Flat Corannulene: When a Transition State Becomes a Stable Molecule

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Supporting Information

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1. General Methods

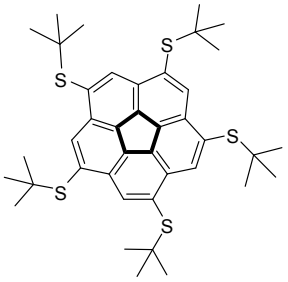
All commercially available chemicals were purchased from Sigma-Aldrich and used without further purification. Dry solvents were either purchased (sure-seal) or purified according to standard procedures.[1] 1,3-Dimethyl-2-imidazolidinone (DMI), was purchased (sure-seal) from Sigma and used without further treatment. Extra-dry 1,4-dioxane was purchased (sure-seal) from Bio-Lab and used without further purification. 1,3,5,7,9-pentachlorocorannulene (**9**) and decaclorocorannulene (**10**) were prepared according to literature procedures.[2,3] ^{1}H NMR and ^{13}C NMR were performed in $CDCl_3$ by using the residual solvent signals: δ_H = 7.26 ppm, δ_C = 77.16 ppm as an internal standard. NMR spectra were recorded with a Bruker Ultrashield AV300 spectrometer (^{1}H 300 MHz, ^{13}C 75.44 MHz) or AV500 (^{1}H 500 MHz, ^{13}C 125.76 MHz). Mass spectra and high resolution mass spectra were recorded with a Water AutoSpec Premier mass spectrometer under chemical ionization (isobutane) or with a MALDI Micromass spectrometer (MALDI-TOF). Gas chromatography (GC) analyses were performed with Varian 3800 GC instrument equipped with a FID detector and a capillary column VB-5 (5% phenyl, 95% methyl polysiloxane, 30m x 0.32mm x 0.25μm). Measurements were carried out in a split mode (split vent flow *vs*. column flow was 30 to 1)., Nitrogen was used as carrier gas at a flow rate of 1.5 ml/min. Analytical TLC was performed on glass sheets pre-coated on silica gel (Merck, Kieselgel 60, F-254, Art. 5715). Flash chromatography was performed Merck on silica gel 60 (230-400 mesh).

2. X-ray crystallography

Single crystals of **8α**, **8β** and **5** were mounted in a Nonius Kappa CCD diffractometer and data were collected by using graphite monochromatized Mo-K_α radiation (λ = 0.71073) at 240 K (**8α**) or 293 K (**8β** and **5**). The following programs were used for data collection and reduction: Nonius 2006 Collect and DENZO HKL2000. Structures were solved by direct methods by using the SHELXS-97 program package and refined in the usual way by using SHELXL-97. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined isotropically. CCDC-1040969 (for **5**), -1040970 (**8α**) and -1040971 (for **8β**) contain the supplementary crystallographic data for this work. These data can be obtained free of charge from the Cambridge Crystallographic Data Center via www.ccdc.cam.ac.il/data_request/cif. Pertinent crystallographic data and refinement parameters for compound **8α**, **8β** and **5** are summarized in Table 3 in the main text.

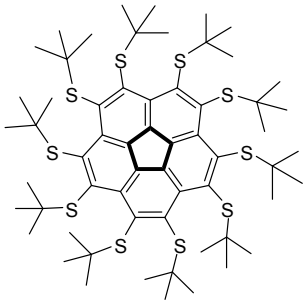
3. Experimental and characterization data

1,3,5,7,9-Penta(*tert*-butylthio)corannulene, 5.



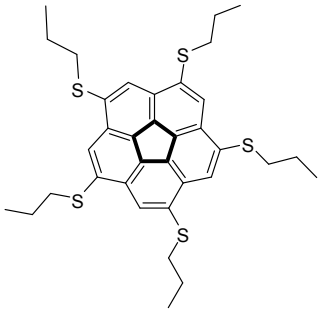
Following the reported procedure,[4] 1,3,5,7,9-Pentachlorocorannulene, **9** (0.3 g, 0.7 mmol) was added to a stirred solution of sodium 2-methylpropane-2-thiolate (1.6 g, 14.2 mmol) in dry DMI (30 ml) under argon. The purple mixture was stirred at room temperature for 48 h. Toluene (50 ml) and water (50 ml) were added and the organic phase was separated, washed with water (2 X 50 ml) and brine (50 ml), dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography (silica-gel, dichlorometane-hexane, 1:4) affording compound **5** (0.11 g, 22%) as a yellow solid, which was recrystallized from dichloromethane. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.50 (s, 5H), 1.51 (s, 45H). ^{13}C NMR (500 MHz, $CDCl_3$): δ = 138.4, 135.6, 134.6, 132.6, 47.5, 31.3 ppm. MS (MALDI-TOF) *m/z*: calcd. 690.25, found 690.60 [M^+].

Deca(*tert*-butylthio)corannulene, 8.



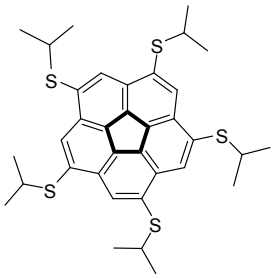
Sodium *tert*-butylthiolate (0.43 g, 3.9 mmol) was added to a stirred solution of decachlorocorannulene, **10** (0.1 g, 168 µmol) in dry DMI (8 ml) under argon. The dark purple mixture was stirred at room temperature for 48 h. Toluene (30 ml) and water (30 ml) were added and the organic phase was separated, washed with water (30 ml X 2) and brine (30 ml), dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography (silica-gel, dichloromethane-hexane, 1:4) affording compound **8** (0.11 g, 60%) as a brown solid, which was recrystallized from either DCM at room temperature or from toluene at 5-8 ˚C. ^{1}H NMR (300 MHz, $CDCl_3$): 1.21 (s, 90H). ^{13}C NMR (500 MHz, $CDCl_3$): δ = 148.1, 138.8, 130.8, 52.2, 31.9. MS (MALDI-TOF) *m/z*: 959.17 [M-3tBu($^-$)], 903.1 [M-4tBu($^-$)], 847.02 [M-5tBu($^-$)], 790.94 [M-6tBu($^-$)], 732.87 [M-7tBu($^-$)], 676.81 [M-8tBu($^-$)], 620.76 [M-9tBu($^-$)], 564.70 [M-10tBu($^-$)].

1,3,5,7,9-Penta(*n*-propylthio)corannulene, 11.



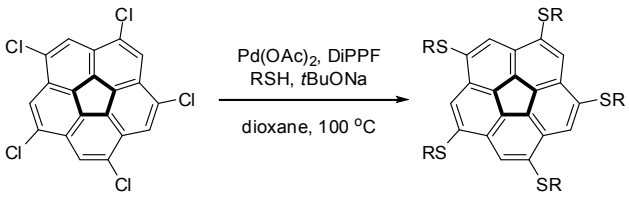
Following the reported procedure,[5] **9** (0.24 g, 0.57 mmol) was reacted with sodium n-propylthiolate (1 g, 10 mmol) to give compound **11** as a yellow oil (0.11 g, 31%). ^{1}H NMR (500 MHz, $CDCl_3$): 7.88 (s, 5H), 3.09 (t, *J* = 10.8 Hz, 10H), 1.71 (m, 10H), 1.06 (t, *J* = 10.3 Hz, 15H). ^{13}C NMR (500 MHz, $CDCl_3$): δ = 136.5, 134.3, 131.1, 124.3, 36.8, 22.5, 13.5 ppm. HRMS (CI) *m/z*: calc. 621.1812, found 621.1790 $[M+H]^+$.

1,3,5,7,9-Penta(*i*-propylthio)corannulene, 12.



Sodium chunks (1.15 g, 50 mmol) were added to a dry 50 ml flask containing ethanol (25 ml) under nitrogen. After stirring at room temperature for 15 min isopropyl mercaptane (4.6 ml, 50 mmol) was added and the mixture was stirred for 2 h. The solvent was removed under reduced pressure and the resulting white solid was filtered and washed with diethyl ether (40 ml). Part of this thiolate (2.2 g, 22 mmol) was added to a stirred solution of **9** (0.47 g, 1.1 mmol) in dry DMI (30 ml) under argon. The dark purple mixture was stirred at room temperature for 72 h. Toluene (50 ml) and water (50 ml) were added, the organic phase was separated, washed with water (2 X 50 ml) and brine (50 ml), dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography (silica-gel, dichlorometane-hexane, 1:9) affording compound **12** (0.41 g, 59%) as a yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.12 (s, 5H), 3.67 (m, 5H), 1.45 (d, 30H). ^{13}C NMR (500 MHz, $CDCl_3$): δ = 135.4, 135.1, 132.4, 129.2, 39.8, 23.5 ppm. HRMS (CI) *m/z*: calc. 621.1812, found 621.1836 $[M+H]^+$.

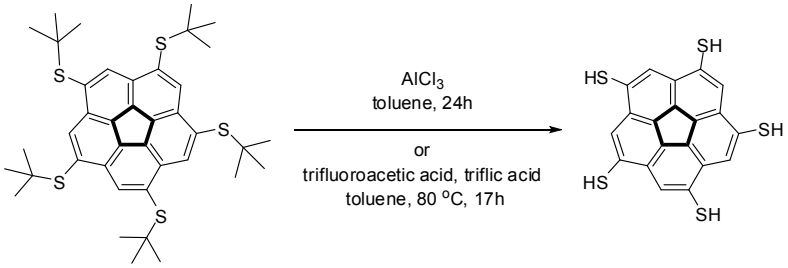
Palladium catalyzed coupling of 9 with thiols[6]



General procedure

A dry flask (25 ml) was charged with solid **9** (1 equiv), palladium(II) acetate (0.1 equiv), diisopropylphosphinoferrocene (diPPF, 0.2 equiv) and sodium *tert*-butoxide (6 equiv). The flask was flashed three times with nitrogen and then 1,4-dioxane (5 ml, extra-dry) was added. The mixture was stirred at room temperature for 30 min, the appropriate thiol (10 equiv) was added and the mixture was stirred at 100 ˚C for 48 h. The mixture was then cooled to room temperature, ethanol (10 ml) was added and the resultant precipitate was removed by filtration. The solution was concentrated under reduced pressure and the residue was purified by column chromatography affording 1,3,5,7,9-penta(*n*-propylthio)corannulene, **11** (54%), 1,3,5,7,9-penta(*i*-propylthio)corannulene, **12** (43%) or 1,3,5,7,9-penta(*tert*-butylthio)corannulene, **5** (75%).

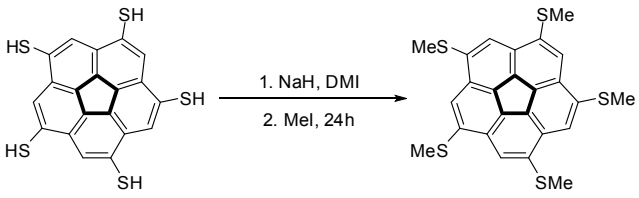
1,3,5,7,9-Pentamercaptocorannulene, 4.



Method A: A solution of **5** (0.1 g, 0.14 mmol) in toluene (5 ml) was added via a syringe at 0 ˚C to $AlCl_3$ (0.07 g, 0.52 mmol) under argon. The mixture was stirred at room temperature for 24 h, quenched with acetic acid-methanol (1:2, 5 ml), the precipitate was collected by filtration and washed with methanol (2 ml) and dichloromethane (2 ml) to give compound **4** as an orange solid (34 mg, 59%), which was slightly soluble in DCM and DMF. ^{1}H NMR (300 MHz, $CDCl_3$): 7.85 (s, 5H), 3.92 (s, 5H). ^{1}H NMR (500 MHz, DMF-d^7): 8.04 (s, 5H), 6.00 (s, 5H). ^{13}C NMR (500 MHz, DMF-d^7): δ= 133.0, 132.6, 130.3, 123.7. MS (MALDI-TOF) *m/z*: calcd. 409.94, found 410.08 [M^+].

Method B: To a stirred solution of **5** (0.23 g, 0.33 mmol) in toluene (10 ml) under argon atmosphere at 80 ˚C were added via a syringe trifluoroacetic acid (2.3 ml, 30 mmol) and triflic acid (2 ml, 22.6 mmol). The mixture was kept at the same temperature for 17 h, cooled to room temperature and diluted with methanol (5 ml). The precipitate was filtered and washed with methanol (2 ml) and dichloromethane (2 ml) to give compound **4** as an orange solid (0.098 g, 73%).

1,3,5,7,9-Penta(methylthio)corannulene, 13.

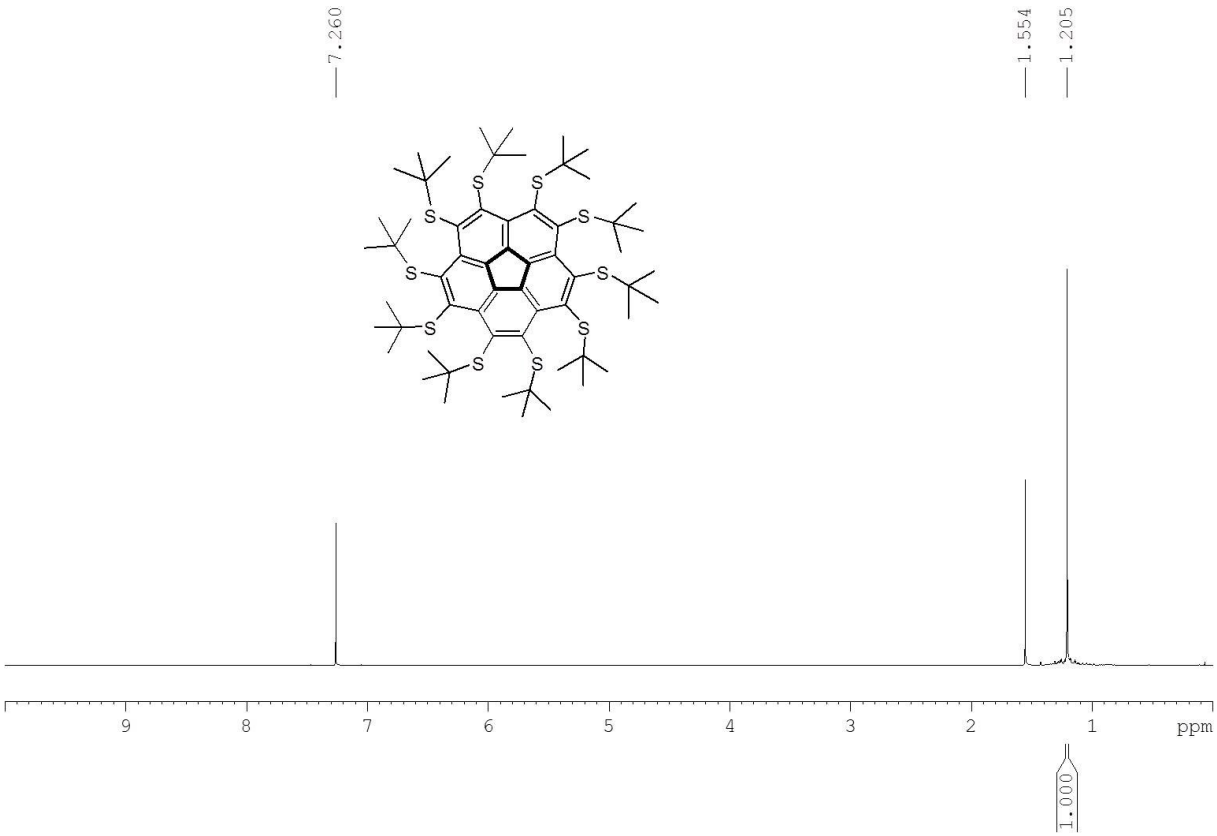


To a stirred solution of **4** (3.7mg, 0.009 mmol) in DMI (0.5 ml) under argon was added sodium hydride (60% suspension in oil, 7 mg, 0.17 mmol). The mixture was stirred for 2.5 h, iodomethane (0.1 ml, 1.8 mmol) was added and the mixture was stirred for 24 h and then quenched by the addition of toluene (2 ml) and water (2 ml). The organic phase was washed with water and brine, dried over $MgSO_4$, and concentrated under reduced pressure. The crude residue was purified by column chromatography (silica-gel, dichloromethane-hexane, 2:3) affording compound **13** (2.1 mg, 49%) as a yellow oil. ^{1}H NMR

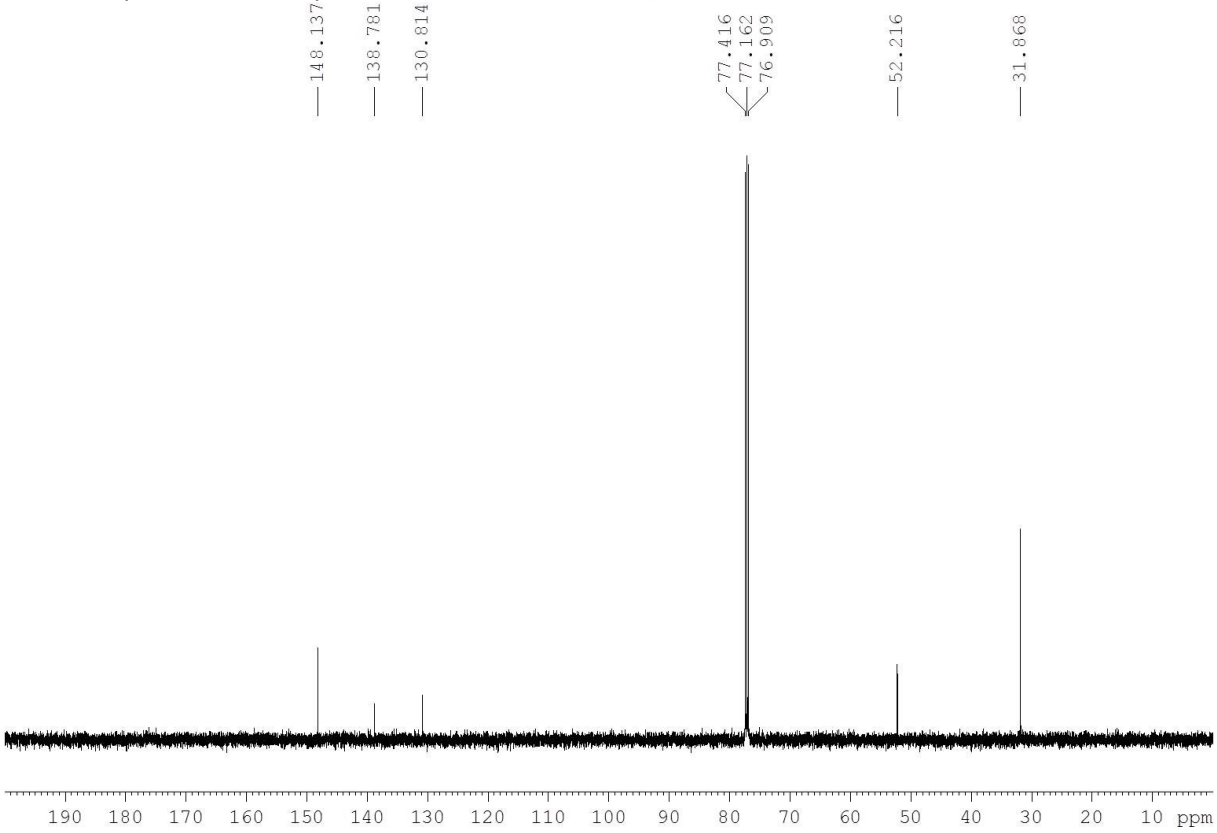
(500 MHz, $CDCl_3$): 7.62 (s, 5H), 2.70 (s, 15H). ^{13}C NMR (500 MHz, $CDCl_3$): δ = 138.5, 134.0, 130.2, 120.1, 16.9. MS (MALDI-TOF) *m/z*: calcd. 480.02, found 480.12 [M^+].

4. ^{1}H and ^{13}C NMR spectra

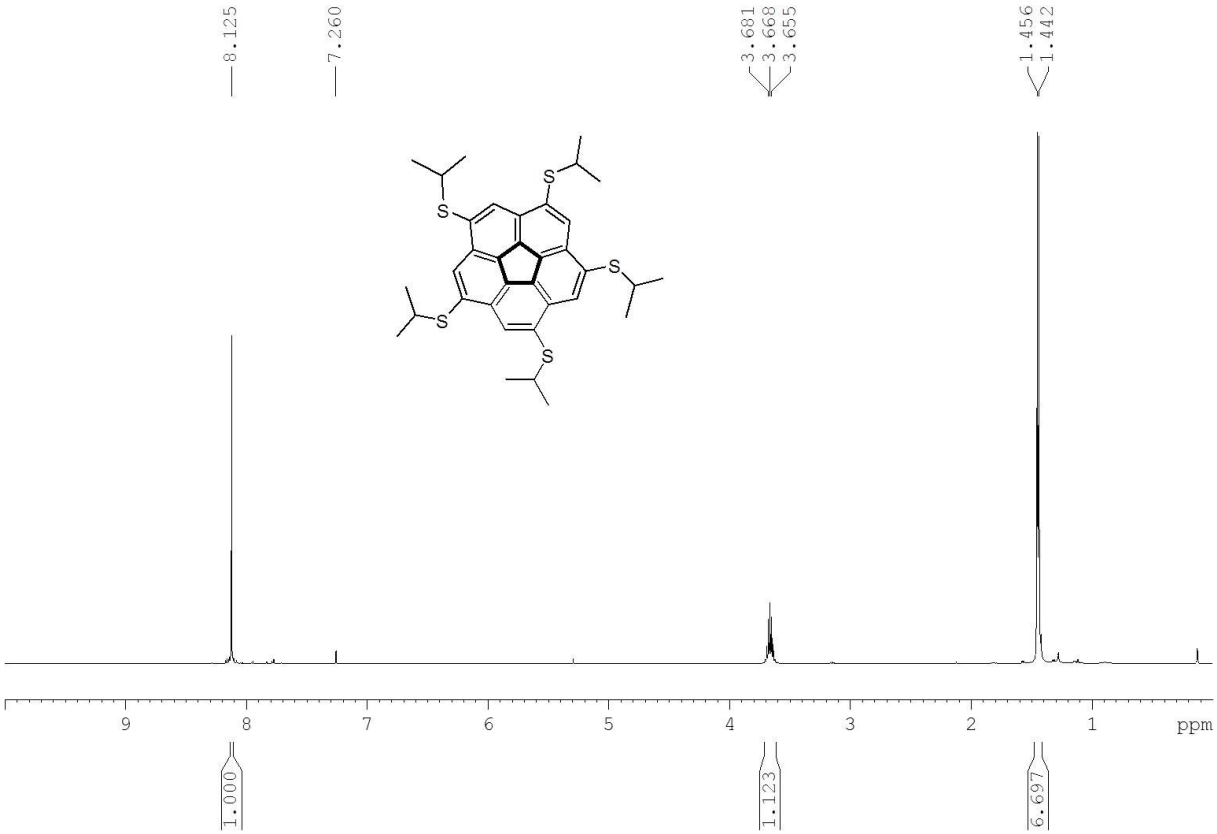
^{1}H NMR spectrum of compound **8** (500 MHz, $CDCl_3$):



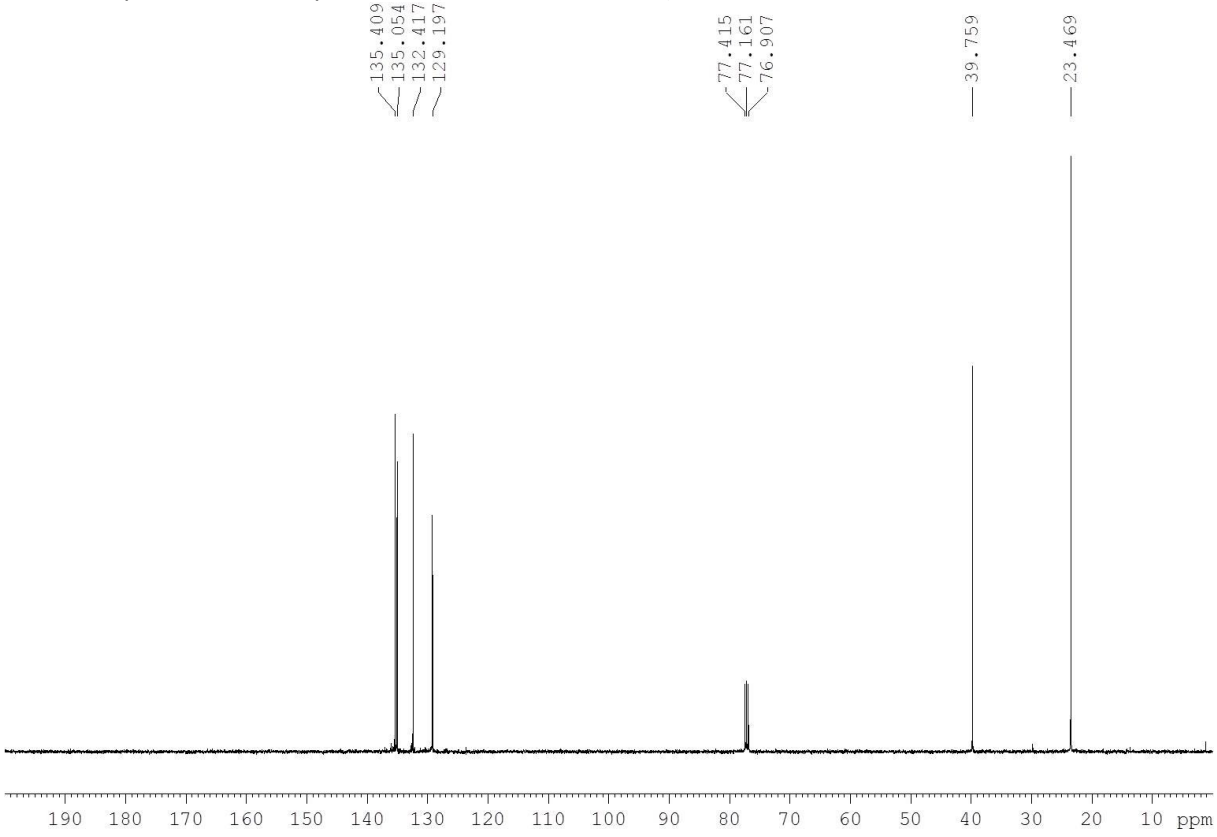
^{13}C NMR spectrum of compound **8** (125.76 MHz, $CDCl_3$):



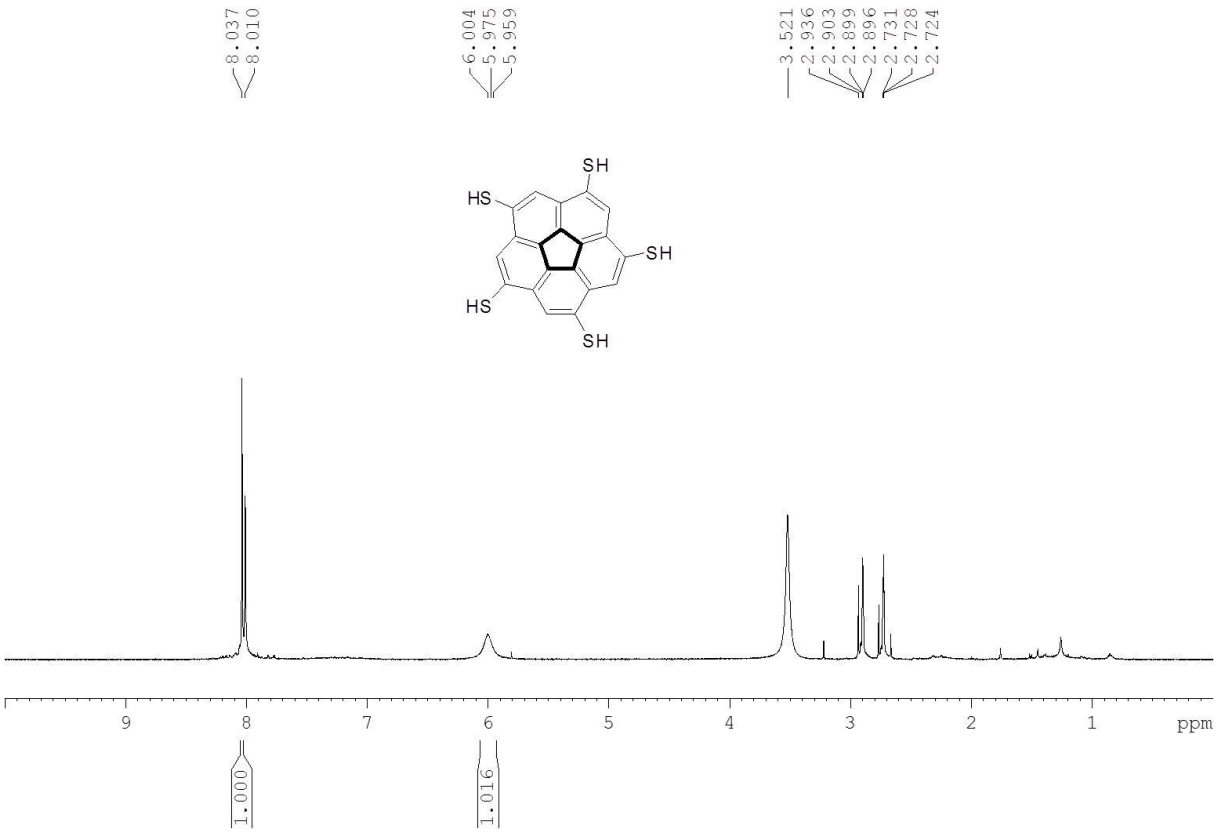
^{1}H NMR spectrum of compound **12** (500 MHz, $CDCl_3$):



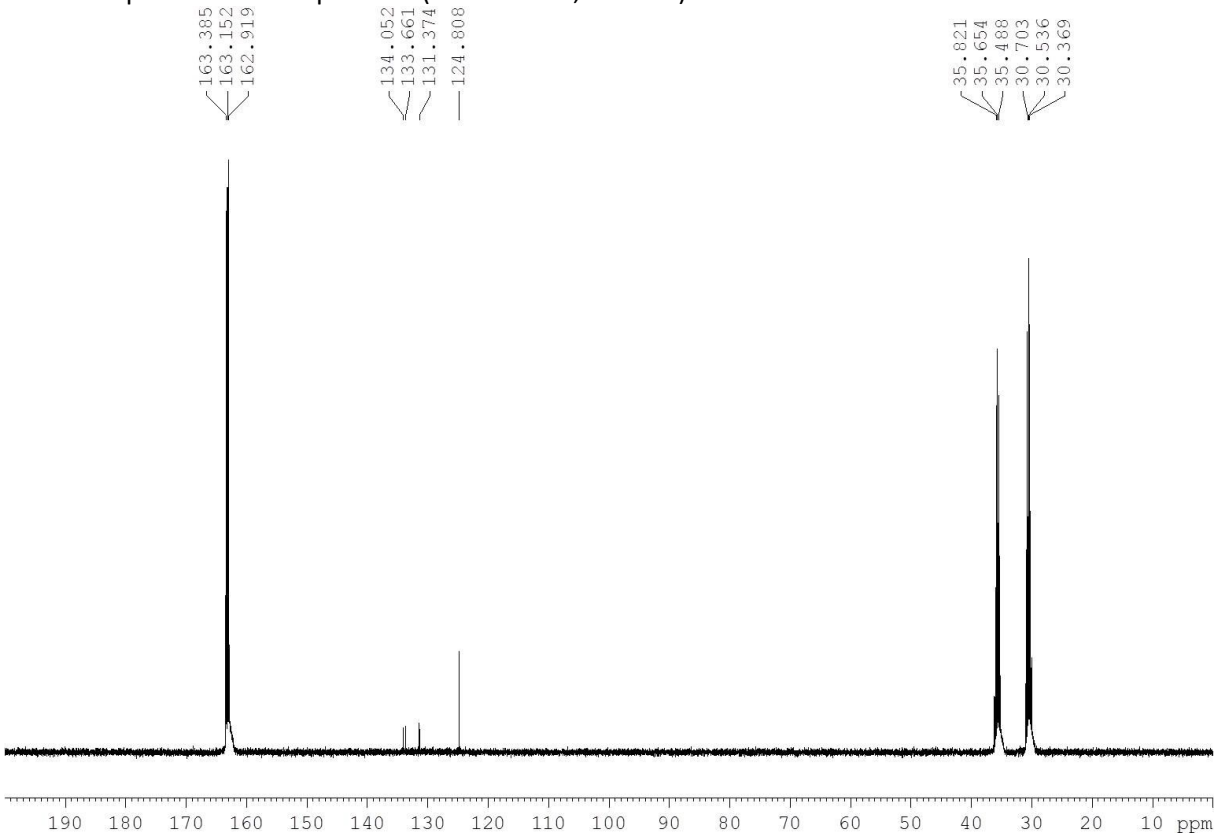
^{13}C NMR spectrum of compound **12** (125.76 MHz, $CDCl_3$):



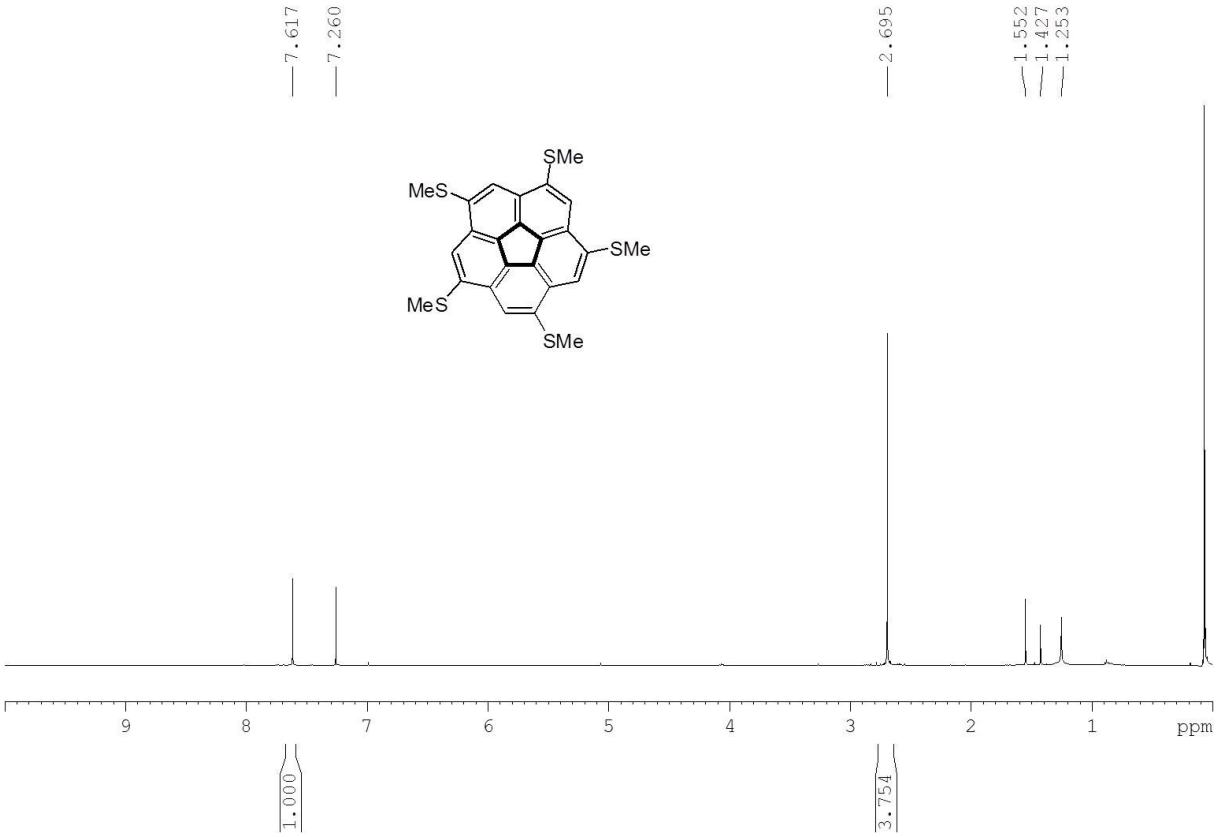
^{1}H-NMR spectrum of compound **4** (500 MHz, DMF-d^{7}):



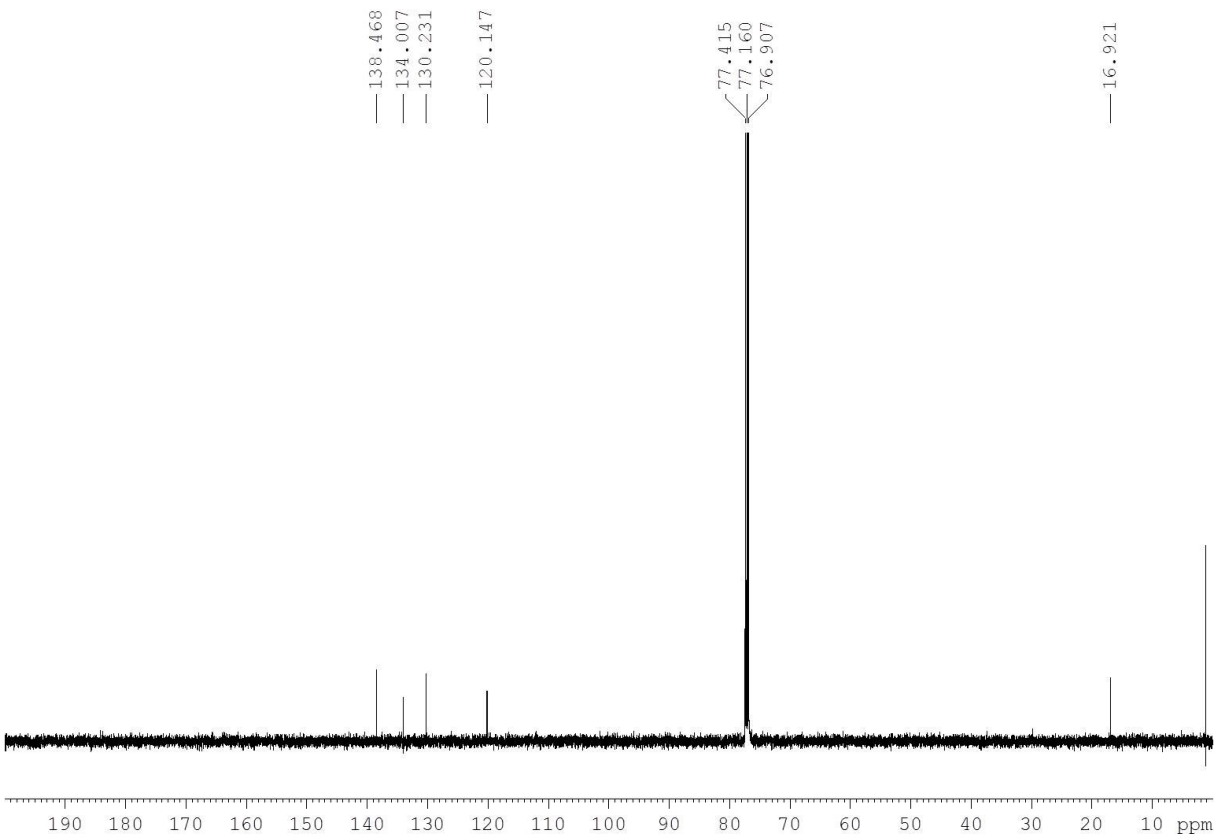
^{13}C-NMR spectrum of compound **4** (125.76 MHz, DMF-d^{7}):



^{1}H-NMR spectrum of compound **13** (500 MHz, $CDCl_3$):



^{13}C-NMR spectrum of compound **13** (125.76 MHz, $CDCl_3$):



5. General Quantum Mechanical Computational Methods

All DFT calculations were carried out using Gaussian16 revision A.03,[7] using geometries with no symmetry constrictions, unless stated otherwise. All minima were characterized with analytical Hessian calculations to ensure real minima (n_{imag}=0) and for obtaining the zero-point energy (ZPE) corrections and thermochemical data. Optimizations of **8** were done with M06-2X/def2-TZVP, and also with B3LYP/def2-TZVP with and without Grimme's D3BJ dispersion correction.[8,9] NBO analysis was done with NBO3.1[10] as implemented in Gaussian16. Single point energy calculations at DLPNO-CCSD(T)[11]/cc-pVTZ (with the default *normalPNO* settings), DLPNO-CCSD(T)/def2-TZVP (with *tightPNO* settings) and at DSDPBEP86[12]/def2-QZVPP (using the RI approximation, with the *tightSCF* convergence criteria) were performed with ORCA 4.2.0.[13,14] NCI plots were generated with NCIPLOT[15] and visualized with Gaussview6.[16]

6. NBO Analysis for 6

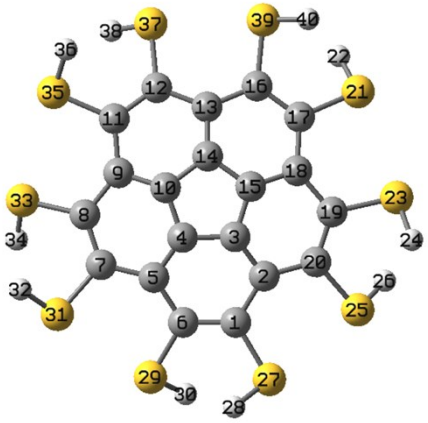


Table S1. The Interactions involving sulfur orbitals from the Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis for decamercaptocorannulene, **6.** The most stable conformer of **6** was used, computed at M06-2X/def2-TZVP. [For each C-C bond, the BD(1) and BD*(1) are σ and σ* orbitals, while the BD(2) and BD*(2) are the π and π* orbitals, respectively. For each sulfur the LP(1)S is an sp^n orbital made of approximately 67% s and 33% p, while the LP(2)S is a p orbital.]

Donor NBO (i)	Acceptor NBO (j)	E(2) (kcal/mol)	E(j)-E(i) (a.u.)	F(i,j) (a.u.)
1. BD (1) C 1 - C 2	/***. BD*(1) C 6 - S 29	4.44	0.98	0.059
3. BD (2) C 1 - C 6	/765. RY*(1) S 27	2.54	1.23	0.053
3. BD (2) C 1 - C 6	/798. RY*(1) S 29	2.61	1.23	0.053
3. BD (2) C 1 - C 6	/***. BD*(1) S 27 - H 28	0.70	0.59	0.019
3. BD (2) C 1 - C 6	/***. BD*(1) S 29 - H 30	0.79	0.59	0.020
4. BD (1) C 1 - S 27	/172. RY*(1) C 2	1.40	1.80	0.045
4. BD (1) C 1 - S 27	/276. RY*(1) C 6	1.03	1.99	0.041
4. BD (1) C 1 - S 27	/997. BD*(1) C 1 - C 6	0.70	1.23	0.026
4. BD (1) C 1 - S 27	/***. BD*(1) C 2 - C 3	3.20	1.34	0.059
4. BD (1) C 1 - S 27	/***. BD*(1) C 5 - C 6	5.70	1.19	0.074
5. BD (1) C 2 - C 3	/999. BD*(1) C 1 - S 27	4.60	1.02	0.061
5. BD (1) C 2 - C 3	/***. BD*(1) C 20 - S 25	4.71	1.02	0.062
7. BD (1) C 2 - C 20	/***. BD*(1) C 19 - S 23	4.35	0.99	0.059

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10. BD (  1) C  4 - C  5     /***. BD*(  1) C  6 - S 29       4.71   1.02   0.062
10. BD (  1) C  4 - C  5     /***. BD*(  1) C  7 - S 31       4.59   1.02   0.061
13. BD (  1) C  5 - C  6     /999. BD*(  1) C  1 - S 27       4.35   0.99   0.059
14. BD (  1) C  5 - C  7     /***. BD*(  1) C  8 - S 33       4.44   0.98   0.059
15. BD (  1) C  6 - S 29     /146. RY*(  1) C  1            0.98   1.93   0.039
15. BD (  1) C  6 - S 29     /250. RY*(  1) C  5            1.49   1.80   0.046
15. BD (  1) C  6 - S 29     /996. BD*(  1) C  1 - C  2       5.64   1.19   0.073
15. BD (  1) C  6 - S 29     /997. BD*(  1) C  1 - C  6       0.73   1.24   0.027
15. BD (  1) C  6 - S 29     /***. BD*(  1) C  4 - C  5       3.37   1.34   0.060
17. BD (  2) C  7 - C  8     /831. RY*(  1) S 31            2.55   1.23   0.053
17. BD (  2) C  7 - C  8     /864. RY*(  1) S 33            2.61   1.23   0.053
17. BD (  2) C  7 - C  8     /***. BD*(  1) S 31 - H 32       0.69   0.59   0.019
17. BD (  2) C  7 - C  8     /***. BD*(  1) S 33 - H 34       0.79   0.58   0.020
18. BD (  1) C  7 - S 31     /250. RY*(  1) C  5            1.40   1.80   0.045
18. BD (  1) C  7 - S 31     /328. RY*(  1) C  8            1.02   2.00   0.040
18. BD (  1) C  7 - S 31     /***. BD*(  1) C  4 - C  5       3.20   1.34   0.059
18. BD (  1) C  7 - S 31     /***. BD*(  1) C  7 - C  8       0.70   1.23   0.026
18. BD (  1) C  7 - S 31     /***. BD*(  1) C  8 - C  9       5.70   1.19   0.074
19. BD (  1) C  8 - C  9     /***. BD*(  1) C  7 - S 31       4.35   0.99   0.059
20. BD (  1) C  8 - S 33     /302. RY*(  1) C  7            0.98   1.93   0.039
20. BD (  1) C  8 - S 33     /354. RY*(  1) C  9            1.49   1.80   0.046
20. BD (  1) C  8 - S 33     /***. BD*(  1) C  5 - C  7       5.64   1.19   0.073
20. BD (  1) C  8 - S 33     /***. BD*(  1) C  7 - C  8       0.74   1.24   0.027
20. BD (  1) C  8 - S 33     /***. BD*(  1) C  9 - C 10       3.37   1.34   0.060
21. BD (  1) C  9 - C 10     /***. BD*(  1) C  8 - S 33       4.70   1.02   0.062
21. BD (  1) C  9 - C 10     /***. BD*(  1) C 11 - S 35       4.60   1.02   0.061
23. BD (  1) C  9 - C 11     /***. BD*(  1) C 12 - S 37       4.44   0.98   0.059
26. BD (  2) C 11 - C 12     /897. RY*(  1) S 35            2.55   1.23   0.053
26. BD (  2) C 11 - C 12     /930. RY*(  1) S 37            2.61   1.23   0.053
26. BD (  2) C 11 - C 12     /***. BD*(  1) S 35 - H 36       0.68   0.59   0.019
26. BD (  2) C 11 - C 12     /***. BD*(  1) S 37 - H 38       0.80   0.58   0.020
27. BD (  1) C 11 - S 35     /354. RY*(  1) C  9            1.40   1.80   0.045
27. BD (  1) C 11 - S 35     /432. RY*(  1) C 12            1.03   2.00   0.041
27. BD (  1) C 11 - S 35     /***. BD*(  1) C  9 - C 10       3.20   1.34   0.059
27. BD (  1) C 11 - S 35     /***. BD*(  1) C 11 - C 12       0.70   1.23   0.026
27. BD (  1) C 11 - S 35     /***. BD*(  1) C 12 - C 13       5.70   1.19   0.074
28. BD (  1) C 12 - C 13     /***. BD*(  1) C 11 - S 35       4.35   0.99   0.059
29. BD (  1) C 12 - S 37     /406. RY*(  1) C 11            0.98   1.93   0.039
29. BD (  1) C 12 - S 37     /458. RY*(  1) C 13            1.49   1.80   0.046
29. BD (  1) C 12 - S 37     /***. BD*(  1) C  9 - C 11       5.65   1.19   0.073
29. BD (  1) C 12 - S 37     /***. BD*(  1) C 11 - C 12       0.73   1.23   0.027
29. BD (  1) C 12 - S 37     /***. BD*(  1) C 13 - C 14       3.37   1.34   0.060
30. BD (  1) C 13 - C 14     /***. BD*(  1) C 12 - S 37       4.71   1.02   0.062
30. BD (  1) C 13 - C 14     /***. BD*(  1) C 16 - S 39       4.59   1.02   0.061
32. BD (  1) C 13 - C 16     /***. BD*(  1) C 17 - S 21       4.44   0.98   0.059
34. BD (  1) C 15 - C 18     /***. BD*(  1) C 17 - S 21       4.71   1.02   0.062
34. BD (  1) C 15 - C 18     /***. BD*(  1) C 19 - S 23       4.60   1.02   0.061
37. BD (  2) C 16 - C 17     /666. RY*(  1) S 21            2.61   1.23   0.053
37. BD (  2) C 16 - C 17     /963. RY*(  1) S 39            2.55   1.23   0.053
37. BD (  2) C 16 - C 17     /***. BD*(  1) S 21 - H 22       0.79   0.59   0.020
37. BD (  2) C 16 - C 17     /***. BD*(  1) S 39 - H 40       0.70   0.59   0.019
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38. BD (1) C 16 - S 39 /458. RY*(1) C 13 1.40 1.80 0.045
38. BD (1) C 16 - S 39 /562. RY*(1) C 17 1.02 1.99 0.040
38. BD (1) C 16 - S 39 /***. BD*(1) C 13 - C 14 3.20 1.34 0.059
38. BD (1) C 16 - S 39 /***. BD*(1) C 16 - C 17 0.70 1.23 0.026
38. BD (1) C 16 - S 39 /***. BD*(1) C 17 - C 18 5.70 1.19 0.074
39. BD (1) C 17 - C 18 /***. BD*(1) C 16 - S 39 4.35 0.99 0.059
40. BD (1) C 17 - S 21 /536. RY*(1) C 16 0.98 1.93 0.039
40. BD (1) C 17 - S 21 /588. RY*(1) C 18 1.49 1.80 0.046
40. BD (1) C 17 - S 21 /***. BD*(1) C 13 - C 16 5.64 1.19 0.073
40. BD (1) C 17 - S 21 /***. BD*(1) C 15 - C 18 3.37 1.34 0.060
40. BD (1) C 17 - S 21 /***. BD*(1) C 16 - C 17 0.74 1.24 0.027
41. BD (1) C 18 - C 19 /***. BD*(1) C 20 - S 25 4.44 0.98 0.059
43. BD (2) C 19 - C 20 /699. RY*(1) S 23 2.54 1.23 0.053
43. BD (2) C 19 - C 20 /732. RY*(1) S 25 2.61 1.23 0.053
43. BD (2) C 19 - C 20 /***. BD*(1) S 23 - H 24 0.69 0.59 0.019
43. BD (2) C 19 - C 20 /***. BD*(1) S 25 - H 26 0.80 0.59 0.020
44. BD (1) C 19 - S 23 /588. RY*(1) C 18 1.40 1.80 0.045
44. BD (1) C 19 - S 23 /640. RY*(1) C 20 1.03 1.99 0.041
44. BD (1) C 19 - S 23 /***. BD*(1) C 2 - C 20 5.70 1.19 0.074
44. BD (1) C 19 - S 23 /***. BD*(1) C 15 - C 18 3.20 1.34 0.059
44. BD (1) C 19 - S 23 /***. BD*(1) C 19 - C 20 0.70 1.23 0.026
45. BD (1) C 20 - S 25 /172. RY*(1) C 2 1.49 1.80 0.046
45. BD (1) C 20 - S 25 /614. RY*(1) C 19 0.98 1.93 0.039
45. BD (1) C 20 - S 25 /***. BD*(1) C 2 - C 3 3.37 1.34 0.060
45. BD (1) C 20 - S 25 /***. BD*(1) C 18 - C 19 5.64 1.19 0.073
45. BD (1) C 20 - S 25 /***. BD*(1) C 19 - C 20 0.74 1.23 0.027
46. BD (1) S 21 - H 22 /564. RY*(3) C 17 0.67 1.50 0.028
46. BD (1) S 21 - H 22 /565. RY*(4) C 17 1.12 2.43 0.047
46. BD (1) S 21 - H 22 /***. BD*(1) C 13 - C 16 0.54 1.09 0.022
46. BD (1) S 21 - H 22 /***. BD*(2) C 16 - C 17 1.44 0.64 0.030
46. BD (1) S 21 - H 22 /***. BD*(1) C 17 - C 18 4.10 1.09 0.060
46. BD (1) S 21 - H 22 /***. BD*(1) C 17 - S 21 0.88 0.83 0.024
47. BD (1) S 23 - H 24 /615. RY*(2) C 19 0.70 1.77 0.032
47. BD (1) S 23 - H 24 /616. RY*(3) C 19 0.56 1.51 0.026
47. BD (1) S 23 - H 24 /617. RY*(4) C 19 1.03 2.46 0.045
47. BD (1) S 23 - H 24 /***. BD*(1) C 2 - C 20 0.55 1.09 0.022
47. BD (1) S 23 - H 24 /***. BD*(1) C 18 - C 19 4.15 1.08 0.060
47. BD (1) S 23 - H 24 /***. BD*(2) C 19 - C 20 1.59 0.64 0.031
47. BD (1) S 23 - H 24 /***. BD*(1) C 19 - S 23 0.81 0.83 0.023
48. BD (1) S 25 - H 26 /642. RY*(3) C 20 0.68 1.50 0.029
48. BD (1) S 25 - H 26 /643. RY*(4) C 20 1.11 2.42 0.047
48. BD (1) S 25 - H 26 /***. BD*(1) C 2 - C 20 4.08 1.09 0.060
48. BD (1) S 25 - H 26 /***. BD*(1) C 18 - C 19 0.54 1.09 0.022
48. BD (1) S 25 - H 26 /***. BD*(2) C 19 - C 20 1.47 0.64 0.030
48. BD (1) S 25 - H 26 /***. BD*(1) C 20 - S 25 0.88 0.83 0.024
49. BD (1) S 27 - H 28 /147. RY*(2) C 1 0.70 1.78 0.032
49. BD (1) S 27 - H 28 /148. RY*(3) C 1 0.57 1.51 0.026
49. BD (1) S 27 - H 28 /149. RY*(4) C 1 1.03 2.46 0.045
49. BD (1) S 27 - H 28 /996. BD*(1) C 1 - C 2 4.14 1.08 0.060
49. BD (1) S 27 - H 28 /998. BD*(2) C 1 - C 6 1.60 0.64 0.031
49. BD (1) S 27 - H 28 /999. BD*(1) C 1 - S 27 0.81 0.83 0.023

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49. BD (  1) S  27 - H  28      /***. BD*(  1) C   5 - C   6        0.55   1.09   0.022
50. BD (  1) S  29 - H  30      /278. RY*(  3) C   6              0.67   1.50   0.029
50. BD (  1) S  29 - H  30      /279. RY*(  4) C   6              1.12   2.42   0.047
50. BD (  1) S  29 - H  30      /996. BD*(  1) C   1 - C   2        0.54   1.09   0.022
50. BD (  1) S  29 - H  30      /998. BD*(  2) C   1 - C   6        1.45   0.64   0.030
50. BD (  1) S  29 - H  30      /***. BD*(  1) C   5 - C   6        4.09   1.09   0.060
50. BD (  1) S  29 - H  30      /***. BD*(  1) C   6 - S  29        0.88   0.83   0.024
51. BD (  1) S  31 - H  32      /303. RY*(  2) C   7              0.70   1.77   0.032
51. BD (  1) S  31 - H  32      /304. RY*(  3) C   7              0.56   1.51   0.026
51. BD (  1) S  31 - H  32      /305. RY*(  4) C   7              1.03   2.46   0.045
51. BD (  1) S  31 - H  32      /***. BD*(  1) C   5 - C   7        4.15   1.08   0.060
51. BD (  1) S  31 - H  32      /***. BD*(  2) C   7 - C   8        1.59   0.64   0.031
51. BD (  1) S  31 - H  32      /***. BD*(  1) C   7 - S  31        0.81   0.83   0.023
51. BD (  1) S  31 - H  32      /***. BD*(  1) C   8 - C   9        0.55   1.09   0.022
52. BD (  1) S  33 - H  34      /330. RY*(  3) C   8              0.67   1.50   0.028
52. BD (  1) S  33 - H  34      /331. RY*(  4) C   8              1.12   2.42   0.047
52. BD (  1) S  33 - H  34      /***. BD*(  1) C   5 - C   7        0.54   1.09   0.022
52. BD (  1) S  33 - H  34      /***. BD*(  2) C   7 - C   8        1.46   0.64   0.030
52. BD (  1) S  33 - H  34      /***. BD*(  1) C   8 - C   9        4.10   1.09   0.060
52. BD (  1) S  33 - H  34      /***. BD*(  1) C   8 - S  33        0.88   0.83   0.024
53. BD (  1) S  35 - H  36      /407. RY*(  2) C  11              0.69   1.77   0.031
53. BD (  1) S  35 - H  36      /408. RY*(  3) C  11              0.55   1.51   0.026
53. BD (  1) S  35 - H  36      /409. RY*(  4) C  11              1.04   2.46   0.045
53. BD (  1) S  35 - H  36      /***. BD*(  1) C   9 - C  11        4.17   1.08   0.060
53. BD (  1) S  35 - H  36      /***. BD*(  2) C  11 - C  12        1.57   0.64   0.031
53. BD (  1) S  35 - H  36      /***. BD*(  1) C  11 - S  35        0.81   0.83   0.023
53. BD (  1) S  35 - H  36      /***. BD*(  1) C  12 - C  13        0.55   1.09   0.022
54. BD (  1) S  37 - H  38      /434. RY*(  3) C  12              0.68   1.50   0.029
54. BD (  1) S  37 - H  38      /435. RY*(  4) C  12              1.11   2.42   0.047
54. BD (  1) S  37 - H  38      /***. BD*(  1) C   9 - C  11        0.54   1.09   0.022
54. BD (  1) S  37 - H  38      /***. BD*(  2) C  11 - C  12        1.47   0.64   0.030
54. BD (  1) S  37 - H  38      /***. BD*(  1) C  12 - C  13        4.07   1.09   0.060
54. BD (  1) S  37 - H  38      /***. BD*(  1) C  12 - S  37        0.88   0.83   0.024
55. BD (  1) S  39 - H  40      /537. RY*(  2) C  16              0.70   1.78   0.032
55. BD (  1) S  39 - H  40      /538. RY*(  3) C  16              0.57   1.51   0.026
55. BD (  1) S  39 - H  40      /539. RY*(  4) C  16              1.03   2.46   0.045
55. BD (  1) S  39 - H  40      /***. BD*(  1) C  13 - C  16        4.14   1.09   0.060
55. BD (  1) S  39 - H  40      /***. BD*(  2) C  16 - C  17        1.60   0.64   0.031
55. BD (  1) S  39 - H  40      /***. BD*(  1) C  16 - S  39        0.81   0.83   0.023
55. BD (  1) S  39 - H  40      /***. BD*(  1) C  17 - C  18        0.55   1.09   0.022
56. CR (  1) C   1          /999. BD*(  1) C   1 - S  27        1.19  10.68   0.101
56. CR (  1) C   1          /***. BD*(  1) C   6 - S  29        0.86  10.68   0.086
57. CR (  1) C   2          /999. BD*(  1) C   1 - S  27        0.70  10.63   0.077
57. CR (  1) C   2          /***. BD*(  1) C  20 - S  25        0.68  10.63   0.077
60. CR (  1) C   5          /***. BD*(  1) C   6 - S  29        0.68  10.63   0.077
60. CR (  1) C   5          /***. BD*(  1) C   7 - S  31        0.70  10.63   0.077
61. CR (  1) C   6          /999. BD*(  1) C   1 - S  27        0.86  10.68   0.086
61. CR (  1) C   6          /***. BD*(  1) C   5 - C   7        1.57  10.93   0.118
61. CR (  1) C   6          /***. BD*(  1) C   6 - S  29        1.17  10.68   0.100
62. CR (  1) C   7          /***. BD*(  1) C   7 - S  31        1.19  10.68   0.101
62. CR (  1) C   7          /***. BD*(  1) C   8 - S  33        0.86  10.68   0.086
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63. CR (1) C 8 /***. BD*(1) C 7 - S 31 0.86 10.68 0.086
63. CR (1) C 8 /***. BD*(1) C 8 - S 33 1.17 10.68 0.100
64. CR (1) C 9 /***. BD*(1) C 8 - S 33 0.68 10.63 0.077
64. CR (1) C 9 /***. BD*(1) C 11 - S 35 0.70 10.63 0.077
66. CR (1) C 11 /***. BD*(1) C 11 - S 35 1.19 10.68 0.101
66. CR (1) C 11 /***. BD*(1) C 12 - S 37 0.86 10.68 0.086
67. CR (1) C 12 /***. BD*(1) C 11 - S 35 0.85 10.68 0.086
67. CR (1) C 12 /***. BD*(1) C 12 - S 37 1.17 10.68 0.100
68. CR (1) C 13 /***. BD*(1) C 12 - S 37 0.69 10.63 0.077
68. CR (1) C 13 /***. BD*(1) C 16 - S 39 0.70 10.63 0.077
71. CR (1) C 16 /***. BD*(1) C 16 - S 39 1.19 10.68 0.101
71. CR (1) C 16 /***. BD*(1) C 17 - S 21 0.86 10.68 0.086
72. CR (1) C 17 /***. BD*(1) C 16 - S 39 0.86 10.68 0.086
72. CR (1) C 17 /***. BD*(1) C 17 - S 21 1.17 10.68 0.100
73. CR (1) C 18 /***. BD*(1) C 17 - S 21 0.68 10.63 0.077
73. CR (1) C 18 /***. BD*(1) C 19 - S 23 0.70 10.63 0.077
74. CR (1) C 19 /***. BD*(1) C 19 - S 23 1.19 10.68 0.101
74. CR (1) C 19 /***. BD*(1) C 20 - S 25 0.86 10.68 0.086
75. CR (1) C 20 /***. BD*(1) C 19 - S 23 0.85 10.68 0.086
75. CR (1) C 20 /***. BD*(1) C 20 - S 25 1.17 10.68 0.100
77. CR (2) S 21 /562. RY*(1) C 17 1.12 10.70 0.098
77. CR (2) S 21 /694. RY*(1) H 22 0.63 10.11 0.071
77. CR (2) S 21 /***. BD*(1) C 16 - C 17 1.68 9.94 0.116
77. CR (2) S 21 /***. BD*(1) C 17 - C 18 0.97 9.90 0.088
82. CR (2) S 23 /614. RY*(1) C 19 0.87 10.63 0.086
82. CR (2) S 23 /727. RY*(1) H 24 0.64 10.12 0.072
82. CR (2) S 23 /***. BD*(1) C 18 - C 19 1.00 9.90 0.090
82. CR (2) S 23 /***. BD*(1) C 19 - C 20 1.61 9.94 0.114
87. CR (2) S 25 /640. RY*(1) C 20 1.11 10.70 0.097
87. CR (2) S 25 /760. RY*(1) H 26 0.63 10.11 0.071
87. CR (2) S 25 /***. BD*(1) C 2 - C 20 0.97 9.90 0.088
87. CR (2) S 25 /***. BD*(1) C 19 - C 20 1.67 9.94 0.116
92. CR (2) S 27 /146. RY*(1) C 1 0.87 10.63 0.086
92. CR (2) S 27 /793. RY*(1) H 28 0.64 10.12 0.072
92. CR (2) S 27 /996. BD*(1) C 1 - C 2 1.00 9.90 0.090
92. CR (2) S 27 /997. BD*(1) C 1 - C 6 1.61 9.94 0.114
97. CR (2) S 29 /276. RY*(1) C 6 1.11 10.70 0.098
97. CR (2) S 29 /826. RY*(1) H 30 0.63 10.11 0.071
97. CR (2) S 29 /997. BD*(1) C 1 - C 6 1.67 9.94 0.116
97. CR (2) S 29 /***. BD*(1) C 5 - C 6 0.97 9.90 0.088
102. CR (2) S 31 /302. RY*(1) C 7 0.87 10.63 0.086
102. CR (2) S 31 /859. RY*(1) H 32 0.64 10.12 0.072
102. CR (2) S 31 /***. BD*(1) C 5 - C 7 1.00 9.90 0.090
102. CR (2) S 31 /***. BD*(1) C 7 - C 8 1.61 9.94 0.114
107. CR (2) S 33 /328. RY*(1) C 8 1.12 10.70 0.098
107. CR (2) S 33 /892. RY*(1) H 34 0.63 10.10 0.071
107. CR (2) S 33 /***. BD*(1) C 7 - C 8 1.68 9.94 0.116
107. CR (2) S 33 /***. BD*(1) C 8 - C 9 0.97 9.90 0.088
112. CR (2) S 35 /406. RY*(1) C 11 0.88 10.63 0.086
112. CR (2) S 35 /925. RY*(1) H 36 0.64 10.12 0.072
112. CR (2) S 35 /***. BD*(1) C 9 - C 11 1.00 9.90 0.090

112. CR (2) S 35 /***. BD*(1) C 11 - C 12 1.61 9.94 0.114
117. CR (2) S 37 /432. RY*(1) C 12 1.11 10.70 0.098
117. CR (2) S 37 /958. RY*(1) H 38 0.62 10.10 0.071
117. CR (2) S 37 /***. BD*(1) C 11 - C 12 1.67 9.94 0.116
117. CR (2) S 37 /***. BD*(1) C 12 - C 13 0.97 9.90 0.088
122. CR (2) S 39 /536. RY*(1) C 16 0.87 10.63 0.086
122. CR (2) S 39 /991. RY*(1) H 40 0.64 10.12 0.072
122. CR (2) S 39 /***. BD*(1) C 13 - C 16 1.00 9.90 0.090
122. CR (2) S 39 /***. BD*(1) C 16 - C 17 1.61 9.94 0.114
126. LP (1) S 21 /562. RY*(1) C 17 0.86 1.98 0.037
126. LP (1) S 21 /***. BD*(1) C 16 - C 17 6.05 1.21 0.077
126. LP (1) S 21 /***. BD*(1) S 23 - H 24 2.00 0.95 0.039
127. LP (2) S 21 /695. RY*(2) H 22 0.66 2.14 0.035
127. LP (2) S 21 /***. BD*(1) C 16 - C 17 2.07 0.82 0.038
127. LP (2) S 21 /***. BD*(2) C 16 - C 17 16.46 0.33 0.070
127. LP (2) S 21 /***. BD*(1) C 17 - C 18 2.30 0.78 0.039
127. LP (2) S 21 /***. BD*(1) S 23 - H 24 1.37 0.56 0.025
127. LP (2) S 21 /***. BD*(1) S 39 - H 40 1.63 0.56 0.028
128. LP (1) S 23 /614. RY*(1) C 19 0.68 1.90 0.032
128. LP (1) S 23 /***. BD*(1) C 19 - C 20 6.21 1.21 0.078
128. LP (1) S 23 /***. BD*(1) S 21 - H 22 1.57 0.94 0.034
129. LP (2) S 23 /728. RY*(2) H 24 0.64 2.15 0.034
129. LP (2) S 23 /***. BD*(1) C 18 - C 19 2.42 0.78 0.040
129. LP (2) S 23 /***. BD*(1) C 19 - C 20 1.29 0.82 0.030
129. LP (2) S 23 /***. BD*(2) C 19 - C 20 17.64 0.33 0.073
129. LP (2) S 23 /***. BD*(1) S 21 - H 22 0.67 0.56 0.018
129. LP (2) S 23 /***. BD*(1) S 25 - H 26 1.71 0.56 0.028
130. LP (1) S 25 /640. RY*(1) C 20 0.86 1.98 0.037
130. LP (1) S 25 /***. BD*(1) C 19 - C 20 6.03 1.21 0.077
130. LP (1) S 25 /***. BD*(1) S 27 - H 28 1.99 0.95 0.039
131. LP (2) S 25 /761. RY*(2) H 26 0.66 2.14 0.035
131. LP (2) S 25 /***. BD*(1) C 2 - C 20 2.34 0.78 0.039
131. LP (2) S 25 /***. BD*(1) C 19 - C 20 2.10 0.82 0.038
131. LP (2) S 25 /***. BD*(2) C 19 - C 20 16.30 0.33 0.070
131. LP (2) S 25 /***. BD*(1) S 23 - H 24 1.66 0.56 0.028
131. LP (2) S 25 /***. BD*(1) S 27 - H 28 1.39 0.56 0.025
132. LP (1) S 27 /146. RY*(1) C 1 0.67 1.91 0.032
132. LP (1) S 27 /997. BD*(1) C 1 - C 6 6.21 1.21 0.078
132. LP (1) S 27 /***. BD*(1) S 25 - H 26 1.56 0.94 0.034
133. LP (2) S 27 /794. RY*(2) H 28 0.64 2.15 0.034
133. LP (2) S 27 /996. BD*(1) C 1 - C 2 2.45 0.78 0.040
133. LP (2) S 27 /997. BD*(1) C 1 - C 6 1.30 0.82 0.030
133. LP (2) S 27 /998. BD*(2) C 1 - C 6 17.57 0.33 0.072
133. LP (2) S 27 /***. BD*(1) S 25 - H 26 0.67 0.56 0.018
133. LP (2) S 27 /***. BD*(1) S 29 - H 30 1.74 0.56 0.028
134. LP (1) S 29 /276. RY*(1) C 6 0.86 1.97 0.037
134. LP (1) S 29 /997. BD*(1) C 1 - C 6 6.04 1.21 0.077
134. LP (1) S 29 /***. BD*(1) S 31 - H 32 2.00 0.95 0.039
135. LP (2) S 29 /827. RY*(2) H 30 0.66 2.14 0.035
135. LP (2) S 29 /997. BD*(1) C 1 - C 6 2.08 0.82 0.038
135. LP (2) S 29 /998. BD*(2) C 1 - C 6 16.39 0.33 0.070

135. LP (2) S 29 /***. BD*(1) C 5 - C 6 2.32 0.78 0.039
135. LP (2) S 29 /***. BD*(1) S 27 - H 28 1.64 0.56 0.028
135. LP (2) S 29 /***. BD*(1) S 31 - H 32 1.38 0.56 0.025
136. LP (1) S 31 /302. RY*(1) C 7 0.68 1.91 0.032
136. LP (1) S 31 /***. BD*(1) C 7 - C 8 6.22 1.21 0.078
136. LP (1) S 31 /***. BD*(1) S 29 - H 30 1.56 0.94 0.034
137. LP (2) S 31 /860. RY*(2) H 32 0.64 2.15 0.034
137. LP (2) S 31 /***. BD*(1) C 5 - C 7 2.42 0.78 0.040
137. LP (2) S 31 /***. BD*(1) C 7 - C 8 1.28 0.82 0.030
137. LP (2) S 31 /***. BD*(2) C 7 - C 8 17.64 0.33 0.073
137. LP (2) S 31 /***. BD*(1) S 29 - H 30 0.67 0.56 0.018
137. LP (2) S 31 /***. BD*(1) S 33 - H 34 1.74 0.55 0.028
138. LP (1) S 33 /328. RY*(1) C 8 0.86 1.98 0.037
138. LP (1) S 33 /***. BD*(1) C 7 - C 8 6.04 1.21 0.077
138. LP (1) S 33 /***. BD*(1) S 35 - H 36 2.01 0.95 0.039
139. LP (2) S 33 /893. RY*(2) H 34 0.66 2.14 0.035
139. LP (2) S 33 /***. BD*(1) C 7 - C 8 2.08 0.82 0.038
139. LP (2) S 33 /***. BD*(2) C 7 - C 8 16.39 0.33 0.070
139. LP (2) S 33 /***. BD*(1) C 8 - C 9 2.32 0.78 0.039
139. LP (2) S 33 /***. BD*(1) S 31 - H 32 1.66 0.56 0.028
139. LP (2) S 33 /***. BD*(1) S 35 - H 36 1.38 0.56 0.025
140. LP (1) S 35 /406. RY*(1) C 11 0.69 1.91 0.032
140. LP (1) S 35 /***. BD*(1) C 11 - C 12 6.22 1.21 0.078
140. LP (1) S 35 /***. BD*(1) S 33 - H 34 1.56 0.94 0.034
141. LP (2) S 35 /926. RY*(2) H 36 0.64 2.15 0.034
141. LP (2) S 35 /***. BD*(1) C 9 - C 11 2.40 0.78 0.039
141. LP (2) S 35 /***. BD*(1) C 11 - C 12 1.26 0.82 0.029
141. LP (2) S 35 /***. BD*(2) C 11 - C 12 17.75 0.33 0.073
141. LP (2) S 35 /***. BD*(1) S 33 - H 34 0.66 0.55 0.017
141. LP (2) S 35 /***. BD*(1) S 37 - H 38 1.71 0.55 0.028
142. LP (1) S 37 /432. RY*(1) C 12 0.86 1.98 0.037
142. LP (1) S 37 /***. BD*(1) C 11 - C 12 6.03 1.21 0.077
142. LP (1) S 37 /***. BD*(1) S 39 - H 40 1.99 0.95 0.039
143. LP (2) S 37 /959. RY*(2) H 38 0.66 2.14 0.035
143. LP (2) S 37 /***. BD*(1) C 11 - C 12 2.10 0.82 0.038
143. LP (2) S 37 /***. BD*(2) C 11 - C 12 16.28 0.33 0.070
143. LP (2) S 37 /***. BD*(1) C 12 - C 13 2.34 0.78 0.039
143. LP (2) S 37 /***. BD*(1) S 35 - H 36 1.70 0.56 0.028
143. LP (2) S 37 /***. BD*(1) S 39 - H 40 1.38 0.56 0.025
144. LP (1) S 39 /536. RY*(1) C 16 0.67 1.90 0.032
144. LP (1) S 39 /***. BD*(1) C 16 - C 17 6.21 1.21 0.078
144. LP (1) S 39 /***. BD*(1) S 37 - H 38 1.56 0.94 0.034
145. LP (2) S 39 /992. RY*(2) H 40 0.64 2.15 0.034
145. LP (2) S 39 /***. BD*(1) C 13 - C 16 2.44 0.78 0.040
145. LP (2) S 39 /***. BD*(1) C 16 - C 17 1.29 0.82 0.030
145. LP (2) S 39 /***. BD*(2) C 16 - C 17 17.57 0.33 0.072
145. LP (2) S 39 /***. BD*(1) S 21 - H 22 1.75 0.56 0.028
145. LP (2) S 39 /***. BD*(1) S 37 - H 38 0.67 0.55 0.018
998. BD*(2) C 1 - C 6 /765. RY*(1) S 27 0.86 0.87 0.058
998. BD*(2) C 1 - C 6 /798. RY*(1) S 29 0.88 0.87 0.058
998. BD*(2) C 1 - C 6 /***. BD*(1) S 27 - H 28 0.72 0.23 0.026

998. BD*(2) C 1 - C 6	/***. BD*(1) S 29 - H 30	0.89	0.22	0.029
***. BD*(2) C 7 - C 8	/831. RY*(1) S 31	0.86	0.87	0.058
***. BD*(2) C 7 - C 8	/864. RY*(1) S 33	0.88	0.87	0.058
***. BD*(2) C 7 - C 8	/***. BD*(1) S 31 - H 32	0.71	0.23	0.026
***. BD*(2) C 7 - C 8	/***. BD*(1) S 33 - H 34	0.89	0.22	0.029
***. BD*(2) C 11 - C 12	/897. RY*(1) S 35	0.86	0.87	0.058
***. BD*(2) C 11 - C 12	/930. RY*(1) S 37	0.88	0.87	0.058
***. BD*(2) C 11 - C 12	/***. BD*(1) S 35 - H 36	0.70	0.23	0.026
***. BD*(2) C 11 - C 12	/***. BD*(1) S 37 - H 38	0.89	0.22	0.029
***. BD*(2) C 16 - C 17	/666. RY*(1) S 21	0.88	0.87	0.058
***. BD*(2) C 16 - C 17	/963. RY*(1) S 39	0.86	0.87	0.058
***. BD*(2) C 16 - C 17	/***. BD*(1) S 21 - H 22	0.88	0.22	0.029
***. BD*(2) C 16 - C 17	/***. BD*(1) S 39 - H 40	0.71	0.23	0.026
***. BD*(2) C 19 - C 20	/699. RY*(1) S 23	0.86	0.87	0.058
***. BD*(2) C 19 - C 20	/732. RY*(1) S 25	0.88	0.87	0.058
***. BD*(2) C 19 - C 20	/***. BD*(1) S 23 - H 24	0.71	0.23	0.026
***. BD*(2) C 19 - C 20	/***. BD*(1) S 25 - H 26	0.89	0.22	0.029

7. Dihedral Scan for 4

To probe the influence of the auxochrome effect on bowl depth, we wanted to examine the change in bowl depth as a function of changing the C_{rim}-C_{rim}-S-R dihedral angles. However, changing these angles could significantly enhance steric congestion between neighboring substituents in **6**. To best isolate the electronic effects and minimize as far as possible steric hindrance between substituents, we turned to study 1,3,5,7,9-pentathiolcorannulene (**4**, R = H). In this molecule, electronic effects are expected to play a more significant role in determining the bowl depth, relative to either decasubstituted corannulenes or to pentasubstituted corannulenes with larger substituents. We calculated the optimized structures of **4**, constricted to C_{5v} symmetry, with dihedral C_{rim}-C_{rim}-S-H angles ranging between 0° and 360° at the M06-2X/def2-TZVP level of theory and checked the changes in bowl depth and in other geometrical parameters (Figure S1).

From inspection of the bond lengths, we can observe minima in the C-S and S-H lengths close to 0° and 180°, while there is a maximum in length for the rim C-C bond around these angles. This is indicative of the expected conjugation between the p orbital of sulfur and the corannulene π system. This conjugation roughly coincides with the two minima in energy of this molecule. However, the bowl depth has only one minimum, around 160°. For the structure with the minimum bowl depth the distance SH-H_{cor} is 2.087 Å, shorter than twice the van der Waals (vDW) radius of hydrogen, suggesting that Pauli repulsion can still play a role in this molecule. As a support for this, we see a maximum in energy and in the C-S-H angle around 160°. In this region both conjugation and steric repulsion are expected to reduce the bowl depth. For the structure at the energy minimum with a dihedral angle of 9°, the shortest SH-H_{cor} distance is 2.289 Å, so the steric hindrance is smaller. We do not observe a low bowl depth in this area, indicating that the conjugation between the sulfur orbitals and the aromatic system probably has an effect on the energy, but it does not exert a strong effect on the bowl depth in this molecule.

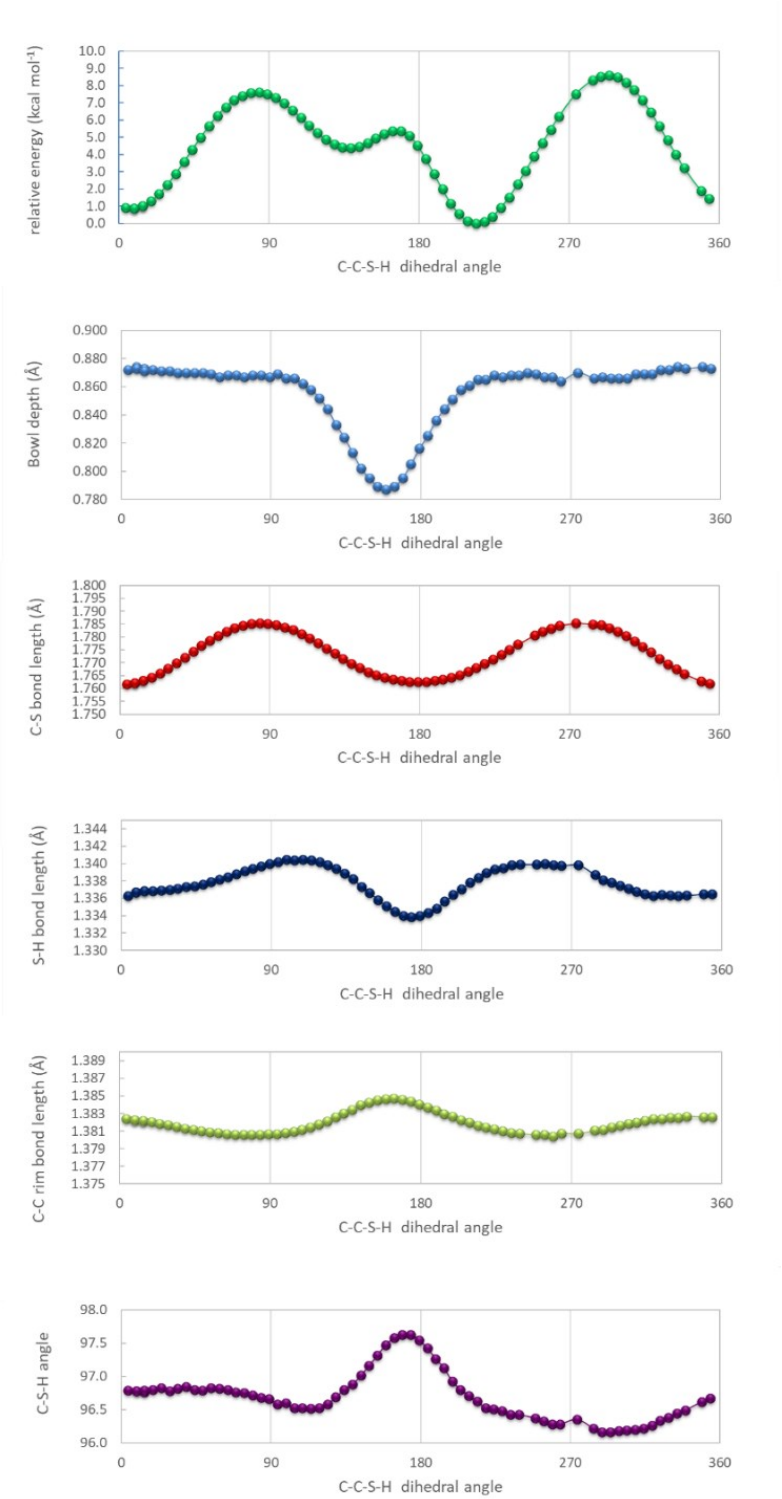

Figure S1 The changes in relative energy, bowl depth, C_{rim}-S, S-H, and C_{rim}-C_{rim} bond lengths as a function of the dihedral angle C_{rim}-C_{rim}-S-H in **4** (M06-2X/def2-TZVP).

8. Cartesian coordinates of calculated molecules

Coordinates of compound **1** optimized at different DFT functionals:

1 from M06-2X/def2-TZVP:

C	1.044334000000	3.069738000000	-0.259623000000
C	2.223944000000	2.359677000000	-0.259685000000
H	3.120341000000	2.845463000000	-0.626986000000
C	2.273230000000	0.962758000000	0.098770000000
C	3.242321000000	-0.044686000000	-0.259300000000
C	2.931501000000	-1.385982000000	-0.259145000000
H	3.670432000000	-2.088360000000	-0.626717000000
C	1.618100000000	-1.864491000000	0.099180000000
C	0.959432000000	-3.097327000000	-0.259472000000
C	-0.412275000000	-3.216183000000	-0.259549000000
H	-0.851973000000	-4.135818000000	-0.627537000000
C	-1.273200000000	-2.115012000000	0.098997000000
C	-2.649275000000	-1.869571000000	-0.259393000000
C	-3.186205000000	-0.601797000000	-0.259313000000
H	-4.196897000000	-0.467793000000	-0.626718000000
C	-2.404997000000	0.557266000000	0.099008000000
C	-2.596815000000	1.941748000000	-0.259415000000
C	-1.556954000000	2.844170000000	-0.259594000000
H	-1.741863000000	3.846696000000	-0.627275000000
C	-0.213179000000	2.459416000000	0.098678000000
C	-0.103750000000	1.197795000000	0.628870000000
C	1.107094000000	0.468912000000	0.628900000000
C	0.787986000000	-0.907942000000	0.629051000000
C	-0.620072000000	-1.029988000000	0.629070000000
C	-1.171196000000	0.271457000000	0.629017000000
H	4.214909000000	0.261147000000	-0.626719000000
H	1.550773000000	-3.927606000000	-0.627443000000
H	-3.256356000000	-2.688593000000	-0.626931000000
H	-3.563418000000	2.265928000000	-0.626840000000
H	1.053916000000	4.089193000000	-0.627143000000

1 from B3LYP/def2-TZVP:

C	-3.181506000000	0.664016000000	-0.256759000000
C	-2.617194000000	1.926911000000	-0.256819000000
H	-3.212089000000	2.756744000000	-0.620872000000
C	-1.235610000000	2.146676000000	0.097311000000
C	-0.351609000000	3.230976000000	-0.256772000000
C	1.023868000000	3.084567000000	-0.256831000000
H	1.629250000000	3.906793000000	-0.620865000000
C	1.659799000000	1.838478000000	0.097221000000
C	2.964181000000	1.332794000000	-0.256862000000
C	3.250033000000	-0.020588000000	-0.256646000000
H	4.219107000000	-0.342281000000	-0.620610000000
C	2.261417000000	-1.010436000000	0.097352000000
C	2.183560000000	-2.407215000000	-0.256798000000
C	0.984735000000	-3.097247000000	-0.256863000000

H	0.978279000000	-4.118292000000	-0.620850000000
C	-0.262167000000	-2.462956000000	0.097207000000
C	-1.614643000000	-2.820559000000	-0.256900000000
C	-2.641379000000	-1.893649000000	-0.256826000000
H	-3.614443000000	-2.203024000000	-0.620827000000
C	-2.423462000000	-0.511774000000	0.097327000000
C	-1.175917000000	-0.248332000000	0.623315000000
C	-0.599548000000	1.041614000000	0.623288000000
C	0.805367000000	0.892091000000	0.623246000000
C	1.097271000000	-0.490262000000	0.623277000000
C	-0.127219000000	-1.195086000000	0.623234000000
H	-0.770352000000	4.162213000000	-0.620795000000
H	3.720463000000	2.018779000000	-0.620894000000
H	3.069713000000	-2.914500000000	-0.620743000000
H	-1.823245000000	-3.820064000000	-0.620952000000
H	-4.196551000000	0.553537000000	-0.620814000000

1 from B3LYP-D3BJ/def2-TZVP:

C	1.899474000000	-2.626131000000	-0.267491000000
C	0.632929000000	-3.178673000000	-0.267582000000
H	0.508218000000	-4.185643000000	-0.647721000000
C	-0.532155000000	-2.414208000000	0.101957000000
C	-1.910641000000	-2.617913000000	-0.267683000000
C	-2.827586000000	-1.584177000000	-0.267290000000
H	-3.823783000000	-1.776671000000	-0.647535000000
C	-2.460669000000	-0.239960000000	0.102647000000
C	-3.080399000000	1.008088000000	-0.267031000000
C	-2.380400000000	2.199481000000	-0.267523000000
H	-2.871338000000	3.087357000000	-0.647913000000
C	-0.988542000000	2.265940000000	0.102166000000
C	0.006873000000	3.241102000000	-0.267447000000
C	1.356295000000	2.943589000000	-0.267698000000
H	2.049044000000	3.684916000000	-0.647927000000
C	1.849585000000	1.640386000000	0.102059000000
C	3.084669000000	0.994975000000	-0.267310000000
C	3.218762000000	-0.380331000000	-0.267337000000
H	4.137916000000	-0.810139000000	-0.647423000000
C	2.131640000000	-1.252124000000	0.102102000000
C	1.038892000000	-0.610226000000	0.648499000000
C	-0.259313000000	-1.176628000000	0.648492000000
C	-1.199136000000	-0.116972000000	0.648749000000
C	-0.481740000000	1.104313000000	0.648578000000
C	0.901447000000	0.799482000000	0.648545000000
H	-2.220810000000	-3.583940000000	-0.647999000000
H	-4.095006000000	1.004493000000	-0.647306000000
H	-0.310088000000	4.204974000000	-0.647632000000
H	3.903473000000	1.594245000000	-0.647417000000
H	2.722465000000	-3.219673000000	-0.647544000000

1 from B97D3/def2-TZVP:

C	-2.521680000000	2.047707000000	-0.274368000000

C	-1.435280000000	2.914071000000	-0.274471000000
H	-1.572334000000	3.919301000000	-0.668559000000
C	-0.111295000000	2.478487000000	0.104575000000
C	1.168274000000	3.030978000000	-0.274498000000
C	2.327996000000	2.265475000000	-0.274410000000
H	3.241700000000	2.706459000000	-0.668436000000
C	2.322849000000	0.871729000000	0.104765000000
C	3.243781000000	-0.174517000000	-0.274166000000
C	2.874034000000	-1.513976000000	-0.274328000000
H	3.575745000000	-2.246701000000	-0.668397000000
C	1.546829000000	-1.939683000000	0.104640000000
C	0.836391000000	-3.138835000000	-0.274440000000
C	-0.551774000000	-3.201182000000	-0.274452000000
H	-1.031776000000	-4.094944000000	-0.668618000000
C	-1.366791000000	-2.070524000000	0.104620000000
C	-2.726767000000	-1.765435000000	-0.274452000000
C	-3.215077000000	-0.464496000000	-0.274233000000
H	-4.213449000000	-0.284166000000	-0.668332000000
C	-2.391597000000	0.660048000000	0.104770000000
C	-1.166221000000	0.321904000000	0.666900000000
C	-0.054233000000	1.208682000000	0.666833000000
C	1.132729000000	0.425161000000	0.666949000000
C	0.754351000000	-0.945867000000	0.666949000000
C	-0.666505000000	-1.009697000000	0.666932000000
H	1.214659000000	4.044439000000	-0.668618000000
H	4.222008000000	0.094534000000	-0.668203000000
H	1.394584000000	-3.986005000000	-0.668537000000
H	-3.359973000000	-2.558077000000	-0.668595000000
H	-3.471243000000	2.404989000000	-0.668401000000

1 from wB97x-D/def2-TZVP:

C	-1.815549000000	2.683157000000	-0.257174000000
C	-0.538104000000	3.194639000000	-0.257227000000
H	-0.386395000000	4.204333000000	-0.621200000000
C	0.604106000000	2.391182000000	0.097667000000
C	1.990881000000	2.555792000000	-0.257351000000
C	2.872081000000	1.498938000000	-0.257239000000
H	3.879267000000	1.666595000000	-0.621158000000
C	2.460841000000	0.164398000000	0.097758000000
C	3.045985000000	-1.103605000000	-0.257100000000
C	2.313147000000	-2.268223000000	-0.257145000000
H	2.783880000000	-3.174289000000	-0.621066000000
C	0.916790000000	-2.289554000000	0.097779000000
C	-0.108311000000	-3.237844000000	-0.257219000000
C	-1.442435000000	-2.900840000000	-0.257298000000
H	-2.158671000000	-3.628482000000	-0.621353000000
C	-1.894241000000	-1.579457000000	0.097702000000
C	-3.112901000000	-0.897546000000	-0.257252000000
C	-3.204655000000	0.475439000000	-0.257182000000
H	-4.118053000000	0.931788000000	-0.621118000000
C	-2.087541000000	1.313431000000	0.097762000000

C	-1.015678000000	0.639098000000	0.623765000000
C	0.293949000000	1.163455000000	0.623734000000
C	1.197323000000	0.080007000000	0.623800000000
C	0.445980000000	-1.113978000000	0.623806000000
C	-0.921706000000	-0.768461000000	0.623765000000
H	2.336909000000	3.516376000000	-0.621403000000
H	4.066515000000	-1.135887000000	-0.621072000000
H	0.176430000000	-4.218337000000	-0.621293000000
H	-3.957442000000	-1.471339000000	-0.621269000000
H	-2.622217000000	3.309079000000	-0.621172000000

Coordinates of compound **2** optimized at different DFT functionals:

2 from M06-2X/def2-TZVP:

C	-0.071779000000	1.197381000000	-0.890827000000
C	-1.160941000000	0.301726000000	-0.890917000000
C	-0.645684000000	-1.010902000000	-0.890868000000
C	0.761893000000	-0.926475000000	-0.890764000000
C	1.116595000000	0.438299000000	-0.890758000000
C	-0.168868000000	2.487951000000	-0.450576000000
C	-1.536756000000	2.887726000000	-0.184509000000
H	-1.728169000000	3.915817000000	0.069822000000
C	-2.623212000000	2.030018000000	-0.172263000000
C	-4.014150000000	2.557774000000	0.192313000000
C	-5.019875000000	2.157944000000	-0.898984000000
H	-4.740213000000	2.610984000000	-1.851956000000
H	-6.017462000000	2.513062000000	-0.632195000000
H	-5.073223000000	1.081793000000	-1.049312000000
C	-4.444971000000	1.996764000000	1.558355000000
H	-4.473952000000	0.909578000000	1.579730000000
H	-5.440373000000	2.367941000000	1.812677000000
H	-3.749789000000	2.324458000000	2.333439000000
C	-4.061693000000	4.084724000000	0.302685000000
H	-3.445873000000	4.455343000000	1.124177000000
H	-5.089387000000	4.393808000000	0.499780000000
H	-3.737560000000	4.565545000000	-0.622182000000
C	-2.418352000000	0.608211000000	-0.450690000000
C	-3.221296000000	-0.569199000000	-0.184726000000
H	-4.258279000000	-0.433612000000	0.069380000000
C	-2.741301000000	-1.867504000000	-0.172381000000
C	-3.673114000000	-3.027222000000	0.192209000000
C	-3.272920000000	-3.610002000000	1.558442000000
H	-3.933700000000	-4.441762000000	1.813038000000
H	-3.369586000000	-2.847301000000	2.333271000000
H	-2.247979000000	-3.973727000000	1.579920000000
C	-3.603498000000	-4.107528000000	-0.898841000000
H	-2.596480000000	-4.490830000000	-1.049027000000
H	-3.947918000000	-3.701790000000	-1.851919000000
H	-4.249501000000	-4.946500000000	-0.631870000000
C	-5.140032000000	-2.600494000000	0.302194000000
H	-5.302442000000	-1.900159000000	1.123529000000

H	-5.751643000000	-3.482331000000	0.499266000000
H	-5.496912000000	-2.143767000000	-0.622835000000
C	-1.325743000000	-2.112042000000	-0.450635000000
C	-0.454119000000	-3.239524000000	-0.184552000000
H	-0.903587000000	-4.183786000000	0.069665000000
C	0.928976000000	-3.184231000000	-0.172189000000
C	1.744058000000	-4.428752000000	0.192451000000
C	0.885006000000	-5.692036000000	0.302767000000
H	0.168838000000	-5.629882000000	1.124158000000
H	1.534761000000	-6.546123000000	0.499996000000
H	0.340288000000	-5.890541000000	-0.622177000000
C	2.792828000000	-4.696540000000	-0.898724000000
H	2.300376000000	-4.899290000000	-1.851609000000
H	3.391446000000	-5.569883000000	-0.631504000000
H	3.468252000000	-3.857115000000	-1.049469000000
C	2.422205000000	-4.228053000000	1.558556000000
H	3.085134000000	-3.365876000000	1.579776000000
H	3.008847000000	-5.113621000000	1.813291000000
H	1.667116000000	-4.083871000000	2.333451000000
C	1.598989000000	-1.913535000000	-0.450542000000
C	2.940666000000	-1.432967000000	-0.184598000000
H	3.699883000000	-2.152201000000	0.069483000000
C	3.315492000000	-0.100479000000	-0.172301000000
C	4.751027000000	0.290119000000	0.192122000000
C	5.687006000000	-0.917294000000	0.302267000000
H	5.406468000000	-1.579293000000	1.123544000000
H	6.700090000000	-0.563378000000	0.499608000000
H	5.707463000000	-1.496559000000	-0.622758000000
C	5.329536000000	1.204871000000	-0.899143000000
H	6.345351000000	1.503959000000	-0.632417000000
H	4.740097000000	2.106845000000	-1.049366000000
H	5.369489000000	0.674065000000	-1.852170000000
C	4.769902000000	0.997060000000	1.558254000000
H	4.400321000000	0.323193000000	2.333316000000
H	4.154125000000	1.893507000000	1.579821000000
H	5.793334000000	1.282064000000	1.812493000000
C	2.314011000000	0.929408000000	-0.450515000000
C	2.271529000000	2.353904000000	-0.184460000000
H	3.190171000000	2.853646000000	0.069796000000
C	1.120078000000	3.122141000000	-0.172205000000
C	1.192193000000	4.608077000000	0.192370000000
C	2.629731000000	5.125126000000	0.302621000000
H	3.172586000000	4.653899000000	1.124018000000
H	2.606164000000	6.198017000000	0.499801000000
H	3.187066000000	4.965462000000	-0.622322000000
C	0.501057000000	5.441076000000	-0.898847000000
H	1.018240000000	5.315127000000	-1.851873000000
H	0.530552000000	6.499568000000	-0.632010000000
H	-0.538933000000	5.159304000000	-1.049105000000
C	0.525626000000	4.844445000000	1.558473000000
H	-0.517265000000	4.535920000000	1.579954000000

H	0.570943000000	5.905846000000	1.812753000000
H	1.052227000000	4.284642000000	2.333533000000

2 from B3LYP/def2-TZVP:

C	-1.195978000000	-0.074020000000	-0.838062000000
C	-0.299146000000	-1.160215000000	-0.837787000000
C	1.011024000000	-0.642922000000	-0.837737000000
C	0.923907000000	0.762964000000	-0.837632000000
C	-0.440088000000	1.114602000000	-0.837843000000
C	-2.497362000000	-0.177130000000	-0.415165000000
C	-2.890944000000	-1.549467000000	-0.161431000000
H	-3.919731000000	-1.745041000000	0.084059000000
C	-2.030095000000	-2.643308000000	-0.152092000000
C	-2.576477000000	-4.045996000000	0.179536000000
C	-2.168052000000	-5.039731000000	-0.930351000000
H	-2.593861000000	-4.737492000000	-1.889365000000
H	-2.543131000000	-6.038612000000	-0.695266000000
H	-1.089933000000	-5.109700000000	-1.058061000000
C	-2.035458000000	-4.517846000000	1.548459000000
H	-0.948977000000	-4.560371000000	1.580500000000
H	-2.417009000000	-5.515889000000	1.778104000000
H	-2.361956000000	-3.841492000000	2.340943000000
C	-4.112010000000	-4.090375000000	0.267566000000
H	-4.498325000000	-3.485756000000	1.089864000000
H	-4.429103000000	-5.119271000000	0.447840000000
H	-4.583576000000	-3.756586000000	-0.658530000000
C	-0.603213000000	-2.429638000000	-0.414475000000
C	0.580346000000	-3.228062000000	-0.160761000000
H	0.448411000000	-4.266842000000	0.085189000000
C	1.886706000000	-2.747453000000	-0.151992000000
C	3.051971000000	-3.700611000000	0.179234000000
C	3.668028000000	-3.332438000000	1.548279000000
H	4.499368000000	-4.003803000000	1.777535000000
H	2.924020000000	-3.434326000000	2.340845000000
H	4.044193000000	-2.312273000000	1.580803000000
C	4.123192000000	-3.618978000000	-0.930713000000
H	4.522838000000	-2.615219000000	-1.058289000000
H	3.704108000000	-3.930356000000	-1.889767000000
H	4.957287000000	-4.284433000000	-0.695815000000
C	2.619716000000	-5.174729000000	0.266831000000
H	1.925352000000	-5.355500000000	1.089120000000
H	3.500285000000	-5.794296000000	0.446878000000
H	2.156521000000	-5.519801000000	-0.659341000000
C	2.124402000000	-1.324394000000	-0.414582000000
C	3.249523000000	-0.445492000000	-0.161165000000
H	4.196847000000	-0.891909000000	0.084245000000
C	3.196109000000	0.945435000000	-0.152305000000
C	4.462962000000	1.758981000000	0.178397000000
C	5.731202000000	0.891990000000	0.265007000000
H	5.688942000000	0.175619000000	1.087199000000
H	6.592891000000	1.537697000000	0.444520000000

H	5.915419000000	0.344910000000	-0.661383000000
C	4.715923000000	2.803094000000	-0.931575000000
H	4.881805000000	2.308327000000	-1.890778000000
H	5.606857000000	3.390489000000	-0.697234000000
H	3.884908000000	3.493612000000	-1.058564000000
C	4.304043000000	2.458319000000	1.547671000000
H	3.450053000000	3.131289000000	1.580863000000
H	5.199592000000	3.041429000000	1.776532000000
H	4.171517000000	1.718999000000	2.340090000000
C	1.916060000000	1.611224000000	-0.414397000000
C	1.427737000000	2.952727000000	-0.160424000000
H	2.144963000000	3.715549000000	0.085757000000
C	0.088392000000	3.331805000000	-0.151755000000
C	-0.293895000000	4.787756000000	0.180075000000
C	0.922617000000	5.725707000000	0.269215000000
H	1.590133000000	5.462768000000	1.091571000000
H	0.574742000000	6.744520000000	0.450010000000
H	1.500677000000	5.733254000000	-0.656649000000
C	-1.207356000000	5.352293000000	-0.930362000000
H	-1.491190000000	6.380788000000	-0.695085000000
H	-2.120572000000	4.775264000000	-1.059228000000
H	-0.684312000000	5.358463000000	-1.888885000000
C	-1.009799000000	4.851463000000	1.548549000000
H	-0.348799000000	4.495702000000	2.341396000000
H	-1.914136000000	4.247739000000	1.579974000000
H	-1.287353000000	5.883263000000	1.778219000000
C	-0.940364000000	2.320328000000	-0.414705000000
C	-2.367273000000	2.270542000000	-0.161491000000
H	-2.871333000000	3.188492000000	0.083921000000
C	-3.141596000000	1.113849000000	-0.152867000000
C	-4.644572000000	1.199879000000	0.178333000000
C	-5.161466000000	2.646502000000	0.265791000000
H	-4.705977000000	3.201107000000	1.087931000000
H	-6.238013000000	2.630072000000	0.445928000000
H	-4.989662000000	3.197806000000	-0.660487000000
C	-5.463150000000	0.504024000000	-0.931588000000
H	-5.307361000000	1.002446000000	-1.890585000000
H	-6.529088000000	0.551753000000	-0.696604000000
H	-5.196213000000	-0.542861000000	-1.059330000000
C	-4.926226000000	0.539851000000	1.547435000000
H	-4.630577000000	-0.506494000000	1.579914000000
H	-5.993384000000	0.594012000000	1.776876000000
H	-4.384208000000	1.059765000000	2.339898000000

2 from B3LYP-D3BJ/def2-TZVP:

C	0.885788000000	-0.813056000000	-0.953304000000
C	1.046981000000	0.591198000000	-0.953235000000
C	-0.238732000000	1.178412000000	-0.953146000000
C	-1.194548000000	0.137094000000	-0.953180000000
C	-0.499553000000	-1.093705000000	-0.953262000000
C	1.850875000000	-1.670768000000	-0.483386000000

C	3.104908000000	-1.008433000000	-0.197295000000
H	3.947644000000	-1.613723000000	0.081494000000
C	3.292343000000	0.367166000000	-0.185452000000
C	4.657599000000	0.949668000000	0.204609000000
C	5.119856000000	1.953183000000	-0.870157000000
H	5.232666000000	1.451428000000	-1.832884000000
H	6.087004000000	2.378313000000	-0.593587000000
H	4.419577000000	2.773412000000	-1.007713000000
C	4.560180000000	1.639071000000	1.581367000000
H	3.829042000000	2.443438000000	1.596967000000
H	5.529978000000	2.058168000000	1.859251000000
H	4.270773000000	0.915462000000	2.345381000000
C	5.753359000000	-0.120705000000	0.314742000000
H	5.558580000000	-0.828474000000	1.121737000000
H	6.706016000000	0.364776000000	0.532232000000
H	5.867819000000	-0.679272000000	-0.615608000000
C	2.161001000000	1.244007000000	-0.483389000000
C	1.918596000000	2.641281000000	-0.197079000000
H	2.754617000000	3.255863000000	0.081631000000
C	0.668159000000	3.244442000000	-0.184813000000
C	0.535880000000	4.722545000000	0.206383000000
C	-0.150099000000	4.841466000000	1.583210000000
H	-0.249670000000	5.893030000000	1.861912000000
H	0.448900000000	4.342382000000	2.346880000000
H	-1.140753000000	4.394049000000	1.598408000000
C	-0.275753000000	5.473133000000	-0.867725000000
H	-1.271873000000	5.060047000000	-1.006198000000
H	0.236687000000	5.426978000000	-1.830332000000
H	-0.382026000000	6.523881000000	-0.589833000000
C	1.892337000000	5.433977000000	0.317401000000
H	2.505173000000	5.029254000000	1.124093000000
H	1.724863000000	6.489805000000	0.535889000000
H	2.459110000000	5.371147000000	-0.612896000000
C	-0.515301000000	2.439528000000	-0.482988000000
C	-1.919137000000	2.640784000000	-0.196843000000
H	-2.245275000000	3.625764000000	0.082044000000
C	-2.879337000000	1.638079000000	-0.185178000000
C	-4.326196000000	1.969327000000	0.205179000000
C	-4.583718000000	3.479391000000	0.314693000000
H	-4.011357000000	3.937558000000	1.122558000000
H	-5.640139000000	3.646629000000	0.530422000000
H	-4.346490000000	3.998443000000	-0.615316000000
C	-5.290547000000	1.428489000000	-0.868752000000
H	-5.087743000000	1.900467000000	-1.831794000000
H	-6.322745000000	1.652798000000	-0.591533000000
H	-5.205825000000	0.353292000000	-1.006019000000
C	-4.651864000000	1.354820000000	1.582332000000
H	-4.532666000000	0.274370000000	1.598162000000
H	-5.682825000000	1.585382000000	1.860458000000
H	-3.992382000000	1.770678000000	2.346002000000
C	-2.479454000000	0.263760000000	-0.483138000000

C	-3.104578000000	-1.009149000000	-0.196705000000
H	-4.142061000000	-1.014955000000	0.082420000000
C	-2.447614000000	-2.232186000000	-0.184972000000
C	-3.209715000000	-3.505902000000	0.205279000000
C	-4.725295000000	-3.284003000000	0.316131000000
H	-4.983320000000	-2.597423000000	1.123707000000
H	-5.210631000000	-4.236837000000	0.533188000000
H	-5.146554000000	-2.898729000000	-0.613777000000
C	-2.994345000000	-4.589429000000	-0.869612000000
H	-3.526465000000	-5.501984000000	-0.592660000000
H	-1.945715000000	-4.841030000000	-1.007926000000
H	-3.381321000000	-4.249931000000	-1.832069000000
C	-2.725188000000	-4.006541000000	1.581843000000
H	-2.915862000000	-3.251010000000	2.345968000000
H	-1.660948000000	-4.227837000000	1.597028000000
H	-3.263558000000	-4.915500000000	1.859906000000
C	-1.017047000000	-2.276630000000	-0.483344000000
C	0.000447000000	-3.264607000000	-0.197248000000
H	-0.314583000000	-4.253238000000	0.081469000000
C	1.366606000000	-3.017579000000	-0.185133000000
C	2.342458000000	-4.135535000000	0.206371000000
C	1.663068000000	-5.508330000000	0.317889000000
H	0.929880000000	-5.540932000000	1.125050000000
H	2.419186000000	-6.264155000000	0.535972000000
H	1.167005000000	-5.790656000000	-0.612082000000
C	3.440325000000	-4.266246000000	-0.867626000000
H	2.998665000000	-4.530218000000	-1.830217000000
H	4.143630000000	-5.054019000000	-0.589464000000
H	4.003739000000	-3.346766000000	-1.006235000000
C	2.967383000000	-3.828045000000	1.583076000000
H	3.506973000000	-2.884392000000	1.597479000000
H	3.665109000000	-4.620773000000	1.862591000000
H	2.189381000000	-3.774790000000	2.346594000000

2 from B97D3/def2-TZVP:

C	1.044742000000	0.605498000000	-0.991392000000
C	-0.252931000000	1.180643000000	-0.991444000000
C	-1.200932000000	0.124215000000	-0.991587000000
C	-0.489159000000	-1.103854000000	-0.991576000000
C	0.898736000000	-0.806421000000	-0.991463000000
C	2.154035000000	1.273196000000	-0.502676000000
C	1.893588000000	2.667320000000	-0.206297000000
H	2.724407000000	3.290389000000	0.086672000000
C	0.629830000000	3.260596000000	-0.193964000000
C	0.481140000000	4.736357000000	0.214247000000
C	-0.345830000000	5.490417000000	-0.852034000000
H	0.166967000000	5.459959000000	-1.819735000000
H	-0.464497000000	6.540627000000	-0.560818000000
H	-1.340507000000	5.063902000000	-0.992212000000
C	-0.201506000000	4.830617000000	1.599704000000
H	-1.190625000000	4.369660000000	1.612537000000

H	-0.311303000000	5.881530000000	1.893314000000
H	0.409737000000	4.325425000000	2.355594000000
C	1.832889000000	5.465672000000	0.327578000000
H	2.454594000000	5.061166000000	1.133407000000
H	1.651926000000	6.521745000000	0.554926000000
H	2.399625000000	5.415513000000	-0.608442000000
C	-0.545192000000	2.441948000000	-0.502699000000
C	-1.951611000000	2.625098000000	-0.206529000000
H	-2.287540000000	3.607806000000	0.086341000000
C	-2.906413000000	1.606536000000	-0.194286000000
C	-4.356048000000	1.921378000000	0.213426000000
C	-4.657530000000	1.301632000000	1.598857000000
H	-5.690624000000	1.523554000000	1.892361000000
H	-3.987615000000	1.725884000000	2.354787000000
H	-4.526514000000	0.218261000000	1.611752000000
C	-5.328432000000	1.367906000000	-0.853131000000
H	-5.230589000000	0.289990000000	-0.992747000000
H	-5.140320000000	1.845697000000	-1.820941000000
H	-6.363966000000	1.580142000000	-0.562512000000
C	-4.631645000000	3.432423000000	0.326484000000
H	-4.055586000000	3.898414000000	1.133036000000
H	-5.692145000000	3.587002000000	0.552666000000
H	-4.407612000000	3.955868000000	-0.609271000000
C	-2.490903000000	0.236054000000	-0.503036000000
C	-3.099644000000	-1.044904000000	-0.206826000000
H	-4.138087000000	-1.060738000000	0.085856000000
C	-2.425991000000	-2.267728000000	-0.194367000000
C	-3.173498000000	-3.548948000000	0.213674000000
C	-4.695680000000	-3.343791000000	0.327310000000
H	-4.960430000000	-2.651563000000	1.133686000000
H	-5.170478000000	-4.304466000000	0.554025000000
H	-5.124597000000	-2.969255000000	-0.608416000000
C	-2.948255000000	-4.644789000000	-0.852994000000
H	-3.345483000000	-4.318348000000	-1.820454000000
H	-3.469588000000	-5.564187000000	-0.561890000000
H	-1.892910000000	-4.884474000000	-0.993503000000
C	-2.676837000000	-4.027294000000	1.598920000000
H	-1.606201000000	-4.238477000000	1.611221000000
H	-3.207809000000	-4.940680000000	1.892957000000
H	-2.872139000000	-3.258717000000	2.354802000000
C	-0.994177000000	-2.296115000000	-0.503034000000
C	0.035965000000	-3.270943000000	-0.206904000000
H	-0.269937000000	-4.263521000000	0.085446000000
C	1.407105000000	-3.008092000000	-0.194194000000
C	2.394688000000	-4.114790000000	0.214157000000
C	1.729346000000	-5.499146000000	0.328006000000
H	0.988799000000	-5.536859000000	1.134041000000
H	2.496292000000	-6.247375000000	0.555307000000
H	1.241052000000	-5.791769000000	-0.607831000000
C	3.506676000000	-4.239398000000	-0.852277000000
H	4.219829000000	-5.019370000000	-0.560942000000

H	4.060913000000	-3.309865000000	-0.992908000000
H	3.073613000000	-4.516416000000	-1.819770000000
C	3.002669000000	-3.789809000000	1.599458000000
H	2.211104000000	-3.738072000000	2.355079000000
H	3.534110000000	-2.836702000000	1.611675000000
H	3.707392000000	-4.576790000000	1.893897000000
C	1.876550000000	-1.655090000000	-0.502750000000
C	3.122020000000	-0.976568000000	-0.206667000000
H	3.971495000000	-1.574200000000	0.085733000000
C	3.295813000000	0.408666000000	-0.194312000000
C	4.653715000000	1.006054000000	0.213095000000
C	5.764997000000	-0.054307000000	0.325738000000
H	5.572538000000	-0.770816000000	1.131398000000
H	6.713587000000	0.443970000000	0.552953000000
H	5.892076000000	-0.608507000000	-0.610508000000
C	5.114726000000	2.025503000000	-0.853481000000
H	5.243406000000	1.528384000000	-1.821289000000
H	6.077190000000	2.462644000000	-0.562958000000
H	4.401827000000	2.839918000000	-0.993117000000
C	4.533511000000	1.684370000000	1.598655000000
H	3.790781000000	2.483859000000	1.611835000000
H	5.499763000000	2.111991000000	1.892195000000
H	4.240918000000	0.947211000000	2.354430000000

2 from wB97x-D/def2-TZVP:

C	0.574878000000	1.050109000000	-0.900908000000
C	-0.821104000000	0.871248000000	-0.900810000000
C	-1.082376000000	-0.511828000000	-0.900530000000
C	0.152233000000	-1.187712000000	-0.900850000000
C	1.176443000000	-0.222384000000	-0.900993000000
C	1.175798000000	2.192001000000	-0.456504000000
C	0.231124000000	3.253507000000	-0.186863000000
H	0.617646000000	4.223486000000	0.073549000000
C	-1.143002000000	3.107339000000	-0.174128000000
C	-2.037119000000	4.298164000000	0.194756000000
C	-3.106680000000	4.498924000000	-0.891947000000
H	-2.635115000000	4.718223000000	-1.851951000000
H	-3.751710000000	5.340843000000	-0.630456000000
H	-3.739094000000	3.623978000000	-1.029181000000
C	-2.695972000000	4.053213000000	1.563970000000
H	-3.310713000000	3.155537000000	1.582589000000
H	-3.331418000000	4.901555000000	1.829388000000
H	-1.931985000000	3.945581000000	2.336428000000
C	-1.260284000000	5.615577000000	0.301578000000
H	-0.535676000000	5.602630000000	1.118039000000
H	-1.961325000000	6.427150000000	0.504838000000
H	-0.735649000000	5.853526000000	-0.625864000000
C	-1.721366000000	1.795557000000	-0.456208000000
C	-3.022883000000	1.225140000000	-0.187089000000
H	-3.826094000000	1.892672000000	0.072126000000
C	-3.308577000000	-0.126964000000	-0.174206000000

C	-4.717776000000	-0.609388000000	0.193416000000
C	-4.689935000000	-1.310748000000	1.563108000000
H	-5.693184000000	-1.653964000000	1.826934000000
H	-4.353703000000	-0.616583000000	2.335773000000
H	-4.025288000000	-2.172085000000	1.583501000000
C	-5.237696000000	-1.565422000000	-0.893239000000
H	-4.600506000000	-2.437090000000	-1.029194000000
H	-5.299666000000	-1.049859000000	-1.853672000000
H	-6.237864000000	-1.919013000000	-0.632635000000
C	-5.731100000000	0.536336000000	0.298148000000
H	-5.495366000000	1.222754000000	1.113654000000
H	-6.719564000000	0.120452000000	0.501606000000
H	-5.795037000000	1.107439000000	-0.630164000000
C	-2.239548000000	-1.082394000000	-0.455604000000
C	-2.098962000000	-2.496386000000	-0.185743000000
H	-2.981546000000	-3.054158000000	0.075185000000
C	-0.901384000000	-3.185862000000	-0.173698000000
C	-0.878353000000	-4.674615000000	0.195906000000
C	-2.281533000000	-5.283050000000	0.302934000000
H	-2.859736000000	-4.846001000000	1.119341000000
H	-2.192065000000	-6.351707000000	0.506343000000
H	-2.845893000000	-5.167067000000	-0.624445000000
C	-0.131285000000	-5.466967000000	-0.890025000000
H	-0.640670000000	-5.366445000000	-1.850506000000
H	-0.106368000000	-6.527260000000	-0.628401000000
H	0.895365000000	-5.132828000000	-1.026480000000
C	-0.201650000000	-4.862873000000	1.565341000000
H	0.823278000000	-4.497858000000	1.583872000000
H	-0.186181000000	-5.922556000000	1.831385000000
H	-0.756649000000	-4.326293000000	2.337335000000
C	0.337512000000	-2.464629000000	-0.456192000000
C	1.725900000000	-2.767983000000	-0.187080000000
H	1.983682000000	-3.779821000000	0.073264000000
C	2.751646000000	-1.841962000000	-0.174946000000
C	4.175192000000	-2.279523000000	0.193184000000
C	4.321500000000	-3.802013000000	0.299330000000
H	3.727944000000	-4.217916000000	1.115767000000
H	5.365793000000	-4.046417000000	0.502158000000
H	4.036762000000	-4.302583000000	-0.628234000000
C	5.157928000000	-1.812290000000	-0.893554000000
H	6.174752000000	-2.114614000000	-0.632880000000
H	5.155338000000	-0.732569000000	-1.029646000000
H	4.904812000000	-2.265865000000	-1.853910000000
C	4.564355000000	-1.694394000000	1.562488000000
H	3.884027000000	-2.057745000000	2.335185000000
H	4.532609000000	-0.606870000000	1.581728000000
H	5.577697000000	-2.005983000000	1.827024000000
C	2.448208000000	-0.440843000000	-0.456759000000
C	3.165818000000	0.785698000000	-0.187427000000
H	4.208208000000	0.718022000000	0.071277000000
C	2.602124000000	2.047337000000	-0.174694000000

C	3.458086000000	3.265482000000	0.195250000000
C	4.950913000000	2.933272000000	0.303162000000
H	5.161157000000	2.238307000000	1.118452000000
H	5.506280000000	3.850160000000	0.508819000000
H	5.340205000000	2.509380000000	-0.624616000000
C	3.319353000000	4.345286000000	-0.890984000000
H	3.672644000000	3.964440000000	-1.851306000000
H	3.922038000000	5.218020000000	-0.629477000000
H	2.292184000000	4.677827000000	-1.027608000000
C	3.020395000000	3.815750000000	1.564352000000
H	1.976484000000	4.122424000000	1.582348000000
H	3.630091000000	4.682626000000	1.830305000000
H	3.154135000000	3.055860000000	2.336753000000

Coordinates of compound **5** optimized at different DFT functionals:

5 from M06-2X/def2-TZVP:

C	0.053988000000	1.200027000000	0.295420000000
C	1.158128000000	0.319126000000	0.295611000000
C	0.661495000000	-1.003203000000	0.295273000000
C	-1.125023000000	0.422162000000	0.294716000000
C	-0.749576000000	-0.939537000000	0.294470000000
C	0.103902000000	2.467613000000	-0.226382000000
C	-2.314870000000	0.861341000000	-0.227661000000
C	2.379057000000	0.663661000000	-0.226047000000
C	1.366591000000	-2.057733000000	-0.226525000000
C	-1.534460000000	-1.935683000000	-0.228230000000
C	2.511758000000	2.056886000000	-0.570030000000
C	1.437937000000	2.929118000000	-0.565811000000
C	-1.180064000000	3.024475000000	-0.570389000000
C	-2.341506000000	2.272942000000	-0.566271000000
C	-3.240726000000	-0.187832000000	-0.572745000000
C	-2.884740000000	-1.524703000000	-0.568520000000
C	-0.822552000000	-3.140779000000	-0.571837000000
C	0.558858000000	-3.215201000000	-0.566518000000
C	2.732707000000	-1.753202000000	-0.570315000000
C	3.230310000000	-0.462314000000	-0.565873000000
S	1.682480000000	4.585993000000	-1.146624000000
S	4.881433000000	-0.182064000000	-1.147121000000
S	1.335578000000	-4.699619000000	-1.145499000000
S	-4.056501000000	-2.720824000000	-1.150192000000
S	-3.841931000000	3.018343000000	-1.145453000000
C	1.877725000000	5.531548000000	0.432175000000
C	5.841851000000	-0.076445000000	0.431290000000
C	1.733706000000	-5.577381000000	0.434392000000
C	-4.772114000000	-3.370605000000	0.428096000000
C	-4.681599000000	3.492953000000	0.434231000000
C	-5.799552000000	-4.400720000000	-0.035186000000
H	-6.288594000000	-4.840168000000	0.836902000000
H	-6.564091000000	-3.938729000000	-0.661288000000
H	-5.323574000000	-5.202094000000	-0.602108000000

C	-3.704424000000	-4.039281000000	1.285283000000
H	-3.203822000000	-4.837957000000	0.736362000000
H	-2.952257000000	-3.322601000000	1.617534000000
H	-4.171234000000	-4.470954000000	2.174859000000
C	-5.455323000000	-2.248629000000	1.199154000000
H	-4.738585000000	-1.485093000000	1.505463000000
H	-6.227089000000	-1.773883000000	0.592030000000
H	-5.922015000000	-2.655598000000	2.100205000000
C	2.392646000000	-6.875367000000	-0.026591000000
H	2.658990000000	-7.474852000000	0.846624000000
H	1.715092000000	-7.459729000000	-0.650628000000
H	3.301772000000	-6.673685000000	-0.594906000000
C	0.456358000000	-5.875932000000	1.208570000000
H	-0.045973000000	-4.956553000000	1.513308000000
H	-0.235881000000	-6.463535000000	0.604291000000
H	0.699691000000	-6.443599000000	2.110714000000
C	2.702729000000	-4.768202000000	1.287683000000
H	3.616430000000	-4.542065000000	0.736478000000
H	2.256132000000	-3.829655000000	1.618613000000
H	2.969584000000	-5.343985000000	2.178116000000
C	5.735030000000	-1.385466000000	1.202729000000
H	4.706328000000	-1.581603000000	1.508972000000
H	6.080344000000	-2.223377000000	0.595867000000
H	6.351674000000	-1.330451000000	2.103865000000
C	7.278623000000	0.152954000000	-0.031806000000
H	7.932532000000	0.220672000000	0.840334000000
H	7.625559000000	-0.670096000000	-0.658073000000
H	7.364735000000	1.081172000000	-0.598510000000
C	5.370847000000	1.092402000000	1.287920000000
H	5.435300000000	2.032615000000	0.738648000000
H	4.341082000000	0.954893000000	1.620257000000
H	6.002216000000	1.167529000000	2.177473000000
C	2.105462000000	6.968818000000	-0.030241000000
H	2.242399000000	7.611295000000	0.842281000000
H	2.996420000000	7.043861000000	-0.655186000000
H	1.250462000000	7.338495000000	-0.598111000000
C	3.088242000000	5.023977000000	1.204891000000
H	2.955554000000	3.985044000000	1.510654000000
H	3.992654000000	5.092749000000	0.599121000000
H	3.225985000000	5.627065000000	2.106346000000
C	0.619321000000	5.445469000000	1.287024000000
H	-0.253738000000	5.798794000000	0.736774000000
H	0.430335000000	4.423432000000	1.617941000000
H	0.742359000000	6.068173000000	2.177347000000
C	-5.975526000000	4.159103000000	-0.027648000000
H	-6.544617000000	4.486119000000	0.845276000000
H	-5.768143000000	5.031413000000	-0.648981000000
H	-6.592407000000	3.464079000000	-0.599092000000
C	-3.823187000000	4.482129000000	1.211893000000
H	-2.878163000000	4.030917000000	1.518128000000
H	-3.605171000000	5.364845000000	0.609486000000

H	-4.355026000000	4.798057000000	2.113364000000
C	-4.993757000000	2.267558000000	1.284419000000
H	-5.601009000000	1.550153000000	0.730895000000
H	-4.082251000000	1.767978000000	1.615036000000
H	-5.548323000000	2.575593000000	2.175018000000
H	-1.234721000000	4.044663000000	-0.929342000000
H	-4.227482000000	0.075312000000	-0.932797000000
H	-1.377460000000	-3.998335000000	-0.931374000000
H	3.376470000000	-2.546062000000	-0.930290000000
H	3.464953000000	2.424182000000	-0.929374000000

5 from B3LYP/def2-TZVP:

C	0.862884000000	-0.835148000000	0.359849000000
C	-0.528607000000	-1.077094000000	0.360134000000
C	-1.188699000000	0.171579000000	0.360315000000
C	1.062774000000	0.563024000000	0.359478000000
C	-0.205191000000	1.185240000000	0.359739000000
C	1.787569000000	-1.718414000000	-0.155498000000
C	2.188338000000	1.169541000000	-0.156211000000
C	-1.082930000000	-2.229558000000	-0.155022000000
C	-2.456130000000	0.342436000000	-0.154604000000
C	-0.434428000000	2.443258000000	-0.155672000000
C	-0.124014000000	-3.247070000000	-0.501291000000
C	1.249061000000	-3.025905000000	-0.495446000000
C	3.051684000000	-1.120874000000	-0.501417000000
C	3.265550000000	0.253382000000	-0.495825000000
C	2.010656000000	2.556473000000	-0.501963000000
C	0.769843000000	3.184627000000	-0.495583000000
C	-1.808510000000	2.702845000000	-0.500968000000
C	-2.789307000000	1.716745000000	-0.494358000000
C	-3.127703000000	-0.884165000000	-0.500025000000
C	-2.492986000000	-2.121668000000	-0.494412000000
S	2.318691000000	-4.307228000000	-1.125967000000
S	-3.381473000000	-3.534780000000	-1.124464000000
S	-4.407648000000	2.124338000000	-1.125109000000
S	0.657678000000	4.850367000000	-1.124772000000
S	4.815159000000	0.874867000000	-1.124721000000
C	2.872467000000	-5.264788000000	0.392130000000
C	-4.118128000000	-4.358773000000	0.394196000000
C	-5.422013000000	2.565423000000	0.392931000000
C	0.770680000000	5.949868000000	0.393939000000
C	5.895553000000	1.101937000000	0.394953000000
C	0.635139000000	7.362025000000	-0.185209000000
H	0.701464000000	8.094757000000	0.622997000000
H	1.429805000000	7.576411000000	-0.901643000000
H	-0.324734000000	7.496123000000	-0.686389000000
C	-0.367542000000	5.662965000000	1.372020000000
H	-1.340073000000	5.793730000000	0.897049000000
H	-0.311947000000	4.648626000000	1.768187000000
H	-0.306389000000	6.352914000000	2.219215000000
C	2.127348000000	5.780911000000	1.076199000000

H	2.262671000000	4.766145000000	1.451761000000
H	2.944271000000	6.003961000000	0.389109000000
H	2.199946000000	6.463652000000	1.928299000000
C	-6.804289000000	2.879953000000	-0.188789000000
H	-7.482493000000	3.166572000000	0.618922000000
H	-6.758165000000	3.706029000000	-0.900276000000
H	-7.229185000000	2.012586000000	-0.696398000000
C	-4.840904000000	3.798039000000	1.084263000000
H	-3.836517000000	3.607973000000	1.464085000000
H	-4.794238000000	4.647269000000	0.401726000000
H	-5.471047000000	4.075897000000	1.934675000000
C	-5.507324000000	1.388970000000	1.364191000000
H	-5.933629000000	0.508303000000	0.883288000000
H	-4.527327000000	1.123154000000	1.761463000000
H	-6.146022000000	1.657550000000	2.211209000000
C	-5.113495000000	-3.423405000000	1.079024000000
H	-4.623912000000	-2.524837000000	1.455819000000
H	-5.905366000000	-3.120384000000	0.393211000000
H	-5.573998000000	-3.933597000000	1.930573000000
C	-4.841935000000	-5.578847000000	-0.185236000000
H	-5.326534000000	-6.132460000000	0.622962000000
H	-5.611104000000	-5.282828000000	-0.900430000000
H	-4.146316000000	-6.252545000000	-0.687990000000
C	-3.028379000000	-4.799174000000	1.370554000000
H	-2.319953000000	-5.477358000000	0.894355000000
H	-2.475265000000	-3.947300000000	1.767104000000
H	-3.483509000000	-5.321512000000	2.217618000000
C	3.808202000000	-6.330851000000	-0.187578000000
H	4.183640000000	-6.963885000000	0.620386000000
H	3.288703000000	-6.969693000000	-0.903645000000
H	4.664787000000	-5.878056000000	-0.689333000000
C	1.673983000000	-5.921393000000	1.075543000000
H	0.971702000000	-5.177499000000	1.453065000000
H	1.140349000000	-6.579067000000	0.388592000000
H	2.015606000000	-6.518683000000	1.926440000000
C	3.628585000000	-4.366049000000	1.369495000000
H	4.493316000000	-3.902816000000	0.893831000000
H	2.990209000000	-3.576070000000	1.766123000000
H	3.983489000000	-4.961155000000	2.216488000000
C	7.198145000000	1.666739000000	-0.181815000000
H	7.915494000000	1.826791000000	0.627102000000
H	7.646974000000	0.978531000000	-0.899907000000
H	7.030928000000	2.622724000000	-0.680477000000
C	6.151246000000	-0.242809000000	1.073810000000
H	5.226994000000	-0.684062000000	1.448195000000
H	6.614266000000	-0.950013000000	0.384843000000
H	6.823295000000	-0.104369000000	1.926236000000
C	5.271667000000	2.094253000000	1.375079000000
H	5.097938000000	3.061323000000	0.902650000000
H	4.322830000000	1.728646000000	1.768781000000
H	5.945852000000	2.245531000000	2.223653000000

H	3.846042000000	-1.753730000000	-0.871707000000
H	2.857831000000	3.115991000000	-0.873224000000
H	-2.079527000000	3.681538000000	-0.871566000000
H	-4.142333000000	-0.839274000000	-0.870306000000
H	-0.480492000000	-4.198030000000	-0.871727000000

5 from B3LYP-D3BJ/def2-TZVP:

C	-0.863362000000	0.840710000000	0.331908000000
C	0.532396000000	1.080767000000	0.331812000000
C	1.191961000000	-0.172487000000	0.331799000000
C	-1.066428000000	-0.560873000000	0.331826000000
C	0.203856000000	-1.187062000000	0.332025000000
C	-1.777955000000	1.719657000000	-0.208442000000
C	-2.184864000000	-1.159150000000	-0.208808000000
C	1.085601000000	2.222235000000	-0.208674000000
C	2.448404000000	-0.346034000000	-0.208847000000
C	0.427233000000	-2.435760000000	-0.208223000000
C	0.134539000000	3.241021000000	-0.564959000000
C	-1.235946000000	3.019620000000	-0.559427000000
C	-3.040397000000	1.129984000000	-0.565804000000
C	-3.253316000000	-0.241862000000	-0.560883000000
C	-2.014173000000	-2.542311000000	-0.565289000000
C	-0.775305000000	-3.168750000000	-0.559639000000
C	1.795307000000	-2.700989000000	-0.564876000000
C	2.773896000000	-1.716330000000	-0.560002000000
C	3.123071000000	0.873062000000	-0.566243000000
C	2.489187000000	2.108139000000	-0.560670000000
S	-2.310816000000	4.304660000000	-1.151386000000
S	3.378994000000	3.526843000000	-1.154580000000
S	4.398151000000	-2.124272000000	-1.153838000000
S	-0.660973000000	-4.840062000000	-1.151957000000
S	-4.806674000000	-0.866672000000	-1.155777000000
C	-2.886926000000	5.116454000000	0.431661000000
C	3.981127000000	4.322111000000	0.427181000000
C	5.343253000000	-2.443605000000	0.427992000000
C	-0.675275000000	-5.835438000000	0.431057000000
C	-5.760905000000	-1.160065000000	0.425393000000
C	-0.590057000000	-7.283834000000	-0.051726000000
H	-0.601817000000	-7.955872000000	0.809452000000
H	-1.435386000000	-7.537474000000	-0.692795000000
H	0.330993000000	-7.460887000000	-0.608850000000
C	0.527190000000	-5.492737000000	1.305836000000
H	1.463173000000	-5.655316000000	0.771829000000
H	0.497845000000	-4.455593000000	1.638187000000
H	0.524588000000	-6.128069000000	2.196069000000
C	-1.978956000000	-5.595876000000	1.186391000000
H	-2.073886000000	-4.554579000000	1.494249000000
H	-2.841129000000	-5.849808000000	0.569455000000
H	-2.003075000000	-6.216179000000	2.086785000000
C	6.746092000000	-2.810765000000	-0.057120000000
H	7.383340000000	-3.028412000000	0.803066000000

H	6.724784000000	-3.693951000000	-0.696967000000
H	7.197927000000	-1.990240000000	-0.616271000000
C	4.713849000000	-3.608493000000	1.185763000000
H	3.694813000000	-3.376517000000	1.495353000000
H	4.687573000000	-4.507546000000	0.569790000000
H	5.298057000000	-3.822264000000	2.085245000000
C	5.390925000000	-1.193147000000	1.301384000000
H	5.833426000000	-0.353642000000	0.765571000000
H	4.396338000000	-0.900295000000	1.635953000000
H	5.996536000000	-1.390983000000	2.190363000000
C	4.895056000000	3.360017000000	1.179923000000
H	4.358835000000	2.462662000000	1.488696000000
H	5.739785000000	3.057364000000	0.560845000000
H	5.282226000000	3.846584000000	2.079604000000
C	4.764577000000	5.542658000000	-0.057160000000
H	5.172338000000	6.078361000000	0.803152000000
H	5.595336000000	5.249627000000	-0.700479000000
H	4.123338000000	6.228652000000	-0.612390000000
C	2.809908000000	4.753574000000	1.305046000000
H	2.148141000000	5.436495000000	0.772806000000
H	2.223371000000	3.898241000000	1.638752000000
H	3.188582000000	5.265242000000	2.194412000000
C	-3.809066000000	6.236524000000	-0.051334000000
H	-4.196294000000	6.786008000000	0.809778000000
H	-3.275171000000	6.939898000000	-0.691728000000
H	-4.657078000000	5.836938000000	-0.609258000000
C	-1.693119000000	5.691000000000	1.188133000000
H	-1.002968000000	4.905667000000	1.496375000000
H	-1.145743000000	6.404434000000	0.571841000000
H	-2.039932000000	6.206066000000	2.088407000000
C	-3.657161000000	4.130678000000	1.305596000000
H	-4.508908000000	3.710700000000	0.770981000000
H	-3.022671000000	3.309828000000	1.638150000000
H	-4.029982000000	4.645224000000	2.195779000000
C	-7.110415000000	-1.690631000000	-0.059875000000
H	-7.754893000000	-1.886975000000	0.800061000000
H	-7.612193000000	-0.966238000000	-0.702802000000
H	-6.991891000000	-2.621733000000	-0.615815000000
C	-5.938864000000	0.154404000000	1.179011000000
H	-4.978866000000	0.567801000000	1.488247000000
H	-6.446377000000	0.894676000000	0.560269000000
H	-6.537819000000	-0.014010000000	2.078432000000
C	-5.064247000000	-2.196232000000	1.302680000000
H	-4.927401000000	-3.136912000000	0.769746000000
H	-4.088079000000	-1.846550000000	1.637056000000
H	-5.671101000000	-2.390031000000	2.191691000000
H	-3.830827000000	1.765659000000	-0.937847000000
H	-2.862922000000	-3.098152000000	-0.936706000000
H	2.061397000000	-3.680125000000	-0.936056000000
H	4.136151000000	0.823444000000	-0.938344000000
H	0.494477000000	4.189742000000	-0.936017000000

5 from B97D3/def2-TZVP:

C	-0.169236000000	1.196815000000	0.353465000000
C	1.086457000000	0.529287000000	0.354028000000
C	0.839294000000	-0.871161000000	0.353559000000
C	-1.192310000000	0.208956000000	0.352707000000
C	-0.569003000000	-1.069183000000	0.353322000000
C	-0.355684000000	2.455914000000	-0.200974000000
C	-2.447081000000	0.420439000000	-0.202787000000
C	2.226357000000	1.095840000000	-0.200273000000
C	1.730081000000	-1.780021000000	-0.201564000000
C	-1.158116000000	-2.197501000000	-0.201362000000
C	2.097094000000	2.484112000000	-0.564001000000
C	0.870676000000	3.153083000000	-0.558781000000
C	-1.715399000000	2.761756000000	-0.566395000000
C	-2.730454000000	1.802093000000	-0.562296000000
C	-3.158900000000	-0.778616000000	-0.566009000000
C	-2.560071000000	-2.040583000000	-0.560041000000
C	-0.237731000000	-3.244755000000	-0.565083000000
C	1.147555000000	-3.064730000000	-0.560505000000
C	3.010276000000	-1.228373000000	-0.565435000000
C	3.267828000000	0.144584000000	-0.559700000000
S	0.807132000000	4.824347000000	-1.158788000000
S	4.837200000000	0.720198000000	-1.162314000000
S	2.181181000000	-4.379559000000	-1.160890000000
S	-3.491504000000	-3.429816000000	-1.159543000000
S	-4.339022000000	2.258721000000	-1.163412000000
C	0.854358000000	5.825351000000	0.431143000000
C	5.805221000000	0.989500000000	0.425851000000
C	2.738163000000	-5.212094000000	0.429047000000
C	-4.116833000000	-4.211572000000	0.430752000000
C	-5.276532000000	2.613586000000	0.425982000000
C	-4.953654000000	-5.400333000000	-0.055640000000
H	-5.374997000000	-5.925895000000	0.809764000000
H	-5.781213000000	-5.069122000000	-0.691494000000
H	-4.341771000000	-6.110046000000	-0.622264000000
C	-2.952711000000	-4.692035000000	1.298508000000
H	-2.320715000000	-5.400987000000	0.756024000000
H	-2.328814000000	-3.856977000000	1.629055000000
H	-3.345389000000	-5.192650000000	2.193477000000
C	-4.986988000000	-3.210881000000	1.192267000000
H	-4.407520000000	-2.336097000000	1.502139000000
H	-5.823009000000	-2.868142000000	0.574937000000
H	-5.392315000000	-3.685958000000	2.095392000000
C	3.615044000000	-6.371371000000	-0.057953000000
H	3.987914000000	-6.932637000000	0.807249000000
H	3.046941000000	-7.058783000000	-0.693259000000
H	4.476962000000	-6.004792000000	-0.625319000000
C	1.521135000000	-5.735957000000	1.192397000000
H	0.864234000000	-4.917677000000	1.502083000000
H	0.939907000000	-6.428626000000	0.576081000000

H	1.851395000000	-6.265845000000	2.095598000000
C	3.551700000000	-4.248798000000	1.294881000000
H	4.419347000000	-3.864309000000	0.751053000000
H	2.947344000000	-3.399090000000	1.624403000000
H	3.909183000000	-4.774089000000	2.190463000000
C	5.928507000000	-0.330832000000	1.187308000000
H	4.947887000000	-0.701944000000	1.499891000000
H	6.404941000000	-1.097612000000	0.568817000000
H	6.537539000000	-0.181968000000	2.088696000000
C	7.177784000000	1.465426000000	-0.063500000000
H	7.828865000000	1.644787000000	0.800540000000
H	7.654163000000	0.713635000000	-0.701263000000
H	7.094538000000	2.399455000000	-0.629008000000
C	5.143154000000	2.059735000000	1.295013000000
H	5.045926000000	3.004874000000	0.753228000000
H	4.148404000000	1.747772000000	1.625190000000
H	5.754727000000	2.234922000000	2.190050000000
C	0.828492000000	7.278570000000	-0.055993000000
H	0.859430000000	7.951876000000	0.809071000000
H	1.691514000000	7.498938000000	-0.692771000000
H	-0.084819000000	7.490170000000	-0.621871000000
C	2.148171000000	5.531009000000	1.191324000000
H	2.195767000000	4.483709000000	1.504209000000
H	3.024655000000	5.744794000000	0.572031000000
H	2.197412000000	6.156174000000	2.092647000000
C	-0.368059000000	5.527481000000	1.300830000000
H	-1.297210000000	5.730553000000	0.760576000000
H	-0.380990000000	4.484268000000	1.628561000000
H	-0.343159000000	6.161009000000	2.197381000000
C	-6.667702000000	3.034316000000	-0.061336000000
H	-7.298287000000	3.273257000000	0.803489000000
H	-6.612501000000	3.921523000000	-0.700614000000
H	-7.150334000000	2.228735000000	-0.624596000000
C	-4.598499000000	3.755791000000	1.183667000000
H	-3.586383000000	3.480328000000	1.494887000000
H	-4.534519000000	4.654965000000	0.563270000000
H	-5.176825000000	3.995135000000	2.085813000000
C	-5.368051000000	1.360315000000	1.298033000000
H	-5.845956000000	0.537071000000	0.759246000000
H	-4.379311000000	1.028574000000	1.627014000000
H	-5.963898000000	1.580029000000	2.193846000000
H	-1.949720000000	3.750079000000	-0.948067000000
H	-4.171582000000	-0.696226000000	-0.946690000000
H	-0.628915000000	-4.182991000000	-0.944680000000
H	3.780786000000	-1.890231000000	-0.946844000000
H	2.964564000000	3.012816000000	-0.945009000000

5 from wB97x-D/def2-TZVP:

C	1.018359000000	-0.632056000000	0.255105000000
C	-0.286791000000	-1.164272000000	0.255139000000
C	-1.196291000000	-0.087480000000	0.254988000000

C	0.915460000000	0.773637000000	0.254847000000
C	-0.453277000000	1.110255000000	0.254680000000
C	2.100397000000	-1.294034000000	-0.259243000000
C	1.879563000000	1.598066000000	-0.259443000000
C	-0.581954000000	-2.398082000000	-0.258957000000
C	-2.460835000000	-0.188077000000	-0.259199000000
C	-0.939486000000	2.281786000000	-0.259825000000
C	0.568924000000	-3.193509000000	-0.595343000000
C	1.853140000000	-2.683983000000	-0.590780000000
C	3.212764000000	-0.445506000000	-0.595187000000
C	3.125303000000	0.933322000000	-0.590280000000
C	1.416098000000	2.918040000000	-0.596000000000
C	0.077632000000	3.260717000000	-0.591368000000
C	-2.338164000000	2.248961000000	-0.595682000000
C	-3.077618000000	1.081804000000	-0.590714000000
C	-2.861852000000	-1.528579000000	-0.594933000000
C	-1.980428000000	-2.592504000000	-0.589861000000
S	3.181204000000	-3.718227000000	-1.145012000000
S	-2.554136000000	-4.175873000000	-1.141593000000
S	-4.760404000000	1.138625000000	-1.143133000000
S	-0.388464000000	4.878556000000	-1.144353000000
S	4.520354000000	1.877291000000	-1.141132000000
C	3.899165000000	-4.343881000000	0.444981000000
C	-2.933205000000	-5.046838000000	0.449946000000
C	-5.706156000000	1.225984000000	0.448282000000
C	-0.595877000000	5.806583000000	0.446419000000
C	5.337822000000	2.358544000000	0.451116000000
C	-0.991435000000	7.212999000000	-0.001282000000
H	-1.128523000000	7.848026000000	0.877018000000
H	-0.218723000000	7.661400000000	-0.627950000000
H	-1.927697000000	7.201180000000	-0.561904000000
C	-1.699349000000	5.197647000000	1.305464000000
H	-2.644432000000	5.154958000000	0.762757000000
H	-1.444056000000	4.188511000000	1.630848000000
H	-1.844044000000	5.808792000000	2.200705000000
C	0.721004000000	5.844199000000	1.213870000000
H	1.038131000000	4.842975000000	1.509387000000
H	1.513010000000	6.290617000000	0.611174000000
H	0.600345000000	6.440237000000	2.122730000000
C	-7.165854000000	1.292482000000	0.001202000000
H	-7.811622000000	1.357464000000	0.879967000000
H	-7.349937000000	2.169321000000	-0.621789000000
H	-7.447931000000	0.401919000000	-0.563027000000
C	-5.329218000000	2.485370000000	1.220500000000
H	-4.279072000000	2.471751000000	1.516017000000
H	-5.504985000000	3.379675000000	0.621229000000
H	-5.933045000000	2.554084000000	2.129630000000
C	-5.473364000000	-0.016001000000	1.302479000000
H	-5.730014000000	-0.924784000000	0.756819000000
H	-4.434851000000	-0.091519000000	1.626884000000
H	-6.098288000000	0.035040000000	2.198472000000

C	-4.020715000000	-4.302133000000	1.216294000000
H	-3.688745000000	-3.305633000000	1.511290000000
H	-4.923613000000	-4.198047000000	0.613169000000
H	-4.273907000000	-4.854510000000	2.125478000000
C	-3.440459000000	-6.417353000000	0.003388000000
H	-3.703342000000	-7.010735000000	0.882176000000
H	-4.328960000000	-6.326060000000	-0.623596000000
H	-2.676162000000	-6.959005000000	-0.556528000000
C	-1.683004000000	-5.202643000000	1.309665000000
H	-0.893863000000	-5.725945000000	0.768457000000
H	-1.295391000000	-4.235871000000	1.632987000000
H	-1.926105000000	-5.779926000000	2.206080000000
C	5.042679000000	-5.252435000000	-0.004355000000
H	5.529404000000	-5.683871000000	0.873389000000
H	4.677435000000	-6.070615000000	-0.627302000000
H	5.792004000000	-4.695398000000	-0.569385000000
C	2.857292000000	-5.144507000000	1.218321000000
H	2.014341000000	-4.518742000000	1.515226000000
H	2.475460000000	-5.972209000000	0.619224000000
H	3.307830000000	-5.554050000000	2.126694000000
C	4.439231000000	-3.201417000000	1.299144000000
H	5.177545000000	-2.613741000000	0.752269000000
H	3.641831000000	-2.533199000000	1.626295000000
H	4.918532000000	-3.609494000000	2.193365000000
C	6.558189000000	3.163102000000	0.005746000000
H	7.119328000000	3.487571000000	0.885125000000
H	7.221975000000	2.563110000000	-0.618980000000
H	6.263199000000	4.050949000000	-0.556149000000
C	5.772722000000	1.116162000000	1.220450000000
H	4.914854000000	0.509575000000	1.514462000000
H	6.440405000000	0.497216000000	0.619684000000
H	6.301675000000	1.413142000000	2.130315000000
C	4.419816000000	3.224842000000	1.307408000000
H	4.094073000000	4.112655000000	0.764095000000
H	3.534801000000	2.674994000000	1.629534000000
H	4.955201000000	3.547942000000	2.204550000000
H	4.134051000000	-0.895487000000	-0.941231000000
H	2.128667000000	3.655059000000	-0.942516000000
H	-2.819225000000	3.154280000000	-0.942114000000
H	-3.871656000000	-1.706365000000	-0.941019000000
H	0.425831000000	-4.208466000000	-0.942351000000

Coordinates of the most stable conformer of **6** optimized at M06-2X/def2-TZVP:

C	2.305295000000	-2.402460000000	-0.123903000000
C	0.856703000000	-2.355772000000	-0.306003000000
C	0.406785000000	-1.124353000000	-0.682359000000
C	1.195173000000	0.039549000000	-0.682665000000
C	2.505548000000	0.086874000000	-0.306891000000
C	3.076621000000	-1.229808000000	-0.052308000000
C	2.997602000000	1.450182000000	-0.124756000000
C	2.120554000000	2.546058000000	-0.052514000000

C	0.691775000000	2.409722000000	-0.306598000000
C	0.331770000000	1.148942000000	-0.682552000000
C	-0.452873000000	3.298712000000	-0.123146000000
C	-1.765985000000	2.803067000000	-0.050728000000
C	-2.077998000000	1.402459000000	-0.306360000000
C	-0.990116000000	0.670683000000	-0.682550000000
C	-0.943751000000	-0.734271000000	-0.682403000000
C	-3.277470000000	0.588774000000	-0.124576000000
C	-3.212139000000	-0.813253000000	-0.052287000000
C	-1.976026000000	-1.542647000000	-0.306353000000
C	-1.572499000000	-2.934770000000	-0.123539000000
C	-0.218864000000	-3.305605000000	-0.050788000000
S	-4.635875000000	-1.753486000000	0.414247000000
H	-5.145170000000	-0.819102000000	1.231910000000
S	-2.843293000000	-4.165112000000	-0.017400000000
H	-2.123232000000	-5.120681000000	-0.627316000000
S	0.234946000000	-4.949387000000	0.419745000000
H	-0.806999000000	-5.138415000000	1.243737000000
S	3.082072000000	-3.991474000000	-0.017663000000
H	4.211417000000	-3.603514000000	-0.632531000000
S	4.780788000000	-1.306835000000	0.415445000000
H	4.640930000000	-2.358809000000	1.236759000000
S	4.748922000000	1.697800000000	-0.019281000000
H	4.728156000000	2.893754000000	-0.629878000000
S	2.719695000000	4.143098000000	0.415412000000
H	3.677530000000	3.684459000000	1.235881000000
S	-0.147627000000	5.040744000000	-0.015723000000
H	-1.294480000000	5.391477000000	-0.619825000000
S	-3.099268000000	3.866184000000	0.419891000000
H	-2.367932000000	4.631194000000	1.245092000000
S	-4.840137000000	1.417716000000	-0.021455000000
H	-5.524408000000	0.439169000000	-0.635640000000

Coordinates of compound **8** optimized at different DFT functionals:

8α from M06-2X/def2-TZVP:

C	-0.943289000000	0.729645000000	-0.008494000000
C	-0.985281000000	-0.671587000000	-0.008156000000
C	0.334353000000	-1.144549000000	-0.008395000000
C	0.402348000000	1.122603000000	-0.008551000000
C	1.191961000000	-0.035708000000	-0.008571000000
C	-2.020579000000	1.562691000000	-0.003640000000
C	0.861753000000	2.404524000000	-0.003224000000
C	-2.110364000000	-1.438799000000	-0.002486000000
C	0.716269000000	-2.451687000000	-0.003545000000
C	2.553130000000	-0.076518000000	-0.003480000000
C	-3.331340000000	-0.609302000000	0.038948000000
C	-3.289119000000	0.807465000000	-0.039322000000
C	-1.608962000000	2.980364000000	0.036339000000
C	-0.248230000000	3.377694000000	-0.040726000000
C	2.337154000000	2.451091000000	0.039079000000

C	3.135699000000	1.279958000000	-0.038506000000
C	3.053371000000	-1.465272000000	0.036756000000
C	2.186261000000	-2.586546000000	-0.041152000000
C	-0.449843000000	-3.356668000000	0.038122000000
C	-1.784371000000	-2.878665000000	-0.038484000000
S	-4.833237000000	1.682161000000	-0.226491000000
S	-4.924402000000	-1.390352000000	0.229723000000
S	-3.093936000000	-4.076751000000	-0.222993000000
S	-0.199117000000	-5.113236000000	0.227395000000
S	2.920816000000	-4.201870000000	-0.229610000000
S	4.801596000000	-1.769805000000	0.225011000000
S	4.899447000000	1.479099000000	-0.221631000000
S	3.167191000000	4.019092000000	0.230817000000
S	0.107403000000	5.116313000000	-0.228194000000
S	-2.843952000000	4.254953000000	0.223175000000
C	-5.022990000000	1.802654000000	-2.064882000000
C	-5.118409000000	-1.499310000000	2.068328000000
C	-3.271129000000	-4.221167000000	-2.060874000000
C	-0.152633000000	-5.332999000000	2.065652000000
C	3.000177000000	-4.411528000000	-2.068103000000
C	5.025828000000	-1.796014000000	2.063201000000
C	5.128804000000	1.494502000000	-2.059267000000
C	3.255556000000	4.222266000000	2.069562000000
C	0.165902000000	5.333708000000	-2.066435000000
C	-3.012088000000	4.407810000000	2.061123000000
C	1.873611000000	4.213761000000	2.707335000000
H	1.249570000000	5.006434000000	2.297175000000
H	1.371322000000	3.255908000000	2.556818000000
H	1.971656000000	4.371476000000	3.785332000000
C	3.895998000000	5.600084000000	2.227372000000
H	4.004540000000	5.825680000000	3.290596000000
H	4.884914000000	5.628107000000	1.767434000000
H	3.274555000000	6.372599000000	1.771756000000
C	4.134177000000	3.151477000000	2.698917000000
H	3.696832000000	2.161178000000	2.565385000000
H	5.131916000000	3.150909000000	2.260830000000
H	4.217998000000	3.336628000000	3.773752000000
C	6.646355000000	1.582833000000	-2.209895000000
H	6.900813000000	1.609141000000	-3.271820000000
H	7.035188000000	2.488000000000	-1.741042000000
H	7.132997000000	0.716624000000	-1.758879000000
C	4.614510000000	0.216205000000	-2.706215000000
H	5.117623000000	-0.658569000000	-2.296750000000
H	3.537804000000	0.102835000000	-2.563993000000
H	4.804838000000	0.254160000000	-3.782713000000
C	4.459663000000	2.709036000000	-2.685247000000
H	3.377315000000	2.666002000000	-2.556963000000
H	4.823860000000	3.634676000000	-2.240299000000
H	4.667680000000	2.724631000000	-3.759074000000
C	6.535292000000	-1.972331000000	2.217392000000
H	7.072718000000	-1.137530000000	1.764776000000

H	6.785601000000	-2.009795000000	3.279969000000
H	6.871493000000	-2.900217000000	1.752302000000
C	4.285828000000	-2.968613000000	2.689374000000
H	3.208033000000	-2.862146000000	2.559842000000
H	4.595822000000	-3.914324000000	2.245629000000
H	4.491357000000	-2.995450000000	3.763454000000
C	4.585048000000	-0.489055000000	2.706950000000
H	5.141609000000	0.354026000000	2.300208000000
H	3.517810000000	-0.311929000000	2.558384000000
H	4.766572000000	-0.537689000000	3.784537000000
C	3.559812000000	-5.824410000000	-2.223279000000
H	3.656708000000	-6.057345000000	-3.286040000000
H	4.544606000000	-5.909222000000	-1.761522000000
H	2.893683000000	-6.558914000000	-1.767900000000
C	3.940734000000	-3.394482000000	-2.697160000000
H	3.560735000000	-2.380213000000	-2.567667000000
H	4.935599000000	-3.450182000000	-2.256095000000
H	4.016940000000	-3.587042000000	-3.771257000000
C	1.622161000000	-4.323569000000	-2.708659000000
H	0.952015000000	-5.077810000000	-2.298661000000
H	1.176295000000	-3.337821000000	-2.560614000000
H	1.713012000000	-4.488193000000	-3.786243000000
C	0.962633000000	-4.518202000000	2.705190000000
H	1.932619000000	-4.794678000000	2.294472000000
H	0.809041000000	-3.447297000000	2.556855000000
H	0.975387000000	-4.705648000000	3.782799000000
C	0.135017000000	-6.825190000000	2.220771000000
H	1.091436000000	-7.086473000000	1.765172000000
H	0.178497000000	-7.073743000000	3.283523000000
H	-0.649869000000	-7.426191000000	1.759207000000
C	-1.492067000000	-4.980484000000	2.695212000000
H	-1.717253000000	-3.921328000000	2.563682000000
H	-2.301227000000	-5.563184000000	2.255734000000
H	-1.451883000000	-5.181748000000	3.769668000000
C	-2.016460000000	-4.809588000000	-2.688673000000
H	-1.165684000000	-4.139228000000	-2.559836000000
H	-1.767204000000	-5.773379000000	-2.245536000000
H	-2.176393000000	-4.942521000000	-3.762606000000
C	-4.447250000000	-5.184102000000	-2.212740000000
H	-4.639570000000	-5.351038000000	-3.274936000000
H	-4.229014000000	-6.146624000000	-1.747743000000
H	-5.349312000000	-4.770932000000	-1.758696000000
C	-3.606634000000	-2.883363000000	-2.704658000000
H	-4.528808000000	-2.473669000000	-2.295162000000
H	-2.803188000000	-2.158325000000	-2.558982000000
H	-3.736704000000	-3.022865000000	-3.781768000000
C	-3.994068000000	-2.299625000000	2.710358000000
H	-3.950711000000	-3.308311000000	2.302203000000
H	-3.025981000000	-1.816891000000	2.561426000000
H	-4.168573000000	-2.368147000000	3.788022000000
C	-6.444274000000	-2.241486000000	2.225272000000

H	-6.391024000000	-3.232984000000	1.772867000000
H	-6.666962000000	-2.357530000000	3.288321000000
H	-7.261606000000	-1.687143000000	1.761614000000
C	-5.205294000000	-0.115294000000	2.694141000000
H	-4.270390000000	0.430860000000	2.561971000000
H	-6.012294000000	0.468653000000	2.252373000000
H	-5.384583000000	-0.213780000000	3.768740000000
C	-6.301506000000	2.624056000000	-2.219964000000
H	-6.518270000000	2.753323000000	-3.282701000000
H	-7.150320000000	2.120486000000	-1.754969000000
H	-6.187347000000	3.610514000000	-1.767819000000
C	-5.194878000000	0.426448000000	-2.690373000000
H	-4.294741000000	-0.175562000000	-2.559451000000
H	-6.035200000000	-0.107272000000	-2.247220000000
H	-5.369469000000	0.535542000000	-3.764718000000
C	-3.853052000000	2.533112000000	-2.708731000000
H	-3.746787000000	3.536650000000	-2.299460000000
H	-2.916151000000	1.991513000000	-2.562833000000
H	-4.025603000000	2.613610000000	-3.785884000000
C	-3.428762000000	3.092288000000	2.703416000000
H	-4.375213000000	2.741099000000	2.295034000000
H	-2.671978000000	2.319157000000	2.555150000000
H	-3.548125000000	3.237753000000	3.780977000000
C	-4.126773000000	5.440936000000	2.214417000000
H	-5.052426000000	5.085024000000	1.759383000000
H	-4.308839000000	5.617376000000	3.276884000000
H	-3.849472000000	6.389043000000	1.751287000000
C	-1.723626000000	4.917272000000	2.689500000000
H	-0.915872000000	4.195893000000	2.559728000000
H	-1.415648000000	5.864462000000	2.247506000000
H	-1.875053000000	5.058511000000	3.763612000000
C	0.545494000000	6.805295000000	-2.220967000000
H	0.603021000000	7.051387000000	-3.283624000000
H	-0.199904000000	7.453490000000	-1.757855000000
H	1.516930000000	7.006352000000	-1.766565000000
C	-1.193101000000	5.065490000000	-2.695595000000
H	-1.483653000000	4.022271000000	-2.564756000000
H	-1.964364000000	5.697061000000	-2.255498000000
H	-1.140902000000	5.264660000000	-3.769924000000
C	1.228297000000	4.451722000000	-2.706933000000
H	2.213112000000	4.665215000000	-2.293902000000
H	1.007121000000	3.392277000000	-2.561727000000
H	1.254501000000	4.640762000000	-3.784006000000

8β from M06-2X/def2-TZVP:

C	-0.232792000000	-1.176148000000	-0.796529000000
C	1.046402000000	-0.585020000000	-0.796715000000
C	0.879536000000	0.814259000000	-0.796499000000
C	-1.190260000000	-0.142179000000	-0.796561000000
C	-0.502829000000	1.087970000000	-0.796617000000
C	-0.477193000000	-2.464929000000	-0.399702000000

C	-2.491527000000	-0.307920000000	-0.399958000000
C	2.196655000000	-1.215772000000	-0.400264000000
C	1.834855000000	1.713129000000	-0.399652000000
C	-1.062565000000	2.274407000000	-0.400080000000
C	2.004113000000	-2.632965000000	-0.105544000000
C	0.747896000000	-3.257228000000	-0.248395000000
C	-1.884547000000	-2.719554000000	-0.104593000000
C	-2.866435000000	-1.717815000000	-0.248129000000
C	-3.168740000000	0.951934000000	-0.105475000000
C	-2.519391000000	2.195329000000	-0.248797000000
C	-0.073611000000	3.307593000000	-0.104995000000
C	1.309554000000	3.074112000000	-0.247953000000
C	3.123225000000	1.091956000000	-0.105156000000
C	3.328737000000	-0.295528000000	-0.248915000000
S	0.695489000000	-5.032445000000	-0.406451000000
S	3.335781000000	-3.556457000000	0.614175000000
S	5.000720000000	-0.894050000000	-0.407557000000
S	4.412965000000	2.072628000000	0.615261000000
S	2.395840000000	4.479218000000	-0.404928000000
S	-0.607757000000	4.836775000000	0.616446000000
S	-3.520614000000	3.662259000000	-0.406193000000
S	-4.788437000000	0.916201000000	0.615383000000
S	-4.570956000000	-2.216701000000	-0.405983000000
S	-2.350971000000	-4.270367000000	0.617586000000
C	0.386183000000	-5.250297000000	-2.219533000000
C	2.811929000000	-3.767951000000	2.386794000000
C	5.112802000000	-1.250940000000	-2.221583000000
C	4.453857000000	1.505851000000	2.386825000000
C	2.771555000000	4.476604000000	-2.218534000000
C	-0.057913000000	4.697992000000	2.388283000000
C	-3.401637000000	4.019347000000	-2.219808000000
C	-4.488355000000	1.398163000000	2.387132000000
C	-4.873286000000	-1.992749000000	-2.219463000000
C	-2.715885000000	-3.834591000000	2.389103000000
C	-3.263968000000	0.681978000000	2.940033000000
H	-3.377159000000	-0.399171000000	2.867298000000
H	-2.353696000000	0.971023000000	2.411581000000
H	-3.137459000000	0.945563000000	3.994049000000
C	-5.752163000000	0.888096000000	3.081529000000
H	-5.700746000000	1.131479000000	4.145146000000
H	-6.645138000000	1.360504000000	2.668081000000
H	-5.849831000000	-0.192708000000	2.973316000000
C	-4.364858000000	2.902025000000	2.591922000000
H	-3.449446000000	3.298098000000	2.152411000000
H	-5.209123000000	3.432487000000	2.152133000000
H	-4.334883000000	3.113659000000	3.665251000000
C	-4.491440000000	5.072673000000	-2.420087000000
H	-4.497009000000	5.386969000000	-3.466100000000
H	-5.474737000000	4.672917000000	-2.170910000000
H	-4.304990000000	5.952138000000	-1.801213000000
C	-2.048159000000	4.592566000000	-2.614910000000

H	-1.796638000000	5.466172000000	-2.011744000000
H	-1.258154000000	3.852422000000	-2.499920000000
H	-2.070834000000	4.890695000000	-3.667512000000
C	-3.713679000000	2.773369000000	-3.035467000000
H	-2.931725000000	2.020203000000	-2.918495000000
H	-4.664374000000	2.334960000000	-2.729366000000
H	-3.770781000000	3.035622000000	-4.095611000000
C	-0.932634000000	5.742693000000	3.083248000000
H	-1.990960000000	5.503179000000	2.973860000000
H	-0.686090000000	5.767320000000	4.147101000000
H	-0.757582000000	6.738213000000	2.671169000000
C	1.410838000000	5.043213000000	2.593802000000
H	2.069372000000	4.294997000000	2.152751000000
H	1.655524000000	6.010604000000	2.155789000000
H	1.621527000000	5.077807000000	3.667180000000
C	-0.362565000000	3.311961000000	2.939605000000
H	-1.426044000000	3.086910000000	2.866316000000
H	0.192804000000	2.535407000000	2.410498000000
H	-0.073140000000	3.271640000000	3.993667000000
C	3.443315000000	5.835468000000	-2.417492000000
H	3.739963000000	5.937932000000	-3.463653000000
H	2.763673000000	6.650222000000	-2.166439000000
H	4.338423000000	5.924434000000	-1.799362000000
C	1.489372000000	4.395622000000	-3.033737000000
H	1.009684000000	3.421603000000	-2.917184000000
H	0.782728000000	5.167788000000	-2.726876000000
H	1.721448000000	4.530426000000	-4.093888000000
C	3.729235000000	3.362120000000	-2.615427000000
H	4.637838000000	3.386698000000	-2.011974000000
H	3.264167000000	2.384291000000	-2.502560000000
H	4.006680000000	3.476393000000	-3.667732000000
C	3.042500000000	1.365566000000	2.940296000000
H	2.498023000000	2.306400000000	2.866811000000
H	2.476134000000	0.595860000000	2.412910000000
H	3.095561000000	1.079062000000	3.994584000000
C	5.176802000000	2.661076000000	3.081319000000
H	4.620507000000	3.592923000000	2.973658000000
H	5.278663000000	2.433548000000	4.144818000000
H	6.176757000000	2.803911000000	2.667563000000
C	5.237804000000	0.216436000000	2.591006000000
H	4.730546000000	-0.641794000000	2.150269000000
H	6.232970000000	0.284113000000	2.152074000000
H	5.337161000000	0.026602000000	3.664230000000
C	4.637749000000	-0.056435000000	-3.035622000000
H	3.563036000000	0.097396000000	-2.918485000000
H	5.152815000000	0.854602000000	-2.728288000000
H	4.837399000000	-0.234421000000	-4.096005000000
C	6.612684000000	-1.468663000000	-2.422324000000
H	6.800723000000	-1.719013000000	-3.468706000000
H	7.177130000000	-0.570059000000	-2.171980000000
H	6.975348000000	-2.292158000000	-1.804630000000

C	4.349266000000	-2.506406000000	-2.618381000000
H	4.654962000000	-3.363199000000	-2.016095000000
H	3.275641000000	-2.367205000000	-2.503833000000
H	4.542348000000	-2.733940000000	-3.671148000000
C	2.242512000000	-2.468409000000	2.938815000000
H	2.968898000000	-1.659900000000	2.863660000000
H	1.335049000000	-2.168564000000	2.411587000000
H	1.987191000000	-2.605943000000	3.993489000000
C	4.135189000000	-4.096704000000	3.079906000000
H	4.849181000000	-3.279796000000	2.969190000000
H	3.952081000000	-4.261534000000	4.144083000000
H	4.579500000000	-5.004421000000	2.667415000000
C	1.828777000000	-4.912152000000	2.594181000000
H	0.854866000000	-4.695647000000	2.155230000000
H	2.200119000000	-5.838029000000	2.155496000000
H	1.681151000000	-5.064229000000	3.667870000000
C	0.646614000000	-6.743259000000	-2.420868000000
H	0.464938000000	-7.000051000000	-3.466813000000
H	1.677038000000	-6.999275000000	-2.172964000000
H	-0.021224000000	-7.344626000000	-1.801550000000
C	1.370605000000	-4.426283000000	-3.036267000000
H	1.181892000000	-3.357252000000	-2.918199000000
H	2.397711000000	-4.631574000000	-2.731896000000
H	1.260713000000	-4.671154000000	-4.096412000000
C	-1.045920000000	-4.916470000000	-2.612207000000
H	-1.762793000000	-5.474131000000	-2.007716000000
H	-1.248233000000	-3.852996000000	-2.497123000000
H	-1.205023000000	-5.170985000000	-3.664484000000
C	-1.655635000000	-2.891769000000	2.941164000000
H	-0.662686000000	-3.334240000000	2.868644000000
H	-1.648618000000	-1.937083000000	2.412115000000
H	-1.866955000000	-2.689160000000	3.995074000000
C	-2.621917000000	-5.193779000000	3.084339000000
H	-1.624563000000	-5.621429000000	2.975803000000
H	-2.836732000000	-5.068756000000	4.148006000000
H	-3.347921000000	-5.896801000000	2.671804000000
C	-4.107584000000	-3.251541000000	2.594053000000
H	-4.201301000000	-2.258838000000	2.153821000000
H	-4.873408000000	-3.890699000000	2.155223000000
H	-4.299001000000	-3.156673000000	3.667408000000
C	-6.212320000000	-2.702752000000	-2.419985000000
H	-6.512480000000	-2.611193000000	-3.466156000000
H	-6.136946000000	-3.761400000000	-2.170278000000
H	-6.990964000000	-2.252738000000	-1.801590000000
C	-3.785043000000	-2.675065000000	-3.035128000000
H	-2.826919000000	-2.164424000000	-2.918291000000
H	-3.662208000000	-3.714716000000	-2.728928000000
H	-4.052163000000	-2.648323000000	-4.095258000000
C	-4.999080000000	-0.528213000000	-2.614298000000
H	-5.751704000000	-0.018441000000	-2.010985000000
H	-4.050572000000	-0.006420000000	-2.499251000000

H	-5.289667000000	-0.457218000000	-3.666865000000

8α from B3LYP/def2-TZVP:

C	-0.944976000000	0.728147000000	-0.001594000000
C	-0.984453000000	-0.673934000000	-0.001643000000
C	0.336816000000	-1.144690000000	-0.001533000000
C	0.400696000000	1.123842000000	-0.001223000000
C	1.192908000000	-0.033646000000	-0.001236000000
C	-2.029574000000	1.563804000000	-0.001435000000
C	0.860267000000	2.413573000000	-0.000441000000
C	-2.114333000000	-1.447286000000	-0.001144000000
C	0.723100000000	-2.458235000000	-0.001158000000
C	2.561575000000	-0.072220000000	-0.000578000000
C	-3.339079000000	-0.619539000000	0.050555000000
C	-3.298954000000	0.806218000000	-0.052938000000
C	-1.620773000000	2.984382000000	0.050256000000
C	-0.252345000000	3.386748000000	-0.052660000000
C	2.337561000000	2.463770000000	0.052689000000
C	3.143230000000	1.286825000000	-0.050698000000
C	3.065859000000	-1.461806000000	0.050112000000
C	2.195211000000	-2.591571000000	-0.053386000000
C	-0.442428000000	-3.367259000000	0.051383000000
C	-1.786093000000	-2.888658000000	-0.051757000000
S	-4.853162000000	1.679512000000	-0.256583000000
S	-4.939789000000	-1.404047000000	0.255842000000
S	-3.096868000000	-4.097391000000	-0.252987000000
S	-0.190542000000	-5.131972000000	0.256877000000
S	2.938900000000	-4.211606000000	-0.258951000000
S	4.822184000000	-1.768699000000	0.252700000000
S	4.914233000000	1.494225000000	-0.251798000000
S	3.171357000000	4.039070000000	0.259225000000
S	0.098261000000	5.134679000000	-0.256484000000
S	-2.861494000000	4.264628000000	0.253408000000
C	-5.147106000000	1.809670000000	-2.109427000000
C	-5.241132000000	-1.512764000000	2.108839000000
C	-3.314875000000	-4.336982000000	-2.105391000000
C	-0.179433000000	-5.451504000000	2.109925000000
C	3.098260000000	-4.488037000000	-2.112147000000
C	5.132365000000	-1.859209000000	2.105205000000
C	5.231198000000	1.563507000000	-2.104008000000
C	3.348461000000	4.303644000000	2.112630000000
C	0.131693000000	5.454346000000	-2.109267000000
C	-3.060870000000	4.518161000000	2.106073000000
C	2.001692000000	4.254832000000	2.828485000000
H	1.311740000000	4.989861000000	2.419373000000
H	1.543908000000	3.267377000000	2.755951000000
H	2.145625000000	4.472892000000	3.891497000000
C	3.931529000000	5.720563000000	2.178511000000
H	4.104628000000	5.991097000000	3.223336000000
H	4.885437000000	5.782938000000	1.652024000000
H	3.248019000000	6.451814000000	1.745318000000

C	4.318986000000	3.303679000000	2.734923000000
H	3.933166000000	2.286692000000	2.675628000000
H	5.290030000000	3.330380000000	2.243127000000
H	4.457204000000	3.541771000000	3.794725000000
C	6.763419000000	1.588040000000	-2.164943000000
H	7.081807000000	1.651728000000	-3.208606000000
H	7.168494000000	2.452405000000	-1.635981000000
H	7.192423000000	0.683891000000	-1.731467000000
C	4.695234000000	0.328788000000	-2.822925000000
H	5.125624000000	-0.582829000000	-2.413560000000
H	3.608568000000	0.263926000000	-2.753830000000
H	4.954113000000	0.384116000000	-3.884994000000
C	4.657521000000	2.833236000000	-2.726726000000
H	3.569664000000	2.845745000000	-2.671538000000
H	5.035380000000	3.726666000000	-2.232143000000
H	4.933644000000	2.876551000000	-3.785444000000
C	6.660314000000	-1.976356000000	2.167628000000
H	7.143668000000	-1.099689000000	1.734908000000
H	6.973225000000	-2.059301000000	3.211679000000
H	7.012936000000	-2.863460000000	1.638880000000
C	4.482283000000	-3.092459000000	2.726161000000
H	3.395790000000	-3.039169000000	2.669376000000
H	4.806321000000	-4.006657000000	2.231367000000
H	4.753875000000	-3.152964000000	3.785127000000
C	4.671297000000	-0.594922000000	2.824726000000
H	5.156732000000	0.289351000000	2.416789000000
H	3.590645000000	-0.464199000000	2.754055000000
H	4.924838000000	-0.666804000000	3.887095000000
C	3.598848000000	-5.936251000000	-2.176829000000
H	3.753858000000	-6.217896000000	-3.221559000000
H	4.548626000000	-6.052377000000	-1.652067000000
H	2.875316000000	-6.626303000000	-1.741002000000
C	4.123918000000	-3.546332000000	-2.736933000000
H	3.797171000000	-2.508760000000	-2.678647000000
H	5.092420000000	-3.628120000000	-2.246213000000
H	4.247021000000	-3.793370000000	-3.796563000000
C	1.755650000000	-4.362641000000	-2.826513000000
H	1.024798000000	-5.055938000000	-2.415274000000
H	1.355832000000	-3.350322000000	-2.754924000000
H	1.885237000000	-4.590258000000	-3.889288000000
C	0.880654000000	-4.620168000000	2.826741000000
H	1.871232000000	-4.808465000000	2.417699000000
H	0.670018000000	-3.552361000000	2.754473000000
H	0.892283000000	-4.881623000000	3.889597000000
C	0.182605000000	-6.940391000000	2.174782000000
H	1.165215000000	-7.129344000000	1.740810000000
H	0.202505000000	-7.261478000000	3.219387000000
H	-0.552488000000	-7.551581000000	1.648320000000
C	-1.552678000000	-5.214350000000	2.731884000000
H	-1.838915000000	-4.164917000000	2.673377000000
H	-2.322038000000	-5.806726000000	2.239129000000

H	-1.524910000000	-5.489224000000	3.791389000000
C	-2.103879000000	-5.023046000000	-2.731571000000
H	-1.217767000000	-4.391864000000	-2.676599000000
H	-1.881630000000	-5.968488000000	-2.239364000000
H	-2.303283000000	-5.218548000000	-3.790245000000
C	-4.538011000000	-5.260200000000	-2.166003000000
H	-4.759896000000	-5.496767000000	-3.209755000000
H	-4.354505000000	-6.198433000000	-1.639640000000
H	-5.416850000000	-4.783964000000	-1.729538000000
C	-3.611418000000	-3.022513000000	-2.821452000000
H	-4.496008000000	-2.540905000000	-2.409686000000
H	-2.772023000000	-2.329350000000	-2.752435000000
H	-3.789622000000	-3.217901000000	-3.883658000000
C	-4.121592000000	-2.260418000000	2.827285000000
H	-3.991672000000	-3.260843000000	2.419702000000
H	-3.172429000000	-1.727729000000	2.755254000000
H	-4.367354000000	-2.351482000000	3.890036000000
C	-6.543264000000	-2.320442000000	2.173624000000
H	-6.416272000000	-3.313810000000	1.741577000000
H	-6.843580000000	-2.437242000000	3.218071000000
H	-7.352480000000	-1.813260000000	1.645320000000
C	-5.443890000000	-0.133233000000	2.729151000000
H	-4.535679000000	0.465397000000	2.670650000000
H	-6.245927000000	0.412918000000	2.235148000000
H	-5.697275000000	-0.243929000000	3.788595000000
C	-6.402631000000	2.688086000000	-2.172564000000
H	-6.695848000000	2.823381000000	-3.216813000000
H	-7.238614000000	2.225217000000	-1.645381000000
H	-6.221041000000	3.672016000000	-1.738594000000
C	-5.425485000000	0.444869000000	-2.733078000000
H	-4.551800000000	-0.203237000000	-2.676003000000
H	-6.256658000000	-0.057314000000	-2.240481000000
H	-5.672186000000	0.572031000000	-3.792288000000
C	-3.987742000000	2.496038000000	-2.825943000000
H	-3.802624000000	3.486630000000	-2.415658000000
H	-3.069462000000	1.911459000000	-2.755622000000
H	-4.228063000000	2.603550000000	-3.888411000000
C	-3.431116000000	3.223412000000	2.823873000000
H	-4.342938000000	2.793501000000	2.414538000000
H	-2.633353000000	2.482899000000	2.753403000000
H	-3.595146000000	3.429491000000	3.886364000000
C	-4.228617000000	5.510392000000	2.168588000000
H	-5.134547000000	5.085294000000	1.734846000000
H	-4.433915000000	5.760305000000	3.212742000000
H	-3.992531000000	6.436025000000	1.640866000000
C	-1.810865000000	5.133720000000	2.728654000000
H	-0.962807000000	4.452425000000	2.672213000000
H	-1.535614000000	6.064367000000	2.235021000000
H	-1.996102000000	5.341346000000	3.787705000000
C	0.579408000000	6.919806000000	-2.172254000000
H	0.619131000000	7.240186000000	-3.216495000000

H	-0.119794000000	7.572166000000	-1.646243000000
H	1.570701000000	7.051158000000	-1.736850000000
C	-1.252055000000	5.297535000000	-2.733570000000
H	-1.598471000000	4.266288000000	-2.676656000000
H	-1.986691000000	5.932849000000	-2.241325000000
H	-1.206868000000	5.571316000000	-3.792725000000
C	1.142991000000	4.563791000000	-2.825308000000
H	2.142161000000	4.694274000000	-2.414975000000
H	0.870930000000	3.509848000000	-2.754543000000
H	1.171154000000	4.825150000000	-3.887854000000

8β from B3LYP/def2-TZVP:

C	1.002434000000	0.649475000000	-0.632152000000
C	-0.307949000000	1.154119000000	-0.632113000000
C	-1.192808000000	0.063795000000	-0.632096000000
C	0.927462000000	-0.752729000000	-0.632211000000
C	-0.429296000000	-1.114723000000	-0.632131000000
C	2.111329000000	1.383950000000	-0.305762000000
C	1.968735000000	-1.580386000000	-0.305976000000
C	-0.663740000000	2.435737000000	-0.305755000000
C	-2.521610000000	0.121417000000	-0.305642000000
C	-0.894729000000	-2.360777000000	-0.305889000000
C	0.491361000000	3.296844000000	-0.040730000000
C	1.820489000000	2.820941000000	-0.211088000000
C	3.287178000000	0.551577000000	-0.040474000000
C	3.245488000000	-0.859604000000	-0.210919000000
C	1.540393000000	-2.955977000000	-0.040948000000
C	0.185308000000	-3.352302000000	-0.211112000000
C	-2.335368000000	-2.378464000000	-0.040772000000
C	-3.130915000000	-1.212077000000	-0.210860000000
C	-2.983607000000	1.486011000000	-0.040453000000
C	-2.120266000000	2.603120000000	-0.210756000000
S	3.162988000000	3.968840000000	-0.510624000000
S	0.193850000000	4.924559000000	0.641536000000
S	-2.797243000000	4.234765000000	-0.509115000000
S	-4.623303000000	1.705780000000	0.642681000000
S	-4.891967000000	-1.351453000000	-0.509091000000
S	-3.051406000000	-3.870383000000	0.641219000000
S	-0.225669000000	-5.070349000000	-0.509563000000
S	2.738204000000	-4.097852000000	0.640869000000
S	4.752499000000	-1.781273000000	-0.509459000000
S	4.742870000000	1.338065000000	0.642174000000
C	2.930920000000	4.494517000000	-2.307466000000
C	0.755679000000	4.868834000000	2.442826000000
C	-3.370399000000	4.177675000000	-2.305478000000
C	-4.395651000000	2.222132000000	2.444028000000
C	-5.014930000000	-1.912610000000	-2.305970000000
C	-3.472869000000	-3.495607000000	2.442715000000
C	0.269841000000	-5.360317000000	-2.306533000000
C	2.251639000000	-4.383096000000	2.442341000000
C	5.182198000000	-1.398237000000	-2.305976000000

C	4.863446000000	0.786548000000	2.443531000000
C	1.933212000000	-3.061875000000	3.137067000000
H	2.770144000000	-2.367853000000	3.073300000000
H	1.053728000000	-2.582295000000	2.707298000000
H	1.725049000000	-3.247211000000	4.195265000000
C	3.541316000000	-4.987907000000	3.015047000000
H	3.388231000000	-5.227384000000	4.070486000000
H	3.811038000000	-5.911308000000	2.498923000000
H	4.378869000000	-4.294487000000	2.937289000000
C	1.103996000000	-5.375536000000	2.613003000000
H	0.163341000000	-4.980745000000	2.234952000000
H	1.305237000000	-6.311343000000	2.093324000000
H	0.972467000000	-5.591209000000	3.678570000000
C	-0.360142000000	-6.730547000000	-2.588268000000
H	-0.124147000000	-7.032095000000	-3.612047000000
H	0.031829000000	-7.495049000000	-1.914978000000
H	-1.444980000000	-6.700866000000	-2.480851000000
C	-0.335164000000	-4.300976000000	-3.225238000000
H	-1.418592000000	-4.253209000000	-3.117602000000
H	0.075129000000	-3.310951000000	-3.025013000000
H	-0.106771000000	-4.548417000000	-4.266515000000
C	1.783145000000	-5.434192000000	-2.492394000000
H	2.261825000000	-4.480017000000	-2.277556000000
H	2.228591000000	-6.186993000000	-1.843638000000
H	2.008358000000	-5.692491000000	-3.532418000000
C	-3.650491000000	-4.908992000000	3.015274000000
H	-2.732583000000	-5.491872000000	2.937428000000
H	-3.925477000000	-4.837322000000	4.070727000000
H	-4.445722000000	-5.450277000000	2.499117000000
C	-4.770864000000	-2.709989000000	2.613374000000
H	-4.685183000000	-1.693178000000	2.236039000000
H	-5.598786000000	-3.189648000000	2.093046000000
H	-5.016999000000	-2.652022000000	3.678884000000
C	-2.314285000000	-2.785295000000	3.137565000000
H	-1.395984000000	-3.367413000000	3.073849000000
H	-2.129241000000	-1.800733000000	2.707923000000
H	-2.554868000000	-2.644505000000	4.195756000000
C	-6.512948000000	-1.737753000000	-2.587291000000
H	-6.727012000000	-2.055967000000	-3.610848000000
H	-7.118381000000	-2.346759000000	-1.913508000000
H	-6.820454000000	-0.696944000000	-2.480302000000
C	-4.616710000000	-3.374434000000	-2.491776000000
H	-3.561397000000	-3.534263000000	-2.276106000000
H	-5.195179000000	-4.031144000000	-1.843601000000
H	-4.791829000000	-3.668345000000	-3.531981000000
C	-4.195119000000	-1.009504000000	-3.224995000000
H	-4.484475000000	0.035615000000	-3.116855000000
H	-3.126620000000	-1.093780000000	-3.025528000000
H	-4.360538000000	-1.302885000000	-4.266251000000
C	-3.360778000000	1.340337000000	3.137645000000
H	-3.629995000000	0.286928000000	3.074027000000

H	-2.367769000000	1.469289000000	2.706960000000
H	-3.300290000000	1.612531000000	4.195810000000
C	-5.794007000000	1.953342000000	3.017972000000
H	-6.063963000000	0.900020000000	2.940621000000
H	-5.810056000000	2.237270000000	4.073369000000
H	-6.555488000000	2.541672000000	2.502388000000
C	-4.050466000000	3.699646000000	2.614582000000
H	-3.057424000000	3.933275000000	2.236535000000
H	-4.763386000000	4.338354000000	2.094879000000
H	-4.070786000000	3.951517000000	3.680131000000
C	-4.639857000000	3.350152000000	-2.489336000000
H	-4.468229000000	2.296844000000	-2.272961000000
H	-5.441661000000	3.699860000000	-1.840607000000
H	-4.974410000000	3.425892000000	-3.529256000000
C	-3.663640000000	5.656792000000	-2.588270000000
H	-4.033227000000	5.761716000000	-3.611571000000
H	-4.428318000000	6.047083000000	-1.914197000000
H	-2.767185000000	6.268790000000	-2.482870000000
C	-2.260130000000	3.673279000000	-3.224809000000
H	-1.354021000000	4.269309000000	-3.118085000000
H	-2.012505000000	2.630648000000	-3.024363000000
H	-2.590977000000	3.739596000000	-4.265858000000
C	0.236775000000	3.612682000000	3.137432000000
H	-0.848235000000	3.542991000000	3.073611000000
H	0.666535000000	2.707834000000	2.707611000000
H	0.514106000000	3.640209000000	4.195632000000
C	0.068070000000	6.116169000000	3.015877000000
H	-1.017119000000	6.047618000000	2.938161000000
H	0.332772000000	6.219676000000	4.071321000000
H	0.392713000000	7.021805000000	2.499903000000
C	2.267552000000	4.996927000000	2.613243000000
H	2.796474000000	4.124608000000	2.235163000000
H	2.654815000000	5.872302000000	2.093579000000
H	2.500882000000	5.094014000000	3.678789000000
C	4.246025000000	5.232069000000	-2.590813000000
H	4.231403000000	5.614534000000	-3.614657000000
H	4.379385000000	6.081059000000	-1.917859000000
H	5.106075000000	4.570076000000	-2.484189000000
C	1.750341000000	5.444364000000	-2.492214000000
H	0.802210000000	4.954166000000	-2.276583000000
H	1.833328000000	6.315085000000	-1.843384000000
H	1.719269000000	5.785877000000	-3.532156000000
C	2.796034000000	3.281736000000	-3.225769000000
H	3.644289000000	2.605870000000	-3.119160000000
H	1.882173000000	2.722418000000	-3.024282000000
H	2.755497000000	3.616007000000	-4.267053000000
C	3.508131000000	0.890624000000	3.137736000000
H	3.105747000000	1.900684000000	3.073958000000
H	2.781082000000	0.201719000000	2.707630000000
H	3.619943000000	0.635354000000	4.195945000000
C	5.836074000000	1.826879000000	3.016926000000

H	5.434532000000	2.837384000000	2.939374000000
H	6.016370000000	1.607102000000	4.072352000000
H	6.797827000000	1.799095000000	2.501108000000
C	5.453817000000	-0.611164000000	2.614052000000
H	4.788157000000	-1.384334000000	2.236265000000
H	6.405918000000	-0.708248000000	2.094086000000
H	5.618765000000	-0.802754000000	3.679573000000
C	6.290578000000	-2.420814000000	-2.588062000000
H	6.650320000000	-2.289242000000	-3.611791000000
H	7.138776000000	-2.284568000000	-1.914698000000
H	5.927028000000	-3.443398000000	-2.481027000000
C	5.720371000000	0.018209000000	-2.490529000000
H	4.960803000000	0.768212000000	-2.275438000000
H	6.573660000000	0.208678000000	-1.841200000000
H	6.036116000000	0.153315000000	-3.530307000000
C	3.987955000000	-1.645309000000	-3.225254000000
H	3.607257000000	-2.660855000000	-3.118389000000
H	3.173421000000	-0.948908000000	-3.024867000000
H	4.294279000000	-1.504041000000	-4.266339000000

8α from B3LYP-D3BJ/def2-TZVP:

C	1.018760000000	-0.623548000000	-0.031834000000
C	0.907657000000	0.775717000000	-0.031482000000
C	-0.457464000000	1.102464000000	-0.031877000000
C	-0.277716000000	-1.161489000000	-0.031684000000
C	-1.190109000000	-0.094844000000	-0.031781000000
C	2.184265000000	-1.336551000000	-0.013842000000
C	-0.595521000000	-2.490234000000	-0.012414000000
C	1.945701000000	1.664003000000	-0.011795000000
C	-0.981413000000	2.364279000000	-0.013625000000
C	-2.552084000000	-0.203270000000	-0.013208000000
C	3.248647000000	0.972850000000	0.038036000000
C	3.362031000000	-0.447715000000	-0.044974000000
C	1.929715000000	-2.789350000000	0.034406000000
C	0.613405000000	-3.335994000000	-0.046144000000
C	-2.055555000000	-2.697135000000	0.040682000000
C	-2.982641000000	-1.614700000000	-0.041595000000
C	-3.200123000000	1.121708000000	0.033546000000
C	-2.456611000000	2.337615000000	-0.047884000000
C	0.078258000000	3.389988000000	0.038104000000
C	1.464662000000	3.058984000000	-0.041999000000
S	4.993225000000	-1.147193000000	-0.229316000000
S	4.747397000000	1.920835000000	0.235857000000
S	2.635064000000	4.394419000000	-0.218077000000
S	-0.361026000000	5.108395000000	0.234625000000
S	-3.364211000000	3.862291000000	-0.235650000000
S	-4.970924000000	1.234964000000	0.221702000000
S	-4.714083000000	-2.007740000000	-0.217965000000
S	-2.709773000000	-4.344950000000	0.244053000000
S	0.451539000000	-5.103280000000	-0.231342000000
S	3.295305000000	-3.922477000000	0.223754000000

C	5.212560000000	-1.273195000000	-2.080648000000
C	4.940909000000	2.068045000000	2.088341000000
C	2.831462000000	4.569650000000	-2.067866000000
C	-0.447686000000	5.338784000000	2.086688000000
C	-3.459637000000	4.093300000000	-2.087407000000
C	-5.225775000000	1.233834000000	2.072598000000
C	-4.974519000000	-2.037984000000	-2.068063000000
C	-2.774381000000	-4.573746000000	2.097104000000
C	0.391945000000	-5.349572000000	-2.082601000000
C	3.504263000000	-4.066932000000	2.074556000000
C	-1.403025000000	-4.394673000000	2.735657000000
H	-0.682117000000	-5.090652000000	2.314811000000
H	-1.029021000000	-3.380087000000	2.597659000000
H	-1.474294000000	-4.577754000000	3.811741000000
C	-3.238843000000	-6.024702000000	2.235953000000
H	-3.329445000000	-6.276221000000	3.295215000000
H	-4.212344000000	-6.173940000000	1.766571000000
H	-2.523588000000	-6.710531000000	1.780489000000
C	-3.782052000000	-3.623121000000	2.730033000000
H	-3.468362000000	-2.587479000000	2.612814000000
H	-4.768515000000	-3.734639000000	2.283805000000
H	-3.854581000000	-3.827470000000	3.802517000000
C	-6.485423000000	-2.245713000000	-2.187246000000
H	-6.760859000000	-2.304339000000	-3.242808000000
H	-6.795823000000	-3.173043000000	-1.703382000000
H	-7.031512000000	-1.416998000000	-1.735187000000
C	-4.569567000000	-0.723417000000	-2.722908000000
H	-5.124304000000	0.111167000000	-2.302332000000
H	-3.503674000000	-0.529463000000	-2.603021000000
H	-4.778120000000	-0.771934000000	-3.795592000000
C	-4.219128000000	-3.199525000000	-2.701399000000
H	-3.143583000000	-3.068369000000	-2.597591000000
H	-4.493330000000	-4.148499000000	-2.244182000000
H	-4.445531000000	-3.244229000000	-3.771009000000
C	-6.750111000000	1.201513000000	2.197570000000
H	-7.160860000000	0.297077000000	1.747402000000
H	-7.027279000000	1.216342000000	3.254205000000
H	-7.204247000000	2.068339000000	1.715134000000
C	-4.660328000000	2.501005000000	2.700577000000
H	-3.578005000000	2.539787000000	2.592866000000
H	-5.081887000000	3.394013000000	2.242844000000
H	-4.887081000000	2.512070000000	3.770985000000
C	-4.616351000000	0.000737000000	2.727270000000
H	-5.037460000000	-0.911053000000	2.312118000000
H	-3.534159000000	-0.025087000000	2.598798000000
H	-4.821626000000	0.019210000000	3.801538000000
C	-4.141744000000	5.456522000000	-2.216845000000
H	-4.270479000000	5.698272000000	-3.274441000000
H	-5.126463000000	5.451408000000	-1.747155000000
H	-3.540054000000	6.240923000000	-1.756327000000
C	-4.309687000000	3.002767000000	-2.726708000000

H	-3.840572000000	2.026748000000	-2.615842000000
H	-5.301021000000	2.958492000000	-2.279463000000
H	-4.413941000000	3.200258000000	-3.797864000000
C	-2.077917000000	4.131984000000	-2.727725000000
H	-1.471256000000	4.926775000000	-2.301713000000
H	-1.552318000000	3.185694000000	-2.599626000000
H	-2.179041000000	4.311386000000	-3.802015000000
C	-1.452588000000	4.390050000000	2.727427000000
H	-2.444269000000	4.527481000000	2.304556000000
H	-1.158366000000	3.348908000000	2.594460000000
H	-1.504313000000	4.584622000000	3.802619000000
C	-0.926253000000	6.785808000000	2.218741000000
H	-1.906961000000	6.917641000000	1.760222000000
H	-1.003723000000	7.046452000000	3.276836000000
H	-0.225796000000	7.477611000000	1.748596000000
C	0.925031000000	5.165637000000	2.723535000000
H	1.281242000000	4.143252000000	2.611438000000
H	1.658153000000	5.834473000000	2.276492000000
H	0.860723000000	5.377956000000	3.794999000000
C	1.535835000000	5.053507000000	-2.706492000000
H	0.747948000000	4.309758000000	-2.602164000000
H	1.191984000000	5.981547000000	-2.253439000000
H	1.694416000000	5.220165000000	-3.776236000000
C	3.923758000000	5.634050000000	-2.186712000000
H	4.115133000000	5.840281000000	-3.242343000000
H	3.620297000000	6.566346000000	-1.708075000000
H	4.853560000000	5.294045000000	-1.729308000000
C	3.288754000000	3.269647000000	-2.717109000000
H	4.229195000000	2.929384000000	-2.291763000000
H	2.546136000000	2.480955000000	-2.596525000000
H	3.431244000000	3.428617000000	-3.789919000000
C	3.722280000000	2.714435000000	2.734726000000
H	3.535049000000	3.700477000000	2.317877000000
H	2.829176000000	2.104084000000	2.600101000000
H	3.892321000000	2.819469000000	3.810174000000
C	6.160048000000	2.982302000000	2.222982000000
H	5.970525000000	3.957034000000	1.772053000000
H	6.385994000000	3.131135000000	3.281436000000
H	7.037709000000	2.542615000000	1.746828000000
C	5.215200000000	0.708294000000	2.717394000000
H	4.358906000000	0.046126000000	2.603624000000
H	6.081346000000	0.228370000000	2.265535000000
H	5.398566000000	0.830902000000	3.789132000000
C	6.561376000000	-1.983722000000	-2.207502000000
H	6.812045000000	-2.099079000000	-3.264569000000
H	7.356634000000	-1.408824000000	-1.730591000000
H	6.526774000000	-2.974371000000	-1.752782000000
C	5.270926000000	0.110755000000	-2.714584000000
H	4.320562000000	0.630182000000	-2.605712000000
H	6.048939000000	0.722684000000	-2.261788000000
H	5.475119000000	0.015075000000	-3.785300000000

C	4.113853000000	-2.106352000000	-2.728353000000
H	4.079973000000	-3.106878000000	-2.305335000000
H	3.135587000000	-1.642129000000	-2.603484000000
H	4.305519000000	-2.190484000000	-3.801977000000
C	3.750332000000	-2.710654000000	2.722975000000
H	4.627896000000	-2.228671000000	2.300342000000
H	2.894209000000	-2.047772000000	2.596845000000
H	3.910927000000	-2.843150000000	3.796840000000
C	4.748206000000	-4.948427000000	2.200339000000
H	5.615833000000	-4.469400000000	1.745236000000
H	4.965103000000	-5.119859000000	3.257252000000
H	4.594924000000	-5.917600000000	1.723327000000
C	2.297121000000	-4.745826000000	2.708376000000
H	1.403488000000	-4.134333000000	2.598688000000
H	2.104605000000	-5.717301000000	2.256866000000
H	2.474647000000	-4.883277000000	3.779304000000
C	0.153499000000	-6.855366000000	-2.209378000000
H	0.115767000000	-7.128311000000	-3.266536000000
H	0.958266000000	-7.423208000000	-1.740152000000
H	-0.791411000000	-7.142995000000	-1.746978000000
C	1.716307000000	-4.958290000000	-2.725743000000
H	1.903384000000	-3.891500000000	-2.616590000000
H	2.549524000000	-5.498974000000	-2.280631000000
H	1.683069000000	-5.180652000000	-3.796573000000
C	-0.755582000000	-4.577928000000	-2.721693000000
H	-1.710482000000	-4.869276000000	-2.292111000000
H	-0.631053000000	-3.502359000000	-2.596520000000
H	-0.781071000000	-4.785184000000	-3.795442000000

8β from B3LYP-D3BJ/def2-TZVP:

C	-0.707264000000	-0.971942000000	-0.874984000000
C	0.705987000000	-0.972868000000	-0.875069000000
C	1.143576000000	0.370923000000	-0.875245000000
C	-1.143145000000	0.372380000000	-0.875236000000
C	0.000748000000	1.202305000000	-0.875405000000
C	-1.467891000000	-2.038399000000	-0.446182000000
C	-2.392522000000	0.766256000000	-0.446606000000
C	1.485302000000	-2.025882000000	-0.446535000000
C	2.385843000000	0.786703000000	-0.446575000000
C	-0.010793000000	2.512224000000	-0.446711000000
C	0.720476000000	-3.222511000000	-0.127086000000
C	-0.688047000000	-3.265516000000	-0.275667000000
C	-2.842160000000	-1.680826000000	-0.126480000000
C	-3.318499000000	-0.354628000000	-0.275518000000
C	-2.477166000000	2.183853000000	-0.127289000000
C	-1.362999000000	3.046618000000	-0.276301000000
C	1.311083000000	3.030751000000	-0.126712000000
C	2.476018000000	2.237885000000	-0.275603000000
C	3.287544000000	-0.310442000000	-0.127084000000
C	2.893375000000	-1.663347000000	-0.275982000000
S	-1.480300000000	-4.853910000000	-0.396257000000

S	1.529530000000	-4.618536000000	0.607690000000
S	4.159471000000	-2.907308000000	-0.397010000000
S	4.865064000000	0.027930000000	0.607965000000
S	4.050110000000	3.058244000000	-0.395690000000
S	1.476301000000	4.635078000000	0.609598000000
S	-1.655718000000	4.797222000000	-0.397385000000
S	-3.952129000000	2.837342000000	0.608034000000
S	-5.074056000000	-0.092605000000	-0.396044000000
S	-3.919308000000	-2.881669000000	0.609163000000
C	-1.932654000000	-4.958473000000	-2.209905000000
C	0.987280000000	-4.585978000000	2.404912000000
C	4.118663000000	-3.369415000000	-2.210761000000
C	4.666170000000	-0.477559000000	2.405185000000
C	4.478494000000	2.875630000000	-2.209003000000
C	1.895947000000	4.288907000000	2.406617000000
C	-1.352039000000	5.146785000000	-2.211365000000
C	-3.493371000000	3.128926000000	2.405260000000
C	-5.312515000000	0.305677000000	-2.209820000000
C	-4.055656000000	-2.355413000000	2.406374000000
C	-2.671834000000	1.960652000000	2.936075000000
H	-3.213009000000	1.023481000000	2.834756000000
H	-1.721779000000	1.865744000000	2.412877000000
H	-2.454970000000	2.118888000000	3.996140000000
C	-4.865009000000	3.165932000000	3.085832000000
H	-4.733923000000	3.354180000000	4.154120000000
H	-5.486816000000	3.965010000000	2.678141000000
H	-5.393783000000	2.221277000000	2.961476000000
C	-2.768424000000	4.450535000000	2.631445000000
H	-1.779287000000	4.454203000000	2.179082000000
H	-3.329711000000	5.286346000000	2.216323000000
H	-2.642481000000	4.614238000000	3.706212000000
C	-1.873217000000	6.579358000000	-2.353322000000
H	-1.743372000000	6.909456000000	-3.386590000000
H	-2.932202000000	6.642389000000	-2.101720000000
H	-1.322188000000	7.265190000000	-1.707702000000
C	0.121424000000	5.086683000000	-2.594159000000
H	0.724810000000	5.737146000000	-1.962382000000
H	0.511077000000	4.075368000000	-2.516158000000
H	0.241575000000	5.407101000000	-3.633416000000
C	-2.169562000000	4.191737000000	-3.073111000000
H	-1.817302000000	3.165784000000	-2.968295000000
H	-3.223471000000	4.220707000000	-2.800798000000
H	-2.072840000000	4.471826000000	-4.126066000000
C	1.504269000000	5.603707000000	3.087786000000
H	0.441817000000	5.812007000000	2.964347000000
H	1.724691000000	5.537439000000	4.155908000000
H	2.069665000000	6.443609000000	2.680016000000
C	3.377513000000	4.011232000000	2.633246000000
H	3.688881000000	3.071740000000	2.182257000000
H	3.997325000000	4.804144000000	2.217199000000
H	3.572125000000	3.943857000000	3.708133000000

C	1.040980000000	3.144632000000	2.936756000000
H	-0.017931000000	3.367664000000	2.834968000000
H	1.246405000000	2.212344000000	2.413347000000
H	1.258334000000	2.987385000000	3.996872000000
C	5.677924000000	3.816452000000	-2.351311000000
H	6.033648000000	3.793494000000	-3.383978000000
H	5.407879000000	4.842995000000	-2.102308000000
H	6.500159000000	3.507619000000	-1.703702000000
C	3.317122000000	3.354124000000	-3.072378000000
H	2.451653000000	2.700154000000	-2.967610000000
H	3.016279000000	4.364988000000	-2.801547000000
H	3.614385000000	3.348225000000	-4.125048000000
C	4.880103000000	1.456072000000	-2.589243000000
H	5.687170000000	1.086744000000	-1.957977000000
H	4.040741000000	0.770882000000	-2.508258000000
H	5.220319000000	1.439469000000	-3.629019000000
C	3.314615000000	-0.016159000000	2.936005000000
H	3.201307000000	1.060094000000	2.834699000000
H	2.490503000000	-0.498074000000	2.412576000000
H	3.232170000000	-0.271782000000	3.996033000000
C	5.797094000000	0.299717000000	3.085562000000
H	5.668423000000	1.374711000000	2.962042000000
H	5.802465000000	0.069768000000	4.153718000000
H	6.769951000000	0.020023000000	2.677259000000
C	4.858026000000	-1.972636000000	2.631791000000
H	4.059761000000	-2.557888000000	2.181037000000
H	5.803022000000	-2.318340000000	2.215356000000
H	4.854205000000	-2.178537000000	3.706667000000
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H	3.327989000000	-1.494045000000	-2.967062000000
H	5.085840000000	-1.519436000000	-2.801554000000
H	4.301927000000	-2.399807000000	-4.125837000000
C	5.383472000000	-4.220315000000	-2.353164000000
H	5.472174000000	-4.564288000000	-3.386259000000
H	6.276599000000	-3.647397000000	-2.102538000000
H	5.342474000000	-5.098658000000	-1.706883000000
C	2.892293000000	-4.188791000000	-2.592418000000
H	2.789136000000	-5.070412000000	-1.961258000000
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C	1.008975000000	-3.158199000000	2.936348000000
H	1.997132000000	-2.717276000000	2.833563000000
H	0.294778000000	-2.523533000000	2.414386000000
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C	2.075704000000	-5.422054000000	3.084840000000
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H	1.858713000000	-5.498697000000	4.152969000000
H	2.110049000000	-6.433524000000	2.676023000000
C	-0.375727000000	-5.229663000000	2.631447000000
H	-1.178692000000	-4.650760000000	2.180701000000
H	-0.413169000000	-6.235225000000	2.215042000000

H	-0.572758000000	-5.289525000000	3.706341000000
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H	-0.953366000000	-4.837685000000	-4.125018000000
C	-3.089638000000	-4.043966000000	-2.592188000000
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H	-2.811049000000	-2.996687000000	-2.513188000000
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C	-2.690840000000	-1.935507000000	2.937791000000
H	-1.966976000000	-2.740067000000	2.836905000000
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C	-5.088500000000	-1.257497000000	2.632565000000
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H	-4.887914000000	-0.584771000000	-4.125043000000
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H	-5.242807000000	2.463444000000	-1.959541000000
H	-3.723201000000	1.753666000000	-2.507922000000
H	-5.069538000000	1.903448000000	-3.630173000000

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