65387300	3.36000700	-0.79971000
C	0.94099700	1.62684800	-1.45559200
C	-1.48223700	1.16561600	-1.48039700
C	-1.71273600	2.50028000	-1.11713200
C	0.65387300	2.94551200	-1.07374700
H	-2.73765800	2.83063500	-0.95700400
H	1.48003800	3.62876800	-0.88684100
C	0.13547300	-0.69863500	-1.56175100
C	0.65387300	-3.36000700	-0.79971000
C	1.48223700	-1.16561600	-1.48039700
C	-0.94099700	-1.62684800	-1.45559200
C	-0.65387300	-2.94551200	-1.07374700
C	1.71273600	-2.50028000	-1.11713200

H	-1.48003800	-3.62876800	-0.88684100
H	2.73765800	-2.83063500	-0.95700400
C	-2.28755300	-1.13344200	-1.57815900
H	-3.10339900	-1.85242400	-1.58798100
C	-2.54675800	0.20352500	-1.59699500
H	-3.57200700	0.56516500	-1.62233400
C	2.54675800	-0.20352500	-1.59699500
H	3.57200700	-0.56516500	-1.62233400
C	2.28755300	1.13344200	-1.57815900
H	3.10339900	1.85242400	-1.58798100
C	0.89433500	-4.60013200	0.03102400
C	-0.89433500	4.60013200	0.03102400
C	0.23524100	-3.24718200	2.20252300
H	0.00604300	-3.59474700	3.21851600
C	0.78107600	-1.80234800	2.27879800
H	1.54692900	-1.75160200	3.06733100
H	1.29850700	-1.56625100	1.34269800
C	-0.78107600	1.80234800	2.27879800
H	-1.54692900	1.75160200	3.06733100
C	-0.23524100	3.24718200	2.20252300
H	-1.29850700	1.56625100	1.34269800
C	-0.28530200	-0.71761100	2.51337500
H	-0.82297300	-0.90589900	3.45452400
H	-1.03470100	-0.79839600	1.71330400
C	0.28530200	0.71761100	2.51337500
H	0.82297300	0.90589900	3.45452400
H	1.03470100	0.79839600	1.71330400
H	0.72325700	3.24286600	1.66690900
H	-0.00604300	3.59474700	3.21851600
C	-1.20332500	4.25489800	1.52180600
H	-1.20972500	5.20228900	2.07599100
H	-0.72325700	-3.24286600	1.66690900
C	1.20332500	-4.25489800	1.52180600
H	1.20972500	-5.20228900	2.07599100
H	2.22750200	-3.86356300	1.58517100
H	-2.22750200	3.86356300	1.58517100
H	-0.00561300	5.24258500	-0.00778600
H	-1.73016100	5.19082500	-0.36676000
H	0.00561300	-5.24258500	-0.00778600
H	1.73016100	-5.19082500	-0.36676000

Compound **3a**: E(RB3LYP) = -922.10440831 a.u.

C	0.01345000	0.71717200	-1.63601500
C	0.05359000	2.70161100	0.25089500

C	1.25647100	1.35437200	-1.34371700
C	-1.20475500	1.39795600	-1.33865300
C	-1.16241300	2.42397800	-0.38409300
C	1.25826300	2.37072400	-0.37543700
H	-2.08883800	2.79780100	0.04391400
H	2.19417100	2.68744500	0.07649300
C	-0.01345000	-0.71717200	-1.63601500
C	-0.05359000	-2.70161100	0.25089500
C	1.20475500	-1.39795600	-1.33865300
C	-1.25647100	-1.35437200	-1.34371700
C	-1.25826300	-2.37072400	-0.37543700
C	1.16241300	-2.42397800	-0.38409300
H	-2.19417100	-2.68744500	0.07649300
H	2.08883800	-2.79780100	0.04391400
C	-2.47646100	-0.63254900	-1.65574200
H	-3.41589100	-1.17562300	-1.72210300
C	-2.45114500	0.72515200	-1.65385900
H	-3.36955700	1.30327300	-1.71896700
C	2.45114500	-0.72515200	-1.65385900
H	3.36955700	-1.30327300	-1.71896700
C	2.47646100	0.63254900	-1.65574200
H	3.41589100	1.17562300	-1.72210300
O	-0.07329400	-3.05653700	1.58869700
O	0.07329400	3.05653700	1.58869700
C	0.42367600	-1.96387400	2.42831100
H	1.45511500	-1.74115200	2.13022200
H	0.45175400	-2.40349400	3.42843300
C	-0.42367600	-0.65267700	2.41743600
H	-1.05416400	-0.64704800	1.52284200
H	-1.10901900	-0.66045200	3.27483500
C	0.42367600	0.65267700	2.41743600
H	1.05416400	0.64704800	1.52284200
H	1.10901900	0.66045200	3.27483500
C	-0.42367600	1.96387400	2.42831100
H	-0.45175400	2.40349400	3.42843300
H	-1.45511500	1.74115200	2.13022200

Compound **3b**: E(RB3LYP) = -961.44975577 a.u.

C	0.00347300	-0.02786000	2.91206300
H	0.07173600	2.12371800	2.93402800
C	0.50425500	1.21679900	2.51997800
C	1.48064800	-1.17228300	1.38906800
C	1.33137100	1.28939900	1.39022200
C	0.63984200	-1.20351600	2.51042500

C	1.65261400	0.07382100	0.71490700
C	1.52591300	2.53462500	0.67959500
H	0.29662100	-2.15288100	2.91173000
C	1.52591300	2.53462500	-0.67959500
H	1.51768600	3.46834300	1.23652100
H	1.51768600	3.46834300	-1.23652100
C	1.33137100	1.28939900	-1.39022200
C	0.50425500	1.21679900	-2.51997800
C	1.65261400	0.07382100	-0.71490700
C	0.00347300	-0.02786000	-2.91206300
H	0.07173600	2.12371800	-2.93402800
C	0.63984200	-1.20351600	-2.51042500
H	0.29662100	-2.15288100	-2.91173000
C	1.48064800	-1.17228300	-1.38906800
C	1.82330100	-2.38535200	0.67945900
H	1.92700700	-3.31274400	1.23728200
C	1.82330100	-2.38535200	-0.67945900
H	1.92700700	-3.31274400	-1.23728200
O	-1.22633200	-0.12530200	-3.53070200
O	-1.22633200	-0.12530200	3.53070200
C	-2.31831600	0.25384300	-2.64197800
H	-3.19986500	0.09256000	-3.26720300
H	-2.24970900	1.32978300	-2.43370600
C	-2.46307100	-0.54045800	-1.30322800
H	-1.85951600	-1.45333400	-1.36480900
H	-3.50724100	-0.87707200	-1.23892100
C	-2.31831600	0.25384300	2.64197800
H	-2.24970900	1.32978300	2.43370600
H	-3.19986500	0.09256000	3.26720300
C	-2.46307100	-0.54045800	1.30322800
H	-3.50724100	-0.87707200	1.23892100
H	-1.85951600	-1.45333400	1.36480900
C	-2.12715600	0.23435500	0.00000000
H	-2.69827100	1.17509400	0.00000000
H	-1.07127800	0.51866500	0.00000000

Compound **3c**:

E(RB3LYP) = -1000.79019555 a.u.

C	0.00125700	0.71265200	-1.62089100
C	-0.00125700	3.11937900	-0.26176700
C	1.23628500	1.40226500	-1.42563200
C	-1.23256800	1.40662600	-1.43897700
C	-1.21157900	2.63202100	-0.75824900
C	1.21361400	2.62918100	-0.74718100
H	-2.13794400	3.09483200	-0.42992400

H	2.14371800	3.09028100	-0.42578500
C	-0.00125700	-0.71265200	-1.62089100
C	0.00125700	-3.11937900	-0.26176700
C	1.23256800	-1.40662600	-1.43897700
C	-1.23628500	-1.40226500	-1.42563200
C	-1.21361400	-2.62918100	-0.74718100
C	1.21157900	-2.63202100	-0.75824900
H	-2.14371800	-3.09028100	-0.42578500
H	2.13794400	-3.09483200	-0.42992400
C	-2.46494600	-0.67763000	-1.64287900
H	-3.40073400	-1.23038100	-1.67334200
C	-2.46293700	0.68284700	-1.65090000
H	-3.39695400	1.23805900	-1.68813400
C	2.46293700	-0.68284700	-1.65090000
H	3.39695400	-1.23805900	-1.68813400
C	2.46494600	0.67763000	-1.64287900
H	3.40073400	1.23038100	-1.67334200
O	0.03312100	-3.95651900	0.83375700
O	-0.03312100	3.95651900	0.83375700
C	-0.36574200	-3.27037800	2.05763400
H	-1.44658400	-3.07818000	2.01952400
C	0.42574000	0.64587100	2.28172700
H	1.02626500	0.66433100	1.36434500
C	-0.40170600	1.95436500	2.38692600
H	1.14327400	0.61391600	3.11518400
C	0.40170600	-1.95436500	2.38692600
H	1.27859900	-1.89102700	1.73345300
H	0.79828300	-2.03573400	3.40757500
C	-0.42574000	-0.64587100	2.28172700
H	-1.02626500	-0.66433100	1.36434500
H	-1.14327400	-0.61391600	3.11518400
H	-0.79828300	2.03573400	3.40757500
H	-1.27859900	1.89102700	1.73345300
C	0.36574200	3.27037800	2.05763400
H	1.44658400	3.07818000	2.01952400
H	0.18876500	4.02472900	2.82817400
H	-0.18876500	-4.02472900	2.82817400

Compound **3d**: E(RB3LYP) = -1040.12647949 a.u.

C	-1.60410600	-0.05118400	0.71243800
C	-0.48860200	-0.01783500	3.25553900
C	-1.50051900	1.18694900	1.41675500
C	-1.41102000	-1.28173000	1.41046200
C	-0.85445700	-1.24206500	2.69518200

C	-0.95176100	1.18165900	2.70876000
H	-0.54953500	-2.15810800	3.19280200
H	-0.72721100	2.11962400	3.20947200
C	-1.60410600	-0.05118400	-0.71243800
C	-0.48860200	-0.01783500	-3.25553900
C	-1.50051900	1.18694900	-1.41675500
C	-1.41102000	-1.28173000	-1.41046200
C	-0.85445700	-1.24206500	-2.69518200
C	-0.95176100	1.18165900	-2.70876000
H	-0.54953500	-2.15810800	-3.19280200
H	-0.72721100	2.11962400	-3.20947200
C	-1.54533000	-2.51662400	-0.68015700
H	-1.54107800	-3.45216900	-1.23401400
C	-1.54533000	-2.51662400	0.68015700
H	-1.54107800	-3.45216900	1.23401400
C	-1.71702000	2.40741500	-0.68092000
H	-1.77533100	3.34339100	-1.23120900
C	-1.71702000	2.40741500	0.68092000
H	-1.77533100	3.34339100	1.23120900
O	0.43494300	-0.02296600	-4.27884000
O	0.43494300	-0.02296600	4.27884000
C	2.35463900	-0.34196200	-2.61984400
H	3.42832300	-0.48557100	-2.80455900
C	2.17036000	0.39868300	-1.27521100
H	2.76013700	1.32728600	-1.30557800
H	1.12776600	0.71262600	-1.18013600
C	2.35463900	-0.34196200	2.61984400
H	3.42832300	-0.48557100	2.80455900
C	1.76614600	0.38448800	3.85894600
H	1.92133800	-1.34842200	2.56799500
C	2.53902700	-0.39143800	0.00000000
H	3.60910900	-0.64663500	0.00000000
H	1.99264300	-1.34527700	0.00000000
C	2.17036000	0.39868300	1.27521100
H	2.76013700	1.32728600	1.30557800
H	1.12776600	0.71262600	1.18013600
H	1.77399600	1.47158400	3.69494800
H	1.92133800	-1.34842200	-2.56799500
C	1.76614600	0.38448800	-3.85894600
H	2.37412100	0.17699400	-4.74333700
H	1.77399600	1.47158400	-3.69494800
H	2.37412100	0.17699400	4.74333700

Compound **3e**: E(RB3LYP) = -1079.45472186 a.u.

C	-0.01867300	-0.71157100	-1.57434000
C	-0.08776800	-3.36444100	-0.71518500
C	-1.27241000	-1.38456100	-1.45995600
C	1.19700600	-1.45509400	-1.47249200
C	1.13977300	-2.79469300	-1.06092200
C	-1.28422700	-2.71825600	-1.02861500
H	2.05699800	-3.34740900	-0.87619200
H	-2.22253800	-3.22020200	-0.81097100
C	0.01867300	0.71157100	-1.57434000
C	0.08776800	3.36444100	-0.71518500
C	-1.19700600	1.45509400	-1.47249200
C	1.27241000	1.38456100	-1.45995600
C	1.28422700	2.71825600	-1.02861500
C	-1.13977300	2.79469300	-1.06092200
H	2.22253800	3.22020200	-0.81097100
H	-2.05699800	3.34740900	-0.87619200
C	2.48018300	0.61299800	-1.59804000
H	3.43161400	1.13890900	-1.61673300
C	2.44392300	-0.74811300	-1.60808600
H	3.36623200	-1.32336500	-1.63549400
C	-2.44392300	0.74811300	-1.60808600
H	-3.36623200	1.32336500	-1.63549400
C	-2.48018300	-0.61299800	-1.59804000
H	-3.43161400	-1.13890900	-1.61673300
O	0.14834700	4.52981700	0.01759000
O	-0.14834700	-4.52981700	0.01759000
C	0.39815200	3.23098500	2.18140300
H	0.60519600	3.58972200	3.19842400
C	-0.41847900	1.91739600	2.26232700
H	-1.18637500	2.02128300	3.04297200
H	-0.96274800	1.77112800	1.32441700
C	0.41847900	-1.91739600	2.26232700
H	1.18637500	-2.02128300	3.04297200
C	-0.39815200	-3.23098500	2.18140300
H	0.96274800	-1.77112800	1.32441700
C	0.41847900	0.64976600	2.51706600
H	0.97227200	0.73864700	3.46310100
H	1.17726000	0.58014600	1.72497800
C	-0.41847900	-0.64976600	2.51706600
H	-0.97227200	-0.73864700	3.46310100
H	-1.17726000	-0.58014600	1.72497800
H	-1.37871300	-3.04185500	1.72758900
H	-0.60519600	-3.58972200	3.19842400
C	0.27654700	-4.38332700	1.39796300

H	0.02132000	-5.35092900	1.83778700
H	1.37871300	3.04185500	1.72758900
C	-0.27654700	4.38332700	1.39796300
H	-0.02132000	5.35092900	1.83778700
H	-1.37049800	4.27827600	1.43266500
H	1.37049800	-4.27827600	1.43266500

Compound **7a**: E(RB3LYP) = -3003.55455908 a.u.

C	-1.30418600	4.45010300	1.29259900
C	-2.29440200	3.41921000	-1.13115700
C	-0.67046200	4.75909200	0.05605600
C	-2.28241900	3.44971700	1.27707300
C	-2.59102700	2.78363300	0.08175300
C	-1.33335300	4.43839000	-1.16604800
H	-2.60365200	3.01920600	2.22278400
H	-2.62923900	2.98084800	-2.06730000
C	0.76511600	4.76658400	0.03679200
C	2.68399300	2.79454400	-0.03847700
C	1.42882200	4.41758100	1.25086600
C	1.40164900	4.49350000	-1.20665900
C	2.38133600	3.49346100	-1.21640200
C	2.38981400	3.39995000	1.19041600
H	2.69819900	3.08402100	-2.17287200
H	2.72141800	2.93522500	2.11506700
C	-0.59422800	4.76111500	2.52215200
H	-1.14408700	4.83215300	3.45739600
C	0.76169700	4.73426400	2.50235000
H	1.34067500	4.78325700	3.42128200
C	-0.66756900	4.78940400	-2.40887100
H	-1.24645000	4.85557300	-3.32679900
C	0.68819800	4.82843700	-2.42804800
H	1.23674800	4.92535100	-3.36172200
C	2.96903700	1.32824000	-0.15915700
C	3.58612900	-1.33765300	-0.77990300
C	4.26222000	0.83123000	0.07974200
C	1.91315800	0.46761700	-0.59902300
C	2.27758200	-0.84354000	-1.00681000
C	4.56355400	-0.51937300	-0.18018900
C	-2.91294700	1.32339300	0.17223900
C	-3.62136600	-1.32545000	0.76880900
C	-1.89055000	0.42889700	0.62239800
C	-4.21540500	0.86575000	-0.09414700
C	-4.56187200	-0.47650400	0.15341100
C	-2.30225500	-0.87205100	1.02002200

C	-0.38288200	0.79802400	0.71113300
H	-0.25293100	1.74257900	1.24423900
H	0.10354800	0.03620500	1.31926300
C	0.41805900	0.88730600	-0.65620500
H	0.32506200	1.90212500	-1.04474600
H	-0.08460000	0.23757300	-1.37226600
C	5.32724300	1.77026600	0.56675800
C	7.30426800	3.55772800	1.47168300
C	5.65977700	1.84275400	1.92651800
C	6.00225500	2.60781500	-0.33201600
C	6.98331300	3.49326500	0.11492900
C	6.63893100	2.72947600	2.37657200
H	5.14560400	1.19923400	2.63537600
H	5.75416700	2.56346600	-1.38907000
H	7.49631400	4.13374600	-0.59790900
H	6.88207800	2.77179000	3.43522700
H	8.06754600	4.24798300	1.82109600
C	5.94474200	-1.04256000	0.08646500
C	8.54070000	-2.00434900	0.59435000
C	6.29575300	-1.52407100	1.35514300
C	6.91610300	-1.05091900	-0.92360800
C	8.20312900	-1.52716700	-0.67293400
C	7.58187100	-2.00209400	1.60835300
H	5.55225000	-1.52607100	2.14810900
H	6.65836800	-0.68273500	-1.91275400
H	8.94265600	-1.52516300	-1.46958700
H	7.83419000	-2.37221100	2.59886400
H	9.54326600	-2.37549600	0.79007800
C	3.97308500	-2.72236900	-1.21580400
C	4.74047700	-5.30382700	-2.03596100
C	4.13137400	-3.75460500	-0.28063700
C	4.20913200	-3.00477900	-2.56871600
C	4.58987400	-4.28321900	-2.97614800
C	4.50911700	-5.03507500	-0.68620000
H	3.95485800	-3.55050800	0.77175600
H	4.08697000	-2.21627100	-3.30612300
H	4.76857600	-4.48157600	-4.02989000
H	4.62500900	-5.82224400	0.05452500
H	5.03673200	-6.30042400	-2.35269100
C	1.33238500	-1.69559800	-1.80581600
C	-0.32073200	-3.30225200	-3.43313300
C	0.93916100	-1.26826200	-3.08620000
C	0.88565500	-2.94684700	-1.36316600
C	0.06779500	-3.74234100	-2.16756900
C	0.11942200	-2.05900600	-3.89080000
H	1.28964100	-0.30685200	-3.45345900

H	1.18618100	-3.30140800	-0.38420600
H	-0.26068400	-4.71301500	-1.80426400
H	-0.16819700	-1.70632200	-4.87804100
H	-0.95434900	-3.92444900	-4.05975300
C	-5.24538400	1.83880400	-0.59029000
C	-7.15583100	3.68986600	-1.51030800
C	-5.53426600	1.95122000	-1.95728400
C	-5.93044600	2.66848700	0.30806700
C	-6.87841300	3.58561500	-0.14645400
C	-6.48040800	2.86940900	-2.41484600
H	-5.01174300	1.31410800	-2.66592500
H	-5.71600500	2.59341100	1.37072900
H	-7.39961200	4.21973200	0.56612500
H	-6.68995100	2.94236600	-3.47901000
H	-7.89325600	4.40482200	-1.86551900
C	-5.95303400	-0.95583800	-0.14188300
C	-8.56723700	-1.83397000	-0.70479000
C	-6.93455600	-0.97172500	0.85830800
C	-6.30336600	-1.38684900	-1.42882800
C	-7.59841900	-1.82381300	-1.70918400
C	-8.23071900	-1.40609400	0.58025200
H	-6.67763100	-0.64232800	1.86120200
H	-5.55218400	-1.38233700	-2.21447900
H	-7.84994700	-2.15550400	-2.71341000
H	-8.97809200	-1.41034100	1.36953500
H	-9.57680300	-2.17295000	-0.92175100
C	-4.05819800	-2.69880100	1.19276900
C	-4.91879000	-5.25852600	1.98831800
C	-4.30760300	-2.98456900	2.54268700
C	-4.25105900	-3.71646800	0.24806000
C	-4.67459800	-4.98632100	0.64149800
C	-4.73465800	-4.25211200	2.93783800
H	-4.15893300	-2.20766300	3.28748300
H	-4.06541300	-3.50906100	-0.80208500
H	-4.81648900	-5.76234900	-0.10641600
H	-4.92299200	-4.45319400	3.98938200
H	-5.25082000	-6.24677500	2.29558100
C	-1.39824600	-1.75314100	1.83537000
C	0.18501400	-3.40369300	3.48896500
C	-1.00090900	-1.33011700	3.11587100
C	-0.99252000	-3.02365500	1.40689800
C	-0.20837500	-3.84020700	2.22342400
C	-0.21596700	-2.14268000	3.93348800
H	-1.31877000	-0.35350200	3.47241100
H	-1.29876800	-3.37556200	0.42882400
H	0.08985200	-4.82407600	1.86973400

H	0.07580000	-1.79217400	4.92028500
H	0.79219000	-4.04214600	4.12532400

Compound **7b**: E(RB3LYP) = -3042.91074870 a.u.

C	-1.59877700	-3.93394600	-0.64779300
C	-2.50432700	-2.94382300	1.82855800
C	-0.85162100	-4.16718900	0.54284800
C	-2.68389000	-3.05831900	-0.57355900
C	-3.00240200	-2.41733400	0.63319300
C	-1.42090700	-3.83708100	1.80802000
H	-3.14117600	-2.70857600	-1.49536600
H	-2.81436500	-2.51784400	2.78005300
C	0.56927700	-4.25799000	0.44204400
C	2.85934600	-2.71811200	0.26351000
C	1.16380100	-4.05706200	-0.84034100
C	1.34827100	-4.05500300	1.61591900
C	2.51890200	-3.29232400	1.49478000
C	2.31365800	-3.26308400	-0.90695400
H	3.00739000	-2.93783900	2.39988200
H	2.65222400	-2.90463200	-1.87526900
C	-0.99337900	-4.26607500	-1.91980600
H	-1.62030800	-4.31485600	-2.80671500
C	0.36001300	-4.31621100	-2.01567400
H	0.85059900	-4.40491600	-2.98189000
C	-0.64298000	-4.11330200	2.99485500
H	-1.13166900	-4.08158000	3.96574000
C	0.70869100	-4.23369900	2.90097400
H	1.32475600	-4.29730600	3.79468000
C	3.48211100	-1.35657900	0.24616900
C	4.64476800	1.19905000	0.32935200
C	4.76512000	-1.14894400	-0.29837500
C	2.71554500	-0.27205600	0.76903300
C	3.35992200	0.98554500	0.87976900
C	5.33647300	0.14072100	-0.29776300
C	-3.57919300	-1.03992000	0.49413100
C	-4.54205000	1.45107000	-0.36641400
C	-2.67039500	0.06140700	0.44465600
C	-4.94325200	-0.88099000	0.18988700
C	-5.44035300	0.37650800	-0.21495200
C	-3.17083300	1.29078000	-0.04116800
C	-1.25454900	-0.00131000	1.07662100
H	-1.12479800	0.95084800	1.60645200
H	-1.28748900	-0.77032400	1.85309700
C	1.26463900	-0.40589900	1.28369100
H	1.12896900	-1.36855200	1.77708900

C	5.49864200	-2.31248100	-0.89567200
C	6.84862000	-4.51263500	-2.02224100
C	5.75220300	-2.37061500	-2.27427500
C	5.93231600	-3.37762900	-0.09246700
C	6.60475800	-4.46597000	-0.64877600
C	6.41840100	-3.46112400	-2.83331500
H	5.42909600	-1.55099800	-2.90965900
H	5.74238000	-3.34963100	0.97686000
H	6.93635600	-5.27877900	-0.00773300
H	6.60340500	-3.48718900	-3.90413200
H	7.37020700	-5.36121900	-2.45699000
C	6.67957500	0.37733600	-0.92033700
C	9.19559100	0.82560400	-2.10405500
C	6.80571300	1.19613200	-2.05234100
C	7.83756400	-0.21212100	-0.39205800
C	9.08426100	0.01156900	-0.97570700
C	8.05072500	1.41596200	-2.64145600
H	5.91965500	1.66477600	-2.47121700
H	7.75812200	-0.85311800	0.48123000
H	9.96936800	-0.45278400	-0.54844400
H	8.12572000	2.05184700	-3.51990100
H	10.16658600	0.99858800	-2.56067800
C	5.29033800	2.54874700	0.44212000
C	6.50678200	5.08079200	0.64765300
C	4.77047900	3.65400900	-0.24679300
C	6.43150700	2.73572500	1.23558200
C	7.03309800	3.98936300	1.34044000
C	5.37356300	4.90798300	-0.14822300
H	3.88717000	3.52646800	-0.86630700
H	6.85042800	1.88958100	1.77249600
H	7.91527400	4.11250900	1.96345900
H	4.95604200	5.75084000	-0.69323300
H	6.97626800	6.05780800	0.72705600
C	2.77924400	2.06187900	1.75714300
C	1.79927200	4.02387700	3.52526100
C	3.27345000	2.16652200	3.06825600
C	1.78202800	2.95547300	1.34932000
C	1.29964400	3.92980700	2.22654700
C	2.78932900	3.13514400	3.94596500
H	4.04727200	1.47806700	3.39719100
H	1.37936200	2.89693800	0.34248900
H	0.52839600	4.61288800	1.88694700
H	3.18789900	3.19602900	4.95553700
H	1.41999900	4.78354500	4.20393600
C	-5.84775800	-2.07314400	0.27590600
C	-7.51328200	-4.33812400	0.44700400

C	-6.08290800	-2.70194500	1.50759900
C	-6.46421100	-2.59986500	-0.86879500
C	-7.28651100	-3.72305100	-0.78536600
C	-6.91024100	-3.82154700	1.59469100
H	-5.61742800	-2.30290000	2.40475000
H	-6.29762000	-2.12369200	-1.83063100
H	-7.75123200	-4.11747500	-1.68532800
H	-7.08229500	-4.29072400	2.56001600
H	-8.15578100	-5.21221500	0.51241700
C	-6.90345700	0.55180400	-0.49181000
C	-9.65793000	0.86693900	-0.98742900
C	-7.37461300	0.81795500	-1.78586300
C	-7.83809700	0.44445800	0.54872000
C	-9.20209100	0.60389100	0.30523800
C	-8.73865800	0.97173700	-2.03254100
H	-6.66533000	0.90792800	-2.60342600
H	-7.49039300	0.23231900	1.55587100
H	-9.90893600	0.51954600	1.12671000
H	-9.08279400	1.17518500	-3.04335900
H	-10.72079700	0.98868200	-1.17903300
C	-5.05565900	2.77938600	-0.84394100
C	-6.03723000	5.26386000	-1.73587200
C	-4.73895000	3.25946400	-2.12288600
C	-5.87558300	3.56523500	-0.02127800
C	-6.36035500	4.79705900	-0.46093100
C	-5.22589300	4.48905500	-2.56631000
H	-4.10390600	2.66483000	-2.77341600
H	-6.13762000	3.20375200	0.96916700
H	-6.99328700	5.39094400	0.19351700
H	-4.96968800	4.84188800	-3.56207000
H	-6.41567500	6.22277400	-2.08010500
C	-2.26713700	2.46895800	-0.25901600
C	-0.75913200	4.77054900	-0.86838400
C	-1.39011000	2.48643900	-1.35474600
C	-2.35846500	3.61897800	0.53829600
C	-1.61686000	4.76057800	0.23382100
C	-0.64194400	3.62560800	-1.65834700
H	-1.32197500	1.60897600	-1.99203200
H	-3.03985900	3.62736900	1.38383200
H	-1.71994800	5.64907200	0.85171800
H	0.01854000	3.62296300	-2.52182900
H	-0.19023800	5.66413200	-1.11106600
H	1.13288300	0.34982100	2.06286100
C	0.07254300	-0.23264700	0.27360300
H	0.26114400	0.62242300	-0.38316400
H	-0.00609900	-1.11901800	-0.36491600

Compound **7c**: $E(\text{RB3LYP}) = -3082.26442946 \text{ a.u.}$

C	-1.43510500	-1.19890200	-3.54495600
C	0.78443900	-2.77860600	-2.84447900
C	-0.11014900	-0.70380900	-3.72429400
C	-1.59999200	-2.41834400	-2.87305400
C	-0.49137200	-3.10799200	-2.36837100
C	1.00147200	-1.57590700	-3.52895600
H	-2.60055300	-2.71874700	-2.56950000
H	1.64146700	-3.36366900	-2.52101500
C	0.11014900	0.70380900	-3.72429400
C	0.49137200	3.10799200	-2.36837100
C	-1.00147200	1.57590700	-3.52895600
C	1.43510500	1.19890200	-3.54495600
C	1.59999200	2.41834400	-2.87305400
C	-0.78443900	2.77860600	-2.84447900
H	2.60055300	2.71874700	-2.56950000
H	-1.64146700	3.36366900	-2.52101500
C	-2.53905400	-0.29288300	-3.75361000
H	-3.54845000	-0.69584800	-3.78850400
C	-2.32911500	1.05139700	-3.74144700
H	-3.16707400	1.74382600	-3.76607200
C	2.32911500	-1.05139700	-3.74144700
H	3.16707400	-1.74382600	-3.76607200
C	2.53905400	0.29288300	-3.75361000
H	3.54845000	0.69584800	-3.78850400
C	0.59989300	3.92724800	-1.11667300
C	0.58304400	5.37315800	1.29428500
C	0.43440600	5.32440800	-1.13861100
C	0.75675500	3.22247800	0.11071300
C	0.73800100	3.96733400	1.31120500
C	0.43307200	6.05671700	0.06929700
C	-0.59989300	-3.92724800	-1.11667300
C	-0.58304400	-5.37315800	1.29428500
C	-0.75675500	-3.22247800	0.11071300
C	-0.43440600	-5.32440800	-1.13861100
C	-0.43307200	-6.05671700	0.06929700
C	-0.73800100	-3.96733400	1.31120500
C	-1.01517200	-1.70650200	0.16938600
C	1.01517200	1.70650200	0.16938600
C	0.23659100	6.01274200	-2.45550400
C	-0.14483500	7.27345600	-4.94506800
C	-0.97843800	6.64324800	-2.76295200
C	1.25579000	6.02446500	-3.41924000
C	1.06953600	6.65162600	-4.65126300
C	-1.16878400	7.26574600	-3.99640800

H	-1.77712000	6.64815100	-2.02683100
H	2.20344700	5.54174000	-3.19706200
H	1.87420800	6.65292200	-5.38205000
H	-2.11879500	7.74638500	-4.21543600
H	-0.29216300	7.76033700	-5.90547800
C	0.27900400	7.54797600	0.04564900
C	-0.00911000	10.34912300	-0.01163200
C	-0.85622200	8.16489000	0.59164700
C	1.26689200	8.36059100	-0.52985500
C	1.12671700	9.74797100	-0.55620000
C	-1.00111000	9.55173000	0.56139900
H	-1.62999800	7.55142400	1.04414900
H	2.15007300	7.89899300	-0.96223200
H	1.90570200	10.35908800	-1.00486900
H	-1.89020500	10.00916200	0.98785800
H	-0.12041400	11.43003000	-0.03363900
C	0.61796000	6.14434300	2.58156400
C	0.69666400	7.59766100	4.99240700
C	-0.43307200	6.05951200	3.50589700
C	1.70867500	6.97128500	2.88666600
C	1.75017800	7.68953100	4.08151000
C	-0.39641400	6.78100400	4.69917700
H	-1.28588800	5.42359500	3.28604800
H	2.52824700	7.05319300	2.17828000
H	2.60603100	8.32337700	4.29907300
H	-1.22315300	6.70332000	5.40070600
H	0.72678000	8.15866400	5.92278900
C	0.93462700	3.27256300	2.62926500
C	1.32237500	1.97889500	5.10100800
C	2.18699500	3.29112500	3.26144200
C	-0.11902800	2.59409000	3.25819200
C	0.07138200	1.95213200	4.48299800
C	2.38045500	2.65013100	4.48519500
H	3.01242400	3.81618000	2.78861100
H	-1.09778300	2.57663700	2.78652100
H	-0.75818200	1.42808800	4.94983600
H	3.35822900	2.67844300	4.95927800
H	1.47141400	1.48415800	6.05737700
C	-0.23659100	-6.01274200	-2.45550400
C	0.14483500	-7.27345600	-4.94506800
C	0.97843800	-6.64324800	-2.76295200
C	-1.25579000	-6.02446500	-3.41924000
C	-1.06953600	-6.65162600	-4.65126300
C	1.16878400	-7.26574600	-3.99640800
H	1.77712000	-6.64815100	-2.02683100
H	-2.20344700	-5.54174000	-3.19706200

H	-1.87420800	-6.65292200	-5.38205000
H	2.11879500	-7.74638500	-4.21543600
H	0.29216300	-7.76033700	-5.90547800
C	-0.27900400	-7.54797600	0.04564900
C	0.00911000	-10.34912300	-0.01163200
C	-1.26689200	-8.36059100	-0.52985500
C	0.85622200	-8.16489000	0.59164700
C	1.00111000	-9.55173000	0.56139900
C	-1.12671700	-9.74797100	-0.55620000
H	-2.15007300	-7.89899300	-0.96223200
H	1.62999800	-7.55142400	1.04414900
H	1.89020500	-10.00916200	0.98785800
H	-1.90570200	-10.35908800	-1.00486900
H	0.12041400	-11.43003000	-0.03363900
C	-0.61796000	-6.14434300	2.58156400
C	-0.69666400	-7.59766100	4.99240700
C	-1.70867500	-6.97128500	2.88666600
C	0.43307200	-6.05951200	3.50589700
C	0.39641400	-6.78100400	4.69917700
C	-1.75017800	-7.68953100	4.08151000
H	-2.52824700	-7.05319300	2.17828000
H	1.28588800	-5.42359500	3.28604800
H	1.22315300	-6.70332000	5.40070600
H	-2.60603100	-8.32337700	4.29907300
H	-0.72678000	-8.15866400	5.92278900
C	-0.93462700	-3.27256300	2.62926500
C	-1.32237500	-1.97889500	5.10100800
C	-2.18699500	-3.29112500	3.26144200
C	0.11902800	-2.59409000	3.25819200
C	-0.07138200	-1.95213200	4.48299800
C	-2.38045500	-2.65013100	4.48519500
H	-3.01242400	-3.81618000	2.78861100
H	1.09778300	-2.57663700	2.78652100
H	0.75818200	-1.42808800	4.94983600
H	-3.35822900	-2.67844300	4.95927800
H	-1.47141400	-1.48415800	6.05737700
H	1.65436600	1.42402600	-0.66991000
H	1.59657600	1.50339400	1.07395200
C	-0.20808200	0.74662700	0.17035000
H	-0.83520700	0.94795900	-0.70543000
H	-1.59657600	-1.50339400	1.07395200
C	0.20808200	-0.74662700	0.17035000
H	0.83520700	-0.94795900	-0.70543000
H	0.82794500	-0.94797000	1.05345900
H	-1.65436600	-1.42402600	-0.66991000
H	-0.82794500	0.94797000	1.05345900

Compound **7d**: $E(\text{RB3LYP}) = -3121.59761365 \text{ a.u.}$

C	-2.77482400	1.88778100	1.41516700
C	-2.43983800	-0.58793200	2.70668600
C	-3.01365300	0.67070200	0.71162700
C	-2.24912900	1.81643200	2.71412700
C	-1.94329400	0.58195800	3.29738800
C	-2.97541600	-0.57080300	1.41319300
H	-1.93285400	2.73450700	3.20444700
H	-2.26425300	-1.54406700	3.19264300
C	-3.01365300	0.67070200	-0.71162700
C	-1.94329400	0.58195800	-3.29738800
C	-2.77482400	1.88778100	-1.41516700
C	-2.97541600	-0.57080300	-1.41319300
C	-2.43983800	-0.58793200	-2.70668600
C	-2.24912900	1.81643200	-2.71412700
H	-2.26425300	-1.54406700	-3.19264300
H	-1.93285400	2.73450700	-3.20444700
C	-2.84228300	3.12584100	0.68105100
H	-2.79094100	4.06187400	1.23222400
C	-2.84228300	3.12584100	-0.68105100
H	-2.79094100	4.06187400	-1.23222400
C	-3.23959900	-1.78334300	0.68029500
H	-3.33831900	-2.71391000	1.23394800
C	-3.23959900	-1.78334300	-0.68029500
H	-3.33831900	-2.71391000	-1.23394800
C	-0.87896300	0.44570500	-4.34593100
C	1.18548600	-0.10304200	-6.17547400
C	-1.19370600	0.04355700	-5.65706300
C	0.47188900	0.59574400	-3.92859000
C	1.49523500	0.29345200	-4.85319000
C	-0.15979800	-0.21701200	-6.58503700
C	-0.87896300	0.44570500	4.34593100
C	1.18548600	-0.10304200	6.17547400
C	0.47188900	0.59574400	3.92859000
C	-1.19370600	0.04355700	5.65706300
C	-0.15979800	-0.21701200	6.58503700
C	1.49523500	0.29345200	4.85319000
C	-2.63243800	-0.12308100	-6.04265200
C	-5.34634200	-0.43857000	-6.72730200
C	-3.50365400	0.97637000	-6.05465400
C	-3.14660000	-1.38395000	-6.38024100
C	-4.49086100	-1.54158900	-6.71639700
C	-4.84714700	0.82207400	-6.39670900
H	-3.12184300	1.96063900	-5.79805200
H	-2.48536200	-2.24561100	-6.38122900

H	-4.86939000	-2.52795200	-6.97187400
H	-5.50396000	1.68817300	-6.40356800
H	-6.39339100	-0.56045800	-6.99178900
C	-0.49565400	-0.60868700	-7.99295900
C	-1.13777600	-1.33327500	-10.63788700
C	-1.14366300	0.29435400	-8.84878700
C	-0.17634300	-1.88217300	-8.48670400
C	-0.49613100	-2.24264500	-9.79556300
C	-1.45939500	-0.06214500	-10.15971200
H	-1.40354300	1.28281600	-8.48056500
H	0.32932900	-2.59318700	-7.83975700
H	-0.24173300	-3.23557100	-10.15747300
H	-1.95911900	0.65422200	-10.80675600
H	-1.38536200	-1.61316800	-11.65848400
C	2.29249500	-0.36657600	-7.15418100
C	4.36827000	-0.84701700	-8.99549100
C	2.51315200	0.50400300	-8.23135300
C	3.13095800	-1.48199300	-7.01595200
C	4.15766000	-1.72255900	-7.92915600
C	3.54229500	0.26837100	-9.14270200
H	1.86855800	1.36942800	-8.35628500
H	2.97591600	-2.16481600	-6.18552300
H	4.79430500	-2.59493300	-7.80551500
H	3.69694500	0.95655400	-9.96977900
H	5.16929300	-1.03286100	-9.70617400
C	2.93456200	0.41912500	-4.44216600
C	5.63031000	0.65643800	-3.66003200
C	3.53137100	-0.54540200	-3.61670800
C	3.71348300	1.50444100	-4.86944500
C	5.04804800	1.62367900	-4.48123000
C	4.86736600	-0.42981300	-3.22965400
H	2.94357100	-1.39672200	-3.28363200
H	3.26749600	2.25808900	-5.51236400
H	5.63401900	2.47298600	-4.82299100
H	5.31153200	-1.19060400	-2.59276100
H	6.67058900	0.74815600	-3.35923000
C	-2.63243800	-0.12308100	6.04265200
C	-5.34634200	-0.43857000	6.72730200
C	-3.14660000	-1.38395000	6.38024100
C	-3.50365400	0.97637000	6.05465400
C	-4.84714700	0.82207400	6.39670900
C	-4.49086100	-1.54158900	6.71639700
H	-2.48536200	-2.24561100	6.38122900
H	-3.12184300	1.96063900	5.79805200
H	-5.50396000	1.68817300	6.40356800
H	-4.86939000	-2.52795200	6.97187400

H	-6.39339100	-0.56045800	6.99178900
C	-0.49565400	-0.60868700	7.99295900
C	-1.13777600	-1.33327500	10.63788700
C	-1.14366300	0.29435400	8.84878700
C	-0.17634300	-1.88217300	8.48670400
C	-0.49613100	-2.24264500	9.79556300
C	-1.45939500	-0.06214500	10.15971200
H	-1.40354300	1.28281600	8.48056500
H	0.32932900	-2.59318700	7.83975700
H	-0.24173300	-3.23557100	10.15747300
H	-1.95911900	0.65422200	10.80675600
H	-1.38536200	-1.61316800	11.65848400
C	2.29249500	-0.36657600	7.15418100
C	4.36827000	-0.84701700	8.99549100
C	2.51315200	0.50400300	8.23135300
C	3.13095800	-1.48199300	7.01595200
C	4.15766000	-1.72255900	7.92915600
C	3.54229500	0.26837100	9.14270200
H	1.86855800	1.36942800	8.35628500
H	2.97591600	-2.16481600	6.18552300
H	4.79430500	-2.59493300	7.80551500
H	3.69694500	0.95655400	9.96977900
H	5.16929300	-1.03286100	9.70617400
C	2.93456200	0.41912500	4.44216600
C	5.63031000	0.65643800	3.66003200
C	3.71348300	1.50444100	4.86944500
C	3.53137100	-0.54540200	3.61670800
C	4.86736600	-0.42981300	3.22965400
C	5.04804800	1.62367900	4.48123000
H	3.26749600	2.25808900	5.51236400
H	2.94357100	-1.39672200	3.28363200
H	5.31153200	-1.19060400	2.59276100
H	5.63401900	2.47298600	4.82299100
H	6.67058900	0.74815600	3.35923000
C	0.83684800	1.15672000	2.54721500
H	1.84421500	1.57819400	2.60935900
C	0.78809400	0.21888700	1.30990500
H	-0.17391600	-0.30177300	1.27362500
C	0.83684800	1.15672000	-2.54721500
H	1.84421500	1.57819400	-2.60935900
C	0.78809400	0.21888700	-1.30990500
H	-0.17391600	-0.30177300	-1.27362500
C	0.98816200	1.01361500	0.00000000
H	1.99008700	1.46807100	0.00000000
H	0.27668200	1.85190500	0.00000000
H	0.17361500	2.00066900	-2.33822600

H	1.56064400	-0.55568500	1.40348200
H	1.56064400	-0.55568500	-1.40348200
H	0.17361500	2.00066900	2.33822600

Compound **7e**: E(RB3LYP) = -3160.92635404 a.u.

C	-1.12565600	-1.50765600	-2.30882900
C	1.40759100	-2.66838400	-1.91526800
C	0.05238100	-0.70944700	-2.41396000
C	-0.99803400	-2.84277400	-1.89948700
C	0.25385000	-3.39050800	-1.58865300
C	1.33501200	-1.32572700	-2.31558200
H	-1.89556900	-3.42287200	-1.70142300
H	2.38446200	-3.11167700	-1.73549200
C	-0.05238100	0.70944700	-2.41396000
C	-0.25385000	3.39050800	-1.58865300
C	-1.33501200	1.32572700	-2.31558200
C	1.12565600	1.50765600	-2.30882900
C	0.99803400	2.84277400	-1.89948700
C	-1.40759100	2.66838400	-1.91526800
H	1.89556900	3.42287200	-1.70142300
H	-2.38446200	3.11167700	-1.73549200
C	-2.40557300	-0.86117200	-2.43686600
H	-3.29979600	-1.47943000	-2.45222700
C	-2.50577800	0.49770100	-2.44309300
H	-3.48155100	0.97729700	-2.46320600
C	2.50577800	-0.49770100	-2.44309300
H	3.48155100	-0.97729700	-2.46320600
C	2.40557300	0.86117200	-2.43686600
H	3.29979600	1.47943000	-2.45222700
C	-0.31917300	4.60796400	-0.71323200
C	-0.22311100	6.81609600	1.02766000
C	-0.00191200	5.88454900	-1.21689600
C	-0.59804400	4.41535400	0.66570800
C	-0.52063200	5.52722600	1.53040700
C	0.03090100	6.99926500	-0.34827000
C	0.31917300	-4.60796400	-0.71323200
C	0.22311100	-6.81609600	1.02766000
C	0.59804400	-4.41535400	0.66570800
C	0.00191200	-5.88454900	-1.21689600
C	-0.03090100	-6.99926500	-0.34827000
C	0.52063200	-5.52722600	1.53040700
C	0.31917300	6.04011800	-2.67301000
C	0.93287200	6.30643800	-5.40913900
C	-0.64984000	5.78758700	-3.65522000

C	1.60220300	6.42765300	-3.08764600
C	1.90778800	6.55690900	-4.44216700
C	-0.34823100	5.92283600	-5.01056700
H	-1.64904300	5.48702400	-3.35270700
H	2.36347600	6.63267000	-2.34070800
H	2.90899800	6.85575800	-4.74173300
H	-1.11549500	5.72656500	-5.75510100
H	1.16972500	6.40940300	-6.46482900
C	0.32880900	8.36498700	-0.88992500
C	0.88353600	10.92720300	-1.92005000
C	-0.54733400	8.98105000	-1.79549500
C	1.48939600	9.05625200	-0.51144300
C	1.76610700	10.32398400	-1.02248700
C	-0.27543800	10.25086400	-2.30374900
H	-1.44747900	8.45757300	-2.10489900
H	2.17793100	8.59554000	0.19079400
H	2.67231400	10.84094800	-0.71740100
H	-0.96984900	10.71081900	-3.00217200
H	1.09752500	11.91592300	-2.31745500
C	-0.22139900	7.99531400	1.95565900
C	-0.24945200	10.21070700	3.69452400
C	-1.22442800	8.97157100	1.86046000
C	0.76563200	8.14810900	2.93984200
C	0.75455800	9.24701600	3.79940800
C	-1.24025300	10.06811000	2.72199200
H	-1.99499100	8.87016500	1.10150800
H	1.54741900	7.39958100	3.03175700
H	1.53149500	9.34814200	4.55288500
H	-2.02722100	10.81253500	2.63164800
H	-0.25973800	11.06571800	4.36543800
C	-0.78539200	5.35007900	2.99763200
C	-1.27808000	4.99829500	5.74813700
C	0.17504500	4.75636100	3.82996700
C	-1.99618100	5.76789800	3.56918900
C	-2.24177600	5.59177400	4.93087600
C	-0.06721900	4.58233700	5.19336500
H	1.12156000	4.43534700	3.40326300
H	-2.74832400	6.23498600	2.93965400
H	-3.18735500	5.92071800	5.35412600
H	0.69170800	4.12261000	5.82135400
H	-1.46879900	4.86334600	6.80953700
C	-0.31917300	-6.04011800	-2.67301000
C	-0.93287200	-6.30643800	-5.40913900
C	0.64984000	-5.78758700	-3.65522000
C	-1.60220300	-6.42765300	-3.08764600
C	-1.90778800	-6.55690900	-4.44216700

C	0.34823100	-5.92283600	-5.01056700
H	1.64904300	-5.48702400	-3.35270700
H	-2.36347600	-6.63267000	-2.34070800
H	-2.90899800	-6.85575800	-4.74173300
H	1.11549500	-5.72656500	-5.75510100
H	-1.16972500	-6.40940300	-6.46482900
C	-0.32880900	-8.36498700	-0.88992500
C	-0.88353600	-10.92720300	-1.92005000
C	-1.48939600	-9.05625200	-0.51144300
C	0.54733400	-8.98105000	-1.79549500
C	0.27543800	-10.25086400	-2.30374900
C	-1.76610700	-10.32398400	-1.02248700
H	-2.17793100	-8.59554000	0.19079400
H	1.44747900	-8.45757300	-2.10489900
H	0.96984900	-10.71081900	-3.00217200
H	-2.67231400	-10.84094800	-0.71740100
H	-1.09752500	-11.91592300	-2.31745500
C	0.22139900	-7.99531400	1.95565900
C	0.24945200	-10.21070700	3.69452400
C	-0.76563200	-8.14810900	2.93984200
C	1.22442800	-8.97157100	1.86046000
C	1.24025300	-10.06811000	2.72199200
C	-0.75455800	-9.24701600	3.79940800
H	-1.54741900	-7.39958100	3.03175700
H	1.99499100	-8.87016500	1.10150800
H	2.02722100	-10.81253500	2.63164800
H	-1.53149500	-9.34814200	4.55288500
H	0.25973800	-11.06571800	4.36543800
C	0.78539200	-5.35007900	2.99763200
C	1.27808000	-4.99829500	5.74813700
C	-0.17504500	-4.75636100	3.82996700
C	1.99618100	-5.76789800	3.56918900
C	2.24177600	-5.59177400	4.93087600
C	0.06721900	-4.58233700	5.19336500
H	-1.12156000	-4.43534700	3.40326300
H	2.74832400	-6.23498600	2.93965400
H	3.18735500	-5.92071800	5.35412600
H	-0.69170800	-4.12261000	5.82135400
H	1.46879900	-4.86334600	6.80953700
C	-0.05706300	-1.97926600	1.42725300
H	-0.65222500	-2.24045300	2.31225900
C	0.52936700	-0.55972800	1.58159600
H	1.21958600	-0.38040000	0.74540400
C	-1.04037100	3.05172700	1.20610500
H	-1.57256100	3.20515900	2.14892700
C	0.05706300	1.97926600	1.42725300

H	0.74785500	1.98116800	0.57805300
C	-0.52936700	0.55972800	1.58159600
H	-1.13735500	0.50412200	2.49648700
H	-1.21958600	0.38040000	0.74540400
H	-1.77570600	2.63186200	0.51378300
H	1.13735500	-0.50412200	2.49648700
H	0.65222500	2.24045300	2.31225900
H	-0.74785500	-1.98116800	0.57805300
C	1.04037100	-3.05172700	1.20610500
H	1.57256100	-3.20515900	2.14892700
H	1.77570600	-2.63186200	0.51378300

Compound **13a**: E(RB3LYP) = -3803.64284607 a.u.

C	-1.69339800	4.28725500	1.12028100
C	-2.05234400	2.83854000	-1.25286900
C	-1.55627500	4.90820400	-0.12365000
C	-2.04720000	2.93686700	1.15542900
C	-2.24497900	2.20129200	-0.02162700
C	-1.70127500	4.19172100	-1.31530000
H	-2.16566500	2.44096100	2.11544200
H	-2.17233800	2.27377000	-2.17298000
C	1.55628600	4.90820300	0.12365300
C	2.24498500	2.20129000	0.02163200
C	1.70128500	4.19172000	1.31530500
C	1.69340800	4.28725300	-1.12027700
C	2.04720700	2.93686400	-1.15542400
C	2.05235200	2.83853900	1.25287400
H	2.16567100	2.44095700	-2.11543600
H	2.17234500	2.27376900	2.17298500
C	2.70605100	0.77883700	-0.10900200
C	3.73346200	-1.75802200	-0.76667800
C	4.05418400	0.47088900	0.16822900
C	1.83767900	-0.20544100	-0.63516700
C	2.37591400	-1.45455700	-1.02307400
C	4.56146000	-0.81068400	-0.13025400
C	-2.70604900	0.77884000	0.10900800
C	-3.73346600	-1.75801700	0.76667900
C	-1.83768000	-0.20543900	0.63517500
C	-4.05418100	0.47089500	-0.16822800
C	-4.56146000	-0.81067600	0.13025300
C	-2.37591800	-1.45455500	1.02307900
C	-0.33549600	0.04983300	0.70630300
H	-0.12377900	1.00371400	1.19825600
H	0.13643700	-0.72730800	1.30816100

C	0.33549600	0.04983500	-0.70629400
H	0.12378100	1.00371800	-1.19824300
H	-0.13643900	-0.72730300	-1.30815400
C	4.96942400	1.52559000	0.72177700
C	6.67876700	3.51534200	1.74388200
C	5.16524800	1.66296800	2.10286900
C	5.64693500	2.39999800	-0.13873700
C	6.49395600	3.38686400	0.36656600
C	6.01164100	2.64904900	2.61128500
H	4.64844300	0.99084000	2.78297400
H	5.50508100	2.30532300	-1.21186600
H	7.01080600	4.05511000	-0.31754700
H	6.15114300	2.73829500	3.68573500
H	7.33925100	4.28316700	2.13819200
C	6.00073700	-1.13118800	0.15162500
C	8.70023600	-1.73369500	0.67642100
C	6.42174700	-1.47183400	1.44453000
C	6.95592000	-1.09616200	-0.87365300
C	8.29408100	-1.39320800	-0.61463300
C	7.75881000	-1.77272100	1.70582400
H	5.69300700	-1.50576700	2.25001400
H	6.64487300	-0.83703100	-1.88186300
H	9.01932000	-1.35983900	-1.42363900
H	8.06437200	-2.03738600	2.71495200
H	9.74228400	-1.96706400	0.87874300
C	4.31022700	-3.07787800	-1.18884400
C	5.40487400	-5.54662200	-1.98546200
C	4.64181700	-4.05545200	-0.24001200
C	4.53799100	-3.35845600	-2.54380500
C	5.08169800	-4.58035600	-2.93944500
C	5.18161600	-5.28008000	-0.63385600
H	4.47377000	-3.85302500	0.81398300
H	4.28169100	-2.61356100	-3.29193000
H	5.25133700	-4.77749500	-3.99491400
H	5.42969400	-6.02550900	0.11746500
H	5.82712000	-6.49973900	-2.29301600
C	1.54119800	-2.44583700	-1.78031800
C	0.05223200	-4.30334400	-3.28907100
C	1.10986600	-2.13942600	-3.08194200
C	1.21035300	-3.69953900	-1.24922800
C	0.47380100	-4.61968500	-1.99679400
C	0.37194900	-3.05673300	-3.82984900
H	1.36329900	-1.17253600	-3.50963700
H	1.53294300	-3.95514100	-0.24562100
H	0.23260300	-5.58927700	-1.56818100
H	0.05217900	-2.79886000	-4.83629800

H	-0.51807100	-5.02289600	-3.87070900
C	-4.96941700	1.52559900	-0.72177900
C	-6.67875000	3.51535500	-1.74389100
C	-5.16523300	1.66297800	-2.10287200
C	-5.64693000	2.40000700	0.13873200
C	-6.49394700	3.38687500	-0.36657400
C	-6.01162100	2.64906100	-2.61129100
H	-4.64842500	0.99085000	-2.78297500
H	-5.50508100	2.30533100	1.21186200
H	-7.01079800	4.05512200	0.31753700
H	-6.15111800	2.73831000	-3.68574200
H	-7.33923100	4.28318200	-2.13820400
C	-6.00073700	-1.13117800	-0.15163100
C	-8.70023500	-1.73368000	-0.67643800
C	-6.95592400	-1.09615100	0.87364300
C	-6.42174200	-1.47182300	-1.44453800
C	-7.75880500	-1.77270700	-1.70583700
C	-8.29408500	-1.39319400	0.61461700
H	-6.64488000	-0.83702000	1.88185300
H	-5.69300000	-1.50575600	-2.25002000
H	-8.06436400	-2.03737100	-2.71496700
H	-9.01932600	-1.35982400	1.42362100
H	-9.74228300	-1.96704600	-0.87876400
C	-4.31023600	-3.07787200	1.18884300
C	-5.40489000	-5.54661400	1.98545500
C	-4.53800400	-3.35845100	2.54380200
C	-4.64182500	-4.05544400	0.24000900
C	-5.18162700	-5.28007100	0.63385000
C	-5.08171500	-4.58035000	2.93944000
H	-4.28170400	-2.61355600	3.29192900
H	-4.47377400	-3.85301700	-0.81398600
H	-5.42970500	-6.02550000	-0.11747200
H	-5.25135700	-4.77748900	3.99490800
H	-5.82713900	-6.49973000	2.29300800
C	-1.54120700	-2.44583800	1.78032600
C	-0.05225300	-4.30335100	3.28908400
C	-1.10988300	-2.13943000	3.08195200
C	-1.21036300	-3.69953900	1.24923500
C	-0.47381700	-4.61968800	1.99680300
C	-0.37197100	-3.05674000	3.82986200
H	-1.36331600	-1.17254100	3.50964900
H	-1.53294800	-3.95513900	0.24562600
H	-0.23261800	-5.58928000	1.56819000
H	-0.05220600	-2.79886900	4.83631300
H	0.51804500	-5.02290500	3.87072300
H	-1.29662900	5.96405300	-0.16658300

H	1.29664100	5.96405200	0.16658700
C	-1.44995400	5.06030200	2.39720000
H	-2.33487300	5.03739700	3.04386700
H	-1.24012000	6.11352800	2.18197300
C	1.44535800	4.87325800	2.63727400
H	1.46202800	5.96225800	2.52252400
H	2.21502200	4.61140200	3.37156500
S	-0.12201000	4.40542000	3.50839300
C	-1.44534700	4.87325700	-2.63727000
H	-1.46201700	5.96225800	-2.52252100
H	-2.21501200	4.61140200	-3.37156100
C	1.44996400	5.06030000	-2.39719700
H	2.33488400	5.03739300	-3.04386400
H	1.24013200	6.11352500	-2.18197100
S	0.12201900	4.40541800	-3.50838900

Compound **13b**: E(RB3LYP) = -3842.95657475 a.u.

C	1.43423700	-4.43777900	1.44559300
C	1.85055100	-2.96800100	-0.89759500
C	1.12581200	-4.98501300	0.19881600
C	2.05159100	-3.18466100	1.49064800
C	2.25155900	-2.42141900	0.33181900
C	1.32122400	-4.25989700	-0.98091100
H	2.35493000	-2.78079600	2.45274100
H	1.97674800	-2.38749800	-1.80606500
C	-1.97810400	-4.69341800	0.43855700
C	-2.66029000	-1.98860900	0.26861000
C	-2.08314000	-3.93961400	1.61189900
C	-2.14501900	-4.11093600	-0.81895000
C	-2.50068500	-2.76250900	-0.88712000
C	-2.42894700	-2.58490500	1.51558400
H	-2.63576700	-2.29409900	-1.85844100
H	-2.51703100	-1.98884600	2.42045800
C	-3.06727800	-0.55148200	0.08504700
C	-3.86660200	2.05333400	-0.62672200
C	-4.43836600	-0.23094900	0.01656600
C	-2.08446400	0.43310200	-0.16388900
C	-2.49200400	1.73077900	-0.54337100
C	-4.84158300	1.07747500	-0.32723500
C	2.90396600	-1.07041300	0.42007800
C	4.23326400	1.41557900	0.61886000
C	2.37098800	-0.05352000	1.25268100
C	4.09509900	-0.83572500	-0.31209500
C	4.74135800	0.41580100	-0.23719200

C	3.07363600	1.16775900	1.37998100
C	1.07097800	-0.23755000	2.02938300
H	1.22931600	0.09682200	3.06053500
C	-0.61956400	0.09688900	0.07127500
H	0.02297200	0.59561600	-0.65837600
C	-5.46843400	-1.29463500	0.26280400
C	-7.39953700	-3.29282700	0.71784100
C	-5.75151000	-1.73687800	1.56271200
C	-6.16915800	-1.87197700	-0.80532300
C	-7.12454700	-2.86347100	-0.58144100
C	-6.71019600	-2.72475200	1.79010700
H	-5.22015700	-1.29610600	2.40206400
H	-5.96388900	-1.53728600	-1.81829000
H	-7.65653500	-3.29846100	-1.42369300
H	-6.91883100	-3.04972100	2.80635000
H	-8.14625800	-4.06277800	0.89350500
C	-6.30201200	1.40951200	-0.41363500
C	-9.04769800	2.01453100	-0.57655800
C	-7.09639200	1.45952800	0.74089300
C	-6.90856000	1.66756900	-1.65149500
C	-8.26868300	1.96508800	-1.73368800
C	-8.45588100	1.76179100	0.66185500
H	-6.64316700	1.25862100	1.70751200
H	-6.30682900	1.63684300	-2.55536500
H	-8.71934600	2.15970500	-2.70355300
H	-9.05290800	1.79780900	1.56955500
H	-10.10727400	2.24822300	-0.63944100
C	-4.29525100	3.43476500	-1.02704400
C	-5.09848400	6.02849000	-1.77429400
C	-4.91450300	4.28910700	-0.10314400
C	-4.08767000	3.90274300	-2.33263100
C	-4.48695500	5.18648900	-2.70441100
C	-5.31002400	5.57503700	-0.47132800
H	-5.08905300	3.93976800	0.91055900
H	-3.60700400	3.25505100	-3.06035900
H	-4.31827100	5.52887900	-3.72223100
H	-5.78637300	6.22189900	0.26098500
H	-5.40831400	7.02954400	-2.06265000
C	-1.47150800	2.78000200	-0.87712900
C	0.39083300	4.78270800	-1.56373000
C	-0.68560100	2.66781200	-2.03502100
C	-1.30240100	3.91281300	-0.06736900
C	-0.38443300	4.90696800	-0.40878900
C	0.23854700	3.65665400	-2.37525200
H	-0.81167200	1.80153500	-2.67958800
H	-1.90584600	4.02012900	0.82887300

H	-0.27890300	5.78293300	0.22626200
H	0.83150800	3.55138600	-3.28016300
H	1.10055500	5.56052000	-1.83315200
C	4.70471600	-1.92385100	-1.14821600
C	5.86202700	-3.96798900	-2.70305000
C	4.74734900	-1.82609700	-2.54661500
C	5.25802500	-3.06176100	-0.54289100
C	5.83312900	-4.07367400	-1.31134800
C	5.31634700	-2.83974500	-3.31804800
H	4.33182400	-0.94739100	-3.03144500
H	5.23017600	-3.15423900	0.53932100
H	6.25860500	-4.94597900	-0.82161600
H	5.33664000	-2.74486100	-4.40073500
H	6.30895800	-4.75640200	-3.30302400
C	5.99720400	0.67475100	-1.01720800
C	8.35401800	1.17483600	-2.47516900
C	7.20272600	0.04798000	-0.67043500
C	5.99440300	1.55810600	-2.10606900
C	7.16064900	1.80500900	-2.83068000
C	8.37083400	0.29591000	-1.39105900
H	7.22211300	-0.64149700	0.16876900
H	5.06953300	2.05522400	-2.38492400
H	7.13607200	2.49195100	-3.67282300
H	9.29518100	-0.19921600	-1.10458100
H	9.26372100	1.36764400	-3.03779300
C	4.96073500	2.72160500	0.75805600
C	6.33068200	5.16677800	1.01801500
C	6.11077400	2.81797900	1.55323500
C	4.50825600	3.87109600	0.09497800
C	5.18773100	5.08300100	0.22169400
C	6.78948600	4.02974000	1.68438800
H	6.47529900	1.93546200	2.07170800
H	3.61739300	3.81281300	-0.52504700
H	4.82229600	5.96303900	-0.30165900
H	7.67871200	4.08416700	2.30720800
H	6.85981500	6.11081500	1.11855500
C	2.66032600	2.17214400	2.42081400
C	1.96005000	4.01990000	4.42934500
C	3.08212400	1.98962700	3.74719000
C	1.88539300	3.29907000	2.11846300
C	1.53781500	4.21407500	3.11392500
C	2.73567800	2.90273900	4.74352400
H	3.68973200	1.12289000	3.99545000
H	1.55162200	3.46363000	1.09912400
H	0.93513600	5.08151400	2.85680300
H	3.07462300	2.74200400	5.76379700

H	1.68946800	4.73380500	5.20293500
H	0.70230600	-5.98572900	0.14530200
H	-1.73233900	-5.75072200	0.50756600
C	1.05827200	-5.15247700	2.72170500
H	1.91511300	-5.23798000	3.39974600
H	0.70231700	-6.16836600	2.52053900
C	-1.82518700	-4.60403000	2.94403500
H	-1.94800100	-5.68906500	2.86093400
H	-2.53882700	-4.25585200	3.69869600
S	-0.19696100	-4.27577400	3.77245400
C	0.97643700	-4.88522500	-2.31253600
H	0.90974800	-5.97421600	-2.21587400
H	1.75958300	-4.67370100	-3.04850700
C	-1.91996500	-4.90854500	-2.08154800
H	-2.79718200	-4.86206500	-2.73678300
H	-1.74288900	-5.96568000	-1.85610200
S	-0.55451100	-4.29617500	-3.17119300
H	0.80948800	-1.29255800	2.08869400
H	-0.46905300	-0.97657100	-0.06185100
C	-0.17871200	0.50155300	1.49768400
H	-0.99190000	0.26909300	2.19765800
H	-0.04123700	1.58619700	1.54319200

Compound **13c**: $E(\text{RB3LYP}) = -3882.26929970 \text{ a.u.}$

C	1.70665700	-4.10648300	1.45918000
C	2.48499100	-2.71873800	-0.83851900
C	1.58131300	-4.69086800	0.19698500
C	2.29996500	-2.84373900	1.55963600
C	2.69332000	-2.13214600	0.41963200
C	1.94478600	-4.00199800	-0.96387300
H	2.44684900	-2.40521000	2.54311000
H	2.76349900	-2.16907200	-1.73278500
C	-1.52528800	-4.67772400	-0.25930800
C	-2.63764500	-2.11284600	-0.41184300
C	-1.89033100	-4.02098100	0.91956000
C	-1.64775700	-4.05849000	-1.50501200
C	-2.23795600	-2.79216300	-1.56999900
C	-2.43291100	-2.73547400	0.82903400
H	-2.38219000	-2.32356300	-2.54043700
H	-2.71713100	-2.21435600	1.73840600
C	-3.30173200	-0.76726900	-0.49837400
C	-4.62580500	1.72377000	-0.62913600
C	-4.63863000	-0.64464100	-0.04631100
C	-2.62224300	0.35783400	-1.02600400

C	-3.30233000	1.59653100	-1.09767000
C	-5.29696700	0.60153300	-0.09999500
C	3.34099000	-0.78065100	0.53016300
C	4.60808800	1.73604200	0.66488600
C	2.63958300	0.32293100	1.07579100
C	4.66862200	-0.62723400	0.06757700
C	5.30187400	0.63309200	0.12756200
C	3.28800000	1.57750100	1.14052600
C	1.22496500	0.17756800	1.63444100
H	0.94575100	1.11790000	2.11380700
C	-1.18363300	0.28152200	-1.52683100
H	-1.10060200	0.90243900	-2.42406700
C	-5.37842400	-1.84460400	0.47061800
C	-6.77612200	-4.09470100	1.42881700
C	-5.73647400	-1.94566100	1.82275600
C	-5.73851900	-2.88887100	-0.39357900
C	-6.43266200	-4.00256900	0.07898900
C	-6.42494100	-3.06147600	2.29929100
H	-5.47363600	-1.14191100	2.50459300
H	-5.46777400	-2.82662300	-1.44391700
H	-6.70464200	-4.79926400	-0.60882200
H	-6.69081600	-3.12050000	3.35165700
H	-7.31603600	-4.96245500	1.79866700
C	-6.71753700	0.73308700	0.36505200
C	-9.38392200	0.99179300	1.23267000
C	-7.02657300	1.44119300	1.53514600
C	-7.76868600	0.15840400	-0.36375700
C	-9.08991400	0.28758700	0.06394200
C	-8.34672700	1.56777400	1.96761300
H	-6.22408500	1.89557800	2.10940500
H	-7.54657300	-0.39648800	-1.27091500
H	-9.89016900	-0.16411800	-0.51675100
H	-8.56419300	2.11911300	2.87885600
H	-10.41312400	1.09147900	1.56742300
C	-5.34373700	3.03712400	-0.74936300
C	-6.69817100	5.49397400	-0.98931300
C	-5.10814400	4.07831300	0.15890300
C	-6.27067300	3.24795900	-1.77957900
C	-6.94093000	4.46538100	-1.90072100
C	-5.77968900	5.29568700	0.04246700
H	-4.39584900	3.93024400	0.96616900
H	-6.46745600	2.44968800	-2.48996500
H	-7.65457800	4.60895200	-2.70799700
H	-5.58407000	6.08941000	0.75902300
H	-7.22103900	6.44225300	-1.08200500
C	-2.65120400	2.78250500	-1.75552200

C	-1.47758000	5.00070900	-3.03890000
C	-2.76300900	2.95479200	-3.14365700
C	-1.94378000	3.74497200	-1.02197300
C	-1.36309700	4.84433700	-1.65714300
C	-2.18074000	4.05080100	-3.78120100
H	-3.31478500	2.22073900	-3.72533000
H	-1.85252600	3.63582500	0.05502700
H	-0.82554500	5.58447700	-1.06952500
H	-2.28056600	4.16371000	-4.85769000
H	-1.02612700	5.85718800	-3.53255400
C	5.42511500	-1.80800300	-0.46872000
C	6.85153400	-4.02470500	-1.46175100
C	5.77757200	-1.88689500	-1.82387400
C	5.80496800	-2.85757200	0.38051100
C	6.51353200	-3.95471100	-0.10927900
C	6.48026400	-2.98615200	-2.31756800
H	5.49964100	-1.07862200	-2.49428000
H	5.53878800	-2.81225300	1.43289700
H	6.80071600	-4.75580500	0.56714500
H	6.74164400	-3.02813200	-3.37187400
H	7.40259600	-4.87950200	-1.84509100
C	6.71186100	0.79907100	-0.35759300
C	9.35708200	1.12065500	-1.26858000
C	7.78499500	0.21816700	0.33344300
C	6.98824500	1.54479000	-1.51256100
C	8.29775700	1.70261200	-1.96638000
C	9.09568900	0.37878800	-0.11551100
H	7.58869000	-0.36655500	1.22770900
H	6.16862900	2.00510000	-2.05704900
H	8.48959300	2.28308100	-2.86519700
H	9.91325300	-0.07813700	0.43628600
H	10.37806100	1.24463800	-1.61999000
C	5.29216900	3.06746100	0.77838100
C	6.58579500	5.55828400	1.00429900
C	6.28611700	3.27534700	1.74529000
C	4.95829800	4.12947800	-0.07350800
C	5.60003600	5.36340100	0.03581800
C	6.92621700	4.50932800	1.85963000
H	6.55970600	2.46104200	2.41042900
H	4.19095400	3.98522900	-0.82900500
H	5.32813800	6.17304800	-0.63666300
H	7.69293800	4.64998700	2.61724700
H	7.08516500	6.51969700	1.09135400
C	2.61027000	2.75794500	1.78143700
C	1.36788200	4.96242900	3.02047600
C	2.82943600	3.03866700	3.13797800

C	1.75951300	3.60335600	1.05510800
C	1.14444300	4.69586100	1.66888600
C	2.21357800	4.12893900	3.75365200
H	3.48895700	2.39421800	3.71307700
H	1.57640800	3.40340800	0.00325400
H	0.49266700	5.34275800	1.08705100
H	2.39710200	4.32752500	4.80648700
H	0.88888100	5.81330700	3.49769300
H	1.17528400	-5.69597800	0.11541800
H	-1.12135200	-5.68558300	-0.20508800
C	1.17301300	-4.80728400	2.68321100
H	1.87257200	-4.72725700	3.52248100
H	1.01222300	-5.87406800	2.49429800
C	-1.72467600	-4.71057300	2.25470400
H	-1.58052600	-5.78768800	2.11763700
H	-2.62706900	-4.58260100	2.86226200
S	-0.39103200	-4.09748100	3.38873900
C	1.77799300	-4.65315100	-2.31794300
H	1.62759900	-5.73288500	-2.21178800
H	2.68229900	-4.51301500	-2.91992200
C	-1.11608300	-4.72526800	-2.74861600
H	-1.81596600	-4.61995800	-3.58480100
H	-0.95754300	-5.79734600	-2.59016800
S	0.44935500	-3.99923700	-3.43345900
H	1.22893900	-0.57020700	2.43502500
H	-0.93993500	-0.73631100	-1.83498700
C	-0.09571000	0.74140100	-0.52688200
H	-0.32537200	1.74757800	-0.15886100
H	0.84593800	0.82497600	-1.08672400
C	0.10274100	-0.21606900	0.64984900
H	0.27827400	-1.22409900	0.26546400
H	-0.82350200	-0.27344900	1.23500500

Compound **13d**: E(RB3LYP) = -3921.57857190 a.u.

C	-1.95175700	-3.66141700	-1.15978300
C	-2.76413700	-2.34153200	1.17541800
C	-1.71179300	-4.21951300	0.09738100
C	-2.66938700	-2.46443100	-1.22956700
C	-3.10142500	-1.80086300	-0.07369800
C	-2.07073300	-3.55481400	1.27360100
H	-2.89969800	-2.03486200	-2.20195900
H	-3.07091800	-1.82473700	2.08086900
C	1.45578900	-4.27206100	0.18243700
C	2.97367800	-1.92850500	0.42205800

C	1.81667400	-3.57176400	-0.97169700
C	1.76546600	-3.78693900	1.45384500
C	2.57832700	-2.65158200	1.55655600
C	2.53711300	-2.38200200	-0.83394300
H	2.90925100	-2.33095000	2.54063600
H	2.80838700	-1.82138500	-1.72292400
C	3.88968700	-0.73785600	0.50739700
C	5.64064100	1.48250000	0.50410200
C	5.11790400	-0.79302400	-0.20129300
C	3.55423300	0.42013700	1.25330500
C	4.44094600	1.52274600	1.24271600
C	5.98794100	0.31730900	-0.21069900
C	-3.93379400	-0.55734000	-0.21627300
C	-5.55105800	1.71604900	-0.62214900
C	-3.35310100	0.63491500	-0.70561700
C	-5.30942300	-0.60515900	0.09782500
C	-6.11978200	0.53437100	-0.09997900
C	-4.17061400	1.76604400	-0.91215800
C	-1.85177000	0.71408100	-0.93028400
H	-1.62448000	1.43460500	-1.72150800
C	2.30413200	0.49553900	2.12421800
H	2.59637700	0.93241000	3.08561700
C	5.53365600	-2.04772400	-0.91490800
C	6.33820800	-4.40387900	-2.23402400
C	5.65030800	-2.08537600	-2.31210800
C	5.83361500	-3.21095600	-0.19075000
C	6.23386800	-4.37753400	-0.84234700
C	6.04378800	-3.25256900	-2.96690000
H	5.43144500	-1.19123300	-2.88868900
H	5.74647800	-3.19983300	0.89220400
H	6.46415800	-5.26684500	-0.26105400
H	6.12564200	-3.25981400	-4.05082400
H	6.64903300	-5.31247800	-2.74304400
C	7.29704200	0.25614200	-0.94226100
C	9.75886700	0.15133200	-2.30567400
C	7.50968800	1.01735500	-2.10043500
C	8.34093700	-0.55718700	-0.47824100
C	9.56124200	-0.60845300	-1.15162000
C	8.72770000	0.96431500	-2.77835900
H	6.71298000	1.65606700	-2.47100200
H	8.19115100	-1.15748400	0.41465300
H	10.35781200	-1.24456300	-0.77416800
H	8.87057500	1.56079900	-3.67579100
H	10.70890600	0.11045400	-2.83198700
C	6.58220500	2.65175300	0.53172800
C	8.36107400	4.83309900	0.58282400

C	6.34421000	3.79026900	-0.25055800
C	7.72708500	2.62489300	1.33998900
C	8.60859700	3.70563200	1.36727100
C	7.22574000	4.87129900	-0.22775300
H	5.46315600	3.82565100	-0.88563900
H	7.92790700	1.74744600	1.94843000
H	9.49044000	3.66523900	2.00152700
H	7.02447500	5.74376000	-0.84421000
H	9.04819200	5.67494700	0.60232200
C	4.15744200	2.73496600	2.08707000
C	3.68101200	5.00171900	3.69190300
C	4.59587300	2.77913900	3.41893200
C	3.48006800	3.84968500	1.57364000
C	3.24397900	4.97360100	2.36703600
C	4.35851400	3.89975900	4.21585800
H	5.13059900	1.92653200	3.82984000
H	3.13897700	3.83625000	0.54201600
H	2.71910500	5.82801600	1.94746700
H	4.70727800	3.91242900	5.24530100
H	3.49773000	5.87640100	4.31029900
C	-5.91109300	-1.86329600	0.65300900
C	-7.03238500	-4.21996500	1.71126900
C	-6.31850900	-1.92585900	1.99350900
C	-6.07709400	-3.00215800	-0.14816200
C	-6.63454400	-4.16926200	0.37437000
C	-6.87141300	-3.09353600	2.51962500
H	-6.20287300	-1.04991100	2.62563400
H	-5.76429700	-2.97175500	-1.18806800
H	-6.75775600	-5.04000400	-0.26472300
H	-7.17967900	-3.12119000	3.56168300
H	-7.46609800	-5.12919700	2.11936200
C	-7.58338500	0.48548400	0.22539900
C	-10.33032800	0.39608800	0.84082900
C	-8.46514000	-0.29594500	-0.53527900
C	-8.10356400	1.22218700	1.29944100
C	-9.46326500	1.17637900	1.60709100
C	-9.82613500	-0.33901700	-0.23314900
H	-8.07896500	-0.87537900	-1.36912000
H	-7.43523100	1.83591300	1.89686900
H	-9.84515800	1.75317800	2.44562100
H	-10.49252200	-0.94930500	-0.83740500
H	-11.39035900	0.36157000	1.07836100
C	-6.42084500	2.90565100	-0.90618200
C	-8.05625500	5.12899800	-1.46403900
C	-7.31177400	2.88831900	-1.98888000
C	-6.36501300	4.05622800	-0.10736100

C	-7.17623400	5.15764600	-0.38128900
C	-8.12052800	3.98992400	-2.26787400
H	-7.37056700	2.00199600	-2.61442800
H	-5.68162900	4.08626000	0.73651200
H	-7.11921400	6.03907700	0.25234900
H	-8.80275600	3.95665300	-3.11349900
H	-8.68736100	5.98727100	-1.67928600
C	-3.58071200	3.01766700	-1.49938100
C	-2.47402600	5.34716000	-2.63323700
C	-3.62710700	3.23514100	-2.88433100
C	-2.97292700	3.99062800	-0.69288200
C	-2.42392600	5.14510000	-1.25348600
C	-3.07862900	4.38793700	-3.44732900
H	-4.09831000	2.49225500	-3.52229300
H	-2.93592600	3.84343800	0.38307500
H	-1.95910300	5.88759400	-0.60977700
H	-3.12516200	4.53651400	-4.52310900
H	-2.04733200	6.24589000	-3.07071800
H	-1.22502700	-5.18806700	0.16524900
H	0.91896300	-5.21125000	0.08741400
C	-1.43351200	-4.31735100	-2.41537500
H	-2.19705300	-4.31613000	-3.20052100
H	-1.15253700	-5.36082900	-2.23735600
C	1.48364900	-4.13177100	-2.33472800
H	1.37256600	-5.22044000	-2.28439700
H	2.29943300	-3.92520700	-3.03508700
S	0.00241900	-3.46080100	-3.22437100
C	-1.73357400	-4.16592200	2.61358700
H	-1.65275900	-5.25531000	2.53356700
H	-2.52452200	-3.95470900	3.34062300
C	1.20823100	-4.44949500	2.68877500
H	1.95487400	-4.48617900	3.48921400
H	0.89332300	-5.47916200	2.48893900
S	-0.21388000	-3.55371000	3.49206400
H	-1.47250800	-0.25280600	-1.26892800
H	1.94087900	-0.50666500	2.34659900
C	1.08882100	1.29650700	1.60927800
H	1.35662500	2.34565400	1.44608700
H	0.36730000	1.29867900	2.43885800
C	0.38763700	0.73461900	0.36130600
H	0.46949900	-0.35925100	0.34025900
H	0.87979400	1.09787700	-0.55161600
C	-1.09898200	1.11193000	0.35813700
H	-1.21249100	2.19114900	0.52453200
H	-1.57314100	0.62002300	1.21790000

Compound **13e**: E(RB3LYP) = -3960.89700111 a.u.

C	-2.04190200	-3.26852900	-1.22765600
C	-3.04247000	-2.15574400	1.13907700
C	-1.70379200	-3.80568700	0.01696200
C	-2.93839800	-2.19526500	-1.26864400
C	-3.47181500	-1.64698400	-0.09322300
C	-2.14403700	-3.22749000	1.20920700
H	-3.23627100	-1.78132500	-2.22968300
H	-3.42508100	-1.71631700	2.05674900
C	1.52854800	-3.64918800	0.21981000
C	3.33742200	-1.52254700	0.21942900
C	1.97366600	-3.13887000	-1.00073000
C	1.88258200	-3.06171700	1.43667100
C	2.80128000	-2.00525300	1.42320700
C	2.88339100	-2.07510000	-0.98575200
H	3.13001400	-1.56836500	2.36380700
H	3.27556900	-1.69206600	-1.92426100
C	4.42484900	-0.48280900	0.21805900
C	6.50806100	1.41930000	0.21403200
C	5.74332300	-0.87861000	-0.10148800
C	4.13899300	0.86675600	0.51960100
C	5.18665700	1.81278300	0.51456000
C	6.78708700	0.07276500	-0.10458700
C	-4.48755100	-0.53967400	-0.15986600
C	-6.41146600	1.51375800	-0.30302300
C	-4.07520900	0.78570500	-0.42208700
C	-5.85037700	-0.83671000	0.05176800
C	-6.81618600	0.19152500	-0.01940400
C	-5.04368700	1.80840600	-0.49211600
C	-2.59750700	1.09607600	-0.58628200
C	2.71491600	1.30070400	0.81894800
H	2.72559600	2.20450200	1.43584000
C	6.03944100	-2.30844800	-0.45009900
C	6.60280500	-4.98716200	-1.11411400
C	6.38586400	-2.66625500	-1.76119300
C	5.98224100	-3.31705500	0.52247600
C	6.26320700	-4.64378400	0.19536800
C	6.66222300	-3.99281500	-2.09193100
H	6.44290100	-1.89579800	-2.52491900
H	5.71616200	-3.05736500	1.54318700
H	6.21759900	-5.40949200	0.96572500
H	6.92834300	-4.24839100	-3.11445100
H	6.82197400	-6.02051000	-1.37003700
C	8.18927200	-0.34505600	-0.43540900
C	10.82319400	-1.12277900	-1.05926900

C	8.80866400	0.09577100	-1.61398000
C	8.91396300	-1.18250600	0.42499300
C	10.21938000	-1.56619500	0.11841000
C	10.11207800	-0.29085500	-1.92540400
H	8.26281200	0.74793600	-2.28989700
H	8.44814000	-1.53625300	1.34036400
H	10.76435500	-2.21370700	0.80059600
H	10.57242700	0.06023300	-2.84543300
H	11.83972300	-1.42285500	-1.29988400
C	7.62165000	2.42337600	0.27602200
C	9.71556600	4.30095300	0.41686900
C	7.75157000	3.42787400	-0.69330200
C	8.56028800	2.37595500	1.31683400
C	9.59644800	3.30677800	1.38914400
C	8.78972900	4.35731600	-0.62589500
H	7.03391300	3.47873000	-1.50717800
H	8.47674200	1.60068000	2.07331400
H	10.31225400	3.25335500	2.20545500
H	8.87378900	5.12657100	-1.38932400
H	10.52366700	5.02572100	0.47097700
C	4.90651400	3.24207600	0.88506000
C	4.37577700	5.91143100	1.61128700
C	5.12123100	3.68585300	2.19828400
C	4.42365600	4.16088500	-0.05795800
C	4.16019600	5.48393800	0.30060100
C	4.85768100	5.00747200	2.55938200
H	5.49844400	2.98671600	2.93972700
H	4.25953600	3.83668600	-1.08216400
H	3.78775000	6.18033900	-0.44633200
H	5.03096400	5.33102600	3.58254200
H	4.17105400	6.94128900	1.89167700
C	-6.27043800	-2.24013600	0.37800700
C	-7.04867500	-4.87186600	1.01054900
C	-6.70021600	-2.57101700	1.67133100
C	-6.23854700	-3.25139400	-0.59268700
C	-6.62593500	-4.55493000	-0.28119400
C	-7.08381900	-3.87452000	1.98643500
H	-6.73720500	-1.79735300	2.43313800
H	-5.90818300	-3.01243600	-1.59961800
H	-6.59780700	-5.32324400	-1.04978600
H	-7.41345800	-4.10967500	2.99524900
H	-7.35041600	-5.88719000	1.25422700
C	-8.26657100	-0.12084900	0.20147100
C	-10.98939000	-0.70517100	0.62096700
C	-8.98627900	-0.89288100	-0.72205900
C	-8.93629000	0.35318400	1.33893200

C	-10.28413100	0.06232400	1.54911800
C	-10.33550100	-1.18074000	-0.51666400
H	-8.48240900	-1.27052400	-1.60726600
H	-8.39469900	0.95609200	2.06234400
H	-10.78358300	0.43777700	2.43861900
H	-10.87552400	-1.77864800	-1.24641200
H	-12.04024000	-0.93064300	0.78273600
C	-7.43859700	2.59945000	-0.43816100
C	-9.37267400	4.62746600	-0.71293600
C	-8.29621100	2.62878900	-1.54731700
C	-7.56679000	3.60499000	0.53036600
C	-8.52627700	4.60876000	0.39653600
C	-9.25352400	3.63362700	-1.68555600
H	-8.21279700	1.85413100	-2.30450200
H	-6.91018300	3.59802100	1.39573900
H	-8.61101800	5.37749400	1.16043600
H	-9.90754400	3.63851800	-2.55379000
H	-10.11925100	5.41024900	-0.81850200
C	-4.62424600	3.21436500	-0.81484500
C	-3.83368700	5.84368900	-1.44297400
C	-4.72112200	3.69945000	-2.12724100
C	-4.12626300	4.07122000	0.17753700
C	-3.73471300	5.37462800	-0.13245500
C	-4.32849000	5.00120900	-2.43992400
H	-5.10842900	3.04830800	-2.90616700
H	-4.05135700	3.71337700	1.20090700
H	-3.35320100	6.02338600	0.65189700
H	-4.41121000	5.35744300	-3.46354500
H	-3.52880800	6.85828600	-1.68540300
H	-1.07454900	-4.68870700	0.05732800
H	0.89059500	-4.52511600	0.22454300
C	-1.43216500	-3.82308700	-2.49200700
H	-2.14035900	-3.75822500	-3.32423700
H	-1.16245600	-4.87830000	-2.37666900
C	1.50836500	-3.74590400	-2.30204500
H	1.25818100	-4.80482200	-2.17816900
H	2.30166500	-3.68777200	-3.05364400
S	0.06346300	-2.92584600	-3.14266900
C	-1.64714700	-3.73830500	2.53994700
H	-1.32151100	-4.78168600	2.47175300
H	-2.44257500	-3.69519500	3.29056200
C	1.29678300	-3.57850300	2.72908000
H	1.99212000	-3.41479700	3.55852900
H	1.10605100	-4.65579600	2.67523100
S	-0.26715100	-2.76591400	3.32862400
H	-2.11409300	0.27876500	-1.12991900

H	2.21614400	0.52672000	1.40638800
C	1.88080500	1.57224100	-0.45109600
H	1.85426700	0.66106100	-1.06291200
H	2.38448900	2.33758300	-1.05457800
C	0.43919900	2.02074900	-0.16040400
H	-0.06646100	2.18042600	-1.12214300
C	-1.86419800	1.27563400	0.76630000
H	-2.28886300	0.57904200	1.49801100
C	-0.35457900	1.01380400	0.68457700
H	0.04586300	0.99812100	1.70595300
H	-0.19919300	0.00194300	0.28374800
H	-2.05660400	2.28515300	1.15381300
H	-2.47309200	1.99367300	-1.19697500
H	0.44820400	2.99752200	0.34598000