Supporting Information for:

Switching of Non-Helical Overcrowded Heptafulvalene Derivatives

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1. Synthesis

General: The reagents and starting materials employed were commercially available and used without any further purification or made following reported methods. Anhydrous and oxygen-free diethyl ether and THF were purified by an Advanced Technology Pure-Solv PS-MD-4 system. ¹H-NMR or ¹³C-NMR spectra were recorded on a Brucker ADVANCE III 400MHz spectrometer. Mass spectra were recorded on a Therno Finnigan MAT 95 XL spectrometer. X-ray crystallography data were collected on a Bruker AXS Kappa ApexII Duo Diffractometer. UV-vis absorption spectra were recorded on a Varian CARY 1E UV-vis spectrophotometer. Melting points, without correction, were measured using a Nikon Polarizing Microscope ECLIPSE 50i POL equipped with an INTEC HCS302 heating stage or using differential scanning calorimetry (PERKIN ELMER DSC 6) as indicated.

Scheme 1 Synthesis and reaction of 2.



10,11-dihydro-5H-dibenzo[a,d]cycloheptene-5-thione (14)

10,11-dihydro-5H-dibenzo[a,d]cycloheptene-5-thione (14) was synthesized following the reported procedures ¹ with minor modifications. A mixture of the dibenzosuberone (2.08 g, 10 mmol) and Lawesson's reagent (0.7 eq, 2.83 g, 7 mmol) in 100 mL of toluene was heated to reflux for 8 hours. Then the dark-blue solution was concentrated under reduced pressure, and the crude product was purified by column chromatography on silica gel with

^{1.} M. I. Hegab, A. B. A. El-Gazzar, I. S. Farag, F. A. Gad, Sulfur Lett. 2002, 25, 79-85

CH₂Cl₂/hexane 1/1 (V/V) as eluent. 10,11-dihydro-5H-dibenzo[a,d]cycloheptene-5-thione (**14**) was collected as a blue solid (2.0 g, 89%). ¹H-NMR (CDCl₃) δ (ppm): 7.76 (d, J = 7.6 Hz, 2H), 7.34 (t, J = 7.6 Hz, 2H), 7.18 (t, J = 7.6 Hz, 2H), 7.11 (d, J = 7.6 Hz, 2H), 3.18 (s, 4H). ¹³C-NMR (CDCl₃) δ (ppm): 246.7, 149.5, 136.5, 131.0, 129.6, 129.0, 126.4, 33.9.

10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-one hydrazone (15)

To a solution of 10,11-dihydro-5H-dibenzo[a,d]cycloheptene-5-thione (**14**) (672 mg, 3 mmol) in 50 ml CHCl₃ was added 3 ml of 35% hydrazine hydrate with stirring at room temperature. The resulting light yellow solution was kept stirred for 30 minutes. Then the solution was washed with water and brine, dried with anhydrous Na₂SO₄, and concentrated under reduced pressure. 647 mg of hydrazone **15** was collected in a yield of 97%. ¹H-NMR (DMSO-d₆) δ (ppm): 7.06-7.50 (8H), 6.28 (s, 2H), 2.94 (br, 4H). ¹³C-NMR (CDCl₃) δ (ppm): 149.8, 140.3, 137.8, 137.2, 133.8, 130.5, 129.5, 128.9, 128.7, 128.3, 127.3, 126.4, 126.3, 34.2, 32.2. MS (EI⁺): cald. for C₁₅H₁₄N₂ ([M]⁺): 222.1152, found: 222.1155.

5-diazo-10,11-dihydro-5H-dibenzo[a,d]cycloheptene (16)

A suspension of hydrazone **15** (666 mg, 3 mmol), anhydrous sodium sulfate (400 mg, 2.8 mmol), and red HgO (1.3 g, 6 mmol) in 30 ml of anhydrous Et_2O was stirred in a round-bottom flask attached to a drying tube of anhydrous $CaCl_2$. To this suspension was added 2 ml of a freshly prepared concentrated solution of KOH in ethanol. The reaction mixture was kept stirred at room temperature for 12 hours. The resulting suspension was filtered and the solid residue was washed with Et_2O . The filtrates were combined and concentrated under reduced pressure yielding diazo compound **16**, which was used in the next step without further purification.

4,5,4',5'-tetrahydro-2,3;6,7,2',3';6,'7'-tetrabenzoheptafulvalene episulfide (6)

To a solution of thioketone **14** (560 mg, 2.5 mmol) in 30 ml anhydrous THF was added a solution of diazo compound **16** (660 mg, crude) in 20 ml of anhydrous THF with stirring at room temperature. The solution was kept stirred overnight in a round-bottom flask equipped with a drying tube of anhydrous CaCl₂. Then the resulting reaction mixture was concentrated under reduced pressure. The crude product was triturated with ethanol, filtered, and repeated for 3 times then purified by column chromatography on silica gel with CH₂Cl₂/hexane 1/1 (V/V) as eluent. 773 mg of episulfide **6** was obtained as white powders in a yield of 62% for the two steps. Although the product appeared as only one spot on TLC, its ¹H-NMR spectrum was not clean. This phenomenon may result from slow ring-flipping, which was reported for other molecules with seven-membered rings and discussed Ref. 2 in its supporting information. ¹H-NMR (CDCl₃) δ (ppm): 7.68 (m, 4H), 6.93 (br, 12H), 3.76 (br, 4H), 3.68 (br, 4H). MS (EI⁺): cald. for C₃₀H₂₄S ([M]⁺): 416.1593, found: 416.1599.

Anti-4,5,4',5'-tetrahydro-2,3;6,7;2',3';6,'7'-tetrabenzoheptafulvalene (anti-2)

A mixture of episulfide **6** (416 mg, 1 mmol) and PPh₃ (315 mg, 1.2 mmol) in 50 ml anhydrous toluene were heated to reflux for 12 hours with the condenser connected to a drying tube of anhydrous CaCl₂. The resulting reaction mixture was then concentrated under reduced pressure. The crude product was triturated with ethanol, filtered, and repeated for 3

times to remove the unreacted PPh₃, which has a very similar polarity as *anti*-**2**. Purification by column chromatography on silica gel with CH₂Cl₂/hexane 1/3 (V/V) as eluent yielded 347 mg (90%) of *anti*-**2** as a white solid. Melting point 324.6 °C (measured with DSC). ¹H-NMR (CDCl₃) δ (ppm): 7.11 (d, J = 7.6 Hz, 4H), 6.98 (m, 4H), 6.76 (m, 8H), 3.68 (m, 4H), 3.00 (m, 4H). ¹³C-NMR (CDCl₃) δ (ppm): 141.0, 140.1, 138.5, 129.2, 128.9, 126.8, 125.5, 33.0. MS (EI⁺): cald. for C₃₀H₂₄ ([M]⁺): 384.1873, found: 384.1876.

Scheme 2 Synthesis and reaction of 3.



5H-dibenzo[a,d]cycloheptene-5-thione (17)

5H-dibenzo[a,d]cycloheptene-5-thione **17** was synthesized according to the reported procedures with minor modifications.^[1] A solution of dibenzosubrenone (2.06 g, 10 mmol) and Lawesson's reagent (0.7 eq, 2.83 g, 7 mmol) in 100 mL of toluene was heated to reflux for 8 hours. The resulting dark-green solution was then concentrated reduced pressure. The crude product was purified by column chromatography on silica gel with CH₂Cl₂/hexane 1/1 (V/V) as eluent. 2.02 g (90%) of 5H-dibenzo[a,d]cycloheptene-5-thione **17** was obtained as a green solid. ¹H-NMR (CDCl₃) δ (ppm): 8.02 (dd, J₁ = 7.6 Hz, J₂ = 1.2 Hz, 2H), 7.48 (dt, J₁ = 7.6 Hz, J₂ = 1.2 Hz, 2H), 7.35 (m, 4H), 7.00 (s, 2H). ¹³C-NMR (CDCl₃) δ (ppm): 239.9, 149.3, 131.5, 130.8, 130.6, 129.6, 128.7, 128.7.

5H-dibenzo[a,d]cyclohepten-5-one hydrazone (18)

To a blue solution of 5H-dibenzo[a,d]cycloheptene-5-thione (**17**) (1.11 g, 5 mmol) in 80 ml CHCl₃ was added 5 ml of 35% hydrazine hydrate with stirring at room temperature. The resulting light yellow solution was kept stirred for 30 minutes. Then the solution was washed with water and brine, dried with anhydrous Na₂SO₄, and concentrated under reduced pressure. 1.1 g (100%) of hydrazone **18** was collected as a light yellow gel. ¹H-NMR (CDCl₃) δ (ppm): 7.58 (t, J = 7.2 Hz, 2H), 7.31-7.49 (6H), 6.86 (m, 2H), 5.54 (s, 2H). ¹³C-NMR (CDCl₃) δ (ppm): 148.1, 139.6, 135.2, 134.1, 131.9, 130.7, 130.3, 130.2, 129.0(4), 128.9(8), 128.8, 128.1(2), 128.0(6), 127.7. MS (EI⁺): cald. For C₁₅H₁₂N₂ ([M]⁺): 220.0995 found: 220.0989.

5-diazo-5H-dibenzo[a,d]cycloheptene (19)

A suspension of hydrazone 18 (1.1 g, 5 mmol), anhydrous sodium sulfate (650 mg, 4.6 mmol), and red HgO (2.16 g, 10 mmol) in 50 ml of anhydrous Et_2O was stirred in a

round-bottom flask attached to a drying tube of anhydrous $CaCl_2$. To this suspension was added 5 ml of a freshly prepared concentrated solution of KOH in ethanol. The reaction mixture was kept stirred at room temperature for 12 hours. The resulting suspension was filtered and the solid residue was washed with Et₂O. The filtrates were combined and concentrated under reduced pressure yielding diazo compound **19**, which was used in the next step immediately without further purification.

4,5-dihydro-2,3;6,7,2',3';6,'7'-tetrabenzoheptafulvalene episulfide (7)

To a solution of thioketone **14** (896 mg, 4 mmol) in 40 ml THF was added 30 ml of a solution of diazo **19** (1.1 g, crude) in THF with stirring at room temperature. The solution was kept stirred overnight in a round-bottom flask attached to a drying tube of anhydrous CaCl₂. Then the resulting reaction mixture was concentrated under reduced pressure. The crude product was triturated with ethanol, filtered, and repeated for 3 times then purified by column chromatography on silica gel with CH₂Cl₂/hexane 1/1 (V/V) as eluent. 1.63 g of episulfide **7** was obtained as white powders in a yield of 79% for the two steps. Although the product appeared as only one spot on TLC, its ¹H-NMR spectrum was not clean. This phenomenon may result from slow ring-flipping, which was reported for other molecules with seven-membered rings and discussed Ref. 2 in its supporting information. ¹H-NMR (CDCl₃) δ (ppm): 7.91 (d, J = 8.0 Hz, 2H), 7.67 (d, J = 8.0 Hz, 2H), 7.15 (m, 2H), 7.05 (m, 4H), 6.96 (s, 2H), 6.86 (m, 2H), 6.81 (m, 4H), 3.85 (m, 2H), 2.62 (m, 2H). MS (EI⁺): cald. For C₃₀H₂₂S ([M]⁺): 414.1437, found: 414.1437.

Anti-4,5-dihydro-2,3;6,7,2',3';6,'7'-tetrabenzoheptafulvalene (anti-3)

A mixture of episulfide **7** (828 mg, 2 mmol) and PPh₃ (629 mg, 2.4 mmol) in 100 ml anhydrous toluene were heated to reflux for 12 hours with the condenser connected to a drying tube of anhydrous CaCl₂. The resulting reaction mixture was then concentrated under reduced pressure. The crude product was triturated with ethanol, filtered, and repeated for 3 times to remove the unreacted PPh₃, which has a very similar polarity as *anti*-**3**. Purification by column chromatography on silica gel with CH₂Cl₂/hexane 1/3 (V/V) as eluent yielded 688 mg (90%) of *anti*-**3** as a white solid. Melting point 301.4 °C (measured with DSC). ¹H-NMR (CDCl₃) δ (ppm): 7.31 (d, J = 7.6 Hz, 2H), 7.09 (m, 6H), 6.96 (m, 4H), 6.91 (d, J = 7.6 Hz, 2H), 6.69 (t, J=7.6 Hz, 2H), 6.47 (d, J=7.6 Hz, 2H), 3.71 (m, 2H), 3.02 (m, 2H). ¹³C-NMR (CDCl₃) δ (ppm): 142.4, 140.3, 139.6, 138.6, 138.5, 135.6, 131.5, 129.6, 128.9, 128.8, 128.0, 128.0, 126.8, 126.4, 125.5, 33.0. MS (EI⁺): cald. For C₃₀H₂₂ ([M]⁺): 382.1716, found:382.1706.





10-Bromo-5H-dibenzo[a, d]cyclohepten-5-one (20)

This compound was synthesized according to the reported procedures.²

1,4-dihydro-1,4-epoxy-9H-tribenzo[a,c,e]cyclohepten-9-one (21)

This compound was synthesized according to reported procedures.³ ¹H-NMR (CDCl₃) δ (ppm): 8.13 (d, J = 7.6 Hz, 2H), 7.65 (t, J = 7.6 Hz, 2H), 7.53 (t, J = 7.6 Hz, 2H), 7.46 (d, J = 7.6 Hz, 2H), 7.39 (s, 2H), 6.07 (s, 2H). ¹³C-NMR (CDCl₃) δ (ppm): 194.1, 148.8, 142.4, 138.0, 131.9, 131.7, 130.5, 129.1, 123.4, 85.5.

1,2,3,4-tetrahydro-1,4-epoxy-9H-tribenzo[a,c,e]cyclohepten-9-one (22)

Ketone **22** was prepared following the reported procedures with minor modifications.⁴ ^[4] A suspension of 1,4-dihydro-1,4-epoxy-9H-tribenzo[a,c,e]cyclohepten-9-one (**21**) (5.44 g, 20 mmol) and 10% Pd/C (544 mg) in 100ml ethyl acetate was stirred for 30 minutes under a hydrogen atmosphere provided by a balloon of hydrogen. The resulting mixture was filtered through a pad of celite and washed with ethyl acetate, and the filtrate was concentrated under reduced pressure. 5.48 g (100%) of ketone **22** was obtained as a yellow solid. Yield: ¹H-NMR (CDCl₃) δ (ppm): 8.10 (d, J = 7.6 Hz, 2H), 7.62 (t, J = 7.6 Hz, 2H), 7.52 (t, J = 7.6 Hz, 2H),

^{2.} J. H. Rupard, T. Depaulis, A. Janowsky, H. E. Smith, J. Med. Chem. 1989, 32, 2261-2268.

^{3.} W. Tochtermann, K. Oppenländer, U. Walter, Chem. Ber. 1964, 97, 1318-1328.

^{4.} W. Tochtermann, K. Oppenländer, U. Walter, Chem. Ber. 1964, 97, 1329-1336.

7.44 (d, J = 7.6 Hz, 2H), 5.67 (d, J = 1.6 Hz, 2H), 2.25 (m, 2H), 1.68 (m, 2H). ¹³C-NMR (CDCl₃) δ (ppm): 194.5, 142.0, 138.9, 131.8, 130.8, 130.5, 128.8, 125.0, 81.9, 27.1.

1,2,3,4-tetrahydro-1,4-epoxy-9H-tribenzo[a,c,e]cyclohepten-9-thione (8)

A mixture of the 1,2,3,4-tetrahydro-1,4-epoxy-9H-tribenzo[a,c,e]cyclohepten-9-one **22** (2.74 g, 10 mmol) and Lawesson's reagent (0.7 eq, 2.83 g, 7 mmol) in 100 mL of toluene was heated to reflux for 8 hours. Then the resulting dark-green solution was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel with CH₂Cl₂/hexane 1/1 (V/V) as eluent. 1.86g of **8** was collected as a green solid in a yield of 64%. Melting point 207-208 °C. ¹H-NMR (CDCl₃) δ (ppm): 7.99 (d, J = 7.6 Hz, 2H), 7.49 (t, J = 7.6 Hz, 2H), 7.37 (t, J = 7.6 Hz, 2H), 7.24 (d, J = 7.6 Hz, 2H), 5.55 (s, 2H), 2.23 (d, J = 7.2 Hz, 2H), 1.68 (d, J = 7.2 Hz, 2H). ¹³C-NMR (CDCl₃) δ (ppm): 240.4, 148.5, 142.3, 130.6, 130.2, 128.6, 127.1, 123.4, 81.9, 27.1. MS (EI⁺): cald. For C₁₉H₁₄OS ([M]⁺): 290.0760, found: 290.0769.

1,2,3,4-tetrahydro-1,4-epoxy-9H-tribenzo[a,c,e]cyclohepten-9-one hydrazone (23)

To a dark-green solution of **8** (1.16 g, 4 mmol) in 50 ml CHCl₃ was added 4 ml of 35% hydrazine hydrate with stirring at room temperature. The resulting light yellow solution was kept stirred for 30 minutes. Then the solution was washed with water and brine, dried with anhydrous Na₂SO₄, and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel with ether/hexane 3/1 (V/V) as eluent. 968 mg of **23** was collected as a white solid in a yield of 84%. Melting point: 186-187 °C. ¹H-NMR (CDCl₃) δ (ppm): 7.60 (m, 2H), 7.35-7.46 (m, 5H), 7.20 (d, J = 7.6 Hz, 2H), 5.49 (m, 4H), 2.19 (m, 2H), 1.61 (m, 2H). ¹³C-NMR (CDCl₃) δ (ppm): 147.7, 142.8, 141.1, 138.2, 132.0, 130.8, 129.5, 129.0, 128.9, 128.5, 128.4, 128.1, 128.0, 125.4, 123.9, 82.1, 81.8, 27.3, 27.2. MS (EI⁺): cald. For C₁₉H₁₆N₂O ([M]⁺): 288.1257, found: 288.1256.

9-diazo-1,2,3,4-tetrahydro-1,4-epoxy-9H-tribenzo[a,c,e]cycloheptene (24)

A suspension of hydrazone **23** (864 mg, 3 mmol), anhydrous sodium sulfate (400 mg, 2.8 mmol), and red HgO (1.3 g, 6 mmol) in 30 ml of anhydrous Et_2O was stirred in a round-bottom flask attached to a drying tube of anhydrous $CaCl_2$. To this suspension was added 2 ml of a freshly prepared concentrated solution of KOH in ethanol. The reaction mixture was kept stirred at room temperature for 12 hours. The resulting suspension was filtered and the solid residue was washed with Et_2O . The filtrates were combined and concentrated under reduced pressure yielding 858 mg of **24**, which was used in the next step without further purification

Episulfide 9

To a solution of thicketone **8** (870 mg, 3 mmol) in 30 ml anhydrous THF was added a solution of diazo compound **24** (858 mg, crude) in 20 ml of anhydrous THF with stirring at room temperature. The solution was kept stirred overnight in a round-bottom flask equipped with a drying tube of anhydrous CaCl₂. Then the resulting reaction mixture was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel with ethyl acetate/hexane 1/3 (V/V) as eluent. 887 mg of episulfide **9** was obtained as

white powders in a yield of 54% for the two steps. Melting point: 282-283 °C. ¹H-NMR (CDCl₃) δ (ppm): 7.83 (m, 4H), 7.00 (m, 8H), 6.88 (m, 4H), 5.45 (m, 4H), 2.00 (m, 4H), 1.22 (m, 4H). ¹³C-NMR (CDCl₃) δ (ppm): 141.0, 133.3, 132.3, 131.8, 127.5, 127.1, 123.6, 81.8, 74.9, 28.6. MS (EI⁺): cald. For C₃₈H₂₈O₂S ([M]⁺): 548.1805, found: 548.1809.

Compound 25

A mixture of episulfide **9** (1.1 g, 2 mmol) and PPh₃ (629 mg, 2.4 mmol) in 100 ml anhydrous toluene were heated to reflux for 12 hours with the condenser connected to a drying tube of anhydrous CaCl₂. The resulting reaction mixture was then concentrated under reduced pressure. Purification of the crude product by column chromatography on silica gel with CH₂Cl₂/hexane 1/1 (V/V) as eluent yielded *anti*-**25** (253 mg, 24%) and *syn*-**25** (594 mg, 58%) separately.

Anti-25: white solid. Melting point: 270.4.°C (measured by DSC). ¹H-NMR (CDCl₃) δ (ppm): 7.17 (d, J = 7.6 Hz, 4H), 7.09 (t, J = 7.6 Hz, 4H), 6.91 (t, J = 7.6 Hz, 4H), 6.64 (d, J = 7.6 Hz, 4H), 5.67 (d, J = 1.2 Hz, 4H), 2.23 (m, 4H), 1.60 (m, 4H). ¹³C-NMR (CDCl₃) δ (ppm): 142.3, 142.1, 136.6, 132.3, 130.2, 128.0, 126.6, 82.0, 27.4. MS (EI⁺): cald. For C₃₈H₂₈O₂ ([M]⁺): 516.2084, found: 516.2075.

*Syn-***25**: white solid. Melting point: 312.0 °C (measured by DSC). ¹H-NMR (CDCl₃) δ (ppm): 7.55 (d, J = 7.6 Hz, 4H), 7.15 (t, J = 7.6 Hz, 4H), 7.03 (t, J = 7.6 Hz, 4H), 6.92(d, J = 7.6 Hz, 4H), 5.25 (s, 4H), 2.00 (m, 4H), 1.35 (m, 4H). ¹³C-NMR (CDCl₃) δ (ppm): 141.6, 141.4, 135.5, 130.7, 129.8, 126.5, 126.3, 122.8, 81.2, 27.4. MS (EI⁺): cald. For C₃₈H₂₈O₂ ([M]⁺): 516.2084, found: 516.2073.

2,3;4,5;6,7;2',3';4',5';6',7'-hexabenzoheptafulvalene (4)

Anti-4: A mixture of the *anit*-25 (103 mg, 0.2 mmol) and p-toluenesulfonic acid (76 mg, 0.4 mmol) in 20 ml benzene were heated to reflux for 12 hours. The reaction was cooled to room temperature, quenched with a saturated NaHCO₃ solution and extracted with CH₂Cl₂. The organic layers were combined, washed with water and brine, and dried with anhydrous Na₂SO₄. Then the resulting solution was concentrated under reduced pressure and purified by column chromatography on silica gel with CH₂Cl₂/hexane 1/2 (V/V) as eluent. 90 mg of *anti*-4 was collected as a white solid in a yield of 94%. Melting point: 410.6 °C (measured by DSC). ¹H-NMR (CDCl₃) δ (ppm): 7.75 (m, 4H), 7.57 (m, 4H), 7.51 (d, J = 7.6 Hz, 4H), 7.14 (dt, J₁ = 7.6 Hz, J₂ = 0.8 Hz, 4H), 6.93 (dt, J₁ = 7.6 Hz, J₂ = 0.8 Hz, 4H), 6.52 (d, J = 7.6 Hz, 4H). ¹³C-NMR (CDCl₃) δ (ppm): 143.2, 139.8, 139.3, 138.3, 130.1, 128.7, 127.8, 127.5(3), 127.4(9), 127.1. MS (EI⁺): cald. For C₃₈H₂₄ ([M]⁺): 480.1873, found: 480.1884.

Syn-4: A mixture of the *syn-***25** (103 mg, 0.2 mmol) and p-toluenesulfonic acid (76 mg, 0.4 mmol) in 20 ml benzene were heated to reflux for 12 hours. After work up and purification in the same as described for *anti-***4**, 85 mg *syn-***4** was obtained as a white solid in a yield of 89%. Melting point: 282.3 °C (measured by DSC). ¹H-NMR (CDCl₃) δ (ppm): 7.59 (d, J = 7.6 Hz, 4H), 7.20 (t, J = 7.6 Hz, 8H), 7.09 (dt, J₁ = 7.6 Hz, J₂ = 1.2 Hz, 4H), 7.07 (s, 8H). ¹³C-NMR (CDCl₃) δ (ppm): 142.2, 139.1, 137.7, 137.1, 129.1(2), 129.0(8), 128.1, 127.5, 126.9, 126.5. MS (EI⁺): cald. For C₃₈H₂₄ ([M]⁺): 480.1873, found: 480.1885.

Scheme 4 Synthesis and reaction of 5.



Episulfide 10

To a solution of thioketone **8** (580 mg, 2 mmol) in 30 ml THF was added a solution of diazo compound **19** (536 mg, crude) in 20 ml of THF with stirring at room temperature. The solution was kept stirred overnight in a round-bottom flask equipped with a drying tube of anhydrous CaCl₂. Then the resulting reaction mixture was concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel with ethyl acetate/hexane 1/4 (V/V) as eluent. 630 mg of episulfide **10** was obtained as white powders in a yield of 68% for the two steps. Melting point: 257-258 °C. ¹H-NMR (CDCl₃) δ (ppm): 7.79 (d, J = 8.0 Hz, 2H), 7.67 (d, J = 8.0 Hz, 2H), 6.98 (m, 10H), 6.85 (m, 4H), 5.48 (s, 2H), 2.17 (m, 2H), 1.44 (m, 2H). ¹³C-NMR (CDCl₃) δ (ppm): 141.7, 135.9, 134.5, 132.9, 132.8, 132.7,132.2, 131.5, 127.9, 127.8, 127.6, 127.1, 126.9, 123.1, 82.2, 73.7, 73.6, 28.2. MS (EI⁺): cald. For C₃₄H₂₄OS ([M]⁺): 480.1542, found: 480.1527.

Compound syn-26

A mixture of episulfide **10** (630 mg, 1.36 mmol) and PPh₃ (430 mg, 1.64 mmol) in 60 ml anhydrous toluene was heated to reflux for 12 hours with the condenser connected to a drying tube of anhydrous CaCl₂. The resulting reaction mixture was then concentrated under reduced pressure and purified by column chromatography on silica gel with CH₂Cl₂/hexane 1/1 (V/V) as eluent. 567 mg of *syn*-**26** was obtained as white powders in a yield of 97%. Melting point: 254.9 °C (measured by DSC). ¹H-NMR (CDCl₃) δ (ppm): 7.56 (d, J = 7.6 Hz, 2H), 7.48 (d, J = 7.6 Hz, 2H), 7.12 (m, 4H), 6.98 (m, 6H), 6.92 (d, J = 7.6 Hz, 2H), 6.69 (s, 2H), 5.29 (s, 2H), 2.06 (d, J = 7.6 Hz, 2H), 1.42 (m, 2H). ¹³C-NMR (CDCl₃) δ (ppm): 141.9, 141.5, 140.3, 138.0, 136.0, 133.8, 130.6, 129.8, 128.8, 127.5, 126.7(3), 126.7(1), 126.4, 126.1, 122.8, 81.5, 27.3. MS (EI⁺): cald. For C₃₄H₂₄O ([M]⁺): 448.1822, found: 448.1816.

2,3;4,5;6,7;2',3';6',7'-pentabenzoheptafulvalene (5)

A mixture of the *syn*-**26** (430 mg, 1 mmol) and p-toluenesulfonic acid (760 mg, 4 mmol) in 50 ml benzene were heated to reflux for 12 hours. The reaction was quenched with saturated NaHCO₃ solution and extracted with CH_2Cl_2 . The combined organic phase was washed with water, brine and dried with anhydrous Na₂SO₄. Then the resulting solution was concentrated under reduced pressure. Purification of the crude product by column chromatography on silica gel with CH_2Cl_2 /hexane 1/1 (V/V) as eluent yielded *anti*-**5** (74 mg, 18%) and *syn*-**5** (286 mg, 69%) separately.

Anti-5: white solid. Melting point 312.2 °C (measured by DSC). ¹H-NMR (CDCl₃) δ (ppm): 7.77 (m, 2H), 7.58 (m, 2H), 7.51 (d, J = 7.6 Hz, 2H), 7.27 (d, J = 7.6 Hz, 2H), 7.13 (dt, J₁ =

7.6 Hz, $J_2 = 1.2$ Hz, 2H), 7.06 (m, 4H), 6.90 (m, 4H), 6.60 (d, J = 7.6 Hz, 2H), 6.53 (d, J = 7.6 Hz, 2H). ¹³C-NMR (CDCl₃) δ (ppm): 143.4, 141.8, 139.5, 139.2, 138.7, 138.6, 135.3, 131.4, 130.1, 129.1, 128.8, 128.1, 127.9, 127.8, 127.6, 127.4, 127.0, 126.6. MS (EI⁺): cald. For C₃₄H₂₂ ([M]⁺): 430.1716, found: 430.1719.

*Syn-***5**: white solid. Melting point 248.5 °C (measured by DSC). ¹H-NMR (CDCl₃) δ (ppm): 7.46 (m, 4H), 7.35 (m, 2H), 7.27 (m, 4H), 7.17 (dt, J₁= 7.6 Hz, J₂= 1.2 Hz, 2H), 7.12 (dt, J₁= 7.6 Hz, J₂= 1.6 Hz, 2H), 7.07 (dt, J₁= 7.6 Hz, J₂= 1.6 Hz, 2H), 6.98 (dt, J₁= 7.6 Hz, J₂= 1.2 Hz, 2H), 6.94 (dd, J₁= 7.6 Hz, J₂= 1.2 Hz, 2H), 6.02 (s, 2H). ¹³C-NMR (CDCl₃) δ (ppm): 142.7, 140.3, 139.4, 138.9, 138.1, 137.0, 133.5, 129.5, 128.7, 128.5, 128.4, 127.5, 127.4, 126.9(3), 126.9(1), 126.7, 126.6, 126.3. MS (EI⁺): cald. For C₃₄H₂₂ ([M]⁺): 430.1716, found: 430.1726.

Scheme 5 Correction of the previously claimed synthesis of hexabenzooctalene



9H-Tribenzo[a,c,e]cyclohepten-9-one (27)

A mixture of **22** (1.37 g, 5 mmol) and *p*-toluenesulfonic acid (1.9 g, 10 mmol) in 100 ml of toluene was heated to reflux for 12 hours. The reaction mixture was cooled to room temperature and then quenched with a saturated aqueous solution of NaHCO₃ and extracted with CH₂Cl₂. The organic layer was washed with water, brine and dried with anhydrous Na₂SO₄ subsequently. Then the resulting solution was concentrated under reduced pressure and purified by column chromatography on silica gel with CH₂Cl₂/hexane 1/1 (V/V) as eluent. 1.26 g of **27** was obtained as white solids in a yield of 98%. Melting point: 177-178 °C. ¹H-NMR (CDCl₃) δ (ppm): 7.71 (d, J = 7.6 Hz, 2H), 7.63 (m, 4H), 7.57 (dt, J₁ = 7.6 Hz, J₂ = 1.2 Hz, 2H), 7.45 (m, 4H). ¹³C-NMR (CDCl₃) δ (ppm): 198.9, 143.2, 137.3, 136.8, 131.6, 131.3, 129.3, 128.5, 128.2, 126.7. MS (EI⁺): cald. For C₁₉H₁₃O ([M+H]⁺): 257.0961, found: 257.0967.

[9,9'-Bi-9H-tribenzo[a,c,e]cycloheptene]-9,9'-diol (28)

A mixture of **27** (1.02 g, 4 mmol), magnesium powder (218 mg, 8.8 mmol) and iodine (680 mg, 2.7 mmol) in a mixed solvent of anhydrous ether and toluene (8 ml and 16 ml respectively) was irradiated with ultrasound in the water bath of a sonicator for 4 hours. During this process, the water bath was kept around room temperature by changing the water

every half an hour. The reaction was quenched with 5 ml dilute HCl, and the resulting mixture was filtered to remove the residual magnesium powder. The filtrate was extracted with diethyl ether and washed with saturated aqueous NaHCO₃ solution and brine subsequently, and dried with anhydrous Na₂SO₄. Then the resulting solution was concentrated under reduced pressure, and the crude product was purified by column chromatography on silica gel with CH₂Cl₂/hexane 1/1 (V/V) as eluent. 540 mg of **28** was obtained as white powders in a yield of 53%. Melting point: 230-231 °C. ¹H-NMR (CDCl₃) δ (ppm): 7.27 (dt, J₁ = 8.0 Hz, J₂ = 1.2 Hz, 4H), 7.21 (dt, J₁ = 8.0 Hz, J₂ = 1.2 Hz, 4H), 7.16 (m, 4H), 7.08 (m, 8H), 7.01 (m, 4H), 2.71(s, 2H). ¹³C-NMR (CDCl₃) δ (ppm): 145.4, 138.9, 135.7, 130.5, 128.7, 128.2, 126.7, 123.2, 84.9. MS (EI⁺): cald. For C₃₈H₂₆O₂ ([M]⁺): 514.1927, found: 514.1916

Spiro[9H-tribenzo[a,c,e]cycloheptene-9,9'(10'H)-tribenzo[a,c,e]cycloocten]-10'-one (29)

A mixture of **28** (205 mg, 0.4 mmol), 6 ml of concentrated H₂SO₄ and 30 ml of acetic acid was heated to reflux for 4 hours. The solution mixture was then poured into ice water. The white precipitates were collected by filtration and washed repeatedly wis water. The crude product was further purified by column chromatography on silica gel with CH₂Cl₂/hexane 1/1 (V/V) as eluent. 72 mg of **29** was obtained as white powders in a yield of 36%. Melting point: 268-269 °C. ¹H-NMR (CD₂Cl₂) δ (ppm): 7.85 (dt, J₁ = 8.0 Hz, J₂ = 1.2 Hz, 1H), 7.56 (dt, J₁ = 7.2 Hz, J₂ = 2.0 Hz, 1H), 7.40 (m, 2H), 7.29 (m, 1H), 7.20-7.26 (m, 5H), 7.11-7.18(m, 4H), 7.03 (m, 1H), 6.90 (m, 1H), 6.83 (m, 1H), 6.69 (m, 1H) , 6.62 (m, 2H) , 6.53 (m, 2H) , 6.47 (m, 2H). ¹³C-NMR (CDCl₃) δ (ppm): 208.4, 145.1, 144.1, 143.7, 141.8, 141.5, 140.6(3), 140.6(0), 139.4, 139.2, 138.8, 137.0, 136.7, 132.1, 131.6, 130.3, 130.1, 130.0, 129.3, 129.2, 128.5, 128.4, 128.3, 127.7, 127.6, 127.5, 127.4, 127.3, 127.2, 127.1, 126.7, 126.6, 126.5, 126.4, 126.3, 126.2, 125.4. MS (EI⁺): cald. For C₃₈H₂₄O ([M]⁺): 496.1822, found: 496.1828.

Spiro[9H-tribenzo[a,c,e]cycloheptene-9,9'(10'H)-tribenzo[a,c,e]cycloocten]-10'-ol (11)

A mixture of **29** (57 mg, 0.11 mmol) and LiAlH₄ (43 mg, 1.1 mmol) in 10 ml of anhydrous THF was stirred at room temperature under N₂ for 4 hours. The reaction was quenched with water and extracted with diethyl ether. The organic layer was washed with water, brine and dried with anhydrous Na₂SO₄. Then the resulting solution was concentrated under reduced pressure and purified by column chromatography on silica gel with CH₂Cl₂/hexane 1/1 (V/V) as eluent. 52 mg of **11** was obtained as white powder in a yield of 94%. Melting point: 248-249 °C. ¹H-NMR (CD₂Cl₂) δ (ppm): 8.78 (d, J = 8.0 Hz, 1H), 8.17 (d, J = 8.0 Hz, 1H), 6.64-7.52 (m, 21H), 6.41 (m, 1H), 6.20 (d, J = 2.0 Hz, 1H), 2.49 (d, J = 2.0 Hz, 1H). ¹³C-NMR (CDCl₃) δ (ppm): 149.7, 1445.6, 142.9, 142.0, 141.9, 141.6, 140.4, 140.0, 139.9, 139.4, 138.4, 137.0, 134.1, 132.6, 131.3, 130.2, 130.1, 129.7, 128.9, 128.5, 128.4, 128.2, 128.1, 128.0, 127.8, 127.2, 127.0, 126.9(4), 126.9(1), 126.8, 126.7, 126.6, 126.2, 125.3, 86.8, 59.5. MS (EI⁺): cald. For C₃₈H₂₆O ([M]⁺): 498.1978, found: 498.1992.

Reaction of 11 with acid

A mixture of **11** (50 mg, 0.1 mmol), 2 ml of H_2SO_4 and 10 ml of acetic acid was heated to reflux for 4 hours. After reaction, the solution was poured into ice water. The white precipitates were collected by filtration and washed repeatedly with water. The crude product

was further purified by column chromatography on silica gel with CH_2Cl_2 /hexane 1/3 (V/V) as eluent. 41 mg of *syn-***4** was obtained as white powder in a yield of 85%.

2. Isomerization and Kinetics Study

General Procedure for Photo-isomerization

A standard photochemical reaction vessel with a double-walled quartz immersion well was used for the photo-isomerization, and a circulating chiller was used to provide cooling water (15 to 18 °C) to the quartz immersion well. N₂ was bubbled through a stirred solution of *anti* isomer (0.2 mmol) in 400 ml cyclohexane for 20 minutes before photo-irradiation, and the N₂ flow was maintained throughout irradiation with a 500 W high-pressure mercury vapor lamp placed in the immersion quartz well. The progress of the reaction was monitored by TLC and ¹H NMR spectroscopy. After completion of the reaction, the solvent was evaporated under reduced pressure and the crude product was purified by column chromatography.

Photochemical reaction of *anti-2*: After 12 h of irradiation, the resulting solution was concentrated under reduced pressure, and the crude product was purified by column chromatography on silica gel with CH₂Cl₂/hexane 1/3 (V/V) as eluent. 18 mg of **13** was obtained as white powder in a yield of 23%. Melting point 264.2 °C (measured with DSC). ¹H-NMR (CDCl₃) δ (ppm): 8.68 (d, J = 8.4 Hz, 2H), 7.47 (dd, J₁ = 8.4 Hz, J₂ = 7.2Hz, 2H), 7.40 (d, J = 7.2 Hz, 2H), 7.04 (d, J = 6.4 Hz, 2H), 6.95 (dt, J₁ = 7.2Hz, J₂ = 1.2 Hz 2H), 6.76 (dd, J₁ = 7.6 Hz, J₂ = 1.2 Hz, 2H), 6.67 (dt, J₁ = 7.6 Hz, J₂ = 1.2 Hz, 2H), 3.56 (m, 2H), 3.38 (m, 4H), 2.94 (m, 2H). ¹³C-NMR (CDCl₃) δ (ppm): 144.0, 142.3, 140.2, 139.4, 135.8, 131.6, 131.0, 130.0, 127.6, 125.6, 125.5, 125.4, 122.0, 40.4, 34.2. MS (EI⁺): cald. For C₃₀H₂₂ ([M]⁺): 384.1716, found: 384.1706.

Charaterization of 13

As shown below, similar to 2, 13 can adopt two isomeric structures, namely helical and non-helical isomers. Molecular modeling indicates that the helical isomer is less stable than the non-helical isomer by 0.4 kcal/mol, and the helical isomer has its inner aromatic H atom close to methylene H atoms with short distance within 4.5 Å. 2D ROESY spectrum of 13 (shown in page 18 following its ¹H and ¹³C NMR spectra) exhibited through-space coupling between the inner aromatic H atom and the methylene H atoms, indicating that it is the helical isomer.



Photo-isomerization of *anti*-**3**: After 0.5 hour of irradiation, *anti*-**3** was converted to *syn*-**3** almost quantitatively as indicated by TLC and ¹H NMR. The resulting solution of *syn*-**3** was concentrated under reduced pressure at room temperature as quickly as possible to prevent thermal isomerization of *syn*-**3**. The crude product was purified by column chromatography on silica gel with CH_2Cl_2 /hexane 1/3 (V/V) as eluent, 73 mg of *syn*-**3** was obtained as white solid in a yield of 96%.

Characterization of *syn-***3**: melting point: 231-232 °C. ¹H-NMR (CDCl₃) δ (ppm): 7.55 (d, J = 7.6 Hz, 2H), 7.40 (d, J = 7.6 Hz, 2H), 7.20 (t, J = 7.6 Hz, 2H), 7.16 (d, J = 7.6 Hz, 2H), 7.05 (t, J = 7.6 Hz, 2H), 6.91 (m, 6H), 6.85 (d, J = 7.6 Hz, 2H), 3.29 (m, 2H), 2.53 (m, 2H). Clean ¹³C-NMR of *syn-***3** could not be obtained because *syn-***3** thermally isomerized to *anti-***3** during recording ¹³C-NMR spectrum within a relatively long period of time. MS (EI⁺): cald. For C₃₀H₂₂ ([M]⁺): 382.1716, found: 382.1719.

Photo-isomerization of *anti*-4: After 4 hours of irradiation, *anti*-4 was converted to the *syn*-4 quantitatively.

Photo-isomerization of *anti*-5: After 1 hour of irradiation, *anti*-5 was converted to the *syn*-5 quantitatively.

Thermal Isomerization of syn-4 and syn-5

Samples of *syn*-4 and *syn*-5 were placed in a tube furnace under a flow of N_2 , and heated at 400 °C and 260 °C respectively for 10 minutes. As indicated by TLC and ¹H NMR, *syn*-4 and *syn*-5 were converted to the corresponding *anti* isomers quantitatively.

Kinetic studies for the thermal isomerization of syn-5

In the kinetic experiment, a solution of *syn*-**5** (30 mg) in 3 ml DMSO-d₆ was refluxed under an atmosphere of N₂, and the solution temperature was measured as 186 °C. A small portion of solution was taken from the reaction mixture at regular time intervals (1.5 h) and quenched with cold DMSO-d₆. Then the progress of thermal *syn*-to-*anti* isomerization of *syn*-**5** was monitored with ¹H NMR spectroscopy.



Figure S-1. Selected ¹H NMR spectra of **5** during the progress of thermal *syn*-to-*anti* isomerization in DMSO-d₆ at 186 °C.



Figure S-2. A plot of ln([*syn*-5]₀/[*syn*-5]_t) versus time

3. NMR spectra



¹³C NMR spectrum of **14**



¹³C NMR spectrum of **15**



¹³C NMR spectrum of anti-2



¹³C NMR spectrum of **13**



2D ¹H-¹H ROESY spectrum of 13



¹³C NMR spectrum of **17**



¹³C NMR spectrum of **18**



¹³C NMR spectrum of *anti-***3**



¹H NMR spectrum of *syn*-**3**



¹³C NMR spectrum of **21**



¹³C NMR spectrum of **22**



¹³C NMR spectrum of **8**



¹³C NMR spectrum of **23**



¹³C NMR spectrum of **9**



¹³C NMR spectrum of *anti*-25



¹³C NMR spectrum of *syn*-25



¹³C NMR spectrum of *anti-***4**



¹³C NMR spectrum of *syn-***4**



¹³C NMR spectrum of **10**



¹³C NMR spectrum of *syn-26*





¹³C NMR spectrum of *anti-5*



¹³C NMR spectrum of *syn*-5



¹³C NMR spectrum of **27**



¹³C NMR spectrum of **28**



¹³C NMR spectrum of **29**



¹³C NMR spectrum of **11**

4. UV absorption spectra of syn- and anti- 3-5

All the UV-vis spectra were recorded in hexane at a concentration of 2.5×10^{-5} mol/L.







UV absorption spectra of anti-4 and syn-4



UV-vis spectrum of anti-5 and syn-5

5. Energy-Optimized Geometries of 3-5

Shown below are the geometries of **3-5** with selected fixed dihedral angles between the planes of C4a-C5-C5a and C4a'-C5'-C5a'as optimized at the Becke3LYP level of density functional theory (DFT) with 6-31G* basis set.

Molecule **3** with fixed dihedral angles between the planes of C4a-C5-C5a and C4a'-C5'-C5a'



dihedral angle: 90°

dihedral angle: 100°

dihedral angle: 180° (syn-3)

Molecule 4 with fixed dihedral angles between the planes of C4a-C5-C5a and C4a'-C5'-C5a'



dihedral angle: 0° (anti-4)

dihedral angle: 100°

dihedralangle:180°(*syn-***4**)



Molecule **5** with fixed dihedral angles between the planes of C4a-C5-C5a and C4a'-C5'-C5a'

dihedral angle: 0° (*anti*-5)

dihedral angle: 100°

dihedralangle:180°(*syn-***5**)

Optimized Cartesian coordinates for *anti-3*:

С	0	4.633724	0.322642	0.910239
С	0	3.729719	-0.348111	1.738622
С	0	2.362832	-0.238447	1.499986
С	0	1.865015	0.543673	0.447278
С	0	2.775090	1.266227	-0.362401
С	0	4.155901	1.112038	-0.128520
С	0	0.396200	0.592660	0.183157
С	0	-0.218762	1.945859	0.339428
С	0	0.156669	3.011119	-0.514941
С	0	-1.192697	2.174053	1.322460
С	0	-1.826734	3.407398	1.443592
С	0	-1.499949	4.443930	0.565254
С	0	-0.524091	4.239653	-0.402395
С	0	-0.340162	-0.508451	-0.113777
С	0	-1.820534	-0.443961	-0.332109
С	0	-2.668185	-1.121804	0.564299
С	0	-0.200579	-3.047073	0.261621
С	0	0.262379	-1.862254	-0.353296
С	0	-2.370381	0.229795	-1.428581
С	0	-3.749995	0.241703	-1.635973
С	0	-4.592767	-0.422952	-0.744931
С	0	-4.049022	-1.099289	0.348588
С	0	0.406766	-4.263723	-0.091007
С	0	1.428581	-4.340306	-1.030440
С	0	1.868645	-3.172430	-1.655278
С	0	1.286211	-1.957499	-1.316687
Н	0	5.703673	0.232027	1.076959
Н	0	4.089036	-0.967241	2.556117

Η	0	1.659364	-0.782551	2.122981
Н	0	4.855579	1.643981	-0.769222
Н	0	-1.465686	1.360928	1.987866
Н	0	-2.584185	3.553934	2.208774
Н	0	-2.000089	5.405802	0.639320
Н	0	-0.255268	5.047953	-1.078642
Н	0	-1.709300	0.746552	-2.118346
Н	0	-4.163671	0.769671	-2.491105
Н	0	-5.668709	-0.415258	-0.898456
Н	0	-4.704888	-1.614244	1.047699
Н	0	0.056074	-5.174914	0.390576
Н	0	1.870498	-5.301754	-1.278647
Н	0	2.654369	-3.207553	-2.405132
Н	0	1.614017	-1.049306	-1.811415
С	0	-1.317424	-3.146200	1.296756
Н	0	-2.068132	-3.848729	0.907996
Н	0	-0.907976	-3.623375	2.198589
С	0	-2.048890	-1.861590	1.725217
Н	0	-2.823609	-2.139435	2.449630
Н	0	-1.347307	-1.202822	2.254316
С	0	2.355142	2.165560	-1.436551
С	0	1.228806	2.910388	-1.504860
Н	0	3.095370	2.323082	-2.220125
Н	0	1.151787	3.607618	-2.338237

Optimized Cartesian coordinates for the transition state of **3** with a dihedral angle of 70° between the planes of C4a-C5-C5a and C4a'-C5'-C5a':

С	0	-3.873907	2.967847	-0.941396
С	0	-2.806662	3.472985	-0.194880
С	0	-1.803611	2.614689	0.243751
С	0	-1.812466	1.235976	-0.046103
С	0	-2.962870	0.703599	-0.700037
С	0	-3.943053	1.601839	-1.174719
С	0	-0.686323	0.309750	0.259929
С	0	-0.999621	-0.774899	1.229351
С	0	-2.030025	-1.739978	1.062714
С	0	-0.209469	-0.826254	2.393364
С	0	-0.423492	-1.793807	3.373929
С	0	-1.417647	-2.757990	3.192611
С	0	-2.200928	-2.733579	2.042888
С	0	0.646055	0.304384	-0.234733
С	0	0.931291	-0.840604	-1.152256
С	0	1.950196	-1.797666	-0.945408
С	0	3.053998	0.880187	0.421139

С	0	1.739159	1.275693	0.051810
С	0	0.145094	-0.927553	-2.313763
С	0	0.393484	-1.906789	-3.278076
С	0	1.415797	-2.831127	-3.079216
С	0	2.182451	-2.776943	-1.910691
С	0	3.972744	1.881769	0.785137
С	0	3.678451	3.237908	0.745588
С	0	2.414807	3.632956	0.303128
С	0	1.481531	2.665062	-0.035757
Н	0	-4.654243	3.626738	-1.311747
Н	0	-2.755421	4.531391	0.047151
Н	0	-0.997416	3.013802	0.847014
Н	0	-4.796591	1.191160	-1.709254
Н	0	0.567624	-0.080577	2.525905
Н	0	0.195834	-1.804505	4.266758
Н	0	-1.578416	-3.527662	3.942782
Н	0	-2.966002	-3.492205	1.893908
Н	0	-0.641906	-0.198355	-2.471464
Н	0	-0.216368	-1.946030	-4.176705
Н	0	1.612953	-3.600082	-3.821815
Н	0	2.960364	-3.518529	-1.740883
Η	0	4.966669	1.566491	1.098111
Н	0	4.426149	3.971338	1.034866
Н	0	2.162898	4.686189	0.207863
Н	0	0.523941	2.981727	-0.426258
С	0	3.644850	-0.528467	0.442030
Η	0	4.371554	-0.587243	-0.382222
Η	0	4.239187	-0.624828	1.360651
С	0	2.728892	-1.753341	0.342130
Н	0	3.355754	-2.649177	0.426921
Н	0	2.035552	-1.772176	1.191135
С	0	-3.246879	-0.717035	-0.891965
С	0	-2.882562	-1.763525	-0.117655
Η	0	-3.958024	-0.929233	-1.689136
Н	0	-3.329789	-2.728771	-0.350651

Optimized Cartesian coordinates for the transition state of **3** with a dihedral angle of 80° between the planes of C4a-C5-C5a and C4a²-C5²-C5a²:

С	0	2.309801	-3.275706	-2.355261
С	0	0.963506	-2.907524	-2.366829
С	0	0.541041	-1.800333	-1.645696
С	0	1.407809	-1.034488	-0.811499
С	0	2.808758	-1.361281	-0.899619
С	0	3.207513	-2.482902	-1.651487

С	0	0.787513	-0.000022	-0.000022
С	0	1.407763	1.034493	0.811447
С	0	2.808735	1.361203	0.899712
С	0	0.540949	1.800495	1.645419
С	0	0.963381	2.907751	2.366488
С	0	2.309699	3.275828	2.355074
С	0	3.207452	2.482870	1.651508
С	0	-0.706749	-0.000068	-0.000052
С	0	-1.331433	0.980489	-0.879556
С	0	-2.699247	1.406411	-0.848430
С	0	-2.699145	-1.406640	0.848336
С	0	-1.331356	-0.980668	0.879486
С	0	-0.508361	1.571831	-1.882115
С	0	-0.958168	2.581467	-2.724721
С	0	-2.280425	3.010931	-2.648244
С	0	-3.133721	2.397295	-1.726278
С	0	-3.133757	-2.397163	1.726512
С	0	-2.280556	-3.010507	2.648771
С	0	-0.958266	-2.581141	2.725124
С	0	-0.508348	-1.571796	1.882210
Н	0	2.661155	-4.131734	-2.924126
Н	0	0.245212	-3.461814	-2.964736
Н	0	-0.496065	-1.503888	-1.718215
Н	0	4.267653	-2.721811	-1.683830
Н	0	-0.496214	1.504201	1.717762
Н	0	0.245015	3.462165	2.964190
Н	0	2.661082	4.131880	2.923885
Н	0	4.267602	2.721725	1.684012
Н	0	0.504757	1.210614	-2.003536
Н	0	-0.280674	3.006519	-3.460724
Н	0	-2.656957	3.783469	-3.312996
Н	0	-4.177629	2.701146	-1.684515
Н	0	-4.177664	-2.701017	1.684735
Н	0	-2.657192	-3.782775	3.313775
Н	0	-0.280792	-3.006020	3.461245
Н	0	0.504787	-1.210602	2.003602
С	0	-3.713073	-0.769625	-0.066487
Н	0	-3.527901	-1.033633	-1.117394
Н	0	-4.705139	-1.164033	0.180950
С	0	-3.713381	0.769014	0.065932
Н	0	-4.705465	1.163035	-0.182059
Н	0	-3.528888	1.033151	1.116927
С	0	3.893935	-0.580235	-0.346230
С	0	3.893935	0.579990	0.346582

Н	0	4.879247	-0.978349	-0.582489
Н	0	4.879247	0.977946	0.583088

Optimized Cartesian coordinates for the transition state of **3** with a dihedral angle of 90° between the planes of C4a-C5-C5a and C4a'-C5'-C5a':

С	0	2.318002	3.697071	1.614776
С	0	0.960395	3.375848	1.628483
С	0	0.531662	2.144788	1.154030
С	0	1.409221	1.182493	0.565855
С	0	2.816200	1.504011	0.626262
С	0	3.218150	2.750223	1.140734
С	0	0.797491	0.000303	-0.002484
С	0	1.407152	-1.181553	-0.573781
С	0	2.813112	-1.508564	-0.629852
С	0	0.527963	-2.137790	-1.169347
С	0	0.954047	-3.367344	-1.650502
С	0	2.310422	-3.692911	-1.635188
С	0	3.212368	-2.752669	-1.151125
С	0	-0.720430	-0.000418	0.001085
С	0	-1.329556	-0.572198	1.188038
С	0	-2.703033	-0.968166	1.334864
С	0	-2.712571	0.960985	-1.324732
С	0	-1.336768	0.570467	-1.182426
С	0	-0.490874	-0.786164	2.324539
С	0	-0.941242	-1.400404	3.488167
С	0	-2.272609	-1.787161	3.600614
С	0	-3.134503	-1.546336	2.524410
С	0	-3.147628	1.546532	-2.509368
С	0	-2.288595	1.798200	-3.585370
С	0	-0.956109	1.413708	-3.478659
С	0	-0.501620	0.793213	-2.320026
Н	0	2.673175	4.647047	2.003526
Н	0	0.233644	4.070009	2.041622
Н	0	-0.518908	1.905368	1.228483
Н	0	4.282539	2.970278	1.163440
Н	0	-0.521520	-1.894476	-1.245460
Н	0	0.226095	-4.056624	-2.069643
Н	0	2.663684	-4.641465	-2.029138
Н	0	4.275923	-2.977029	-1.170421
Н	0	0.535314	-0.448784	2.290560
Н	0	-0.251384	-1.546888	4.315259
Н	0	-2.647910	-2.245917	4.511162
Н	0	-4.181528	-1.829701	2.609363
Н	0	-4.196036	1.825750	-2.591075

Н	0	-2.667109	2.262671	-4.491673
Н	0	-0.268537	1.567074	-4.306409
Н	0	0.525530	0.458339	-2.290481
С	0	-3.726124	0.721846	-0.237110
Н	0	-3.544034	1.378560	0.625792
Н	0	-4.719669	0.982309	-0.619096
С	0	-3.717021	-0.743176	0.245038
Н	0	-4.707975	-1.017536	0.623905
Н	0	-3.522867	-1.396882	-0.617487
С	0	3.898923	0.624133	0.248496
С	0	3.897481	-0.637495	-0.236680
Н	0	4.885329	1.051583	0.419988
Н	0	4.882813	-1.072520	-0.394650

Optimized Cartesian coordinates for the transition state of **3** with a dihedral angle of 100° between the planes of C4a-C5-C5a and C4a'-C5'-C5a':

С	0	-2.333554	-3.139894	-2.538002
С	0	-0.969515	-2.948898	-2.319135
С	0	-0.533745	-1.958390	-1.451622
С	0	-1.416104	-1.041469	-0.793914
С	0	-2.827510	-1.270858	-1.021472
С	0	-3.232516	-2.312832	-1.874659
С	0	-0.809271	0.000055	-0.000070
С	0	-1.415893	1.041672	0.793806
С	0	-2.827234	1.271287	1.021520
С	0	-0.533309	1.958476	1.451392
С	0	-0.968818	2.948952	2.319070
С	0	-2.332803	3.140072	2.538195
С	0	-3.231977	2.313226	1.874871
С	0	0.734094	-0.000066	-0.000058
С	0	1.339542	-0.967301	0.891993
С	0	2.723517	-1.012215	1.292658
С	0	2.723699	1.011768	-1.292691
С	0	1.339721	0.967105	-0.892071
С	0	0.492819	-1.951350	1.498011
С	0	0.953569	-2.885582	2.419971
С	0	2.299118	-2.922258	2.765007
С	0	3.161721	-1.984329	2.184238
С	0	3.162120	1.983875	-2.184185
С	0	2.299708	2.922006	-2.764904
С	0	0.954145	2.885578	-2.419891
С	0	0.493193	1.951365	-1.498014
Η	0	-2.692049	-3.930867	-3.190307
Н	0	-0.238306	-3.593768	-2.798849

Η	0	0.526810	-1.866000	-1.276959
Н	0	-4.299166	-2.459659	-2.024159
Η	0	0.527197	1.866016	1.276464
Н	0	-0.237468	3.593730	2.798692
Н	0	-2.691087	3.931004	3.190664
Η	0	-4.298587	2.460200	2.024504
Н	0	-0.554001	-1.980443	1.239658
Н	0	0.253331	-3.599041	2.846812
Η	0	2.681265	-3.662223	3.462639
Н	0	4.216032	-1.997161	2.452444
Н	0	4.216442	1.996536	-2.452353
Н	0	2.682010	3.661944	-3.462480
Н	0	0.254054	3.599208	-2.846689
Η	0	-0.553612	1.980684	-1.239637
С	0	3.739718	0.034039	-0.768667
Н	0	3.554277	-0.974106	-1.167345
Н	0	4.731413	0.329993	-1.128842
С	0	3.739724	-0.034705	0.768613
Η	0	4.731363	-0.330880	1.128769
Η	0	3.554533	0.973483	1.167300
С	0	-3.909861	-0.523023	-0.427654
С	0	-3.909752	0.523761	0.427619
Η	0	-4.895962	-0.879597	-0.719784
Η	0	-4.895780	0.880552	0.719732

Optimized Cartesian coordinates for *syn-3*:

С	0	3.752739	-2.831336	-0.328208
С	0	3.337701	-2.236674	-1.522469
С	0	2.113433	-1.574061	-1.576217
С	0	1.279269	-1.496787	-0.453451
С	0	1.667429	-2.151043	0.742023
С	0	2.925744	-2.782035	0.787702
С	0	-0.003505	-0.730743	-0.480313
С	0	-1.213042	-1.603908	-0.369344
С	0	-1.475596	-2.256747	0.860700
С	0	-2.086834	-1.808978	-1.445112
С	0	-3.244178	-2.571907	-1.304011
С	0	-3.550496	-3.145128	-0.067658
С	0	-2.672573	-2.985961	0.997897
С	0	-0.040035	0.623326	-0.456648
С	0	1.198507	1.467205	-0.392962
С	0	1.537929	2.029106	0.854189
С	0	-1.588216	2.255255	0.740918
С	0	-1.301714	1.431606	-0.371717

С	0	1.964469	1.776238	-1.521200
С	0	3.076752	2.613929	-1.419447
С	0	3.426474	3.155264	-0.183203
С	0	2.655458	2.863174	0.943732
С	0	-2.773584	3.006769	0.724390
С	0	-3.653962	2.983894	-0.352640
С	0	-3.348965	2.202389	-1.466377
С	0	-2.182927	1.443668	-1.467179
Н	0	4.713549	-3.335689	-0.271121
Н	0	3.972534	-2.274279	-2.403596
Н	0	1.797068	-1.096635	-2.498408
Н	0	3.238173	-3.258557	1.714112
Н	0	-1.854661	-1.359304	-2.404963
Н	0	-3.911503	-2.704293	-2.151291
Н	0	-4.461049	-3.724372	0.059270
Н	0	-2.890453	-3.457181	1.953641
Н	0	1.682139	1.365888	-2.486510
Н	0	3.665086	2.841986	-2.304379
Н	0	4.293014	3.805381	-0.094963
Н	0	2.924598	3.288132	1.908572
Н	0	-3.002135	3.632084	1.585704
Н	0	-4.561113	3.582013	-0.327926
Н	0	-4.008165	2.187313	-2.330210
Н	0	-1.927945	0.858894	-2.343944
С	0	-0.713988	2.424055	1.982384
Н	0	-0.553091	3.502944	2.116582
Н	0	-1.295318	2.103056	2.858489
С	0	0.660539	1.727803	2.045787
Н	0	1.157018	2.058176	2.966126
Н	0	0.517427	0.645488	2.136499
С	0	0.814782	-2.219183	1.929761
С	0	-0.537554	-2.254336	1.983293
Н	0	1.346466	-2.364676	2.869413
Н	0	-0.985965	-2.425484	2.961185

Optimized Cartesian coordinates for anti-4:

С	0	2.274352	-3.496856	2.208675
С	0	0.922306	-3.211316	2.405021
С	0	0.361641	-2.087117	1.804101
С	0	1.130566	-1.240071	0.993748
С	0	2.497340	-1.528634	0.783045
С	0	3.046811	-2.663800	1.403978
С	0	0.525152	0.000000	0.424654
С	0	1.130566	1.240071	0.993748

С	0	2.497340	1.528635	0.783043
С	0	3.339410	0.709672	-0.129187
С	0	3.339410	-0.709673	-0.129186
С	0	0.361642	2.087117	1.804101
С	0	0.922307	3.211317	2.405020
С	0	2.274352	3.496857	2.208671
С	0	3.046812	2.663801	1.403975
С	0	-0.525152	0.000000	-0.424651
С	0	-1.130566	1.240071	-0.993745
С	0	-2.497339	1.528635	-0.783043
С	0	-3.339412	0.709672	0.129185
С	0	-3.339412	-0.709673	0.129184
С	0	-2.497339	-1.528635	-0.783045
С	0	-1.130565	-1.240071	-0.993746
С	0	-0.361640	2.087117	-1.804096
С	0	-0.922303	3.211317	-2.405016
С	0	-2.274349	3.496858	-2.208670
С	0	-3.046810	2.663802	-1.403975
С	0	-3.046810	-2.663800	-1.403979
С	0	-2.274349	-3.496856	-2.208675
С	0	-0.922303	-3.211316	-2.405019
С	0	-0.361639	-2.087117	-1.804097
С	0	4.198990	1.381583	-1.018108
С	0	5.041801	0.697453	-1.888242
С	0	5.041802	-0.697456	-1.888240
С	0	4.198992	-1.381585	-1.018104
С	0	-4.198995	1.381583	1.018104
С	0	-5.041807	0.697452	1.888236
С	0	-5.041807	-0.697456	1.888235
С	0	-4.198995	-1.381585	1.018101
Н	0	2.728702	-4.361109	2.685770
Н	0	0.309362	-3.854514	3.030693
Н	0	-0.686474	-1.849893	1.960580
Н	0	4.102382	-2.879999	1.265333
Н	0	-0.686473	1.849893	1.960580
Н	0	0.309364	3.854515	3.030692
Н	0	2.728703	4.361111	2.685766
Н	0	4.102382	2.880000	1.265328
Н	0	0.686475	1.849893	-1.960574
Н	0	-0.309359	3.854515	-3.030687
Н	0	-2.728699	4.361112	-2.685765
Н	0	-4.102380	2.880001	-1.265331
Н	0	-4.102381	-2.879999	-1.265336
Н	0	-2.728699	-4.361108	-2.685771

Н	0	-0.309358	-3.854513	-3.030690
Н	0	0.686476	-1.849893	-1.960574
Н	0	4.184254	2.467553	-1.032735
Н	0	5.683067	1.250089	-2.569599
Н	0	5.683070	-1.250092	-2.569595
Н	0	4.184258	-2.467554	-1.032729
Н	0	-4.184260	2.467553	1.032730
Н	0	-5.683076	1.250088	2.569591
Н	0	-5.683075	-1.250093	2.569589
Н	0	-4.184260	-2.467555	1.032726

Optimized Cartesian coordinates for the transition state of **4** with a dihedral angle of 100° between the planes of C4a-C5-C5a and C4a'-C5'-C5a':

С	0	-3.575988	3.448403	-0.926814
С	0	-2.221540	3.608475	-1.226124
С	0	-1.323142	2.603173	-0.898380
С	0	-1.726647	1.391072	-0.266291
С	0	-3.138911	1.164650	-0.160460
С	0	-4.017348	2.225677	-0.424988
С	0	-0.663232	0.578551	0.309671
С	0	-0.870498	-0.256593	1.504882
С	0	-2.075022	-0.967397	1.785192
С	0	-3.167451	-1.198437	0.807587
С	0	-3.701614	-0.199290	-0.034066
С	0	0.176118	-0.367727	2.459144
С	0	0.033412	-1.043258	3.658008
С	0	-1.180945	-1.663513	3.966669
С	0	-2.197910	-1.629425	3.025678
С	0	0.663233	0.578550	-0.309669
С	0	0.870497	-0.256599	-1.504876
С	0	2.075019	-0.967405	-1.785186
С	0	3.167451	-1.198441	-0.807583
С	0	3.701615	-0.199292	0.034066
С	0	3.138913	1.164648	0.160456
С	0	1.726650	1.391073	0.266288
С	0	-0.176123	-0.367739	-2.459133
С	0	-0.033421	-1.043277	-3.657994
С	0	1.180934	-1.663535	-3.966655
С	0	2.197903	-1.629442	-3.025668
С	0	4.017353	2.225677	0.424975
С	0	3.575995	3.448406	0.926795
С	0	2.221547	3.608481	1.226106
С	0	1.323148	2.603179	0.898369
С	0	-3.729711	-2.489583	0.751132

С	0	-4.807841	-2.794332	-0.071944
С	0	-5.351875	-1.799169	-0.883117
С	0	-4.791319	-0.527450	-0.866668
С	0	3.729711	-2.489588	-0.751128
С	0	4.807842	-2.794335	0.071946
С	0	5.351877	-1.799171	0.883117
С	0	4.791322	-0.527452	0.866667
Н	0	-4.285570	4.249450	-1.114084
Н	0	-1.859098	4.526747	-1.679974
Н	0	-0.267712	2.758890	-1.082811
Н	0	-5.080629	2.068887	-0.268019
Н	0	1.119536	0.121875	2.256027
Н	0	0.863157	-1.069989	4.359472
Н	0	-1.326579	-2.172005	4.915401
Н	0	-3.139961	-2.120921	3.247761
Н	0	-1.119541	0.121864	-2.256015
Н	0	-0.863170	-1.070013	-4.359454
Н	0	1.326565	-2.172034	-4.915384
Н	0	3.139952	-2.120941	-3.247750
Н	0	5.080632	2.068885	0.268004
Н	0	4.285578	4.249454	1.114058
Н	0	1.859107	4.526758	1.679950
Н	0	0.267718	2.758899	1.082800
Н	0	-3.290482	-3.273885	1.358771
Н	0	-5.206906	-3.804846	-0.090866
Н	0	-6.185840	-2.016308	-1.544976
Н	0	-5.177642	0.229446	-1.541530
Н	0	3.290482	-3.273889	-1.358767
Н	0	5.206907	-3.804849	0.090868
Н	0	6.185843	-2.016310	1.544975
Н	0	5.177646	0.229445	1.541527

Optimized Cartesian coordinates for syn-4:

С	0	3.236907	3.457116	-1.127835
С	0	2.523693	3.149543	-2.286296
С	0	1.682577	2.038956	-2.301055
С	0	1.523494	1.231290	-1.167436
С	0	2.257064	1.528128	0.004472
С	0	3.103490	2.650397	-0.001074
С	0	0.675207	0.000288	-1.204608
С	0	1.524569	-1.229976	-1.167669
С	0	2.258515	-1.526359	0.004120
С	0	2.138286	-0.709105	1.240843
С	0	2.137553	0.710479	1.241011

С	0	1.684352	-2.037271	-2.301460
С	0	2.526579	-3.147021	-2.287005
С	0	3.240189	-3.454136	-1.128666
С	0	3.106043	-2.647793	-0.001723
С	0	-0.675197	-0.000288	-1.204607
С	0	-1.524559	1.229979	-1.167667
С	0	-2.258509	1.526356	0.004120
С	0	-2.138278	0.709103	1.240845
С	0	-2.137544	-0.710481	1.241012
С	0	-2.257058	-1.528126	0.004470
С	0	-1.523484	-1.231289	-1.167436
С	0	-1.684347	2.037272	-2.301458
С	0	-2.526581	3.147015	-2.287006
С	0	-3.240197	3.454125	-1.128669
С	0	-3.106046	2.647784	-0.001725
С	0	-3.103493	-2.650388	-0.001080
С	0	-3.236917	-3.457103	-1.127844
С	0	-2.523698	-3.149532	-2.286303
С	0	-1.682575	-2.038950	-2.301058
С	0	2.077198	-1.380687	2.475496
С	0	2.020925	-0.697133	3.684895
С	0	2.020169	0.697782	3.685061
С	0	2.075755	1.381691	2.475829
С	0	-2.077197	1.380684	2.475499
С	0	-2.020937	0.697130	3.684898
С	0	-2.020180	-0.697785	3.685063
С	0	-2.075753	-1.381693	2.475830
Н	0	3.907140	4.312228	-1.104991
Н	0	2.628079	3.763098	-3.177119
Н	0	1.147322	1.781467	-3.209269
Н	0	3.685921	2.872691	0.888337
Η	0	1.148760	-1.780137	-3.209577
Н	0	2.631494	-3.760286	-3.177965
Н	0	3.911266	-4.308591	-1.106052
Н	0	3.688733	-2.869694	0.887616
Н	0	-1.148757	1.780137	-3.209577
Н	0	-2.631498	3.760278	-3.177967
Н	0	-3.911281	4.308575	-1.106056
Н	0	-3.688741	2.869679	0.887612
Н	0	-3.685928	-2.872678	0.888329
Н	0	-3.907158	-4.312209	-1.105003
Н	0	-2.628089	-3.763083	-3.177128
Н	0	-1.147323	-1.781460	-3.209274
Н	0	2.052927	-2.466474	2.474746

Н	0	1.963102	-1.250030	4.618641
Н	0	1.961741	1.250391	4.618939
Н	0	2.050329	2.467451	2.475355
Н	0	-2.052924	2.466471	2.474750
Н	0	-1.963121	1.250027	4.618645
Н	0	-1.961760	-1.250395	4.618941
Н	0	-2.050324	-2.467453	2.475355

Optimized Cartesian coordinates for anti-5:

С	0	2.136531	-3.478108	1.994028
С	0	0.848698	-3.189575	2.448622
С	0	0.178241	-2.073239	1.955594
С	0	0.770452	-1.236017	0.999562
С	0	2.071699	-1.525326	0.532226
С	0	2.734822	-2.653600	1.045166
С	0	0.064597	0.000000	0.545439
С	0	0.770452	1.236017	0.999562
С	0	2.071699	1.525326	0.532227
С	0	2.721273	0.709602	-0.527952
С	0	2.721273	-0.709602	-0.527952
С	0	0.178241	2.073239	1.955594
С	0	0.848698	3.189575	2.448622
С	0	2.136532	3.478108	1.994028
С	0	2.734822	2.653600	1.045166
С	0	-1.125255	0.000000	-0.100148
С	0	-1.806350	1.261608	-0.513519
С	0	-3.099850	1.579649	-0.033344
С	0	-3.895388	0.676121	0.797413
С	0	-3.895388	-0.676121	0.797413
С	0	-3.099850	-1.579649	-0.033344
С	0	-1.806350	-1.261608	-0.513519
С	0	-1.154975	2.159841	-1.371681
С	0	-1.738872	3.372791	-1.726539
С	0	-2.992979	3.715172	-1.213487
С	0	-3.656301	2.828601	-0.373898
С	0	-3.656301	-2.828601	-0.373898
С	0	-2.992979	-3.715172	-1.213487
С	0	-1.738872	-3.372791	-1.726539
С	0	-1.154975	-2.159841	-1.371681
С	0	3.394722	1.381632	-1.564630
С	0	4.054782	0.697473	-2.580526
С	0	4.054782	-0.697473	-2.580526
С	0	3.394722	-1.381632	-1.564630

Н	0	2.677037	-4.337217	2.382274
Н	0	0.371660	-3.825192	3.189785
Н	0	-0.820708	-1.836217	2.309195
Н	0	3.743968	-2.869523	0.705798
Н	0	-0.820708	1.836217	2.309195
Η	0	0.371660	3.825192	3.189785
Н	0	2.677038	4.337217	2.382274
Η	0	3.743968	2.869523	0.705798
Η	0	-0.170410	1.899926	-1.748584
Η	0	-1.211224	4.054846	-2.387708
Η	0	-3.451331	4.666091	-1.471445
Η	0	-4.637948	3.086006	0.017398
Η	0	-4.637948	-3.086006	0.017398
Н	0	-3.451331	-4.666091	-1.471445
Н	0	-1.211224	-4.054846	-2.387708
Η	0	-0.170410	-1.899926	-1.748583
Η	0	3.378495	2.467692	-1.574839
Η	0	4.553916	1.250203	-3.371855
Н	0	4.553916	-1.250203	-3.371855
Н	0	3.378494	-2.467692	-1.574839
Η	0	-4.650511	-1.164820	1.411896
Н	0	-4.650511	1.164820	1.411896

Optimized Cartesian coordinates for the transition state of **5** with a dihedral angle of 90° between the planes of C4a-C5-C5a and C4a'-C5'-C5a':

С	0	1.611817	-2.075259	-3.596552
С	0	0.252705	-1.762434	-3.474636
С	0	-0.210631	-1.137015	-2.332623
С	0	0.631211	-0.823910	-1.223358
С	0	2.041472	-0.984399	-1.436599
С	0	2.477804	-1.652657	-2.598188
С	0	0.004487	-0.398504	0.014635
С	0	0.590111	-0.521650	1.333131
С	0	1.984149	-0.683246	1.646931
С	0	3.062853	-0.165720	0.773711
С	0	3.081593	-0.295439	-0.633136
С	0	-0.318296	-0.640055	2.429491
С	0	0.082650	-1.024936	3.701310
С	0	1.418555	-1.345152	3.938808
С	0	2.347197	-1.152770	2.916038
С	0	-1.370074	0.224909	-0.063772
С	0	-1.343384	1.661238	-0.226539
С	0	-2.462285	2.573748	-0.142061
С	0	-3.854679	2.192764	-0.065360

С	0	-4.450409	0.978955	-0.063410
С	0	-3.897786	-0.355760	-0.034533
С	0	-2.491924	-0.681035	0.032736
С	0	-0.073754	2.265290	-0.484460
С	0	0.124103	3.639413	-0.501340
С	0	-0.956671	4.504419	-0.335273
С	0	-2.227779	3.958775	-0.188252
С	0	-4.849093	-1.393479	-0.003073
С	0	-4.501495	-2.733574	0.106074
С	0	-3.149634	-3.061534	0.240254
С	0	-2.188536	-2.064065	0.239645
С	0	4.119618	0.527682	1.400825
С	0	5.181996	1.067923	0.686679
С	0	5.198296	0.948331	-0.702402
С	0	4.155306	0.288408	-1.340692
Н	0	1.991465	-2.598497	-4.469331
Н	0	-0.445924	-2.015473	-4.267940
Н	0	-1.268550	-0.919073	-2.257856
Н	0	3.542123	-1.835078	-2.710904
Н	0	-1.370654	-0.472926	2.249044
Н	0	-0.658373	-1.118745	4.490727
Н	0	1.741431	-1.715862	4.907580
Н	0	3.398397	-1.339217	3.115792
Н	0	0.775346	1.631028	-0.688592
Н	0	1.121677	4.030266	-0.681719
Н	0	-0.821937	5.581808	-0.365455
Н	0	-3.084769	4.622504	-0.104856
Н	0	-5.899416	-1.119460	-0.064806
Н	0	-5.268995	-3.501703	0.126208
Н	0	-2.844436	-4.095270	0.378020
Н	0	-1.154197	-2.344368	0.384667
Н	0	4.080749	0.667901	2.475868
Н	0	5.972847	1.599851	1.208604
Н	0	6.001901	1.386220	-1.288386
Н	0	4.149292	0.240201	-2.424281
Н	0	-5.538804	0.998784	-0.048018
Н	0	-4.536145	3.041533	-0.048415

Optimized Cartesian coordinates for syn-5:

С	0	3.466925	-2.678534	-1.462417
С	0	3.150637	-1.757111	-2.460917
С	0	2.037578	-0.932307	-2.309331
С	0	1.236036	-1.001662	-1.163572
С	0	1.542120	-1.944082	-0.155079

С	0	2.667368	-2.768006	-0.325718
С	0	0.000565	-0.173209	-1.011919
С	0	-1.220856	-1.022370	-1.162224
С	0	-1.509085	-1.970707	-0.153922
С	0	-0.691988	-2.067203	1.085411
С	0	0.727919	-2.054473	1.084963
С	0	-2.025156	-0.966093	-2.306756
С	0	-3.123866	-1.810092	-2.457433
С	0	-3.422431	-2.737852	-1.459361
С	0	-2.619862	-2.814199	-0.323822
С	0	-0.009944	1.128094	-0.649024
С	0	1.237545	1.897634	-0.363796
С	0	1.556804	2.220532	0.978124
С	0	0.659654	1.948275	2.101576
С	0	-0.692502	1.937407	2.101699
С	0	-1.593957	2.195301	0.978343
С	0	-1.269564	1.877570	-0.363539
С	0	2.105180	2.296716	-1.388634
С	0	3.299798	2.956689	-1.108099
С	0	3.649782	3.221455	0.218135
С	0	2.787083	2.852091	1.243658
С	0	-2.834042	2.807398	1.243832
С	0	-3.702284	3.163436	0.218271
С	0	-3.347990	2.904510	-1.107974
С	0	-2.143155	2.263338	-1.388437
С	0	-1.362145	-2.216485	2.312802
С	0	-0.676125	-2.349914	3.515582
С	0	0.718943	-2.337132	3.515130
С	0	1.401572	-2.191352	2.311865
Н	0	4.325452	-3.335503	-1.573171
Н	0	3.761719	-1.684645	-3.356621
Н	0	1.776426	-0.227101	-3.092469
Н	0	2.899387	-3.506351	0.436600
Н	0	-1.777388	-0.255942	-3.089766
Н	0	-3.737409	-1.747591	-3.352208
Н	0	-4.269399	-3.409756	-1.569528
Н	0	-2.837914	-3.557171	0.438128
Н	0	1.837973	2.078257	-2.417875
Н	0	3.961186	3.248522	-1.919402
Н	0	4.587191	3.720154	0.449372
Н	0	3.047829	3.073572	2.276067
Н	0	-3.098301	3.024666	2.276243
Н	0	-4.647402	3.647374	0.449494
Н	0	-4.013695	3.186185	-1.919337

Н	0	-1.872223	2.049621	-2.417705
Н	0	-2.448244	-2.204184	2.315392
Н	0	-1.227487	-2.451030	4.446645
Н	0	1.272669	-2.428099	4.445837
Н	0	2.487275	-2.159361	2.313591
Η	0	-1.181883	1.826866	3.068207
Н	0	1.150896	1.845541	3.068003