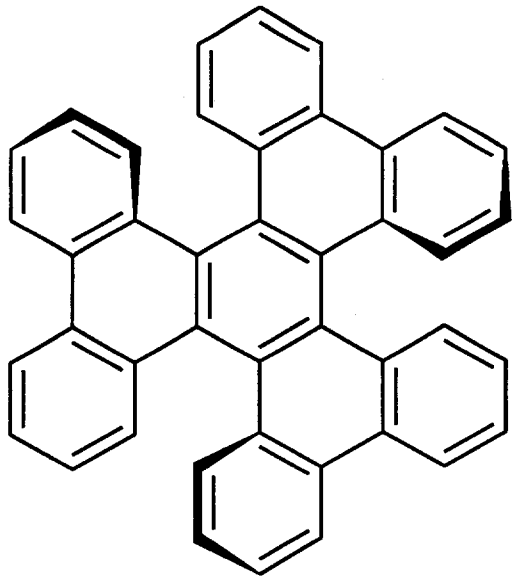
Single Crystal X-ray Structure Report RAP002

Hexabenzotriphenylene

(Dibenzo[*f,j*]phenanthro[9,10-*s*]picene, $C_{42}H_{24}$)



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Experimental

Hexabenzotriphenylene, prepared by chemical synthesis, was crystallized by the slow cooling of a solution in nitrobenzene. An orange plate, 0.04 mm × 0.25 mm × 0.28 mm, was mounted on a glass fiber and transferred to a Nonius KappaCCD diffractometer, where Mo Kα radiation (λ = 0.71074 Å) was employed for data collection at 298 K.[1] Five crystal settings were used for the measurements, which employed 1° oscillations, and a total of 651° of data were collected. A total of 45,305 reflections (θ_{max} = 27.4°) were indexed, integrated, and corrected for Lorentz and polarization effects (but not for absorption) by using the program DENZO-SMN,[2] and then were merged to 6512 reflections (R_{int} = 0.066) by using the program SCALEPACK.[2] Postrefinement of the unit cell parameters gave a = 19.9721(5) Å, b = 7.0005(1) Å, c = 19.5456(5) Å, β = 104.013(1)°, and V = 2651.4(1) Å^3. Systematic absences were consistent with the monoclinic space group $P2_1/c$ (No. 14), so 456 extinctions were discarded to give 6016 unique reflections in the final data set.

The structure was solved by direct methods by using Siemens SHELXTL.[3] All atomic coordinates were refined; carbon atoms were refined anisotropically, and hydrogens isotropically (SHELXTL). The final weighting scheme was $w = 1/[\sigma^2(F_o)^2 + (0.0600P)^2 + 0.4023P]$ where $P = (F_o^2 + 2F_c^2)/3$. The refinement converged to $R(F)$ = 0.0512, $wR(F^2)$ = 0.1091, and S = 1.095 for 3652 reflections with $I > 2\sigma(I)$, and $R(F)$ = 0.1007, $wR(F^2)$ = 0.1327, and S = 1.013 for 6016 unique reflections, 475 parameters, and 0 restraints.[4] The maximum Δ/σ in the final cycle of least squares was less than

0.001, and the residual peaks on the final $\Delta\rho$ map ranged from −0.179 to 0.157 $e/Å^3$. Scattering factors were taken from the *International Tables for Crystallography, Vol. C.*[5,6]

References and Notes

[1] *COLLECT* Data Collection Software. Nonius Company, Bohemia, New York, USA, 1998.

[2] Otwinowski, Z.; Minor, W., "Processing of X-ray Diffraction Data Collected in Oscillation Mode", *Methods Enzymol.* **1997**, *276*, 307-326.

[3] Sheldrick, G. M. *SHELXTL* Version 5. Siemens Analytical X-ray Instruments, Madison, Wisconsin, USA, 1996.

[4] $R(F) = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$,
$wR(F^2) = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$, and
S = goodness-of-fit on $F^2 = [\Sigma w(F_o^2 - F_c^2)^2 / (n - p)]^{1/2}$, where n is the number of reflections and p is the number of parameters refined.

[5] Maslen, E. N.; Fox, A. G.; O'Keefe, M. A., Chapter 6 in *International Tables for Crystallography: Mathematical, Physical and Chemical Tables*, Vol. C; Wilson, A. J. C., Ed.; Kluwer, Dordrecht, The Netherlands, 1992; pp 476-516.

[6] Creagh, D. C.; McAuley, W. J., Chapter 4 in *International Tables for Crystallography: Mathematical, Physical and Chemical Tables*, Vol. C; Wilson, A. J. C., Ed.; Kluwer, Dordrecht, The Netherlands, 1992; pp 206-222.

Miscellaneous Data

1. The "aromatic" rings of hexabenzotriphenylene (the central ring and the six peripheral benzo groups) are much less distorted from planarity than the remaining three "non-aromatic" rings. The equations for the least-squares planes of the seven "aromatic" rings (rings **1-7**), the defining atoms, and the rms deviations of the fitted atoms are listed below, as well as the same data for the three "non-aromatic" rings (**8-10**).

Plane **1**: $8.322(12)x + 5.203(3)y - 11.897(10)z = 4.020(4)$
Atoms: C1 C2 C3 C4 C5 C6 Rms deviation: 0.058 Å

Plane **2**: $0.053(15)x + 6.756(1)y - 4.977(15)z = 4.954(3)$
Atoms: C7 C8 C9 C10 C11 C12 Rms deviation: 0.011 Å

Plane **3**: $4.749(15)x + 6.782(1)y - 2.463(15)z = 5.222(1)$
Atoms: C13 C14 C15 C16 C17 C18 Rms deviation: 0.013 Å

Plane **4**: $5.096(16)x - 2.697(5)y + 18.025(6)z = 1.081(5)$
Atoms: C19 C20 C21 C22 C23 C24 Rms deviation: 0.007 Å

Plane **5**: $0.904(17)x - 3.933(5)y + 15.450(10)z = 0.361(8)$
Atoms: C25 C26 C27 C28 C29 C30 Rms deviation: 0.006 Å

Plane **6**: $16.472(9)x + 3.730(4)y - 7.496(13)z = 6.116(6)$
Atoms: C31 C32 C33 C34 C35 C36 Rms deviation: 0.012 Å

Plane **7**: $16.124(9)x + 2.609(5)y - 12.498(12)z = 3.187(8)$
Atoms: C37 C38 C39 C40 C41 C42 Rms deviation: 0.010 Å

Plane **8**: $4.914(12)x + 6.409(2)y - 7.202(12)z = 4.858(2)$
Atoms: C1 C7 C12 C13 C18 C2 Rms deviation: 0.117 Å

Plane **9**: $4.520(14)x - 4.213(4)y + 15.596(8)z = 1.805(5)$
Atoms: C3 C19 C24 C25 C30 C4 Rms deviation: 0.123 Å

Plane **10**: $13.945(10)x + 4.093(4)y - 11.137(11)z = 4.612(5)$
Atoms: C5 C31 C36 C37 C42 C6 Rms deviation: 0.121 Å

2. One measure of the distortion in hexabenzotriphenylene is found in the dihedral angles between the mean planes of the three peripheral "biphenylene" groups and that of the central ring. These data are listed below, along with the defining atoms of the "biphenylenes" and the rms deviations of these atoms from the corresponding mean plane.

Plane **B1**: $2.696(9)x + 6.812(1)y - 4.176(6)z = 5.129(1)$
Angle to central ring plane (plane **1**) = 28.70(5)°
Atoms: C7 C8 C9 C10 C11 C12 C13 C14 C15 C16 C17 C18
Rms deviation: 0.151 Å

Plane **B2**: $2.291(10)x - 3.434(3)y + 16.925(5)z = 0.496(3)$
Angle to central ring plane (plane **1**) = 30.18(6)°
Atoms: C19 C20 C21 C22 C23 C24 C25 C26 C27 C28 C29 C30
Rms deviation: 0.174 Å

Plane **B3**: $16.275(3)x + 3.303(3)y - 10.242(9)z = 4.681(5)$
Angle to central ring plane (plane **1**) = 29.95(6)°
Atoms: C31 C32 C33 C34 C35 C36 C37 C38 C39 C40 C41 C42
Rms deviation: 0.155 Å

3. Another measure of the distortion in hexabenzotriphenylene is the degree of twist in the three "naphthalene" subunits defined by the central ring and each of the three attached rings. The torsional angles defined by the ends of these "naphthalene" groups are listed below.

C1 - C2 - C13 - C12	-22.4(1)°
C3 - C4 - C25 - C24	-23.9(1)°
C5 - C6 - C37 - C36	-23.2(1)°

Table 1. Crystal data and structure refinement for $C_{42}H_{24}$.

Formula	$C_{42}H_{24}$
Formula weight	528.61
Temperature	298(2) K
Wavelength	0.71074 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 19.9721(5) Å α = 90°
	b = 7.0005(1) Å β = 104.013(1)°
	c = 19.5456(5) Å γ = 90°
Volume	2651.4(1) Å^3
Z	4
Density (calculated)	1.324 Mg/m^3
Absorption coefficient	0.075 mm^{-1}
F(000)	1104
Crystal size	0.28 mm × 0.25 mm × 0.04 mm
θ range for data collection	2.10° to 27.42°
Index ranges	$0 \le h \le 25$, $0 \le k \le 9$, $-25 \le l \le 24$
Reflections collected	45305
Independent reflections	6016
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6016 / 0 / 475
Goodness-of-fit on F^2	1.013
Final R indices [$I > 2\sigma(I)$]	$R1$ = 0.0512, $wR2$ = 0.1091
R indices (all data)	$R1$ = 0.1007, $wR2$ = 0.1327
Largest diff. peak and hole	0.157 and -0.179 e/Å^3

Table 2. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for $C_{42}H_{24}$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	1642(1)	8112(2)	1361(1)	36(1)
C(2)	1875(1)	6887(2)	902(1)	36(1)
C(3)	2553(1)	6082(2)	1113(1)	37(1)
C(4)	3028(1)	6867(2)	1689(1)	39(1)
C(5)	2786(1)	8091(2)	2163(1)	39(1)
C(6)	2131(1)	8904(2)	1955(1)	37(1)
C(7)	891(1)	8281(2)	1263(1)	38(1)
C(8)	597(1)	8673(3)	1834(1)	47(1)
C(9)	-105(1)	8615(3)	1759(1)	57(1)
C(10)	-541(1)	8175(3)	1113(1)	61(1)
C(11)	-270(1)	7744(3)	556(1)	56(1)
C(12)	444(1)	7764(2)	618(1)	43(1)
C(13)	739(1)	7218(2)	37(1)	43(1)
C(14)	354(1)	7214(3)	-664(1)	59(1)
C(15)	648(1)	6790(3)	-1207(1)	65(1)
C(16)	1341(1)	6380(3)	-1072(1)	55(1)
C(17)	1733(1)	6360(2)	-393(1)	44(1)
C(18)	1441(1)	6726(2)	179(1)	38(1)
C(19)	2758(1)	4298(2)	818(1)	41(1)
C(20)	2268(1)	2946(2)	487(1)	49(1)
C(21)	2460(1)	1207(3)	276(1)	60(1)
C(22)	3151(1)	734(3)	397(1)	71(1)
C(23)	3640(1)	1997(3)	731(1)	65(1)
C(24)	3459(1)	3804(3)	949(1)	48(1)
C(25)	3970(1)	5172(3)	1314(1)	48(1)
C(26)	4661(1)	5127(4)	1266(1)	64(1)
C(27)	5126(1)	6487(4)	1588(1)	73(1)
C(28)	4917(1)	7940(4)	1968(1)	67(1)
C(29)	4244(1)	8022(3)	2023(1)	53(1)
C(30)	3762(1)	6634(3)	1709(1)	44(1)
C(31)	3160(1)	8329(3)	2903(1)	43(1)
C(32)	3621(1)	6926(3)	3252(1)	52(1)
C(33)	3917(1)	7039(4)	3963(1)	63(1)
C(34)	3758(1)	8568(4)	4347(1)	66(1)
C(35)	3298(1)	9933(3)	4028(1)	60(1)
C(36)	2980(1)	9836(3)	3305(1)	47(1)
C(37)	2461(1)	11198(3)	2954(1)	48(1)
C(38)	2387(1)	13013(3)	3243(1)	65(1)
C(39)	1902(1)	14284(3)	2894(2)	72(1)
C(40)	1482(1)	13822(3)	2243(1)	64(1)
C(41)	1542(1)	12065(3)	1951(1)	51(1)
C(42)	2021(1)	10702(2)	2302(1)	43(1)

Table 3. Bond lengths [Å] for $C_{42}H_{24}$.

C(1)-C(2)	1.399(2)	C(19)-C(24)	1.404(2)
C(1)-C(6)	1.435(2)	C(20)-C(21)	1.370(3)
C(1)-C(7)	1.471(2)	C(21)-C(22)	1.381(3)
C(2)-C(3)	1.432(2)	C(22)-C(23)	1.362(3)
C(2)-C(18)	1.472(2)	C(23)-C(24)	1.410(3)
C(3)-C(4)	1.397(2)	C(24)-C(25)	1.454(3)
C(3)-C(19)	1.475(2)	C(25)-C(30)	1.403(2)
C(4)-C(5)	1.431(2)	C(25)-C(26)	1.407(3)
C(4)-C(30)	1.467(2)	C(26)-C(27)	1.372(3)
C(5)-C(6)	1.393(2)	C(27)-C(28)	1.382(3)
C(5)-C(31)	1.468(2)	C(28)-C(29)	1.375(3)
C(6)-C(42)	1.472(2)	C(29)-C(30)	1.401(3)
C(7)-C(12)	1.404(2)	C(31)-C(32)	1.405(3)
C(7)-C(8)	1.408(2)	C(31)-C(36)	1.413(2)
C(8)-C(9)	1.376(3)	C(32)-C(33)	1.374(3)
C(9)-C(10)	1.384(3)	C(33)-C(34)	1.388(3)
C(10)-C(11)	1.361(3)	C(34)-C(35)	1.367(3)
C(11)-C(12)	1.402(2)	C(35)-C(36)	1.403(3)
C(12)-C(13)	1.453(2)	C(36)-C(37)	1.452(3)
C(13)-C(14)	1.399(3)	C(37)-C(42)	1.406(2)
C(13)-C(18)	1.404(2)	C(37)-C(38)	1.412(3)
C(14)-C(15)	1.364(3)	C(38)-C(39)	1.369(3)
C(15)-C(16)	1.376(3)	C(39)-C(40)	1.381(3)
C(16)-C(17)	1.367(3)	C(40)-C(41)	1.374(3)
C(17)-C(18)	1.406(2)	C(41)-C(42)	1.406(2)
C(19)-C(20)	1.402(2)		

Table 4. Bond angles [°] for $C_{42}H_{24}$.

C(2)-C(1)-C(6)	119.3(1)	C(20)-C(19)-C(3)	121.5(2)
C(2)-C(1)-C(7)	116.9(1)	C(24)-C(19)-C(3)	119.8(2)
C(6)-C(1)-C(7)	123.1(1)	C(21)-C(20)-C(19)	121.6(2)
C(1)-C(2)-C(3)	119.6(1)	C(20)-C(21)-C(22)	120.2(2)
C(1)-C(2)-C(18)	116.9(1)	C(23)-C(22)-C(21)	119.8(2)
C(3)-C(2)-C(18)	122.9(1)	C(22)-C(23)-C(24)	121.4(2)
C(4)-C(3)-C(2)	119.2(1)	C(19)-C(24)-C(23)	118.8(2)
C(4)-C(3)-C(19)	116.7(1)	C(19)-C(24)-C(25)	118.5(2)
C(2)-C(3)-C(19)	123.6(1)	C(23)-C(24)-C(25)	122.6(2)
C(3)-C(4)-C(5)	119.2(1)	C(30)-C(25)-C(26)	118.7(2)
C(3)-C(4)-C(30)	117.2(1)	C(30)-C(25)-C(24)	118.9(2)
C(5)-C(4)-C(30)	122.8(2)	C(26)-C(25)-C(24)	122.3(2)
C(6)-C(5)-C(4)	119.7(1)	C(27)-C(26)-C(25)	121.2(2)
C(6)-C(5)-C(31)	117.4(1)	C(26)-C(27)-C(28)	120.0(2)
C(4)-C(5)-C(31)	122.4(1)	C(29)-C(28)-C(27)	120.0(2)
C(5)-C(6)-C(1)	119.0(1)	C(28)-C(29)-C(30)	121.2(2)
C(5)-C(6)-C(42)	116.7(1)	C(29)-C(30)-C(25)	118.9(2)
C(1)-C(6)-C(42)	123.7(1)	C(29)-C(30)-C(4)	120.7(2)
C(12)-C(7)-C(8)	117.8(2)	C(25)-C(30)-C(4)	119.6(2)
C(12)-C(7)-C(1)	120.2(2)	C(32)-C(31)-C(36)	118.5(2)
C(8)-C(7)-C(1)	121.4(2)	C(32)-C(31)-C(5)	121.1(2)
C(9)-C(8)-C(7)	121.3(2)	C(36)-C(31)-C(5)	119.7(2)
C(8)-C(9)-C(10)	120.2(2)	C(33)-C(32)-C(31)	121.4(2)
C(11)-C(10)-C(9)	119.7(2)	C(32)-C(33)-C(34)	119.6(2)
C(10)-C(11)-C(12)	121.4(2)	C(35)-C(34)-C(33)	120.5(2)
C(11)-C(12)-C(7)	119.5(2)	C(34)-C(35)-C(36)	121.1(2)
C(11)-C(12)-C(13)	121.8(2)	C(35)-C(36)-C(31)	118.8(2)
C(7)-C(12)-C(13)	118.7(2)	C(35)-C(36)-C(37)	122.8(2)
C(14)-C(13)-C(18)	118.7(2)	C(31)-C(36)-C(37)	118.4(2)
C(14)-C(13)-C(12)	122.4(2)	C(42)-C(37)-C(38)	118.8(2)
C(18)-C(13)-C(12)	118.9(2)	C(42)-C(37)-C(36)	119.0(2)
C(15)-C(14)-C(13)	121.6(2)	C(38)-C(37)-C(36)	122.3(2)
C(14)-C(15)-C(16)	119.9(2)	C(39)-C(38)-C(37)	121.1(2)
C(17)-C(16)-C(15)	120.2(2)	C(38)-C(39)-C(40)	120.3(2)
C(16)-C(17)-C(18)	121.3(2)	C(41)-C(40)-C(39)	119.8(2)
C(13)-C(18)-C(17)	118.3(2)	C(40)-C(41)-C(42)	121.5(2)
C(13)-C(18)-C(2)	120.0(2)	C(37)-C(42)-C(41)	118.5(2)
C(17)-C(18)-C(2)	121.0(2)	C(37)-C(42)-C(6)	119.9(2)
C(20)-C(19)-C(24)	118.2(2)	C(41)-C(42)-C(6)	121.0(2)

Table 5. Bond lengths [Å] involving H atoms for $C_{42}H_{24}$.

C(8)-H(8)	0.99(2)	C(26)-H(26)	1.00(2)
C(9)-H(9)	0.99(2)	C(27)-H(27)	0.96(2)
C(10)-H(10)	1.00(2)	C(28)-H(28)	0.98(2)
C(11)-H(11)	1.02(2)	C(29)-H(29)	0.97(2)
C(14)-H(14)	0.98(2)	C(32)-H(32)	0.98(2)
C(15)-H(15)	1.01(2)	C(33)-H(33)	1.01(2)
C(16)-H(16)	1.00(2)	C(34)-H(34)	0.97(2)
C(17)-H(17)	0.97(2)	C(35)-H(35)	1.01(2)
C(20)-H(20)	0.99(2)	C(38)-H(38)	0.98(2)
C(21)-H(21)	0.99(2)	C(39)-H(39)	1.02(2)
C(22)-H(22)	0.97(2)	C(40)-H(40)	1.03(2)
C(23)-H(23)	0.97(2)	C(41)-H(41)	1.01(2)

Table 6. Bond angles [°] involving H atoms for $C_{42}H_{24}$.

C(9)-C(8)-H(8)	120.7(10)	C(27)-C(26)-H(26)	118.4(12)
C(7)-C(8)-H(8)	118.0(10)	C(25)-C(26)-H(26)	120.4(12)
C(8)-C(9)-H(9)	115.7(11)	C(26)-C(27)-H(27)	118.3(13)
C(10)-C(9)-H(9)	124.0(11)	C(28)-C(27)-H(27)	121.7(14)
C(11)-C(10)-H(10)	120.3(12)	C(29)-C(28)-H(28)	119.2(12)
C(9)-C(10)-H(10)	120.0(12)	C(27)-C(28)-H(28)	120.7(12)
C(10)-C(11)-H(11)	118.9(11)	C(28)-C(29)-H(29)	119.4(11)
C(12)-C(11)-H(11)	119.7(11)	C(30)-C(29)-H(29)	119.3(11)
C(15)-C(14)-H(14)	123.1(12)	C(33)-C(32)-H(32)	120.1(11)
C(13)-C(14)-H(14)	115.3(12)	C(31)-C(32)-H(32)	118.4(11)
C(14)-C(15)-H(15)	119.5(13)	C(32)-C(33)-H(33)	118.2(12)
C(16)-C(15)-H(15)	120.6(13)	C(34)-C(33)-H(33)	122.2(12)
C(17)-C(16)-H(16)	118.9(11)	C(35)-C(34)-H(34)	119.4(13)
C(15)-C(16)-H(16)	120.9(11)	C(33)-C(34)-H(34)	120.1(13)
C(16)-C(17)-H(17)	118.7(10)	C(34)-C(35)-H(35)	119.9(12)
C(18)-C(17)-H(17)	119.9(10)	C(36)-C(35)-H(35)	118.9(12)
C(21)-C(20)-H(20)	119.3(10)	C(39)-C(38)-H(38)	122.5(13)
C(19)-C(20)-H(20)	119.0(10)	C(37)-C(38)-H(38)	116.4(13)
C(20)-C(21)-H(21)	118.2(11)	C(38)-C(39)-H(39)	119.1(13)
C(22)-C(21)-H(21)	121.6(11)	C(40)-C(39)-H(39)	120.5(13)
C(23)-C(22)-H(22)	120.0(13)	C(41)-C(40)-H(40)	120.6(13)
C(21)-C(22)-H(22)	120.1(13)	C(39)-C(40)-H(40)	119.5(12)
C(22)-C(23)-H(23)	123.0(12)	C(40)-C(41)-H(41)	120.0(11)
C(24)-C(23)-H(23)	115.6(12)	C(42)-C(41)-H(41)	118.4(11)

Table 7. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $C_{42}H_{24}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	36(1)	38(1)	34(1)	5(1)	11(1)	3(1)
C(2)	35(1)	37(1)	37(1)	2(1)	12(1)	-1(1)
C(3)	36(1)	41(1)	35(1)	1(1)	12(1)	3(1)
C(4)	36(1)	45(1)	36(1)	1(1)	10(1)	3(1)
C(5)	36(1)	46(1)	36(1)	-2(1)	12(1)	-2(1)
C(6)	37(1)	41(1)	36(1)	-1(1)	14(1)	1(1)
C(7)	36(1)	39(1)	40(1)	6(1)	10(1)	5(1)
C(8)	43(1)	58(1)	42(1)	4(1)	13(1)	6(1)
C(9)	48(1)	71(1)	57(1)	7(1)	24(1)	9(1)
C(10)	35(1)	73(1)	75(2)	0(1)	14(1)	3(1)
C(11)	38(1)	64(1)	63(1)	-9(1)	6(1)	2(1)
C(12)	38(1)	41(1)	47(1)	1(1)	8(1)	5(1)
C(13)	42(1)	42(1)	43(1)	-1(1)	4(1)	3(1)
C(14)	52(1)	68(1)	50(1)	-7(1)	-1(1)	14(1)
C(15)	77(2)	72(1)	39(1)	-7(1)	-1(1)	17(1)
C(16)	69(1)	55(1)	40(1)	-2(1)	13(1)	9(1)
C(17)	48(1)	45(1)	41(1)	1(1)	13(1)	1(1)
C(18)	42(1)	36(1)	36(1)	-2(1)	7(1)	-1(1)
C(19)	51(1)	42(1)	33(1)	4(1)	15(1)	8(1)
C(20)	62(1)	41(1)	47(1)	1(1)	18(1)	0(1)
C(21)	86(2)	42(1)	56(1)	-2(1)	24(1)	-1(1)
C(22)	108(2)	44(1)	68(2)	-1(1)	35(1)	20(1)
C(23)	76(2)	63(1)	61(1)	6(1)	23(1)	31(1)
C(24)	55(1)	53(1)	37(1)	5(1)	15(1)	18(1)
C(25)	42(1)	66(1)	37(1)	6(1)	11(1)	18(1)
C(26)	47(1)	94(2)	51(1)	2(1)	16(1)	23(1)
C(27)	36(1)	124(2)	60(1)	5(1)	15(1)	12(1)
C(28)	42(1)	102(2)	59(1)	-4(1)	15(1)	-7(1)
C(29)	39(1)	76(1)	45(1)	-2(1)	12(1)	-1(1)
C(30)	37(1)	60(1)	36(1)	4(1)	10(1)	6(1)
C(31)	34(1)	60(1)	37(1)	-4(1)	11(1)	-8(1)
C(32)	40(1)	73(1)	42(1)	2(1)	9(1)	-2(1)
C(33)	48(1)	93(2)	45(1)	9(1)	7(1)	-6(1)
C(34)	57(1)	105(2)	36(1)	-6(1)	10(1)	-22(1)
C(35)	54(1)	85(2)	44(1)	-17(1)	19(1)	-20(1)
C(36)	43(1)	62(1)	40(1)	-12(1)	18(1)	-17(1)
C(37)	50(1)	51(1)	50(1)	-12(1)	28(1)	-12(1)
C(38)	74(2)	63(1)	66(2)	-23(1)	34(1)	-20(1)
C(39)	91(2)	47(1)	94(2)	-16(1)	53(2)	-6(1)
C(40)	77(2)	44(1)	83(2)	5(1)	46(1)	4(1)
C(41)	58(1)	44(1)	59(1)	4(1)	29(1)	5(1)
C(42)	45(1)	45(1)	45(1)	-5(1)	24(1)	-4(1)

Table 8. Hydrogen coordinates (× 10^4) and isotropic displacement parameters (Å^2 × 10^3) for $C_{42}H_{24}$.

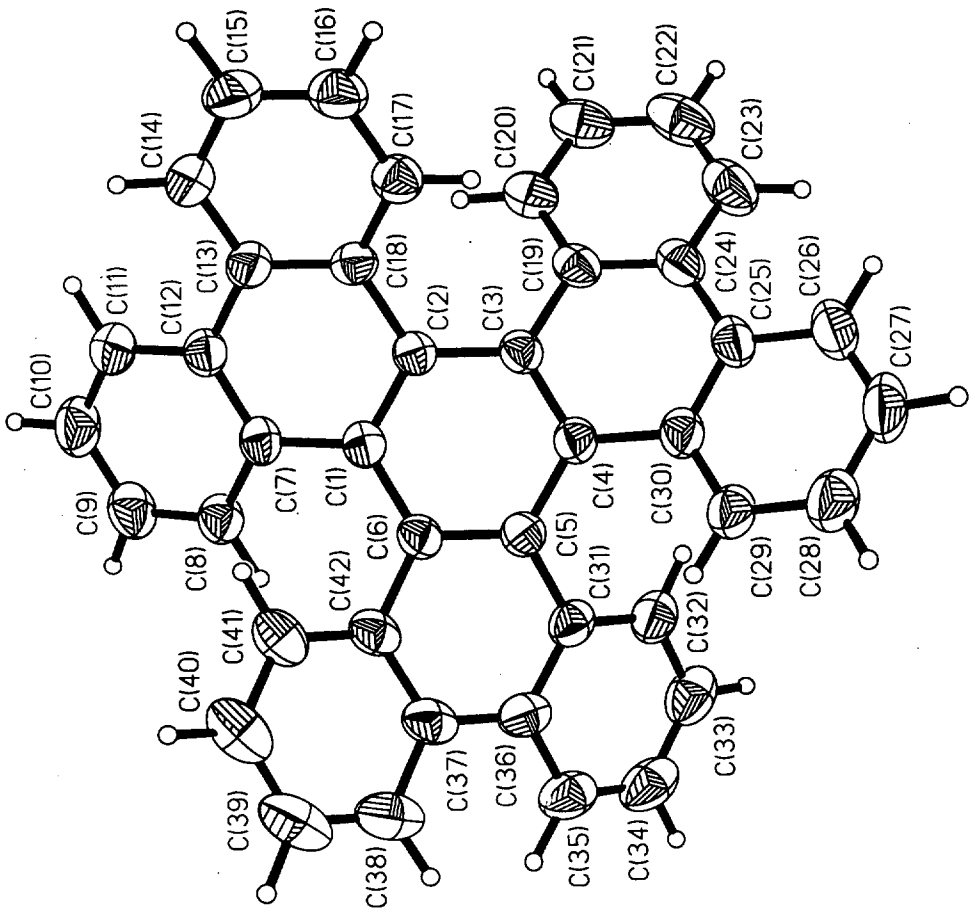
	x	*y*	*z*	*U*(eq)
H(8)	913(9)	8982(23)	2296(10)	47(5)
H(9)	-265(10)	8888(28)	2190(11)	68(6)
H(10)	-1051(11)	8143(28)	1060(11)	74(6)
H(11)	-597(10)	7377(26)	87(11)	64(6)
H(14)	-139(10)	7521(26)	-733(10)	62(6)
H(15)	354(12)	6789(32)	-1705(13)	91(7)
H(16)	1569(10)	6111(28)	-1466(11)	69(6)
H(17)	2228(9)	6166(23)	-312(9)	46(5)
H(20)	1770(9)	3227(24)	432(9)	50(5)
H(21)	2094(10)	306(28)	47(10)	61(6)
H(22)	3286(11)	-484(35)	242(12)	85(7)
H(23)	4133(11)	1716(29)	842(11)	72(6)
H(26)	4821(11)	4115(32)	984(11)	79(7)
H(27)	5589(12)	6416(31)	1530(12)	87(7)
H(28)	5240(11)	8959(30)	2182(11)	72(6)
H(29)	4094(9)	9104(27)	2256(10)	59(6)
H(32)	3716(9)	5823(27)	2979(10)	58(6)
H(33)	4234(10)	5967(29)	4191(11)	72(6)
H(34)	3980(10)	8688(29)	4846(12)	75(6)
H(35)	3163(11)	10996(32)	4319(12)	84(7)
H(38)	2701(11)	13305(30)	3697(12)	76(7)
H(39)	1868(11)	15587(36)	3111(12)	92(7)
H(40)	1147(11)	14826(31)	1970(12)	82(7)
H(41)	1254(9)	11749(27)	1464(11)	62(6)

Table 9. Torsion angles [°] for $C_{42}H_{24}$.

C6	C1	C2	C3	14.8(2)	C3	C19	C20	C21	-173.3(2)
C7	C1	C2	C3	-156.14(14)	C19	C20	C21	C22	1.1(3)
C6	C1	C2	C18	-156.26(14)	C20	C21	C22	C23	0.4(3)
C7	C1	C2	C18	32.8(2)	C21	C22	C23	C24	-0.9(3)
C1	C2	C3	C4	-15.3(2)	C20	C19	C24	C23	1.4(3)
C18	C2	C3	C4	155.22(15)	C3	C19	C24	C23	172.9(2)
C1	C2	C3	C19	156.39(15)	C20	C19	C24	C25	-177.8(2)
C18	C2	C3	C19	-33.1(2)	C3	C19	C24	C25	-6.3(2)
C2	C3	C4	C5	16.4(2)	C22	C23	C24	C19	0.1(3)
C19	C3	C4	C5	-155.86(15)	C22	C23	C24	C25	179.2(2)
C2	C3	C4	C30	-154.05(15)	C19	C24	C25	C30	19.5(2)
C19	C3	C4	C30	33.7(2)	C23	C24	C25	C30	-159.7(2)
C3	C4	C5	C6	-17.6(2)	C19	C24	C25	C26	-158.1(2)
C30	C4	C5	C6	152.3(2)	C23	C24	C25	C26	22.7(3)
C3	C4	C5	C31	153.8(2)	C30	C25	C26	C27	-0.7(3)
C30	C4	C5	C31	-36.3(2)	C24	C25	C26	C27	176.9(2)
C4	C5	C6	C1	17.0(2)	C25	C26	C27	C28	-0.3(3)
C31	C5	C6	C1	-154.74(15)	C26	C27	C28	C29	0.1(4)
C4	C5	C6	C42	-154.57(15)	C27	C28	C29	C30	0.9(3)
C31	C5	C6	C42	33.7(2)	C28	C29	C30	C25	-1.9(3)
C2	C1	C6	C5	-15.8(2)	C28	C29	C30	C4	-171.7(2)
C7	C1	C6	C5	154.56(15)	C26	C25	C30	C29	1.7(3)
C2	C1	C6	C42	155.17(15)	C24	C25	C30	C29	-175.9(2)
C7	C1	C6	C42	-34.5(2)	C26	C25	C30	C4	171.7(2)
C2	C1	C7	C12	-20.2(2)	C24	C25	C30	C4	-6.0(2)
C6	C1	C7	C12	169.19(15)	C3	C4	C30	C29	148.7(2)
C2	C1	C7	C8	149.9(2)	C5	C4	C30	C29	-21.4(3)
C6	C1	C7	C8	-20.6(2)	C3	C4	C30	C25	-21.1(2)
C12	C7	C8	C9	-2.1(3)	C5	C4	C30	C25	168.9(2)
C1	C7	C8	C9	-172.5(2)	C6	C5	C31	C32	148.6(2)
C7	C8	C9	C10	-0.4(3)	C4	C5	C31	C32	-23.0(2)
C8	C9	C10	C11	2.0(3)	C6	C5	C31	C36	-21.7(2)
C9	C10	C11	C12	-1.1(3)	C4	C5	C31	C36	166.8(2)
C10	C11	C12	C7	-1.4(3)	C36	C31	C32	C33	-2.6(3)
C10	C11	C12	C13	177.0(2)	C5	C31	C32	C33	-172.9(2)
C8	C7	C12	C11	2.9(2)	C31	C32	C33	C34	0.0(3)
C1	C7	C12	C11	173.4(2)	C32	C33	C34	C35	1.6(3)
C8	C7	C12	C13	-175.6(2)	C33	C34	C35	C36	-0.5(3)
C1	C7	C12	C13	-5.0(2)	C34	C35	C36	C31	-2.1(3)
C11	C12	C13	C14	20.3(3)	C34	C35	C36	C37	176.6(2)
C7	C12	C13	C14	-161.3(2)	C32	C31	C36	C35	3.6(2)
C11	C12	C13	C18	-161.5(2)	C5	C31	C36	C35	174.1(2)
C7	C12	C13	C18	16.9(2)	C32	C31	C36	C37	-175.1(2)
C18	C13	C14	C15	-1.6(3)	C5	C31	C36	C37	-4.6(2)
C12	C13	C14	C15	176.6(2)	C35	C36	C37	C42	-160.7(2)
C13	C14	C15	C16	-0.9(3)	C31	C36	C37	C42	18.0(2)
C14	C15	C16	C17	1.3(3)	C35	C36	C37	C38	19.9(3)
C15	C16	C17	C18	0.9(3)	C31	C36	C37	C38	-161.5(2)
C14	C13	C18	C17	3.7(2)	C42	C37	C38	C39	-0.8(3)
C12	C13	C18	C17	-174.6(2)	C36	C37	C38	C39	178.7(2)
C14	C13	C18	C2	174.4(2)	C37	C38	C39	C40	-1.2(3)
C12	C13	C18	C2	-3.9(2)	C38	C39	C40	C41	1.4(3)
C16	C17	C18	C13	-3.4(3)	C39	C40	C41	C42	0.4(3)
C16	C17	C18	C2	-174.0(2)	C38	C37	C42	C41	2.5(2)
C1	C2	C18	C13	-21.4(2)	C36	C37	C42	C41	-177.0(2)
C3	C2	C18	C13	167.87(15)	C38	C37	C42	C6	173.8(2)
C1	C2	C18	C17	149.0(2)	C36	C37	C42	C6	-5.7(2)
C3	C2	C18	C17	-21.7(2)	C40	C41	C42	C37	-2.3(3)
C4	C3	C19	C20	150.7(2)	C40	C41	C42	C6	-173.6(2)
C2	C3	C19	C20	-21.1(2)	C5	C6	C42	C37	-20.5(2)
C4	C3	C19	C24	-20.5(2)	C1	C6	C42	C37	168.3(2)
C2	C3	C19	C24	167.6(2)	C5	C6	C42	C41	150.6(2)
C24	C19	C20	C21	-2.0(3)	C1	C6	C42	C41	-20.5(2)

Figures

1. Molecular structure of hexabenzotriphenylene drawn with 50% probability thermal ellipsoids for carbon atoms and spheres of arbitrary size for hydrogen atoms.
2. Molecular structure drawn with 50% probability thermal ellipsoids for all atoms.
3. "Side" view of the molecular structure (nonhydrogen atoms only) drawn with with 50% probability thermal ellipsoids.
4. Stereo "side" view of the molecular structure (nonhydrogen atoms) drawn with with 50% probability thermal ellipsoids.
5. Ball-and-stick drawing of the central triphenylene substructure.
6. Space-filling drawings ("top" and "side" views) of the molecular structure.
7. Unit cell viewed down the *b* axis.
8. Stereo view of the unit cell viewed down the *b* axis.
9. Crystal packing viewed down the *b* axis.
10. Interdigitated layers of hexabenzotriphenylene parallel to the *b* axis.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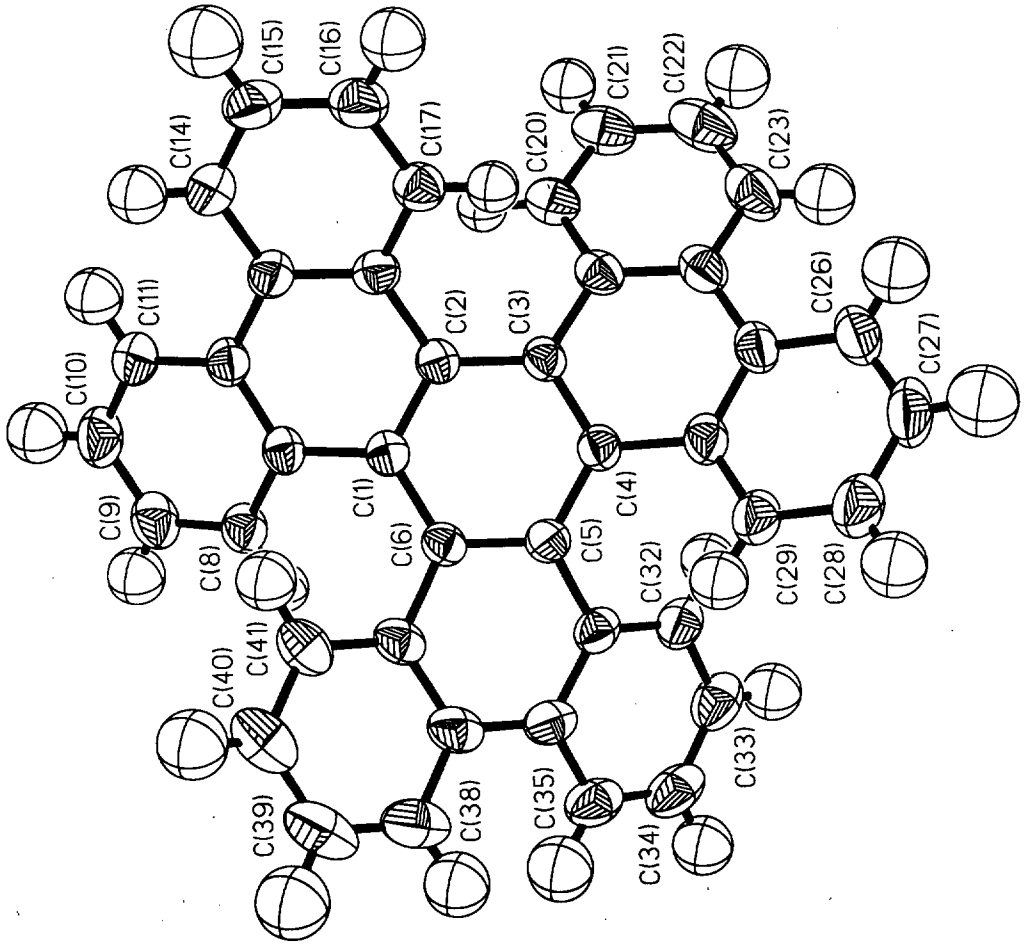
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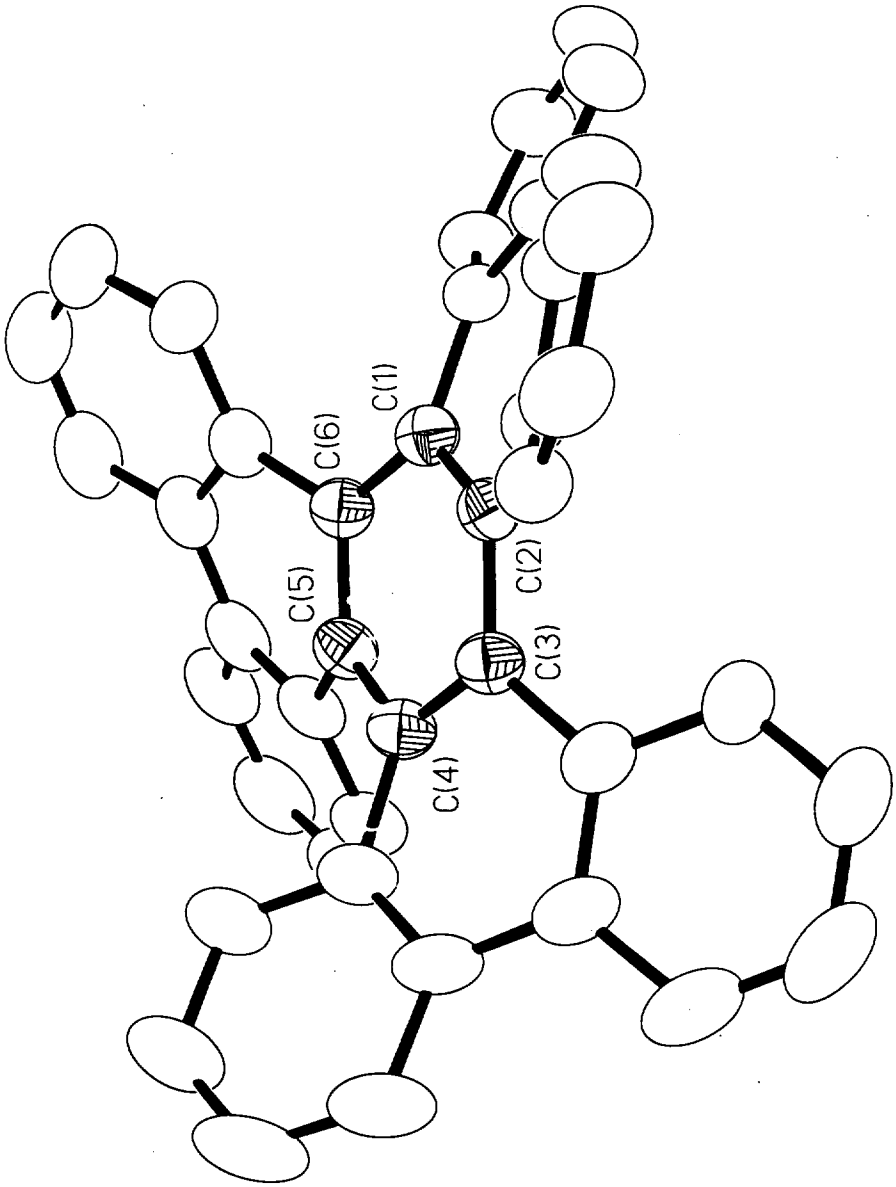
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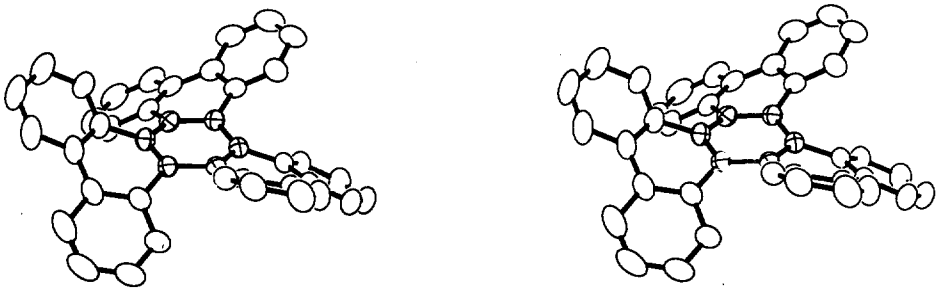

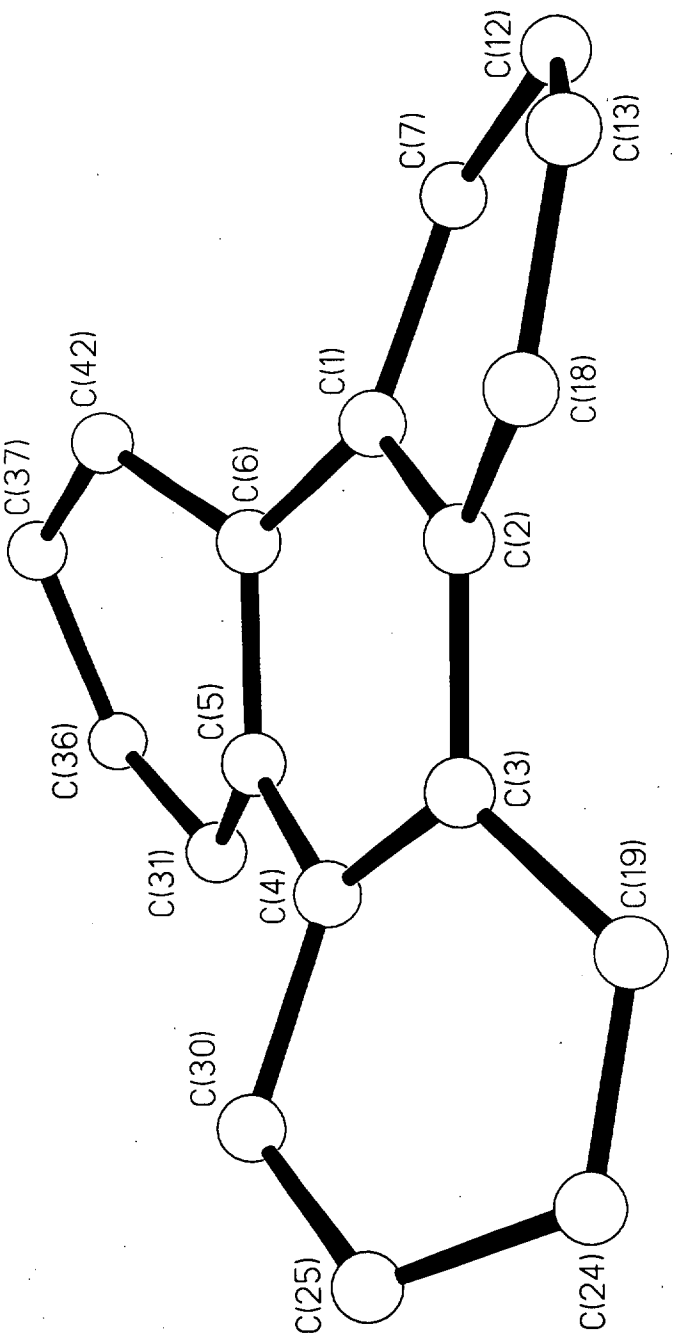
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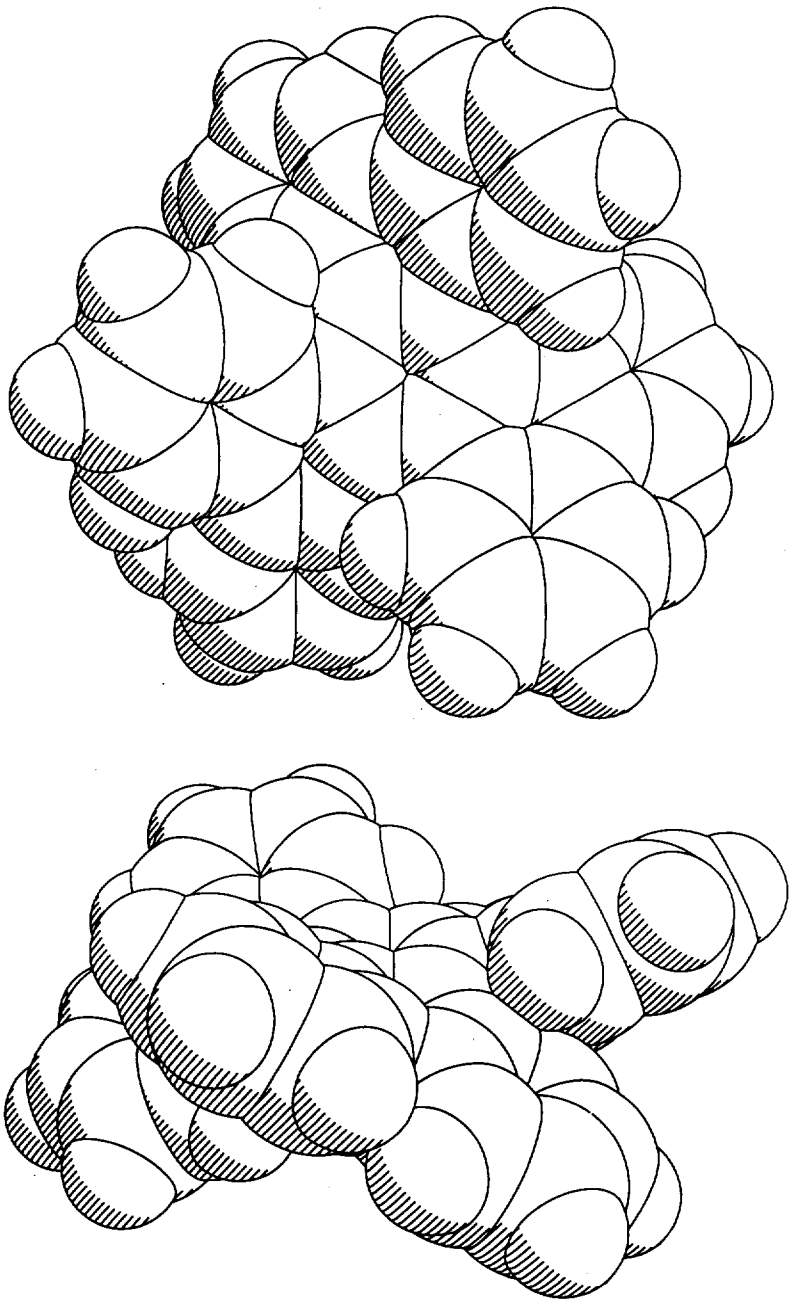

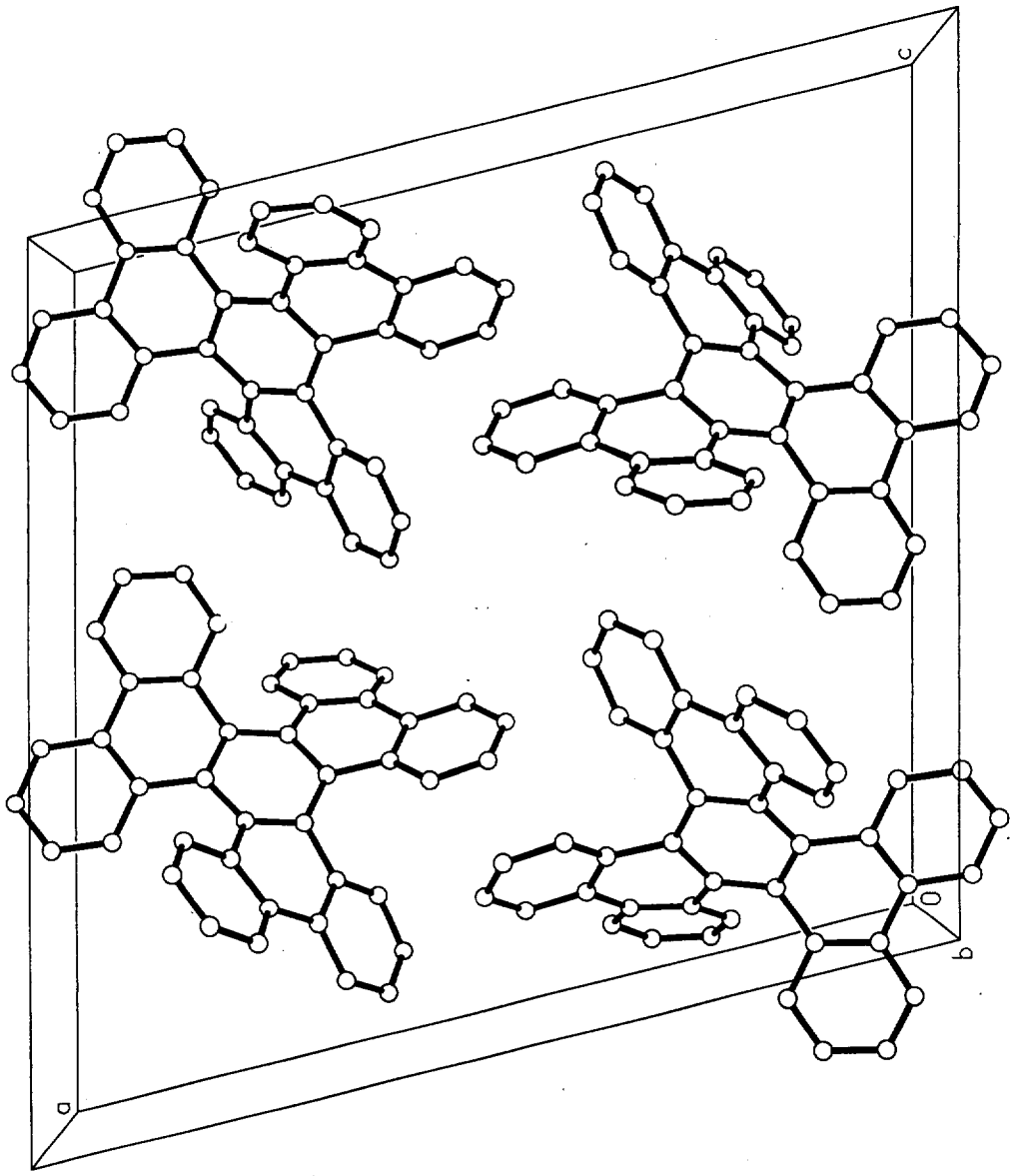
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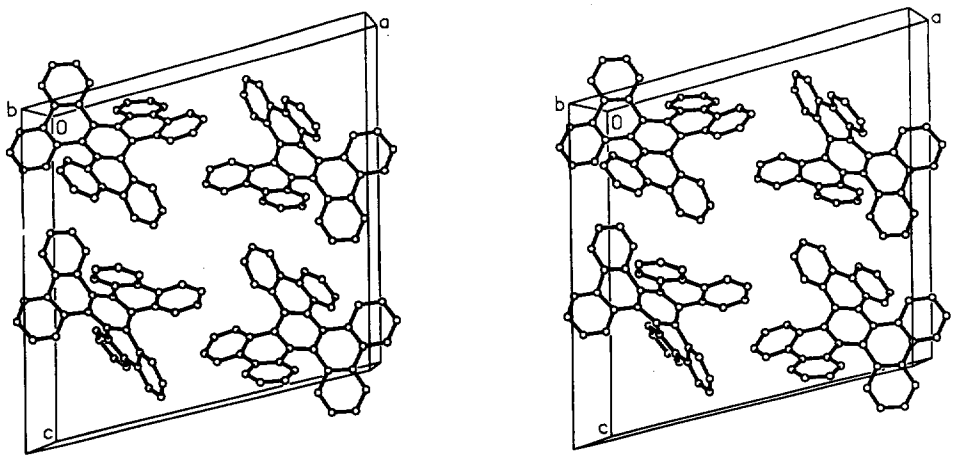
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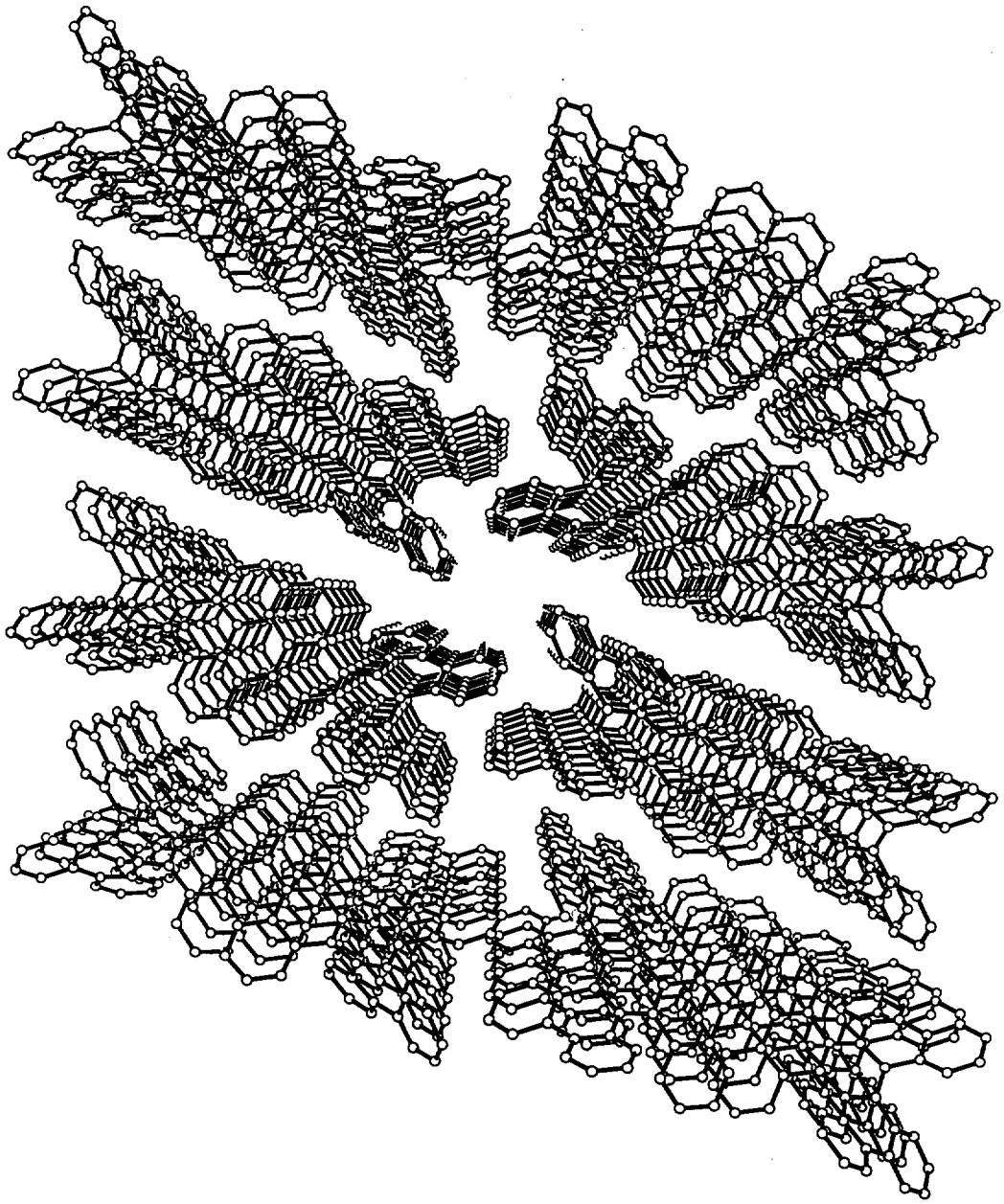
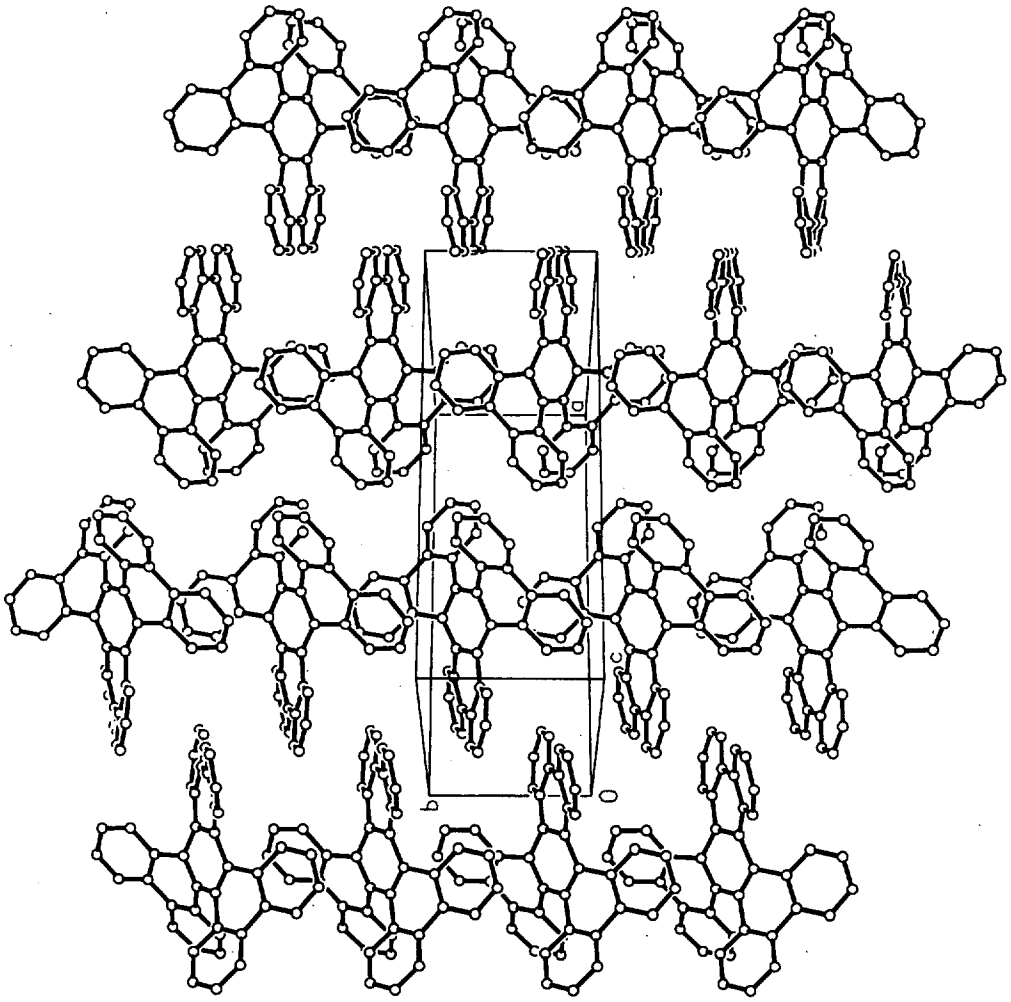


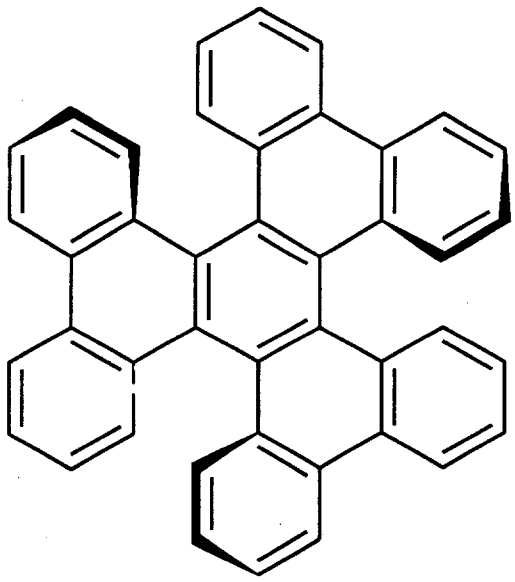


Single Crystal X-ray Structure Report RAP008

Hexabenzotriphenylene

(Dibenzo[*f,j*]phenanthro[9,10-*s*]picene, $C_{42}H_{24}$)

Low Temperature Determination (110 K)



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Experimental

Hexabenzotriphenylene, prepared by chemical synthesis, was crystallized by the slow cooling of a solution in nitrobenzene. An orange plate, 0.04 mm × 0.25 mm × 0.28 mm, was mounted on a glass fiber and transferred to a Nonius KappaCCD diffractometer, where Mo Kα radiation (λ = 0.71074 Å) was employed for data collection at 110 K.[1] Fourteen crystal settings were used for the measurements, which employed 2° oscillations, and a total of 1300° of data were collected. A total of 57,890 reflections (θ_{max} = 27.5°) were indexed, integrated, and corrected for Lorentz and polarization effects (but not for absorption) by using the program DENZO-SMN,[2] and then were merged to 6453 reflections (R_{int} = 0.102) by using the program SCALEPACK.[2] Postrefinement of the unit cell parameters gave a = 19.8971(8) Å, b = 6.9274(2) Å, c = 19.4153(8) Å, β = 103.846(1)°, and V = 2598.3(2) Å^3. Systematic absences were consistent with the monoclinic space group $P2_1/c$ (No. 14), so 501 extinctions were discarded to give 5952 unique reflections in the final data set.

The structure was solved by direct methods by using Siemens SHELXTL.[3] All atomic coordinates were refined; carbon atoms were refined anisotropically, and hydrogens isotropically (SHELXTL). The final weighting scheme was $w = 1/[\sigma^2(F_o)^2 + (0.0901P)^2 + 0.1060P]$ where $P = (F_o^2 + 2F_c^2)/3$. The refinement converged to $R(F)$ = 0.0563, $wR(F^2)$ = 0.1417, and S = 1.176 for 3809 reflections with $I > 2\sigma(I)$, and $R(F)$ = 0.0962, $wR(F^2)$ = 0.1621, and S = 1.054 for 5952 unique reflections, 475 parameters, and 0 restraints.[4] The maximum Δ/σ in the final cycle of least squares was less than

0.001, and the residual peaks on the final $\Delta\rho$ map ranged from -0.284 to 0.268 $e/Å^3$. Scattering factors were taken from the *International Tables for Crystallography, Vol. C.*[5,6]

References and Notes

[1] *COLLECT* Data Collection Software. Nonius Company, Bohemia, New York, USA, 1998.

[2] Otwinowski, Z.; Minor, W., "Processing of X-ray Diffraction Data Collected in Oscillation Mode", *Methods Enzymol.* **1997**, *276*, 307-326.

[3] Sheldrick, G. M. *SHELXTL* Version 5. Siemens Analytical X-ray Instruments, Madison, Wisconsin, USA, 1996.

[4] $R(F) = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$,
$wR(F^2) = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$, and
S = goodness-of-fit on $F^2 = [\Sigma w(F_o^2 - F_c^2)^2 / (n - p)]^{1/2}$, where n is the number of reflections and p is the number of parameters refined.

[5] Maslen, E. N.; Fox, A. G.; O'Keefe, M. A., Chapter 6 in *International Tables for Crystallography: Mathematical, Physical and Chemical Tables*, Vol. C; Wilson, A. J. C., Ed.; Kluwer, Dordrecht, The Netherlands, 1992; pp 476-516.

[6] Creagh, D. C.; McAuley, W. J., Chapter 4 in *International Tables for Crystallography: Mathematical, Physical and Chemical Tables*, Vol. C; Wilson, A. J. C., Ed.; Kluwer, Dordrecht, The Netherlands, 1992; pp 206-222.

Miscellaneous Data

1. The "aromatic" rings of hexabenzotriphenylene (the central ring and the six peripheral benzo groups) are much less distorted from planarity than the remaining three "non-aromatic" rings. The equations for the least-squares planes of the seven "aromatic" rings (rings **1-7**), the defining atoms, and the rms deviations of the fitted atoms are listed below, as well as the same data for the three "non-aromatic" rings (**8-10**).

Plane **1**: $8.354(14)x + 5.117(4)y - 11.893(11)z = 3.977(4)$
Atoms: C1 C2 C3 C4 C5 C6 Rms deviation: 0.058 Å

Plane **2**: $0.150(15)x + 6.672(1)y - 5.104(15)z = 4.904(3)$
Atoms: C7 C8 C9 C10 C11 C12 Rms deviation: 0.011 Å

Plane **3**: $4.780(15)x + 6.700(1)y - 2.684(15)z = 5.156(1)$
Atoms: C13 C14 C15 C16 C17 C18 Rms deviation: 0.014 Å

Plane **4**: $5.165(16)x - 2.660(5)y + 17.911(6)z = 1.099(5)$
Atoms: C19 C20 C21 C22 C23 C24 Rms deviation: 0.005 Å

Plane **5**: $0.829(17)x - 3.861(5)y + 15.439(10)z = 0.376(8)$
Atoms: C25 C26 C27 C28 C29 C30 Rms deviation: 0.007 Å

Plane **6**: $16.421(9)x + 3.663(5)y - 7.571(14)z = 6.023(7)$
Atoms: C31 C32 C33 C34 C35 C36 Rms deviation: 0.013 Å

Plane **7**: $16.027(10)x + 2.610(5)y - 12.366(13)z = 3.216(8)$
Atoms: C37 C38 C39 C40 C41 C42 Rms deviation: 0.010 Å

Plane **8**: $4.963(14)x + 6.314(2)y - 7.326(13)z = 4.794(2)$
Atoms: C1 C7 C12 C13 C18 C2 Rms deviation: 0.116 Å

Plane **9**: $4.506(15)x - 4.154(4)y + 15.522(9)z = 1.778(6)$
Atoms: C3 C19 C24 C25 C30 C4 Rms deviation: 0.121 Å

Plane **10**: $13.929(11)x + 4.023(4)y - 11.088(12)z = 4.570(6)$
Atoms: C5 C31 C36 C37 C42 C6 Rms deviation: 0.121 Å

2. One measure of the distortion in hexabenzotriphenylene is found in the dihedral angles between the mean planes of the three peripheral "biphenylene" groups and that of the central ring. These data are listed below, along with the defining atoms of the "biphenylenes" and the rms deviations of these atoms from the corresponding mean plane.

Plane **B1**: $2.767(9)x + 6.724(1)y - 4.347(6)z = 5.065(1)$
Angle to central ring plane (plane **1**) = 28.49(6)°
Atoms: C7 C8 C9 C10 C11 C12 C13 C14 C15 C16 C17 C18
Rms deviation: 0.150 Å

Plane **B2**: $2.361(11)x - 3.377(3)y + 16.859(5)z = 0.499(3)$
Angle to central ring plane (plane **1**) = 29.99(7)°
Atoms: C19 C20 C21 C22 C23 C24 C25 C26 C27 C28 C29 C30
Rms deviation: 0.174 Å

Plane **B3**: $16.199(3)x + 3.258(3)y - 10.202(10)z = 4.636(6)$
Angle to central ring plane (plane **1**) = 29.68(7)°
Atoms: C31 C32 C33 C34 C35 C36 C37 C38 C39 C40 C41 C42
Rms deviation: 0.150 Å

3. Another measure of the distortion in hexabenzotriphenylene is the degree of twist in the three "naphthalene" subunits defined by the central ring and each of the three attached rings. The torsional angles defined by the ends of these "naphthalene" groups are listed below.

C1 - C2 - C13 - C12	-22.1(1)°
C3 - C4 - C25 - C24	-23.6(1)°
C5 - C6 - C37 - C36	-23.1(1)°

4. The nonbonded distances between the most strongly interacting carbons on adjacent "wings" of the structure are listed below.

C8 - C41	2.992(3) Å
C17 - C20	2.966(3) Å
C29 - C32	3.060(3) Å

Table 1. Crystal data and structure refinement for $C_{42}H_{24}$ (LT).

Formula	$C_{42}H_{24}$
Formula weight	528.61
Temperature	110(2) K
Wavelength	0.71074 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 19.8971(8) Å α = 90°
	b = 6.9274(2) Å β = 103.846(1)°
	c = 19.4153(8) Å γ = 90°
Volume	2598.3(2) Å^3
Z	4
Density (calculated)	1.351 Mg/m^3
Absorption coefficient	0.077 mm^{-1}
F(000)	1104
Crystal size	0.28 mm × 0.25 mm × 0.04 mm
θ range for data collection	1.05° to 27.50°
Index ranges	$-25 \le h \le 25$, $-9 \le k \le 0$, $0 \le l \le 25$
Reflections collected	57890
Independent reflections	5952
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	5952 / 0 / 475
Goodness-of-fit on F^2	1.054
Final R indices [$I > 2\sigma(I)$]	$R1$ = 0.0563, $wR2$ = 0.1417
R indices (all data)	$R1$ = 0.0962, $wR2$ = 0.1621
Largest diff. peak and hole	0.268 and -0.284 e/Å^3

Table 2. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for $C_{42}H_{24}$ (LT). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	*U*(eq)
C(1)	1634(1)	8137(2)	1348(1)	22(1)
C(2)	1872(1)	6881(2)	889(1)	22(1)
C(3)	2553(1)	6070(3)	1108(1)	22(1)
C(4)	3023(1)	6872(3)	1682(1)	23(1)
C(5)	2781(1)	8122(3)	2159(1)	23(1)
C(6)	2122(1)	8944(3)	1945(1)	23(1)
C(7)	880(1)	8310(2)	1248(1)	23(1)
C(8)	585(1)	8726(3)	1821(1)	26(1)
C(9)	-123(1)	8673(3)	1747(1)	29(1)
C(10)	-564(1)	8221(3)	1096(1)	31(1)
C(11)	-286(1)	7767(3)	535(1)	29(1)
C(12)	434(1)	7776(3)	598(1)	25(1)
C(13)	734(1)	7196(2)	15(1)	25(1)
C(14)	343(1)	7187(3)	-689(1)	31(1)
C(15)	640(1)	6718(3)	-1238(1)	32(1)
C(16)	1342(1)	6310(3)	-1096(1)	29(1)
C(17)	1734(1)	6313(3)	-410(1)	25(1)
C(18)	1438(1)	6705(2)	164(1)	23(1)
C(19)	2765(1)	4265(3)	813(1)	24(1)
C(20)	2272(1)	2907(3)	477(1)	26(1)
C(21)	2468(1)	1134(3)	267(1)	32(1)
C(22)	3168(1)	656(3)	394(1)	35(1)
C(23)	3656(1)	1949(3)	734(1)	32(1)
C(24)	3468(1)	3781(3)	948(1)	27(1)
C(25)	3981(1)	5156(3)	1314(1)	27(1)
C(26)	4674(1)	5108(3)	1272(1)	33(1)
C(27)	5140(1)	6491(3)	1592(1)	35(1)
C(28)	4924(1)	7979(3)	1975(1)	33(1)
C(29)	4248(1)	8058(3)	2026(1)	28(1)
C(30)	3763(1)	6644(3)	1711(1)	25(1)
C(31)	3151(1)	8377(3)	2904(1)	25(1)
C(32)	3614(1)	6962(3)	3261(1)	27(1)
C(33)	3912(1)	7094(3)	3972(1)	32(1)
C(34)	3755(1)	8658(3)	4361(1)	32(1)
C(35)	3290(1)	10031(3)	4032(1)	30(1)
C(36)	2970(1)	9911(3)	3305(1)	26(1)
C(37)	2449(1)	11282(3)	2946(1)	27(1)
C(38)	2373(1)	13105(3)	3237(1)	32(1)
C(39)	1884(1)	14400(3)	2889(1)	35(1)
C(40)	1465(1)	13912(3)	2230(1)	33(1)
C(41)	1530(1)	12131(3)	1934(1)	27(1)
C(42)	2011(1)	10765(3)	2290(1)	24(1)

Table 3. Bond lengths [Å] for $C_{42}H_{24}$ (LT).

C(1)-C(2)	1.406(3)	C(19)-C(24)	1.400(3)
C(1)-C(6)	1.435(3)	C(20)-C(21)	1.380(3)
C(1)-C(7)	1.471(3)	C(21)-C(22)	1.396(3)
C(2)-C(3)	1.434(3)	C(22)-C(23)	1.368(3)
C(2)-C(18)	1.469(3)	C(23)-C(24)	1.414(3)
C(3)-C(4)	1.388(3)	C(24)-C(25)	1.451(3)
C(3)-C(19)	1.479(3)	C(25)-C(26)	1.402(3)
C(4)-C(5)	1.434(3)	C(25)-C(30)	1.416(3)
C(4)-C(30)	1.468(3)	C(26)-C(27)	1.374(3)
C(5)-C(6)	1.397(3)	C(27)-C(28)	1.397(3)
C(5)-C(31)	1.468(3)	C(28)-C(29)	1.374(3)
C(6)-C(42)	1.471(3)	C(29)-C(30)	1.407(3)
C(7)-C(12)	1.406(3)	C(31)-C(32)	1.409(3)
C(7)-C(8)	1.407(3)	C(31)-C(36)	1.412(3)
C(8)-C(9)	1.382(3)	C(32)-C(33)	1.369(3)
C(9)-C(10)	1.390(3)	C(33)-C(34)	1.398(3)
C(10)-C(11)	1.371(3)	C(34)-C(35)	1.374(3)
C(11)-C(12)	1.408(3)	C(35)-C(36)	1.406(3)
C(12)-C(13)	1.457(3)	C(36)-C(37)	1.455(3)
C(13)-C(18)	1.402(3)	C(37)-C(38)	1.407(3)
C(13)-C(14)	1.402(3)	C(37)-C(42)	1.407(3)
C(14)-C(15)	1.375(3)	C(38)-C(39)	1.377(3)
C(15)-C(16)	1.386(3)	C(39)-C(40)	1.391(3)
C(16)-C(17)	1.373(3)	C(40)-C(41)	1.380(3)
C(17)-C(18)	1.407(3)	C(41)-C(42)	1.403(3)
C(19)-C(20)	1.403(3)		

Table 4. Bond angles [°] for $C_{42}H_{24}$ (LT).

C(2)-C(1)-C(6)	119.2(2)	C(24)-C(19)-C(3)	119.7(2)
C(2)-C(1)-C(7)	116.9(2)	C(20)-C(19)-C(3)	121.0(2)
C(6)-C(1)-C(7)	123.2(2)	C(21)-C(20)-C(19)	121.3(2)
C(1)-C(2)-C(3)	119.5(2)	C(20)-C(21)-C(22)	120.0(2)
C(1)-C(2)-C(18)	116.7(2)	C(23)-C(22)-C(21)	119.5(2)
C(3)-C(2)-C(18)	123.3(2)	C(22)-C(23)-C(24)	121.5(2)
C(4)-C(3)-C(2)	119.3(2)	C(19)-C(24)-C(23)	118.8(2)
C(4)-C(3)-C(19)	116.7(2)	C(19)-C(24)-C(25)	119.2(2)
C(2)-C(3)-C(19)	123.6(2)	C(23)-C(24)-C(25)	121.9(2)
C(3)-C(4)-C(5)	119.6(2)	C(26)-C(25)-C(30)	118.8(2)
C(3)-C(4)-C(30)	117.7(2)	C(26)-C(25)-C(24)	122.9(2)
C(5)-C(4)-C(30)	122.0(2)	C(30)-C(25)-C(24)	118.2(2)
C(6)-C(5)-C(4)	119.4(2)	C(27)-C(26)-C(25)	121.6(2)
C(6)-C(5)-C(31)	117.2(2)	C(26)-C(27)-C(28)	119.7(2)
C(4)-C(5)-C(31)	122.8(2)	C(29)-C(28)-C(27)	119.9(2)
C(5)-C(6)-C(1)	119.2(2)	C(28)-C(29)-C(30)	121.5(2)
C(5)-C(6)-C(42)	116.5(2)	C(29)-C(30)-C(25)	118.4(2)
C(1)-C(6)-C(42)	123.7(2)	C(29)-C(30)-C(4)	121.2(2)
C(12)-C(7)-C(8)	118.0(2)	C(25)-C(30)-C(4)	119.5(2)
C(12)-C(7)-C(1)	120.1(2)	C(32)-C(31)-C(36)	118.4(2)
C(8)-C(7)-C(1)	121.2(2)	C(32)-C(31)-C(5)	121.0(2)
C(9)-C(8)-C(7)	121.3(2)	C(36)-C(31)-C(5)	120.0(2)
C(8)-C(9)-C(10)	120.4(2)	C(33)-C(32)-C(31)	121.6(2)
C(11)-C(10)-C(9)	119.2(2)	C(32)-C(33)-C(34)	119.9(2)
C(10)-C(11)-C(12)	121.6(2)	C(35)-C(34)-C(33)	119.9(2)
C(7)-C(12)-C(11)	119.3(2)	C(34)-C(35)-C(36)	121.2(2)
C(7)-C(12)-C(13)	118.8(2)	C(35)-C(36)-C(31)	119.0(2)
C(11)-C(12)-C(13)	121.9(2)	C(35)-C(36)-C(37)	122.8(2)
C(18)-C(13)-C(14)	119.6(2)	C(31)-C(36)-C(37)	118.2(2)
C(18)-C(13)-C(12)	118.7(2)	C(38)-C(37)-C(42)	119.3(2)
C(14)-C(13)-C(12)	121.7(2)	C(38)-C(37)-C(36)	121.7(2)
C(15)-C(14)-C(13)	121.1(2)	C(42)-C(37)-C(36)	118.9(2)
C(14)-C(15)-C(16)	119.5(2)	C(39)-C(38)-C(37)	121.2(2)
C(17)-C(16)-C(15)	120.4(2)	C(38)-C(39)-C(40)	119.5(2)
C(16)-C(17)-C(18)	121.3(2)	C(41)-C(40)-C(39)	120.3(2)
C(13)-C(18)-C(17)	118.1(2)	C(40)-C(41)-C(42)	121.3(2)
C(13)-C(18)-C(2)	120.4(2)	C(41)-C(42)-C(37)	118.4(2)
C(17)-C(18)-C(2)	120.9(2)	C(41)-C(42)-C(6)	120.9(2)
C(24)-C(19)-C(20)	118.9(2)	C(37)-C(42)-C(6)	120.1(2)

Table 5. Bond lengths [Å] involving H atoms for $C_{42}H_{24}$ (LT).

C(8)-H(8)	0.96(2)	C(26)-H(26)	1.03(2)
C(9)-H(9)	0.99(2)	C(27)-H(27)	1.02(3)
C(10)-H(10)	1.00(2)	C(28)-H(28)	1.02(2)
C(11)-H(11)	1.00(2)	C(29)-H(29)	1.03(2)
C(14)-H(14)	0.99(2)	C(32)-H(32)	1.03(2)
C(15)-H(15)	1.02(2)	C(33)-H(33)	1.04(2)
C(16)-H(16)	0.99(2)	C(34)-H(34)	0.99(2)
C(17)-H(17)	1.03(2)	C(35)-H(35)	1.03(2)
C(20)-H(20)	1.01(2)	C(38)-H(38)	1.02(2)
C(21)-H(21)	1.01(2)	C(39)-H(39)	1.02(2)
C(22)-H(22)	1.01(2)	C(40)-H(40)	1.00(2)
C(23)-H(23)	1.00(2)	C(41)-H(41)	1.01(2)

Table 6. Bond angles [°] involving H atoms for $C_{42}H_{24}$ (LT).

C(9)-C(8)-H(8)	120.2(12)	C(27)-C(26)-H(26)	120.6(13)
C(7)-C(8)-H(8)	118.5(12)	C(25)-C(26)-H(26)	117.8(13)
C(8)-C(9)-H(9)	117.5(12)	C(26)-C(27)-H(27)	117.4(13)
C(10)-C(9)-H(9)	122.0(12)	C(28)-C(27)-H(27)	122.9(13)
C(11)-C(10)-H(10)	121.2(12)	C(29)-C(28)-H(28)	120.4(13)
C(9)-C(10)-H(10)	119.4(13)	C(27)-C(28)-H(28)	119.7(13)
C(10)-C(11)-H(11)	118.2(12)	C(28)-C(29)-H(29)	119.1(13)
C(12)-C(11)-H(11)	120.1(12)	C(30)-C(29)-H(29)	119.3(13)
C(15)-C(14)-H(14)	121.6(12)	C(33)-C(32)-H(32)	121.3(11)
C(13)-C(14)-H(14)	117.3(12)	C(31)-C(32)-H(32)	117.1(11)
C(14)-C(15)-H(15)	118.2(13)	C(32)-C(33)-H(33)	120.1(12)
C(16)-C(15)-H(15)	122.3(13)	C(34)-C(33)-H(33)	120.0(12)
C(17)-C(16)-H(16)	120.1(12)	C(35)-C(34)-H(34)	120.1(13)
C(15)-C(16)-H(16)	119.6(12)	C(33)-C(34)-H(34)	120.0(13)
C(16)-C(17)-H(17)	118.6(12)	C(34)-C(35)-H(35)	119.9(12)
C(18)-C(17)-H(17)	120.0(12)	C(36)-C(35)-H(35)	118.9(12)
C(21)-C(20)-H(20)	118.0(11)	C(39)-C(38)-H(38)	119.7(12)
C(19)-C(20)-H(20)	120.6(11)	C(37)-C(38)-H(38)	119.1(12)
C(20)-C(21)-H(21)	118.4(11)	C(38)-C(39)-H(39)	119.2(13)
C(22)-C(21)-H(21)	121.6(11)	C(40)-C(39)-H(39)	121.3(13)
C(23)-C(22)-H(22)	121.1(12)	C(41)-C(40)-H(40)	118.0(12)
C(21)-C(22)-H(22)	119.3(12)	C(39)-C(40)-H(40)	121.7(11)
C(22)-C(23)-H(23)	119.4(12)	C(40)-C(41)-H(41)	116.8(11)
C(24)-C(23)-H(23)	119.0(12)	C(42)-C(41)-H(41)	121.9(11)

Table 7. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $C_{42}H_{24}$ (LT). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	22(1)	21(1)	22(1)	2(1)	7(1)	1(1)
C(2)	22(1)	20(1)	23(1)	2(1)	6(1)	-2(1)
C(3)	24(1)	22(1)	22(1)	1(1)	7(1)	1(1)
C(4)	25(1)	22(1)	22(1)	2(1)	5(1)	1(1)
C(5)	24(1)	25(1)	22(1)	1(1)	5(1)	-2(1)
C(6)	25(1)	25(1)	21(1)	2(1)	7(1)	0(1)
C(7)	22(1)	21(1)	27(1)	2(1)	6(1)	3(1)
C(8)	27(1)	27(1)	23(1)	1(1)	6(1)	2(1)
C(9)	28(1)	33(1)	30(1)	3(1)	12(1)	3(1)
C(10)	23(1)	33(1)	38(1)	0(1)	7(1)	1(1)
C(11)	26(1)	29(1)	32(1)	-3(1)	4(1)	1(1)
C(12)	24(1)	22(1)	28(1)	1(1)	4(1)	3(1)
C(13)	27(1)	20(1)	29(1)	1(1)	5(1)	1(1)
C(14)	28(1)	33(1)	30(1)	-2(1)	2(1)	6(1)
C(15)	37(1)	32(1)	24(1)	-1(1)	-1(1)	7(1)
C(16)	35(1)	26(1)	26(1)	-3(1)	8(1)	4(1)
C(17)	27(1)	21(1)	27(1)	1(1)	5(1)	0(1)
C(18)	24(1)	20(1)	24(1)	-1(1)	4(1)	0(1)
C(19)	31(1)	23(1)	18(1)	2(1)	8(1)	2(1)
C(20)	32(1)	24(1)	24(1)	2(1)	9(1)	2(1)
C(21)	42(1)	24(1)	30(1)	1(1)	11(1)	-3(1)
C(22)	51(2)	25(1)	32(1)	0(1)	16(1)	8(1)
C(23)	37(1)	33(1)	28(1)	5(1)	9(1)	11(1)
C(24)	30(1)	30(1)	22(1)	3(1)	7(1)	6(1)
C(25)	27(1)	35(1)	21(1)	4(1)	5(1)	7(1)
C(26)	28(1)	44(1)	26(1)	2(1)	7(1)	7(1)
C(27)	24(1)	56(1)	27(1)	4(1)	9(1)	4(1)
C(28)	26(1)	46(1)	26(1)	-1(1)	6(1)	-5(1)
C(29)	25(1)	36(1)	22(1)	1(1)	6(1)	-1(1)
C(30)	25(1)	30(1)	20(1)	5(1)	6(1)	3(1)
C(31)	22(1)	31(1)	24(1)	-1(1)	6(1)	-4(1)
C(32)	22(1)	34(1)	27(1)	-2(1)	7(1)	-3(1)
C(33)	25(1)	42(1)	28(1)	4(1)	6(1)	-4(1)
C(34)	27(1)	47(1)	23(1)	-3(1)	5(1)	-8(1)
C(35)	28(1)	36(1)	28(1)	-7(1)	11(1)	-8(1)
C(36)	26(1)	29(1)	25(1)	-4(1)	11(1)	-9(1)
C(37)	26(1)	27(1)	31(1)	-2(1)	15(1)	-6(1)
C(38)	37(1)	31(1)	32(1)	-7(1)	15(1)	-8(1)
C(39)	44(1)	26(1)	44(1)	-5(1)	25(1)	-4(1)
C(40)	40(1)	22(1)	42(1)	6(1)	23(1)	1(1)
C(41)	27(1)	26(1)	30(1)	2(1)	12(1)	0(1)
C(42)	25(1)	25(1)	26(1)	-1(1)	13(1)	-4(1)

Table 8. Hydrogen coordinates (× 10^4) and isotropic displacement parameters (Å^2 × 10^3) for $C_{42}H_{24}$ (LT).

	x	*y*	*z*	*U*(eq)
H(8)	889(10)	8998(26)	2277(11)	21(5)
H(9)	-297(11)	8898(29)	2176(12)	33(6)
H(10)	-1076(11)	8138(27)	1055(11)	31(6)
H(11)	-608(10)	7375(27)	77(12)	26(5)
H(14)	-156(11)	7491(27)	-773(11)	25(5)
H(15)	335(12)	6752(29)	-1744(13)	40(6)
H(16)	1560(10)	6032(27)	-1492(11)	24(5)
H(17)	2261(11)	6079(28)	-322(11)	31(6)
H(20)	1763(11)	3172(26)	409(11)	24(5)
H(21)	2095(10)	203(28)	31(10)	26(5)
H(22)	3305(11)	-673(31)	261(12)	34(6)
H(23)	4154(12)	1562(29)	861(12)	36(6)
H(26)	4826(12)	3999(35)	989(13)	48(7)
H(27)	5632(13)	6387(32)	1529(13)	52(7)
H(28)	5267(12)	9010(33)	2208(13)	45(7)
H(29)	4084(12)	9229(33)	2267(13)	44(6)
H(32)	3714(10)	5814(27)	2966(11)	23(5)
H(33)	4262(11)	6048(30)	4222(12)	34(6)
H(34)	3973(12)	8763(30)	4874(13)	40(6)
H(35)	3173(11)	11176(31)	4318(12)	35(6)
H(38)	2694(11)	13478(30)	3708(13)	37(6)
H(39)	1854(11)	15720(33)	3107(12)	42(6)
H(40)	1118(10)	14834(28)	1952(11)	27(5)
H(41)	1222(11)	11869(28)	1452(12)	32(6)