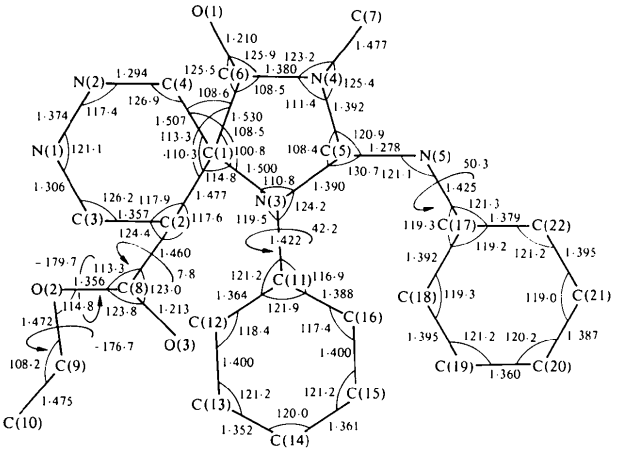

Fig. 1. Atomic numbering, bond distances (Å) and bond angles (°) for non-hydrogen atoms. E.s.d.'s are in the range 0·007–0·014 Å for distances and 0·3–0·5° for angles. Some torsion angles of interest are also given.

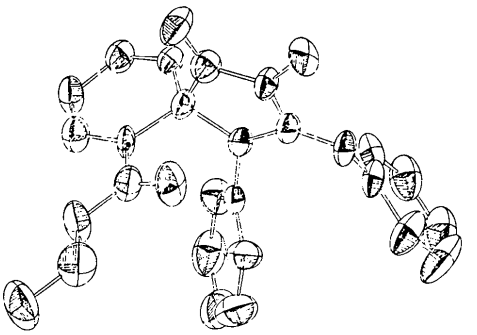

Fig. 2. An *ORTEP* view of the main molecule. Ellipsoids of the non-hydrogen atoms are at 50% probability level.

No special features were found in the molecular packing, all the intermolecular distances being in the normal range. An *ORTEP* drawing (Fig. 2) shows the stereochemistry of the molecule.

The anisotropic temperature factors of the non-hydrogen atoms were analysed by the method of Schoemaker & Trueblood (1968).

As expected, the whole molecule does not behave as a rigid body but a satisfactory fit was obtained for the phenyl rings and the central ring skeleton considered separately, excluding the side chain. For these fragments the r.m.s. values ΔU_{ij} are of the same order as the average value (0·0043 Å^2) of $\sigma(U_{ij})$.

Bond lengths have not been corrected for librational shortening, the corrections being smaller than the corresponding e.s.d.'s.

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Diethyl 2,6-Dimethyl-4-phenyl-1,4-dihydro-3,5-pyridinedicarboxylate

BY A. HEMPEL* AND M. P. GUPTA†

Department of Physics, University of York, York YO1 5DD, England

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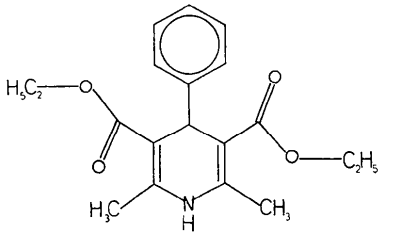
Abstract. $C_{19}H_{23}NO_4$, monoclinic, $P2_1/c$, $a = 9{\cdot}73$ (1), $b = 7{\cdot}39$ (1), $c = 24{\cdot}32$ (2) Å, $\beta = 92{\cdot}62$ (5)°, $V = 1747$ Å^3, $Z = 4$, $D_m = 1{\cdot}26$, $D_x = 1{\cdot}25$ g cm^{-3}, $F(000) = 704$. The structure was solved by direct methods and refined by full-matrix least squares to a final $R = 0{\cdot}077$ for 4014 reflections. The dihydropyridine ring adopts a flat-boat conformation. The phenyl ring is approximately perpendicular to the dihydropyridine ring.

Introduction. This study was undertaken to establish the conformational features of the title compound (I). The crystals were yellow and needle-like and were elongated along the *b* axis. The space group was found

* Present address: Department of Pharmaceutical Technology and Biochemistry, Technical University, 80-952 Gdansk, Poland.

† Present address: Department of Physics, University of Ranchi, Ranchi 834008, India.

from precession photographs. A crystal of approximately 0·4 × 0·6 × 0·3 mm was used to determine the cell parameters and to collect intensity data on a Hilger & Watts Y290 four-circle diffractometer. Lattice parameters were refined by a least-squares fit of 23 high-angle reflections. The θ–2θ scan technique was used to collect 4227 unique intensities up to $\theta_{max} = 28°$ with Mo $K\alpha$ radiation. The structure was solved by direct methods using the *MULTAN* 78 package (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) and refined by full-matrix least-squares methods using *SHELX* 76 (Sheldrick, 1976). All non-methyl H atoms were found from a difference map. The positions of the methyl H atoms were calculated geometrically. During the refinement methyl residues were treated as rigid groups and the remaining H atoms were 'riding' on corresponding atoms. Anisotropic temperature factors for non-hydrogen atoms and a single isotropic temperature factor for all H atoms were refined. Throughout the refinement 4014 structure amplitudes were used. The function minimized was $\sum \|F_o| - |F_c\|^2$. The final R index was 0·077 where $R = \sum \|F_o| - |F_c\| / \sum |F_o|$. The final difference map contained no residual electron density higher than 0·35 e Å^{-3}. All the calculations were carried out on the University of York DEC-10 computer.*



(I)

Discussion. The atomic positional parameters are presented in Tables 1 and 2. Bond lengths and angles are given in Tables 3 and 4. The molecule shows close conformational similarity to diethyl 2,6-dimethyl-4-(3-pyridyl)-1,4-dihydro-3,5-pyridinedicarboxylate (Krajewski, Urbanczyk-Lipkowska & Gluzinski, 1977*a*). The conformational details and atom numbering of (I) are shown in Fig. 1. The 1,4-dihydropyridine ring adopts a flat-boat conformation. This feature was reported earlier for *N*-phenyl-1,4-dihydronicotinamide (Karle, 1961) and for 3,5-diacetyl-2,6-dimethyl-4-(3-pyridyl)-1,4-dihydropyridine (Krajewski, Urbanczyk-Lipkowska & Gluzinski, 1977*b*). The two ethoxycarbonyl groups are twisted in opposite directions and the plane of the phenyl ring is approximately perpendicular to the dihydropyridine ring. The packing of the molecules in the crystal is illustrated in Fig. 2. A weak linear intermolecular hydrogen-bond system involving N(1)—H(10)···O(3) is observed [N(1)···O(3) 2·98 Å.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33999 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional coordinates of non-hydrogen atoms* (×10⁴)

	x	*y*	*z*
N(1)	8358 (3)	6273 (3)	10500 (1)
C(2)	9407 (4)	5947 (4)	10890 (1)
C(3)	9582 (3)	4235 (4)	11079 (1)
C(4)	8484 (3)	2821 (4)	10935 (1)
C(5)	7842 (3)	3200 (4)	10366 (1)
C(6)	7717 (3)	4934 (4)	10190 (1)
C(7)	6942 (4)	5655 (5)	9686 (1)
C(8)	10248 (4)	7601 (5)	11038 (2)
C(9)	10763 (3)	3764 (5)	11452 (1)
C(10)	11856 (4)	1345 (6)	11962 (2)
C(11)	11432 (5)	1624 (8)	12538 (2)
C(12)	7327 (3)	1610 (4)	10067 (1)
C(13)	6011 (4)	448 (4)	9296 (1)
C(14)	5179 (6)	1222 (6)	8824 (2)
C(15)	7429 (3)	2793 (4)	11374 (1)
C(16)	7672 (3)	1782 (5)	11850 (1)
C(17)	6744 (4)	1834 (6)	12276 (1)
C(18)	5574 (4)	2860 (6)	12220 (1)
C(19)	5300 (4)	3844 (5)	11754 (1)
C(20)	6235 (3)	3812 (4)	11328 (1)
O(1)	11637 (3)	4780 (4)	11634 (1)
O(2)	10792 (2)	1974 (3)	11567 (1)
O(3)	7620 (3)	68 (3)	10198 (1)
O(4)	6489 (2)	1962 (3)	9633 (1)

Table 2. *Hydrogen coordinates and thermal parameters* (Å) (*all* × 10⁴)

	x	*y*	*z*	*U*
H(10)	8165 (3)	7387 (3)	10409 (1)	629 (119)
H(40)	8872 (3)	1665 (4)	10953 (1)	228 (68)
H(71)	6427 (4)	4573 (5)	9460 (1)	2267 (221)
H(72)	7607 (4)	6374 (5)	9417 (1)	1935 (206)
H(73)	6186 (4)	6576 (5)	9838 (1)	1416 (181)
H(81)	11184 (4)	7295 (5)	11275 (2)	1744 (196)
H(82)	9553 (4)	8327 (5)	11293 (2)	2088 (218)
H(83)	10484 (4)	8426 (5)	10688 (2)	1246 (180)
H(101)	12713 (4)	2057 (6)	11909 (2)	736 (132)
H(102)	12087 (4)	29 (6)	11813 (2)	1266 (161)
H(111)	10544 (5)	764 (8)	12578 (2)	1148 (172)
H(112)	11185 (5)	2984 (8)	12664 (2)	1279 (188)
H(113)	12277 (5)	1114 (8)	12797 (2)	1432 (183)
H(131)	6868 (4)	−199 (4)	9165 (1)	644 (119)
H(132)	5553 (4)	−379 (4)	9555 (1)	649 (119)
H(141)	4296 (6)	1876 (6)	8990 (2)	1386 (185)
H(142)	4838 (6)	131 (6)	8555 (2)	1276 (163)
H(143)	5750 (6)	2193 (6)	8594 (2)	1005 (149)
H(160)	8553 (3)	1123 (5)	11863 (1)	481 (89)
H(170)	6797 (4)	1022 (6)	12603 (1)	650 (116)
H(180)	5081 (4)	2950 (6)	12547 (1)	575 (104)
H(190)	4385 (4)	4454 (5)	11686 (1)	767 (133)
H(200)	6047 (3)	4468 (4)	10977 (1)	430 (92)

Table 3. *Bond lengths* (Å)

N(1)–C(2)	1·381 (4)	O(2)–C(10)	1·456 (4)
C(2)–C(3)	1·354 (4)	C(5)–C(12)	1·458 (4)
C(2)–C(8)	1·505 (5)	O(3)–C(12)	1·213 (4)
C(3)–C(4)	1·524 (4)	O(4)–C(12)	1·330 (4)
C(3)–C(9)	1·473 (4)	C(13)–C(14)	1·489 (6)
C(4)–C(5)	1·517 (4)	O(4)–C(13)	1·450 (4)
C(4)–C(15)	1·516 (4)	C(4)–C(15)	1·516 (4)
C(5)–C(6)	1·355 (4)	C(15)–C(16)	1·389 (4)
C(5)–C(12)	1·458 (4)	C(15)–C(20)	1·384 (4)
N(1)–C(6)	1·377 (4)	C(16)–C(17)	1·405 (5)
C(6)–C(7)	1·507 (4)	C(17)–C(18)	1·369 (5)
O(1)–C(9)	1·204 (4)	C(18)–C(19)	1·362 (5)
O(2)–C(9)	1·352 (4)	C(20)–C(19)	1·410 (5)
C(10)–C(11)	1·493 (6)		

Table 4. *Bond angles* (°)

C(2)–N(1)–C(6)	123·6 (3)	O(2)–C(9)–C(3)	111·6 (3)
C(3)–C(2)–N(1)	118·2 (3)	O(2)–C(9)–O(1)	121·7 (3)
C(8)–C(2)–N(1)	113·5 (3)	O(2)–C(10)–C(9)	117·2 (3)
C(8)–C(2)–C(3)	128·2 (3)	O(2)–C(10)–C(11)	110·8 (3)
C(4)–C(3)–C(2)	119·1 (3)	O(3)–C(12)–C(5)	123·7 (3)
C(9)–C(3)–C(2)	120·8 (3)	O(4)–C(12)–C(5)	115·2 (2)
C(9)–C(3)–C(4)	119·9 (3)	O(4)–C(12)–O(3)	121·3 (3)
C(5)–C(4)–C(3)	109·7 (2)	O(4)–C(13)–C(14)	106·8 (3)
C(15)–C(4)–C(3)	109·8 (2)	C(16)–C(15)–C(4)	120·0 (3)
C(15)–C(4)–C(5)	112·4 (2)	C(20)–C(15)–C(4)	121·9 (3)
C(6)–C(5)–C(4)	119·4 (2)	C(20)–C(15)–C(16)	118·0 (3)
C(12)–C(5)–C(4)	115·0 (2)	C(17)–C(16)–C(15)	120·6 (3)
C(12)–C(5)–C(6)	125·5 (3)	C(18)–C(17)–C(16)	120·1 (3)
C(5)–C(6)–N(1)	118·3 (3)	C(19)–C(18)–C(17)	120·5 (3)
C(7)–C(6)–N(1)	112·9 (3)	C(20)–C(19)–C(18)	119·6 (3)
C(7)–C(6)–C(5)	128·8 (3)	C(19)–C(20)–C(15)	121·1 (3)
O(1)–C(9)–C(3)	126·7 (3)	C(13)–O(4)–C(12)	117·8 (3)

O(3)···H(10) 2·11 Å, O(3) being at x, 1 + y, z] to form an infinite chain of the molecules along the b axis.

We thank Professor M. M. Woolfson for the use of his laboratory and the University of York for computing facilities. One of us (MPG) is indebted to the Royal Society and the Indian National Science Academy for an award under the Scientists' Exchange Visit Programme. We also thank Professor J. N. Chatterjee of the Patna University, India, for the gift of the crystals.

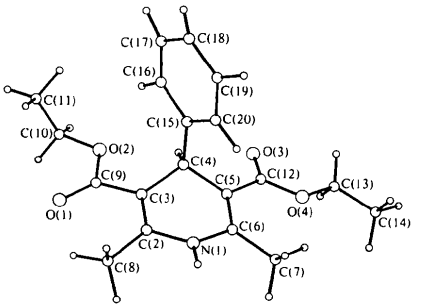


Fig. 1. The molecule and atom numbering.

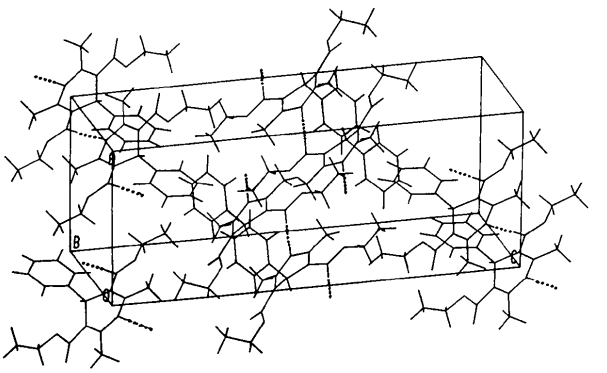


Fig. 2. Packing diagram.

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2,3-Dimethyl-2,3-butanediol (Pinacol)

BY G. A. JEFFREY AND A. ROBBINS

Department of Crystallography, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, *USA*

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Abstract. $C_6H_{14}O_2$, M_r = 118·17, m.p. 39–40°C, monoclinic, $C2/c$, Z = 16, a = 16·456 (1), b = 16·320 (2), c = 11·147 (1) Å, β = 91·54 (1)°, D_x = 1·049, D_m = 1·042 g cm^{-3} (flotation in ether–bromobenzene at 20°C). The structure was solved with *MULTAN* and refined by full-matrix anisotropic least-