Crystal structure of phenanthrene—5,10,15,20-tetraphenyl-21*H*,23*H*-porphyrin (1/1), $C_{58}H_{40}N_4$

J. Blömker^I and W. Frey^{II}^I Universität Stuttgart, Physikalisches Institut, Pfaffenwaldring 57, D-70569 Stuttgart, Germany^{II} Universität Stuttgart, Institut für Organische Chemie, Pfaffenwaldring 55, D-70569 Stuttgart, Germany

Received October 12, 1999, CCDC-No. 1267/310

Fig. 1. TPP layers with molecules of phenanthrene in between.

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	Occ.	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(2N)	2i		0.1246(3)	0.5609(3)	0.4942(2)	0.052
H(2)	2i		0.3944(4)	0.4868(3)	0.8725(3)	0.061
H(3)	2i		0.1487(4)	0.3521(3)	0.8775(3)	0.060
H(7)	2i		0.5624(4)	0.7839(4)	0.5976(3)	0.064
H(8)	2i		0.4269(4)	0.8157(4)	0.4098(3)	0.064
H(12)	2i		0.5173(4)	0.7714(4)	0.9228(3)	0.063
H(13)	2i		0.7692(4)	0.8455(4)	1.0452(3)	0.077
H(14)	2i		0.9470(4)	0.7715(4)	0.9650(4)	0.080
H(15)	2i		0.8727(4)	0.6250(4)	0.7601(4)	0.079
H(16)	2i		0.6205(4)	0.5506(4)	0.6373(3)	0.067
H(18)	2i		0.1886(5)	0.5894(4)	0.1051(4)	0.080

Table 2. Continued.

Atom	Site	Occ.	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(19)	2i		0.2705(5)	0.7055(5)	−0.0198(4)	0.092
H(20)	2i		0.2965(4)	0.9322(4)	0.0282(3)	0.077
H(21)	2i		0.2307(5)	1.0421(4)	0.1962(3)	0.080
H(22)	2i		0.1471(4)	0.9266(4)	0.3204(3)	0.074
H(1P)	2i		0.5902(8)	0.8582(8)	1.2652(6)	0.161
H(2P)	2i		0.647(1)	1.0442(9)	1.2036(7)	0.175
H(3P)	2i		0.888(1)	1.2065(8)	1.2912(7)	0.161
H(4P)	2i	0.5	1.0802	1.1876	1.4482	0.152
H(6P)	2i	0.5	0.7739	0.8360	1.4215	0.165
H(7A)	2i	0.5	1.140(1)	1.2783(9)	1.4466(9)	0.109
H(7B)	2i	0.5	0.691(1)	0.7476(8)	1.4105(9)	0.101

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	Occ.	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
N(1)	2i		0.1110(3)	0.4784(3)	0.6606(2)	0.039(2)	0.046(2)	0.043(2)	0.006(1)	0.014(1)	0.022(1)
C(1)	2i		0.2663(4)	0.5241(3)	0.7186(3)	0.043(2)	0.047(2)	0.043(2)	0.011(2)	0.013(2)	0.019(2)
N(2)	2i		0.2093(3)	0.6153(3)	0.4962(2)	0.039(2)	0.048(2)	0.045(2)	0.006(1)	0.015(1)	0.023(1)
C(2)	2i		0.2980(4)	0.4716(3)	0.8191(3)	0.049(2)	0.054(2)	0.047(2)	0.011(2)	0.007(2)	0.024(2)
C(3)	2i		0.1633(4)	0.3971(3)	0.8216(3)	0.050(2)	0.055(2)	0.049(2)	0.011(2)	0.016(2)	0.031(2)
C(4)	2i		0.0456(4)	0.4000(3)	0.7215(3)	0.044(2)	0.045(2)	0.042(2)	0.012(2)	0.015(2)	0.021(2)
C(5)	2i		0.3776(3)	0.6071(3)	0.6858(3)	0.039(2)	0.044(2)	0.044(2)	0.009(2)	0.013(1)	0.019(2)
C(6)	2i		0.3484(3)	0.6502(3)	0.5834(3)	0.039(2)	0.051(2)	0.043(2)	0.009(2)	0.015(2)	0.021(2)
C(7)	2i		0.4582(4)	0.7431(4)	0.5535(3)	0.041(2)	0.061(2)	0.055(2)	0.004(2)	0.015(2)	0.029(2)
C(8)	2i		0.3831(4)	0.7606(4)	0.4500(3)	0.045(2)	0.064(2)	0.050(2)	0.001(2)	0.016(2)	0.031(2)
C(9)	2i		0.2257(4)	0.6805(3)	0.4123(3)	0.047(2)	0.045(2)	0.043(2)	0.009(2)	0.020(2)	0.020(2)
C(10)	2i		0.1108(4)	0.6717(3)	0.3098(3)	0.045(2)	0.044(2)	0.042(2)	0.013(2)	0.019(2)	0.020(2)
C(11)	2i		0.5410(3)	0.6535(3)	0.7660(3)	0.042(2)	0.043(2)	0.043(2)	0.011(2)	0.012(2)	0.021(2)
C(12)	2i		0.5885(4)	0.7416(4)	0.8892(3)	0.052(2)	0.058(2)	0.046(2)	0.009(2)	0.017(2)	0.022(2)
C(13)	2i		0.7393(4)	0.7858(4)	0.9628(3)	0.064(3)	0.063(3)	0.048(2)	0.000(2)	0.001(2)	0.025(2)
C(14)	2i		0.8453(4)	0.7421(4)	0.9151(4)	0.044(2)	0.076(3)	0.076(3)	0.008(2)	0.003(2)	0.044(2)
C(15)	2i		0.8008(4)	0.6545(4)	0.7931(4)	0.051(2)	0.075(3)	0.082(3)	0.026(2)	0.024(2)	0.037(2)
C(16)	2i		0.6498(4)	0.6104(4)	0.7196(3)	0.051(2)	0.059(2)	0.057(2)	0.020(2)	0.016(2)	0.018(2)
C(17)	2i		0.1610(3)	0.7463(3)	0.2272(3)	0.037(2)	0.045(2)	0.040(2)	0.008(1)	0.011(1)	0.020(2)
C(18)	2i		0.1973(5)	0.6812(4)	0.1247(4)	0.096(3)	0.056(2)	0.076(3)	0.034(2)	0.054(2)	0.036(2)
C(19)	2i		0.2469(5)	0.7510(5)	0.0498(4)	0.102(3)	0.084(3)	0.082(3)	0.041(3)	0.066(3)	0.047(3)
C(20)	2i		0.2610(4)	0.8853(4)	0.0775(3)	0.068(2)	0.068(3)	0.062(2)	0.007(2)	0.029(2)	0.039(2)
C(21)	2i		0.2231(5)	0.9506(4)	0.1776(3)	0.094(3)	0.046(2)	0.053(2)	0.008(2)	0.021(2)	0.023(2)
C(22)	2i		0.1730(4)	0.8810(4)	0.2521(3)	0.087(3)	0.052(2)	0.047(2)	0.014(2)	0.029(2)	0.022(2)
C(1P)	2i		0.6866(8)	0.9249(8)	1.3016(6)	0.139(6)	0.169(8)	0.115(6)	0.060(5)	0.083(5)	0.039(5)
C(2P)	2i		0.721(1)	1.0349(9)	1.2647(7)	0.187(9)	0.182(9)	0.124(6)	0.101(7)	0.103(6)	0.060(6)
C(3P)	2i		0.864(1)	1.1316(8)	1.3165(7)	0.203(8)	0.134(6)	0.137(6)	0.101(6)	0.117(6)	0.064(5)
C(4P)	2i		0.970(1)	1.1139(8)	1.4077(7)	0.185(8)	0.143(7)	0.109(5)	0.105(6)	0.095(6)	0.045(5)
C(5P)	2i		0.9462(8)	1.0079(9)	1.4533(4)	0.165(8)	0.159(6)	0.107(5)	0.108(6)	0.095(6)	0.054(5)
C(6P)	2i		0.798(1)	0.9146(8)	1.3948(7)	0.195(8)	0.164(7)	0.122(6)	0.111(7)	0.112(6)	0.057(6)
C(7A)	2i	0.5	1.111(1)	1.2009(9)	1.4675(9)	0.117(9)	0.063(6)	0.109(9)	0.030(7)	0.078(7)	0.021(6)
C(7B)	2i	0.5	0.786(1)	0.8159(8)	1.4435(9)	0.092(7)	0.066(6)	0.099(8)	0.022(5)	0.060(6)	0.016(6)

Acknowledgment. We thank W. Tuffentsammer for the preparation of the crystal samples.

References

- Byrn, M. P.; Curtis, C. J.; Goldberg, I.; Hsiou, Y.; Khan, S. I.; Sawin, P. A.; Tendick, S. K.; Strouse, C. E.: Porphyrin Sponges: Structural Systematics of the Host Lattice. *J. Am. Chem. Soc.* **113** (1991) 6549–6557.
- Byrn, M. P.; Curtis, C. J.; Khan, S. I.; Sawin, P. A.; Tsurumi, R.; Strouse, C. E.: Tetraarylporphyrin Sponges. Composition, Structural Systematics, and Applications of a Large Class of Programmable Lattice Clathrates. *J. Am. Chem. Soc.* **112** (1990) 1865–1874.
- Silvers, S. J.; Tulinsky, A.: The Triclinic Crystal Form of $\alpha,\beta,\gamma,\delta$ -Tetra-phenylporphine. *J. Am. Chem. Soc.* **86** (1964) 927–928.
- Sheldrick, G. M.: Phase Annealing in SHELX-90: Direct Methods for Larger Structures. *Acta Crystallogr. A* **46** (1990) 476.
- Sheldrick, G. M.: SHELXL-93. Program for the Refinement of Crystal Structures. University of Göttingen, Germany 1993.