Crystal structure of *trans*-1,4,7,10-tetrakis(2,2-dimethylpropyloxy)-5,6,11,12-tetrahydro-5,12[1',2']:6,11[1'',2'']dibenzenodibenzo[*a,e*]cyclooctatetraene, [C₁₄H₈(C₅H₁₁O)₂]₂

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Abstract

C₄₈H₆₀O₄, triclinic, *P* $\bar{1}$ (No. 2), *a* = 10.543(3) Å, *b* = 12.603(3) Å, *c* = 8.932(2) Å, α = 87.20(2)°, β = 110.34(2)°, γ = 108.26(2)°, *V* = 1054.4 Å³, *Z* = 1, *R*_{gt}(*F*) = 0.078, *wR*(*F*) = 0.075, *T* = 293 K.

Source of material

The title compound was prepared, according to [1], by irradiation ($\lambda > 345$ nm) of a solution of bis-1,4-(2,2-dimethylpropyloxy)-anthracene [2] in cyclohexane at room temperature. The irradiated mixture was briefly heated to boiling and allowed to cool overnight. Recrystallization of the product from toluene at 263 K afforded colourless crystals, mp 527 K – 528 K.

Discussion

Due to a partial disorder of two *tert*-butyl groups a split model (see Fig.) could improve our refinements from *R* = 0.09 to *R* = 0.075.

Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.45 × 0.55 × 0.3 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.70 cm ⁻¹
Diffractionmeter, scan mode:	Siemens R3m/V, Wyckoff
2 θ _{max} :	55°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	4881, 4881
Criterion for <i>F</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>F</i> _{obs} > 3 σ (<i>F</i> _{obs}), 3613
<i>N</i> (<i>param</i>) _{refined} :	263
Program:	SHELXTL-plus [3]

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

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(2A)	2i	0.1825(5)	−0.0838(3)	0.3387(5)	0.08
H(3A)	2i	0.1348(4)	0.0704(3)	0.1995(5)	0.08
H(6A)	2i	0.49387	0.2018	−0.00905	0.08
H(8A)	2i	0.7495(5)	0.2988(4)	0.0785(6)	0.08
H(9A)	2i	0.9785(6)	0.3064(5)	0.2487(7)	0.08
H(10A)	2i	1.0187(6)	0.1495(5)	0.3827(6)	0.08
H(11A)	2i	0.8301(5)	−0.0164(5)	0.3437(5)	0.08
H(13A)	2i	0.57367	−0.11082	0.24749	0.08
H(15A)	2i	0.0739(4)	0.1808(3)	−0.0194(5)	0.08
H(15B)	2i	0.1858(4)	0.2621(3)	0.1274(5)	0.08
H(17A)	2i	0.0614(5)	0.4487(4)	−0.1428(6)	0.08
H(17B)	2i	0.0857(5)	0.4119(4)	0.0325(6)	0.08
H(17C)	2i	−0.0320(5)	0.3317(4)	−0.1121(6)	0.08
H(18A)	2i	0.0403(6)	0.2373(4)	−0.2957(5)	0.08
H(18B)	2i	0.2027(6)	0.2606(4)	−0.2646(5)	0.08
H(18C)	2i	0.1327(6)	0.3547(4)	−0.3267(5)	0.08
H(19A)	2i	0.3862(5)	0.3896(4)	−0.0350(6)	0.08
H(19B)	2i	0.3395(5)	0.4462(4)	0.0804(6)	0.08
H(19C)	2i	0.3160(5)	0.4838(4)	−0.0945(6)	0.08
H(20A)	2i	0.3864(6)	−0.1771(4)	0.5425(5)	0.08
H(20B)	2i	0.2355(6)	−0.2458(4)	0.4237(5)	0.08

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

Atom	Site	Occ.	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
O(1)	2i		0.3709(4)	−0.1795(3)	0.3263(5)	0.164(4)	0.092(3)	0.143(3)	0.089(3)	0.119(3)	0.078(2)
C(1)	2i		0.3451(5)	−0.0826(3)	0.2652(5)	0.086(3)	0.053(2)	0.074(3)	0.037(2)	0.049(2)	0.025(2)
C(2)	2i		0.2382(5)	−0.0458(3)	0.2754(5)	0.084(3)	0.053(3)	0.083(3)	0.027(2)	0.056(3)	0.020(2)
C(3)	2i		0.2105(4)	0.0457(3)	0.1941(5)	0.070(3)	0.053(2)	0.081(3)	0.029(2)	0.046(2)	0.015(2)
O(4)	2i		0.2716(3)	0.1901(2)	0.0145(4)	0.083(2)	0.063(2)	0.093(2)	0.046(2)	0.057(2)	0.034(2)
C(4)	2i		0.2923(4)	0.1010(3)	0.1048(5)	0.069(3)	0.045(2)	0.065(2)	0.028(2)	0.036(2)	0.014(2)
C(5)	2i		0.4041(4)	0.0676(3)	0.1007(5)	0.063(3)	0.045(2)	0.060(2)	0.023(2)	0.035(2)	0.012(2)
C(6)	2i		0.4999(4)	0.1261(3)	0.0082(5)	0.073(3)	0.046(2)	0.072(3)	0.030(2)	0.044(2)	0.019(2)
C(7)	2i		0.6523(5)	0.1363(4)	0.1114(5)	0.069(3)	0.058(3)	0.068(3)	0.024(2)	0.040(2)	0.008(2)
C(8)	2i		0.7652(5)	0.2340(4)	0.1331(6)	0.079(3)	0.069(3)	0.089(3)	0.019(3)	0.049(3)	0.004(3)
C(9)	2i		0.9005(6)	0.2385(5)	0.2340(7)	0.072(4)	0.097(4)	0.103(4)	0.004(3)	0.044(3)	−0.018(3)
C(10)	2i		0.9245(6)	0.1455(5)	0.3123(6)	0.070(4)	0.123(5)	0.082(4)	0.033(4)	0.028(3)	−0.009(3)
C(11)	2i		0.8131(5)	0.0482(5)	0.2896(5)	0.076(3)	0.096(4)	0.071(3)	0.041(3)	0.033(3)	0.009(3)
C(12)	2i		0.6769(5)	0.0428(4)	0.1906(5)	0.068(3)	0.067(3)	0.062(3)	0.032(2)	0.036(2)	0.010(2)
C(13)	2i		0.5490(5)	−0.0608(3)	0.1629(5)	0.076(3)	0.061(3)	0.064(3)	0.041(2)	0.039(2)	0.024(2)
C(14)	2i		0.4293(4)	−0.0249(3)	0.1797(5)	0.069(3)	0.050(2)	0.061(2)	0.030(2)	0.037(2)	0.014(2)
C(15)	2i		0.1662(4)	0.2366(3)	0.0198(5)	0.058(3)	0.057(3)	0.073(3)	0.027(2)	0.030(2)	0.013(2)
C(16)	2i		0.1706(4)	0.3344(3)	−0.0871(5)	0.053(2)	0.056(3)	0.068(3)	0.025(2)	0.018(2)	0.013(2)
C(17)	2i		0.0612(5)	0.3864(4)	−0.0765(6)	0.095(4)	0.099(4)	0.118(4)	0.064(3)	0.044(3)	0.042(3)
C(18)	2i		0.1329(6)	0.2929(4)	−0.2595(5)	0.100(4)	0.098(4)	0.074(3)	0.026(3)	0.026(3)	0.020(3)
C(19)	2i		0.3164(5)	0.4214(4)	−0.0286(6)	0.083(4)	0.060(3)	0.099(4)	0.020(3)	0.023(3)	0.021(3)
C(20)	2i		0.3364(6)	−0.2278(4)	0.4487(5)	0.136(5)	0.067(3)	0.066(3)	0.052(3)	0.051(3)	0.020(2)
C(21)	2i		0.3774(6)	−0.3349(4)	0.4812(5)	0.121(4)	0.055(3)	0.066(3)	0.046(3)	0.043(3)	0.023(2)
C(22)	2i	0.5	0.284(2)	−0.425(1)	0.365(2)	0.13(1)	0.042(6)	0.069(9)	0.009(7)	−0.029(8)	0.002(6)
C(23)	2i	0.5	0.393(2)	−0.364(1)	0.653(1)	0.16(1)	0.081(9)	0.057(6)	0.061(9)	0.034(8)	0.030(6)
C(24)	2i	0.5	0.535(2)	−0.313(1)	0.477(2)	0.10(1)	0.11(1)	0.21(2)	0.069(9)	0.09(1)	0.08(1)
C(22A)	2i	0.5	0.508(2)	−0.313(1)	0.588(3)	0.13(2)	0.09(1)	0.18(2)	0.07(1)	−0.08(1)	−0.02(1)
C(23A)	2i	0.5	0.341(3)	−0.393(1)	0.317(2)	0.26(3)	0.08(1)	0.09(1)	0.11(2)	0.06(1)	0.014(8)
C(24A)	2i	0.5	0.256(2)	−0.417(1)	0.542(3)	0.25(2)	0.08(1)	0.30(3)	0.08(1)	0.20(2)	0.10(1)

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