Table 2. *Bond distances* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

C(1)—C(2)	1·507 (6)	C(12)—C(18)	1·471 (6)
C(2)—C(3)	1·506 (5)	C(18)—C(13)	1·399 (6)
C(3)—C(9)	1·509 (5)	C(13)—C(14)	1·383 (6)
C(9)—C(8)	1·383 (6)	C(14)—C(15)	1·412 (6)
C(8)—C(1)	1·506 (5)	C(15)—C(16)	1·404 (7)
C(1)—O(1)	1·217 (5)	C(16)—C(17)	1·391 (6)
C(3)—O(2)	1·215 (5)	C(17)—C(18)	1·424 (5)
C(9)—C(4)	1·419 (5)	C(10)—C(17)	1·496 (6)
C(4)—C(5)	1·388 (7)	C(11)—C(19)	1·541 (5)
C(5)—C(6)	1·391 (7)	C(12)—O(3)	1·230 (4)
C(6)—C(7)	1·399 (5)	C(19)—C(20)	1·482 (5)
C(7)—C(8)	1·403 (6)	C(20)—O(4)	1·187 (5)
C(2)—C(10)	1·383 (5)	C(20)—O(5)	1·338 (4)
C(10)—C(11)	1·538 (5)	C(21)—C(22)	1·499 (18)
C(11)—C(12)	1·535 (5)	C(21)—O(5)	1·481 (11)
C(1)—C(2)—C(3)	104·4 (3)	C(10)—C(11)—C(19)	117·4 (3)
C(1)—C(2)—C(10)	124·6 (3)	C(11)—C(10)—C(17)	106·0 (2)
C(2)—C(1)—C(8)	108·3 (3)	C(10)—C(17)—C(16)	131·2 (3)
C(1)—C(8)—C(7)	129·8 (3)	C(10)—C(17)—C(18)	108·1 (3)
C(1)—C(8)—C(9)	109·6 (3)	C(11)—C(12)—O(3)	126·0 (3)
C(2)—C(1)—O(1)	126·8 (3)	C(12)—C(11)—C(19)	111·2 (3)
C(8)—C(1)—O(1)	124·9 (3)	C(11)—C(19)—C(20)	114·9 (3)
C(2)—C(3)—C(9)	108·4 (3)	C(12)—C(18)—C(13)	126·6 (3)
C(3)—C(2)—C(10)	130·9 (3)	C(12)—C(18)—C(17)	109·4 (3)
C(2)—C(10)—C(11)	123·0 (3)	C(18)—C(12)—O(3)	125·9 (3)
C(2)—C(10)—C(17)	130·8 (3)	C(13)—C(14)—C(15)	119·0 (3)
C(3)—C(9)—C(4)	130·6 (3)	C(14)—C(13)—C(18)	117·5 (3)
C(3)—C(9)—C(8)	109·1 (3)	C(13)—C(18)—C(17)	124·0 (3)
C(9)—C(3)—O(2)	122·7 (3)	C(14)—C(15)—C(16)	123·6 (3)
C(4)—C(5)—C(6)	120·9 (4)	C(15)—C(16)—C(17)	117·8 (3)
C(5)—C(4)—C(9)	118·6 (3)	C(16)—C(17)—C(18)	118·0 (3)
C(4)—C(9)—C(8)	120·4 (3)	C(19)—C(20)—O(4)	126·4 (3)
C(5)—C(6)—C(7)	120·6 (3)	C(19)—C(20)—O(5)	109·7 (3)
C(6)—C(7)—C(8)	118·8 (3)	O(4)—C(20)—O(5)	124·0 (3)
C(7)—C(8)—C(9)	120·7 (3)	C(20)—O(5)—C(21)	116·9 (4)
C(10)—C(11)—C(12)	105·4 (2)	C(22)—C(21)—O(5)	117·2 (7)

The intermolecular contacts (C···O and C···C with minimum values of 3·21 and 3·53 Å, respectively) are van der Waals. Despite the O atoms of the carbonyl functions being involved in the intermolecular bonding, no dipolar bonds are found as in 2-dicyanomethyleneindan-1,3-dione (Silverman, Krukonis & Yannoni, 1974).

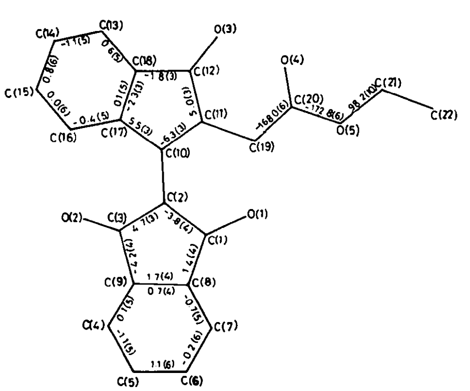

Fig. 2. Selected torsion angles (°) with e.s.d.'s in parentheses. τ[C(10)—C(11)—C(19)—C(20)] = −61·4 (4); τ[C(11)—C(19)—C(20)—O(4)] = 13·4 (5)°.

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2-(4-Oxo-2,3-diphenylindeno[1,2-*b*]pyrrol-1-yl)ethyl Acetate

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Abstract. $C_{27}H_{21}NO_3$, $M_r = 407{\cdot}469$, orthorhombic, $P2_12_12_1$, $a = 5{\cdot}823$ (2), $b = 14{\cdot}933$ (4), $c = 24{\cdot}067$ (3) Å, $V = 2092{\cdot}74$ Å^3, $Z = 4$, $D_x = 1{\cdot}293$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0{\cdot}51$ mm^{-1}, $F(000) = 856$, $T = 293$ K, $R = 0{\cdot}043$ for 987 observed reflections. The C—O bond lengths in the β-acetylethyl side chain indicate the presence of resonance structures of the carbonyl group. The indenopyrrole fragment is

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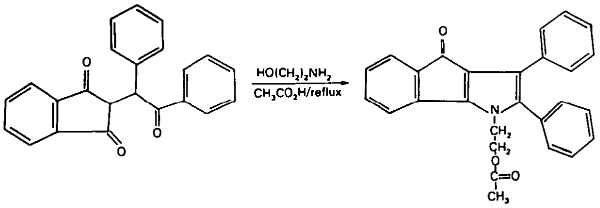
planar and the β-acetylethyl side chain has a folded conformation.

Introduction. The structural study of the title compound is part of a programme of investigations into some novel derivatives of indan-1,3-dione (Varghese, Srinivasan, Padmanabhan & Ramadas, 1986; Varghese, Srinivasan, Ramadas & Padmanabhan, 1986). The compound was synthesized by Padmanabhan and Ramadas (Padmanabhan, 1982).

Experimental. Treatment of 2-desylindan-1,3-dione with ethanolamine in refluxing glacial acetic acid yielded the title compound as the reaction product. Slow recrystallization from ethanol yielded crystals of suitable dimensions for X-ray studies.



Crystal dimensions: 0·40 × 0·20 × 0·65 mm. Enraf–Nonius CAD-4 diffractometer, graphite monochromator. Cell parameters refined by least-squares method using 25 reflections ($2 < 2\theta < 40°$). Two check reflections monitored every 100 reflections did not show significant intensity variations. Lp correction, no absorption corrections, no extinctions. 1724 reflections with $2 < 2\theta < 40°$ (*hkl* range: $h \pm 6, k \pm 18, l \pm 23$), 987 reflections having $I > 3\sigma(I)$. Structure solved by multi-solution direct methods using *MULTAN*80 program (Main *et al.*, 1980) and difference Fourier syntheses using *SHELX*76 (Sheldrick, 1976). Final *R* factor with anisotropic thermal parameters for the non-H atoms and isotropic thermal parameters for H atoms is $R = 0{\cdot}043$ (unit weights) and $wR = 0{\cdot}045$, with $w = k(\sigma|F_o|^2 + g|F_o|^2)^{-1}$, where $g = 0{\cdot}001147$ and $k = 1{\cdot}0000$. The quantity minimized was $\sum w(|F_o| - k|F_c|)^2$. The least-squares refinement was carried out with *SHELX*76 (Sheldrick, 1976). Max. $\Delta/\sigma = 0{\cdot}275$; max. and min. heights in final difference Fourier synthesis, 0·31 and $-0{\cdot}32$ e Å^{-3}. Scattering factors from *SHELX*76.

Discussion. The final atomic parameters are given in Table 1.* An *ORTEP* plot (Johnson, 1965) of the molecule is shown in Fig. 1. Bond lengths and bond angles are given in Table 2, and selected torsion angles in Fig. 2.

In the indenopyrrole fragment, the *ipso* angles of the six-membered ring are expanded and the apical angles contracted, as in related fused-ring systems (Allen, 1981; Varghese, Srinivasan, Padmanabhan & Ramadas, 1986; Varghese, Srinivasan, Ramadas & Padmanabhan, 1986; Csöregh & Eckstein, 1979). In the pyrrole ring, all bond lengths are close to the values found for the C(sp^2)—N distances in 3,6-dimethyl-5-thioformylpyrrolo[2,1-*b*]thiazole (Sharma & Killean, 1974), 6-methyl-5-thioformylpyrrolo[2,1-*b*]thiazole (Killean, Lawrence, Cameron & Sharma, 1975)

Table 1. *Final fractional atomic coordinates* (×10^4 *for non-*H *atoms;* ×10^3 *for* H *atoms) with e.s.d.'s in parentheses*

$$U_{eq} = \sum_{l=1}^{3} U_{ll}/3.$$

	x	y	z	U_{eq}(×10^3 Å^2)
N(1)	5774 (11)	864 (4)	6046 (2)	46 (4)
C(1a)	5205 (13)	861 (4)	6594 (3)	42 (4)
C(2)	4303 (13)	268 (5)	5776 (2)	39 (4)
C(3)	2870 (13)	−124 (4)	6163 (3)	40 (4)
C(3a)	3460 (13)	273 (5)	6696 (2)	41 (4)
C(4)	3018 (15)	276 (5)	7291 (3)	48 (5)
C(4a)	4717 (15)	937 (5)	7527 (3)	50 (5)
C(5)	4954 (16)	1172 (5)	8083 (3)	56 (5)
C(6)	6735 (20)	1815 (6)	8186 (3)	73 (6)
C(7)	8135 (18)	2161 (5)	7775 (3)	67 (5)
C(8a)	6084 (14)	1299 (5)	7108 (3)	44 (5)
C(8)	7807 (17)	1893 (6)	7223 (3)	66 (6)
C(12)	4565 (13)	105 (4)	5176 (3)	39 (4)
C(13)	2830 (15)	345 (5)	4812 (3)	53 (5)
C(14)	3126 (17)	211 (5)	4236 (3)	59 (5)
C(15)	5041 (18)	−179 (6)	4035 (3)	63 (6)
C(16)	6795 (16)	−441 (5)	4392 (3)	57 (5)
C(17)	6520 (14)	−283 (5)	4971 (3)	51 (5)
C(18)	1160 (13)	−844 (4)	6068 (3)	38 (4)
C(19)	1524 (15)	−1491 (4)	5647 (2)	47 (5)
C(20)	−63 (15)	−2176 (5)	5570 (3)	53 (5)
C(21)	−1992 (16)	−2204 (6)	5902 (3)	64 (6)
C(22)	−2354 (15)	−1594 (6)	6311 (3)	56 (5)
C(23)	−759 (14)	−922 (4)	6398 (2)	43 (4)
C(24)	7366 (15)	1470 (5)	5776 (3)	54 (5)
C(25)	6271 (18)	2362 (5)	5635 (3)	66 (6)
C(26)	3342 (20)	2929 (6)	6238 (5)	84 (8)
C(27)	3154 (22)	3403 (7)	6813 (5)	108 (8)
O(1)	1641 (11)	−170 (4)	7564 (2)	77 (4)
O(2)	5577 (11)	2829 (4)	6125 (2)	64 (4)
O(3)	1889 (15)	2679 (7)	5938 (4)	149 (8)
H(5)	394 (16)	75 (4)	839 (3)	79 (32)
H(6)	719 (13)	196 (4)	860 (3)	90 (129)
H(7)	897 (14)	276 (6)	789 (3)	105 (31)
H(8)	882 (14)	235 (4)	697 (3)	101 (30)
H(13)	166 (16)	62 (5)	498 (3)	30 (29)
H(14)	161 (15)	10 (5)	401 (4)	105 (38)
H(15)	503 (17)	−28 (6)	359 (4)	133 (32)
H(16)	837 (15)	−80 (5)	420 (4)	32 (31)
H(17)	797 (14)	−44 (6)	524 (3)	24 (30)
H(19)	231 (16)	−126 (5)	528 (4)	128 (45)
H(20)	31 (17)	−266 (6)	524 (4)	88 (31)
H(21)	−318 (14)	−260 (6)	583 (4)	51 (34)
H(22)	−358 (13)	−156 (5)	657 (3)	46 (22)
H(23)	−91 (16)	−53 (5)	667 (3)	17 (29)
H(24·1)	763 (15)	125 (5)	545 (3)	38 (31)
H(24·2)	832 (16)	139 (5)	600 (4)	8 (32)
H(25·1)	754 (15)	271 (5)	544 (4)	71 (30)
H(25·2)	507 (15)	227 (5)	532 (4)	81 (32)
H(27·1)	218 (14)	355 (5)	669 (4)	44 (30)
H(27·2)	129 (16)	374 (6)	705 (4)	160 (51)
H(27·3)	326 (16)	303 (6)	721 (4)	155 (40)

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* Lists of structure factors, selected torsion angles, details of least-squares planes, intermolecular contact distances, bond lengths and angles involving H atoms, and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43083 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

and 6-*tert*-butyl-3-methyl-5-thioformylpyrrolo[2,1-*b*]-thiazole (Sharma, Lawrence & Killean, 1982). The average values of the endocyclic bond angles are also identical.

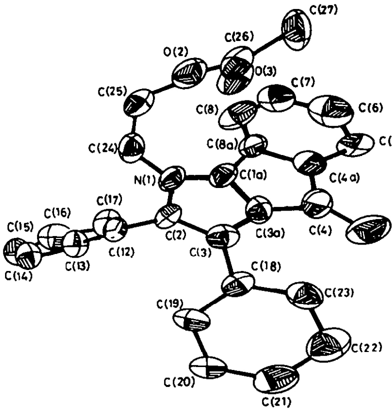

Fig. 1. *ORTEP* plot of the molecule showing thermal ellipsoids.

Table 2. *Bond lengths* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

N(1)—C(1a)	1·360 (9)	C(12)—C(13)	1·384 (11)
N(1)—C(2)	1·399 (9)	C(12)—C(17)	1·369 (11)
N(1)—C(24)	1·449 (10)	C(13)—C(14)	1·411 (10)
C(1a)—C(3a)	1·365 (10)	C(14)—C(15)	1·348 (14)
C(1a)—C(8a)	1·490 (10)	C(15)—C(16)	1·391 (13)
C(2)—C(3)	1·383 (10)	C(16)—C(17)	1·422 (10)
C(2)—C(12)	1·467 (9)	C(18)—C(19)	1·416 (9)
C(3)—C(3a)	1·454 (9)	C(18)—C(23)	1·376 (10)
C(3)—C(18)	1·483 (10)	C(19)—C(20)	1·391 (11)
C(3a)—C(4)	1·455 (9)	C(20)—C(21)	1·379 (12)
C(4)—C(4a)	1·509 (11)	C(21)—C(22)	1·358 (11)
C(4)—O(1)	1·232 (10)	C(22)—C(23)	1·383 (11)
C(4a)—C(5)	1·390 (10)	C(24)—C(25)	1·515 (11)
C(4a)—C(8a)	1·394 (11)	C(25)—O(2)	1·428 (9)
C(5)—C(6)	1·435 (13)	C(26)—C(27)	1·558 (16)
C(6)—C(7)	1·382 (13)	C(26)—O(2)	1·338 (13)
C(7)—C(8)	1·401 (10)	C(26)—O(3)	1·173 (15)
C(8)—C(8a)	1·368 (12)		
N(1)—C(1a)—C(3a)	111·0 (5)	C(4)—C(4a)—C(8a)	110·9 (6)
N(1)—C(1a)—C(8a)	136·1 (5)	C(4a)—C(4)—O(1)	125·4 (6)
C(1a)—N(1)—C(2)	107·6 (4)	C(4a)—C(5)—C(6)	114·0 (6)
N(1)—C(2)—C(3)	108·8 (5)	C(5)—C(4a)—C(8a)	122·8 (6)
N(1)—C(2)—C(12)	120·0 (5)	C(4a)—C(8a)—C(8)	121·6 (6)
C(1a)—N(1)—C(24)	126·3 (5)	C(5)—C(6)—C(7)	123·6 (7)
C(2)—N(1)—C(24)	125·4 (5)	C(6)—C(7)—C(8)	119·5 (6)
N(1)—C(24)—C(25)	112·3 (5)	C(7)—C(8)—C(8a)	118·5 (6)
C(1a)—C(3a)—C(3)	106·2 (5)	C(12)—C(13)—C(14)	119·7 (6)
C(1a)—C(3a)—C(4)	107·9 (5)	C(13)—C(12)—C(17)	119·2 (5)
C(3a)—C(1a)—C(8a)	112·9 (5)	C(12)—C(17)—C(16)	121·1 (6)
C(1a)—C(8a)—C(4a)	103·6 (5)	C(13)—C(14)—C(15)	121·0 (6)
C(1a)—C(8a)—C(8)	134·8 (6)	C(14)—C(15)—C(16)	120·5 (6)
C(2)—C(3)—C(3a)	106·4 (5)	C(15)—C(16)—C(17)	118·4 (6)
C(2)—C(3)—C(18)	127·3 (5)	C(18)—C(19)—C(20)	119·9 (5)
C(3)—C(2)—C(12)	131·1 (5)	C(19)—C(18)—C(23)	118·5 (5)
C(2)—C(12)—C(13)	120·1 (5)	C(19)—C(20)—C(21)	119·1 (6)
C(2)—C(12)—C(17)	120·6 (5)	C(20)—C(21)—C(22)	121·8 (6)
C(3)—C(3a)—C(4)	145·9 (5)	C(21)—C(22)—C(23)	119·5 (6)
C(3a)—C(3)—C(18)	126·2 (5)	C(24)—C(25)—O(2)	111·3 (6)
C(3)—C(18)—C(19)	120·3 (5)	C(25)—O(2)—C(26)	119·8 (6)
C(3)—C(18)—C(23)	121·2 (5)	C(27)—C(26)—O(2)	107·4 (7)
C(3a)—C(4)—C(4a)	104·9 (5)	C(27)—C(26)—O(3)	129·8 (8)
C(3a)—C(4)—O(1)	129·7 (6)	O(2)—C(26)—O(3)	122·7 (7)
C(4)—C(4a)—C(5)	126·4 (6)		

The difference in the O—C(sp^3) distances, between C(26)—O(2) [1·338 (13) Å] and C(25)—O(2) [1·428 (9) Å] in the group $C(27)\text{—}\underset{\underset{\displaystyle O(3)}{\|}}{C}(26)\text{—}O(2)\text{—}C(25)$ of the side chain, is attributed to a partial contribution from the resonance structure $C\text{—}\underset{\underset{\displaystyle O^-}{|}}{C}{=}O^+\text{—}C$ for this group as in ethyl [3-(1,3-dioxoindanylidene)-1-oxoindan-2-yl]acetate (Varghese, Srinivasan, Padmanabhan & Ramadas, 1986). The bond angles of the side chain conform to those reported for carboxylic esters (Dunitz & Schweizer, 1982).

The indenopyrrole fragment is essentially planar as revealed by the endocyclic torsion angles of its rings (Fig. 2). The dihedral angle between its six-membered ring and the pyrrole ring is ~2°. The phenyl rings C(12)···C(17) and C(18)···C(23) are rotated from the plane of this fragment, with the former making ~67° and the latter ~31°. These are attributed to short nonbonded contacts between C(3) and C(13) (3·178 Å) and C(3a) and C(23) (3·120 Å).

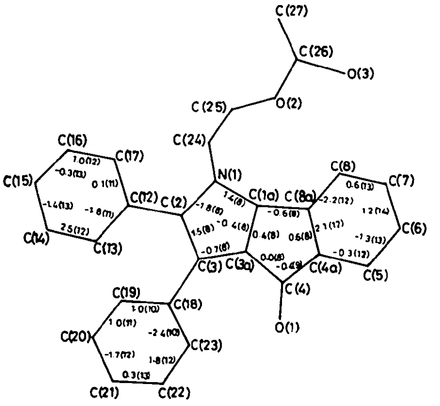

Fig. 2. Selected torsion angles (°) with e.s.d.'s in parentheses.

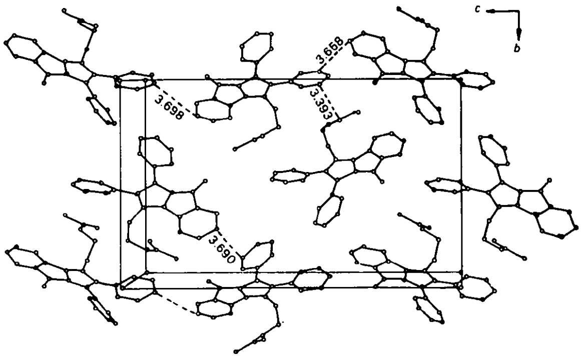

Fig. 3. Packing of molecules in the unit cell. C(23)···C(2) 3·698; C(14)···O(2) 3·393; C(22)···C(6) 3·690; C(16)···C(6) 3·658 Å.

The torsion angles τ[C(2)—N(1)—C(24)—C(25)] +88·3 (8)°, τ[N(1)—C(24)—C(25)—O(2)] +63·5 (8)° and τ[C(24)—C(25)—O(2)—C(26)] −110·4 (8)° show that the side chain assumes a folded conformation. While in the majority of cases, these angles are close to 180°, a few of alkyl-substituted esters have values around 120° (Dunitz & Schweizer, 1982).

The intermolecular contacts (Fig. 3) are van der Waals.

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6,6-Dimethyl-4-oxo-1,2-diphenyl-4,5,6,7-tetrahydroindole

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Abstract. $C_{22}H_{21}NO$, $M_r = 315{\cdot}410$, $P\bar{1}$, $a = 9{\cdot}316$ (2), $b = 9{\cdot}742$ (4), $c = 11{\cdot}057$ (2) Å, $\alpha = 98{\cdot}560$ (14), $\beta = 65{\cdot}690$ (15), $\gamma = 102{\cdot}020$ (25)°, $V = 892{\cdot}2$ Å^3, $Z = 2$, $D_x = 1{\cdot}175$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0{\cdot}32$ mm^{-1}, $F(000) = 336$, $T = 293$ K, $R = 0{\cdot}058$ for 1600 reflections. The presence of conjugation between the pyrrole N atom and the carbonyl O atom, which is believed to cause the lack of activity of the 4-keto function in unsubstituted tetrahydroindoles, is not removed by the substituents in the title compound. The cyclohexene ring assumes a distorted sofa conformation.

Introduction. A majority of 4-ketotetrahydroindoles, particularly the unsubstituted compounds, were found to be inactive, even though a few of them are good analgesic, antipsychotic and antianxiety agents (Remers, Roth & Weiss, 1971). The lack of activity was attributed to the conjugation between the pyrrole nitrogen and the carbonyl function (Weiss, Allen, Gibbs, Pidacks, Poletto & Remers, 1968). The title compound is one of a series of 4-ketotetrahydroindole derivatives prepared with the intention of delocalizing the lone pair of electrons of the N atom into the aromatic nucleus and activating the 4-keto function (Ramadas, Ramana & Padmanabhan, 1978).

Experimental. Title compound prepared by condensing 5,5-dimethyl-2-phenacyl-1,3-cyclohexanedione with aniline in refluxing glacial acetic acid. Recrystallization (by slow evaporation) from ethanol gave plate-shaped crystals. Approximate dimensions of crystal: 0·55 × 0·20 × 0·60 mm. Enraf–Nonius CAD-4 automated diffractometer, graphite monochromator. Intensities measured with NaI(Tl) scintillation counter interfaced with PDP/8a microcomputer. Cell parameters refined by least-squares method on basis of 25 2θ values. $2 < 2\theta < 30°$. No significant variation in intensities of 2 check reflections, monitored every 100 reflections. Lp correction. Absorption neglected. 3054 unique reflections measured, 1600 with $I > 3\sigma(I)$. $h = \pm 7$, $k = \pm 9$, $l = \pm 11$. Space group from intensity statistics. Structure solved by multisolution technique using *MULTAN80* (Main *et al.*, 1980). Refinement of structure by least-squares method, H-atom positions from difference Fourier maps at an intermediate stage

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