Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Synthesis, Structure and Properties of Decakis(phenylthio)corannulene.

SUPPLEMENTARY INFORMATION

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A) Synthesis
B) Crystallographic Methods
C) Computational Details

A) Synthesis

Decakis(thiophenol)corannulene. To a 5 mL round bottom flask equipped with a reflux condenser, 1,3-dimethylimidizolidinone (2 mL, dried over 4 Å MS) is added. Thiophenol (0.056 g, 0.504 mmol) and sodium hydride (0.027 g, 0.672 mmol, 60% in mineral oil) are added and allowed to stir at ambient temperature for 10 minutes. Decachlorocorannulene (0.020 g, 0.034 mmol) is added and the solution is warmed to 60 °C for 12 hours. The solution is cooled, extracted with benzene (10 mL), and washed 4 times with water (10 mL). The organic layer is dried over magnesium sulfate, filtered, and evaporated. The product is purified by passage through a plug of silica with benzene as eluent. The yield of a dark red solid is 20 mg (50 %). ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.80 (t, *J*= 3.5 Hz, 20H), 6.98 (t, *J*= 3.5 Hz, 30H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 125.3, 127.4, 128.5, 133.7, 134.6, 139.7 142.3. HRMS *m/z*: found 1330.1084 calcd ($C_{80}H_{50}S_{10}$) 1330.1120.

B) Crystallographic Methods

A crystal of **5** with dimensions of 0.14 x 0.15 x 0.31 mm^3 was mounted on the tip of a glass fiber using epoxy and placed in a cooled nitrogen gas stream at 153 K on a Bruker SMART 1000 CCD sealed tube diffractometer with graphite monochromated MoK_α (0.71073 Å) radiation[a]. Data were measured at 153 K using a series of combinations of phi and omega scans with 10 s frame exposures and 0.3^o frame widths. Data collection, indexing and initial cell refinements were all carried out using SMART[b] software. Frame integration and final cell refinements were done using SAINT[c] software The structure was solved using Direct methods and difference Fourier techniques (SHELXTL, V6.12).[d] Hydrogen atoms were placed their expected chemical positions using the HFIX command and were included in the final cycles of least squares with isotropic U_{ij} 's related to the atom's ridden upon. All non-hydrogen atoms were refined anisotropically except the carbon atoms in the disordered corannulene core. Scattering factors and anomalous dispersion corrections are taken from the *International Tables for X-ray Crystallography*[e]. Structure solution, refinement, graphics and generation of publication materials were performed by using SHELXTL, V6.12 software.

References

a. Center for Molecular Structure, California State University Fullerton, Fullerton, CA

b Bruker SMART, Bruker AXS Inc., Madison, Wisconsin, USA

c Bruker SAINT, Bruker AXS Inc., Madison, Wisconsin, USA.

d "A short history of SHEL*X*". Sheldrick, G.M. (2008). *Acta Cryst*. A64, 112-122.

e A. J. C. Wilson (ed), *International Tables for X-ray Crystallography, Volume C.* Kynoch, Academic Publishers, Dordrecht, **1992**, Tables 6.1.1.4 (pp. 500-502) and 4.2.6.8 (pp. 219-222).

C) Computational Details

Compound **5** calculated in C5 symmetry at B98 in pdb format

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ATOM      1 S    RES 0 0        -4.700  -1.695  -0.352                       S
ATOM      2 S    RES 0 0         0.159  -4.993  -0.352                       S
ATOM      3 S    RES 0 0         4.798  -1.391  -0.352                       S
ATOM      4 S    RES 0 0         2.806   4.133  -0.352                       S
ATOM      5 S    RES 0 0        -2.773  -4.316   0.366                       S
ATOM      6 S    RES 0 0         3.248  -3.971   0.366                       S
ATOM      7 S    RES 0 0         4.780   1.862   0.366                       S
ATOM      8 S    RES 0 0        -0.294   5.121   0.366                       S
ATOM      9 S    RES 0 0        -4.962   1.303   0.366                       S
ATOM     10 S    RES 0 0        -3.064   3.946  -0.352                       S
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ATOM     14 C    RES 0 0         2.370   4.010  -2.104                       C
ATOM     15 C    RES 0 0        -3.628  -4.019   1.926                       C
ATOM     16 C    RES 0 0         2.701  -4.692   1.926                       C
ATOM     17 C    RES 0 0         5.298   1.119   1.926                       C
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ATOM     19 C    RES 0 0        -4.944   2.208   1.926                       C
ATOM     20 C    RES 0 0        -3.081   3.493  -2.104                       C
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ATOM     22 C    RES 0 0        -0.404  -3.808  -2.862                       C
ATOM     23 C    RES 0 0         3.496  -1.561  -2.862                       C
ATOM     24 C    RES 0 0         2.565   2.843  -2.862                       C
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ATOM     33 H    RES 0 0         2.748  -2.204  -2.394                       H
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ATOM     46 C    RES 0 0         2.242  -4.550   4.304                       C
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ATOM     84 C    RES 0 0         1.630   5.180  -4.100                    C
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ATOM     95 H    RES 0 0        -6.766  -4.368   3.228                    H
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Compound **5** calculated in D5 symmetry at B98 in pdb format

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ATOM      1 S    RES 0 0        -4.905  -1.520  -0.374                      S
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ATOM      8 S    RES 0 0        -0.070   5.135   0.374                      S
ATOM      9 S    RES 0 0        -4.905   1.520   0.374                      S
ATOM     10 S    RES 0 0        -2.962   4.195  -0.374                      S
ATOM     11 C    RES 0 0        -4.610  -2.062  -2.073                      C
ATOM     12 C    RES 0 0         0.536  -5.021  -2.073                      C
ATOM     13 C    RES 0 0         4.941  -1.042  -2.073                      C
ATOM     14 C    RES 0 0         2.518   4.377  -2.073                      C
ATOM     15 C    RES 0 0        -3.385  -3.747   2.073                      C
ATOM     16 C    RES 0 0         2.518  -4.377   2.073                      C
ATOM     17 C    RES 0 0         4.941   1.042   2.073                      C
ATOM     18 C    RES 0 0         0.536   5.021   2.073                      C
ATOM     19 C    RES 0 0        -4.610   2.062   2.073                      C
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ATOM     28 C    RES 0 0        -0.103   4.221   3.037                      C
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ATOM     31 H    RES 0 0        -3.728  -0.199  -2.761                      H
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ATOM     37 H    RES 0 0         3.133   2.030   2.761                      H
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ATOM     42 C    RES 0 0         0.361  -4.220  -4.357                      C
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ATOM     46 C    RES 0 0          2.188  -3.626   4.357                      C
ATOM     47 C    RES 0 0          4.125   0.961   4.357                      C
ATOM     48 C    RES 0 0          0.361   4.220   4.357                      C
ATOM     49 C    RES 0 0         -3.902   1.647   4.357                      C
ATOM     50 C    RES 0 0         -2.772   3.202  -4.357                      C
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ATOM     53 H    RES 0 0          3.373  -1.245  -5.099                      H
ATOM     54 H    RES 0 0          2.226   2.824  -5.099                      H
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ATOM     57 H    RES 0 0          3.373   1.245   5.099                      H
ATOM     58 H    RES 0 0         -0.141   3.593   5.099                      H
ATOM     59 H    RES 0 0         -3.461   0.976   5.099                      H
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ATOM     70 C    RES 0 0         -4.123   3.219  -4.731                      C
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ATOM     72 H    RES 0 0          1.797  -5.029  -5.765                      H
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ATOM     78 H    RES 0 0          1.797   5.029   5.765                      H
ATOM     79 H    RES 0 0         -4.228   3.263   5.765                      H
ATOM     80 H    RES 0 0         -4.410   3.012  -5.765                      H
ATOM     81 C    RES 0 0         -4.913  -3.768  -3.774                      C
ATOM     82 C    RES 0 0          2.066  -5.837  -3.774                      C
ATOM     83 C    RES 0 0          6.190   0.161  -3.774                      C
ATOM     84 C    RES 0 0          1.760   5.936  -3.774                      C
ATOM     85 C    RES 0 0         -5.102  -3.508   3.774                      C
ATOM     86 C    RES 0 0          1.760  -5.936   3.774                      C
ATOM     87 C    RES 0 0          6.190  -0.161   3.774                      C
ATOM     88 C    RES 0 0          2.066   5.837   3.774                      C
ATOM     89 C    RES 0 0         -4.913   3.768   3.774                      C
ATOM     90 C    RES 0 0         -5.102   3.508  -3.774                      C
ATOM     91 H    RES 0 0         -5.253  -4.769  -4.055                      H
ATOM     92 H    RES 0 0          2.912  -6.469  -4.055                      H
ATOM     93 H    RES 0 0          7.053   0.770  -4.055                      H
ATOM     94 H    RES 0 0          1.447   6.945  -4.055                      H
ATOM     95 H    RES 0 0         -6.158  -3.522   4.055                      H
ATOM     96 H    RES 0 0          1.447  -6.945   4.055                      H
ATOM     97 H    RES 0 0          7.053  -0.770   4.055                      H
ATOM     98 H    RES 0 0          2.912   6.469   4.055                      H
ATOM     99 H    RES 0 0         -5.253   4.769   4.055                      H
ATOM    100 H    RES 0 0         -6.158   3.522  -4.055                      H
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ATOM    103 C    RES 0 0          6.045  -0.256  -2.444                      C
ATOM    104 C    RES 0 0          2.112   5.670  -2.444                      C
ATOM    105 C    RES 0 0         -4.740  -3.760   2.444                      C
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ATOM    107 C    RES 0 0          6.045   0.256   2.444                      C
ATOM    108 C    RES 0 0          1.625   5.828   2.444                      C
ATOM    109 C    RES 0 0         -5.041   3.346   2.444                      C
ATOM    110 C    RES 0 0         -4.740   3.760  -2.444                      C
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ATOM    112 H    RES 0 0          2.128  -6.438  -1.692                      H
ATOM    113 H    RES 0 0          6.781   0.034  -1.692                      H
ATOM    114 H    RES 0 0          2.063   6.459  -1.692                      H
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ATOM    116 H    RES 0 0          2.063  -6.459   1.692                      H
ATOM    117 H    RES 0 0          6.781  -0.034   1.692                      H
ATOM    118 H    RES 0 0          2.128   6.438   1.692                      H
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ATOM    123 C    RES 0 0         -0.967  -0.703  -0.000                      C
ATOM    124 C    RES 0 0          0.369  -1.137  -0.000                      C
ATOM    125 C    RES 0 0          1.195   0.000  -0.000                      C
ATOM    126 C    RES 0 0          0.794   2.444  -0.000                      C
ATOM    127 C    RES 0 0         -2.079   1.511  -0.000                      C
ATOM    128 C    RES 0 0         -2.079  -1.511  -0.000                      C
ATOM    129 C    RES 0 0          0.794  -2.444  -0.000                      C
ATOM    130 C    RES 0 0          2.570   0.000  -0.000                      C
ATOM    131 C    RES 0 0         -0.347  -3.375  -0.048                      C
ATOM    132 C    RES 0 0          3.103  -1.373  -0.048                      C
ATOM    133 C    RES 0 0          2.265   2.527  -0.048                      C
ATOM    134 C    RES 0 0         -1.703   2.935  -0.048                      C
ATOM    135 C    RES 0 0         -3.317   0.713   0.048                      C
ATOM    136 C    RES 0 0         -1.703  -2.935   0.048                      C
ATOM    137 C    RES 0 0          2.265  -2.527   0.048                      C
ATOM    138 C    RES 0 0          3.103   1.373   0.048                      C
ATOM    139 C    RES 0 0         -0.347   3.375   0.048                      C
ATOM    140 C    RES 0 0         -3.317  -0.713  -0.048                      C
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