centrosymmetric space group, *Pn* (Yamaguchi & Ueda, 1984), and was later refined more satisfactorily as a disordered model in the centrosymmetric *P2/n* (Marsh, 1986); the disordered model again required that the central N and CH groups of the acridine molecule be equivalent. And the conclusion is the same: on the basis of the diffraction data, there is little choice but to opt for the centrosymmetric, disordered description.

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Acta Cryst. (1990). C**46**, 1357–1358

Structure of 1,2,5,6-tetramethyltricyclo[3.1.0.0^{2,6}]hexane-3,4-dione.

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(*Received* 18 *October* 1989; *accepted* 23 *January* 1990)

Abstract

The crystal structure of the title compound, which was originally described in the non-centrosymmetric space group *Pnc*2 [Spek (1977). *Cryst. Struct. Commun.* **6**, 259–262], has been refined successfully in the centrosymmetric space group *Pnca*. The molecular geometry has been improved significantly. The cell parameters are: a = 12·084 (2), b = 11·295 (2), c = 6·659 (2) Å, with R = 0·049.

The structure of the title compound ($C_{10}H_{12}O_2$, M_r = 164·2, μ = 0·9 cm^{-1}) has been reported (Spek, 1977) in space group *Pnc*2 [CAD-4, Zr-filtered Mo $K\alpha$, θ_{max} = 20°, 341 reflections with $I > 2{\cdot}5\sigma(I)$, R = 0·08]. Molecules are located in this space group on crystallographic twofold axes resulting in two independent half molecules. Examination of the symmetry of the refined structural parameters with the *MISSYM* algorithm (Le Page, 1987) as implemented in the program *PLATON* (Spek, 1982) revealed an additional inversion centre at 0·254, −0·509, −0·244. This inversion centre relates the previously reported two independent half molecules. The correct space group is *Pnca* (non-standard setting of *Pbcn*) [a = 12·084 (2), b = 11·295 (2), c = 6·659 (2) Å, Z = 4]. The structure was refined on F by full-matrix least squares with *SHELX*76 (Sheldrick, 1976). Hydrogen atoms on the methyl groups were included at calculated positions (C—H = 0·98 Å) and refined as rigid groups with two common isotropic thermal parameters. Convergence was reached at R = 0·049 {wR = 0·077, $w^{-1} = \sigma^2(F) + 0{\cdot}0002F^2$, S = 0·58, 333 reflections [$I > 2{\cdot}5\sigma(I)$], 63 parameters, $(\Delta/\sigma)_{max}$ = 0·3}. No residual density outside ±0·15 e Å^{-3}. Final parameters are given in Table 1.* Fig. 1 gives the atom numbering. The additional

Table 1. *Final coordinates, space group Pnca, and equivalent isotropic thermal parameters, with their e.s.d.'s in parentheses*

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}(Å^2)
O(1)	0·3524 (3)	0·0732 (3)	0·2877 (6)	0·070 (2)
C(2)	0·3031 (3)	0·0390 (4)	0·1373 (9)	0·049 (2)
C(3)	0·3261 (3)	0·0566 (3)	−0·0746 (8)	0·046 (2)
C(4)	0·2841 (3)	−0·0524 (3)	−0·1908 (7)	0·047 (2)
C(5)	0·4230 (4)	0·1282 (4)	−0·1511 (8)	0·065 (2)
C(6)	0·3377 (4)	−0·1373 (4)	−0·3320 (7)	0·067 (2)

Table 2. *Bond distances* (Å), *space group Pnca*

Primed atoms are related by $\frac{1}{2} - x, -y, z$.

O(1)—C(2)	1·228 (7)	C(3)—C(4′)	1·540 (6)
C(2)—C(2′)	1·557 (6)	C(3)—C(5)	1·512 (6)
C(2)—C(3)	1·452 (8)	C(4)—C(4′)	1·442 (5)
C(3)—C(4)	1·540 (6)	C(4)—C(6)	1·491 (6)

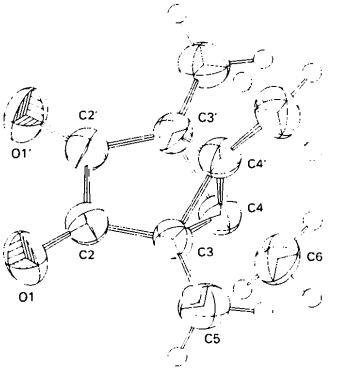

Fig. 1. Thermal motion ellipsoid plot (50% probability level) showing the twofold crystallographic symmetry and atom labelling.

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, bond distances, bond angles and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52626 (6 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

0108-2701/90/071357-02$03.00

a glide generated with the inversion centre is supported by the observed systematic absences ($hk0$, $h = 2n + 1$), apart from a few exceptions [*e.g.* the reflection 540 with $I > 30\sigma(I)$] which were the reason for adopting the space group *Pnc*2 in the previous work. The present geometry is regular as opposed to that of the previous determination which was hampered by the effects (large variations in chemically equivalent bond lengths) of the refinement of a centrosymmetric structure in a non-centrosymmetric space group (Schomaker & Marsh, 1979). Bond distances are given in Table 2. In view of the above it is believed that a description of the structure in the centrosymmetric space group *Pnca* is the best choice and that the small number of 'observed extinctions' must be considered as artifacts. All calculations were carried out on a MicroVAX cluster.

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Acta Cryst. (1990). C**46**, 1358

Structure of bis[(−)-menthyl] acetylenedicarboxylate. Erratum.

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(*Received* 3 *May* 1990)

Abstract

All the data in the paper by Evans, Trotter & Yee [*Acta Cryst.* (1988). C**44**, 878–880] refer to the (+)-menthyl isomer. The (−)-menthyl isomer (on which the crystal structure analysis was actually performed) has space group $P3_221$.

All relevant information is given in the *Abstract*.

0108-2701/90/071358-01$03.00