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Crystal structure of tetramethyl (*M*,*P*)-2,2′-bi-(3,6-heptanooxepine)-4,4′,5,5′-tetracarboxylate, $[C_6HO(CH_2)_7(COOCH_3)_2]_2$

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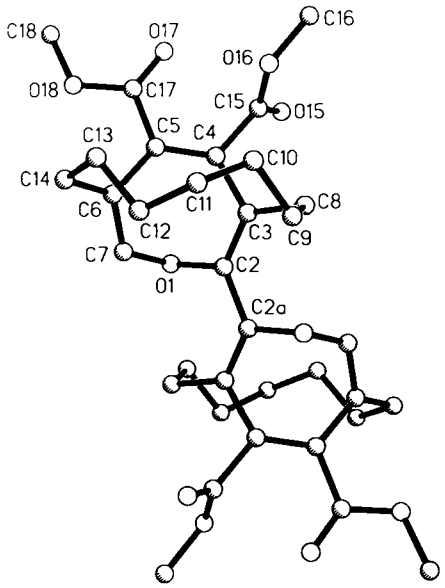

Source of material: The title compound was prepared from 3,4-heptamethylenefuran as described in ref. 1.

$C_{34}H_{42}O_{10}$, monoclinic, $C12/c1$ (No. 15), a =21.535(7) Å, b =8.876(3) Å, c =16.526(4) Å, β =101.56(2)°, V =3094.8 Å^3, Z =4, $R(F)$ =0.057, $R_w(F)$ =0.054.

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless prism, size 0.3 x 0.3 x 0.4 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.00 cm^{-1}
Diffractometer:	Siemens P4
Scan mode:	ω
$T_{measurement}$:	293 K
$2\theta_{max}$:	55°
$N(hkl)_{unique}$:	3574
Criterion for F_o:	$F_o > 3\,\sigma(F_o)$
$N(param)_{refined}$:	200
Program:	SHELXTL-plus

Table 2. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{iso}
H(7A)	8*f*	0.1635(1)	−0.0199(3)	1.0169(1)	0.08
H(8A)	8*f*	0.1882(1)	0.4643(2)	0.8148(1)	0.08
H(8B)	8*f*	0.2296(1)	0.5004(2)	0.9020(1)	0.08
H(9A)	8*f*	0.1372(1)	0.4588(3)	0.9575(2)	0.08
H(9B)	8*f*	0.1346(1)	0.6044(3)	0.9031(2)	0.08
H(10A)	8*f*	0.0549(1)	0.5250(4)	0.8144(2)	0.08
H(10B)	8*f*	0.0822(1)	0.3611(4)	0.8154(2)	0.08
H(11A)	8*f*	−0.0176(1)	0.3818(5)	0.8586(2)	0.08
H(11B)	8*f*	0.0197(1)	0.4584(5)	0.9393(2)	0.08
H(12A)	8*f*	0.0821(1)	0.2323(4)	0.9590(2)	0.08
H(12B)	8*f*	0.0136(1)	0.2218(4)	0.9772(2)	0.08
H(13A)	8*f*	−0.0205(1)	0.0753(4)	0.8709(2)	0.08
H(13B)	8*f*	0.0285(1)	0.1382(4)	0.8210(2)	0.08
H(14A)	8*f*	0.0497(1)	−0.1167(3)	0.8578(2)	0.08
H(14B)	8*f*	0.0614(1)	−0.0709(3)	0.9513(2)	0.08
H(16A)	8*f*	0.1252(1)	0.4022(3)	0.5815(2)	0.08
H(16B)	8*f*	0.1761(1)	0.2761(3)	0.5811(2)	0.08
H(16C)	8*f*	0.1962(1)	0.4317(3)	0.6233(2)	0.08
H(18A)	8*f*	0.0742(1)	−0.3600(3)	0.6924(2)	0.08
H(18B)	8*f*	0.1372(1)	−0.3013(3)	0.6696(2)	0.08
H(18C)	8*f*	0.0727(1)	−0.2216(3)	0.6331(2)	0.08

Table 3. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	8*f*	0.23664(6)	0.0565(2)	0.96476(8)	0.0497(8)	0.0361(8)	0.0401(8)	0.0001(6)	−0.0001(6)	−0.0002(7)
C(2)	8*f*	0.23473(9)	0.2138(2)	0.9614(1)	0.0368(9)	0.035(1)	0.037(1)	−0.0006(8)	0.0062(7)	−0.0011(8)
C(3)	8*f*	0.20631(9)	0.2773(2)	0.8881(1)	0.039(1)	0.040(1)	0.035(1)	−0.0028(9)	0.0062(8)	−0.0002(9)

Table 3. (Continued)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(4)	8*f*	0.18382(8)	0.1768(2)	0.8170(1)	0.0346(9)	0.042(1)	0.034(1)	0.0007(8)	0.0044(7)	0.0008(9)
C(5)	8*f*	0.15204(9)	0.0460(2)	0.8189(1)	0.040(1)	0.044(1)	0.037(1)	–0.0027(9)	0.0024(8)	–0.0006(9)
C(6)	8*f*	0.1330(1)	–0.0049(3)	0.8954(1)	0.055(1)	0.045(1)	0.041(1)	–0.014(1)	0.0061(9)	0.002(1)
C(7)	8*f*	0.1752(1)	0.0062(3)	0.9655(1)	0.061(1)	0.046(1)	0.041(1)	–0.012(1)	0.007(1)	0.006(1)
C(8)	8*f*	0.1938(1)	0.4447(2)	0.8729(1)	0.063(1)	0.040(1)	0.036(1)	0.001(1)	–0.0014(9)	0.0022(9)
C(9)	8*f*	0.1349(1)	0.4962(3)	0.9024(2)	0.085(2)	0.060(2)	0.057(2)	0.023(1)	0.008(1)	–0.001(1)
C(10)	8*f*	0.0727(1)	0.4427(4)	0.8491(2)	0.074(2)	0.095(2)	0.066(2)	0.025(2)	0.011(1)	0.008(2)
C(11)	8*f*	0.0225(1)	0.3873(5)	0.8964(2)	0.074(2)	0.145(3)	0.071(2)	0.037(2)	0.017(2)	–0.000(2)
C(12)	8*f*	0.0377(1)	0.2350(4)	0.9348(2)	0.071(2)	0.132(3)	0.056(2)	0.003(2)	0.023(1)	0.002(2)
C(13)	8*f*	0.0229(1)	0.1037(4)	0.8741(2)	0.047(1)	0.154(3)	0.067(2)	–0.029(2)	0.008(1)	–0.013(2)
C(14)	8*f*	0.0646(1)	–0.0382(3)	0.8969(2)	0.062(2)	0.091(2)	0.053(1)	–0.031(1)	0.014(1)	0.000(1)
C(15)	8*f*	0.20057(9)	0.2345(2)	0.7383(1)	0.048(1)	0.044(1)	0.037(1)	–0.007(1)	0.0089(9)	–0.006(1)
O(15)	8*f*	0.25280(7)	0.2297(2)	0.72463(9)	0.0499(9)	0.083(1)	0.058(1)	–0.0104(9)	0.0218(8)	–0.0076(9)
O(16)	8*f*	0.15121(7)	0.3002(2)	0.68930(9)	0.0631(9)	0.058(1)	0.0353(8)	0.0025(8)	0.0107(7)	0.0095(7)
C(16)	8*f*	0.1632(1)	0.3573(3)	0.6124(2)	0.108(2)	0.077(2)	0.045(1)	0.004(2)	0.024(1)	0.018(1)
C(17)	8*f*	0.1371(1)	–0.0454(2)	0.7408(1)	0.043(1)	0.043(1)	0.043(1)	–0.0021(9)	–0.0009(9)	–0.001(1)
O(17)	8*f*	0.15242(9)	–0.0124(2)	0.6776(1)	0.086(1)	0.058(1)	0.0421(9)	–0.0139(9)	0.0134(8)	–0.0084(8)
O(18)	8*f*	0.10607(8)	–0.1716(2)	0.7508(1)	0.069(1)	0.051(1)	0.053(1)	–0.0191(8)	0.0030(8)	–0.0073(8)
C(18)	8*f*	0.0967(1)	–0.2721(3)	0.6806(2)	0.092(2)	0.059(2)	0.066(2)	–0.021(1)	–0.002(1)	–0.019(1)

References

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