

Tableau 1. Coordonnées atomiques et facteurs d'agitation thermique isotrope équivalents (Å²)

$$U_{eq} = (1/3) \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	U _{eq}
S(1)	0,53344 (3)	0,78940 (6)	0,0185 (1)	0,0529 (5)
S(2)	0,42171 (3)	0,46429 (6)	0,0733 (1)	0,0515 (5)
N(1)	0,36711 (9)	0,7733 (2)	-0,1311 (3)	0,046 (1)
N(2)	0,42196 (9)	0,8030 (2)	-0,0434 (3)	0,047 (2)
N(3)	0,46100 (9)	0,6408 (2)	0,0007 (3)	0,043 (1)
C(1)	0,4681 (1)	0,7443 (2)	-0,0079 (4)	0,042 (2)
C(2)	0,4205 (1)	0,5873 (2)	0,0597 (3)	0,040 (2)
C(3)	0,3739 (1)	0,6484 (2)	0,1088 (4)	0,043 (2)
C(4)	0,3442 (1)	0,7016 (2)	-0,0602 (4)	0,042 (2)
C(5)	0,4285 (1)	0,9120 (3)	-0,0536 (6)	0,065 (3)
C(6)	0,2865 (1)	0,6715 (2)	-0,1510 (4)	0,042 (2)
C(7)	0,2654 (1)	0,5772 (2)	-0,1247 (5)	0,059 (2)
C(8)	0,2112 (1)	0,5512 (3)	-0,2118 (6)	0,069 (3)
C(9)	0,1776 (1)	0,6184 (3)	-0,3244 (5)	0,060 (2)
C(10)	0,1985 (1)	0,7118 (3)	-0,3520 (4)	0,051 (2)
C(11)	0,2523 (1)	0,7386 (2)	-0,2655 (4)	0,046 (2)

Tableau 2. Paramètres géométriques (Å, °)

S(1)—C(1)	1,660 (3)	C(7)—C(8)	1,384 (4)
S(2)—C(2)	1,642 (3)	C(8)—C(9)	1,378 (5)
N(1)—N(2)	1,411 (3)	C(8)—H(8)	1,06 (1)
N(1)—C(4)	1,273 (3)	C(9)—C(10)	1,373 (4)
N(2)—C(1)	1,344 (3)	C(10)—C(11)	1,376 (4)
N(2)—C(5)	1,463 (4)	H(1)—S(2 ⁱ)	2,33 (1)
N(3)—C(1)	1,392 (3)	N(3)—S(2 ⁱ)	3,302 (2)
N(3)—C(2)	1,354 (3)	S(1)—S(2 ⁱ)	3,656 (1)
C(2)—C(3)	1,492 (4)	S(1)—C(9 ⁱⁱ)	3,653 (3)
C(3)—C(4)	1,504 (4)	S(2)—N(3 ⁱⁱⁱ)	3,455 (2)
C(4)—C(6)	1,477 (3)	C(3)—C(10 ^{iv})	3,338 (4)
C(6)—C(7)	1,384 (4)	C(10)—C(11 ^v)	3,386 (4)
C(6)—C(11)	1,391 (4)		
N(2)—N(1)—C(4)	117,4 (2)	N(1)—C(4)—C(3)	122,2 (2)
N(1)—N(2)—C(1)	126,3 (2)	N(1)—C(4)—C(6)	117,3 (2)
N(1)—N(2)—C(5)	110,8 (2)	C(3)—C(4)—C(6)	120,5 (2)
C(1)—N(2)—C(5)	119,6 (2)	C(4)—C(6)—C(7)	121,3 (3)
C(1)—N(3)—C(2)	129,8 (2)	C(4)—C(6)—C(11)	119,8 (3)
S(1)—C(1)—N(2)	122,8 (2)	C(7)—C(6)—C(11)	118,9 (3)
S(1)—C(1)—N(3)	118,4 (2)	C(6)—C(7)—C(8)	119,9 (3)
N(2)—C(1)—N(3)	118,7 (2)	C(7)—C(8)—C(9)	120,7 (3)
S(2)—C(2)—N(3)	122,7 (2)	C(8)—C(9)—C(10)	119,6 (3)
S(2)—C(2)—C(3)	122,3 (2)	C(9)—C(10)—C(11)	120,3 (3)
N(3)—C(2)—C(3)	115,0 (2)	C(6)—C(11)—C(10)	120,7 (3)
C(2)—C(3)—C(4)	107,7 (2)	N(3)—H(1)—S(2 ⁱ)	172 (3)
N(2)—N(1)—C(4)—C(6)	179,25	C(1)—N(3)—C(2)—C(3)	5,51
C(4)—N(1)—N(2)—C(1)	57,92	S(2)—C(2)—N(3)—C(1)	-175,40
N(1)—N(2)—C(1)—N(3)	-22,44	N(3)—C(2)—C(3)—C(4)	62,53
S(1)—C(1)—N(2)—N(1)	155,17	S(2)—C(2)—C(3)—C(4)	-116,57
C(5)—N(2)—N(1)—C(4)	-143,01	C(2)—C(3)—C(4)—C(6)	109,17
N(2)—C(1)—N(3)—C(2)	-33,67	N(1)—C(4)—C(6)—C(11)	-21,73
C(2)—N(3)—C(1)—S(1)	148,61	N(1)—C(4)—C(6)—C(7)	158,21

Codes de symétrie: (i) $1 - x, 1 - y, -z$; (ii) $\frac{1}{2} + x, \frac{3}{2} - y, \frac{1}{2} + z$; (iii) $x, 1 - y, \frac{1}{2} + z$; (iv) $\frac{1}{2} - x, \frac{3}{2} - y, -z$; (v) $\frac{1}{2} - x, \frac{3}{2} - y, -1 - z$.

L'enregistrement a été effectué à l'aide d'un diffractomètre équipé d'un monochromateur en graphite, balayage $\omega/2\theta$; $\Delta\omega = (0,80 + 0,34 \tan\theta)^\circ$; vitesse de balayage variable de 1,8 à 20,1° min⁻¹ en ω en fonction de l'intensité du pic de diffraction. Les atomes S, N et C ont été localisés par les méthodes directes à l'aide du programme *SHELXS86* (Sheldrick, 1985). La structure a été résolue par des synthèses de Fourier différence successives et affinements par moindres carrés en matrice totale, en utilisant le programme *CRYSTALS* (Watkin, Carruthers & Betteridge, 1988), adapté sur un micro-ordinateur Dell 333D (processeur 80386, 33 MHz). Après l'affinement anisotrope de tous les atomes, les atomes d'hydrogène ont été localisés par Fourier différence. Leurs coordonnées, ainsi qu'un facteur d'agitation thermique isotrope commun, ont été

introduits dans l'affinement. Au total, 180 paramètres variables ont été considérés: facteur d'échelle, facteur d'extinction secondaire (Larson, 1970), coordonnées atomiques, facteurs d'agitation thermique, isotrope pour les atomes d'hydrogène et anisotropes pour les autres atomes.

Les listes des facteurs de structure, des facteurs d'agitation thermique anisotrope, des coordonnées des atomes d'hydrogène, des distances et angles des atomes d'hydrogène, ont été déposées au dépôt d'archives de l'UICr (Référence: DU1107). On peut en obtenir des copies en s'adressant à: The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, Angleterre.

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Methyl 1-Hydroxy-2,4,6-trimethoxy-carbonyl-3-oxo-1-cyclohexaneacetate

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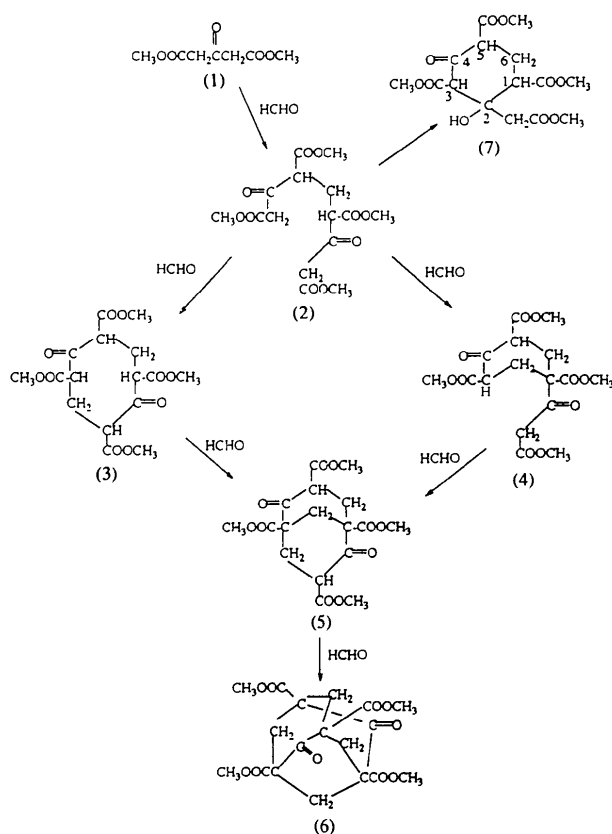
Abstract

The structure of the title compound, C₁₅H₂₀O₁₀, agrees with an earlier determination by ¹H NMR and our own determination by ¹³C NMR. The six-membered ring has

a chair conformation. All but one of the carbonyl O atoms are on one side of the least-squares plane of this ring, while all methoxy O atoms are on the opposite side.

Comment

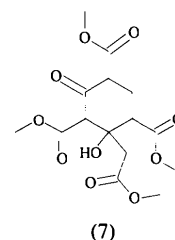
Some years ago, Prelog, Metzler & Jeger (1947) reacted dimethyl acetone-1,3-dicarboxylate, (1), with various 1,3-diketones to form phenol derivatives (see scheme below). Later, Weiss and co-workers (Weiss & Edwards 1968; Weiss *et al.*, 1976) reported that the reaction of (1) with 1,2-diketones leads to substituted bicyclo[3.3.0]octanes. Later still, one of us reported that some 1,3-dialdehydes react with (1) to give bicyclo[3.3.1]nonanes instead of phenols (Sands, 1983).



A logical extension of the above was to see if the reaction of formaldehyde with (1) would produce compounds (3), (4), (5) (Meerwein's ester; Meerwein & Schürmann, 1913) or (6) (an adamantane derivative), all of which would depend on the expected initial formation of (2).

A compound which we hoped to be (2) was isolated. The X-ray structure, however, showed it to be (7), an isomer of (2) resulting from an internal aldol condensation of (2). We then discovered that Haensel

& Haller (1970) had already reported the formation of (7) by this reaction. The present crystal structure and 400 MHz ^{13}C spectrum (assignments supplied in the supplementary material) agree with the structure for (7) that Haensel & Haller were able to establish by ^1H NMR spectroscopy.



Since C atoms (1)–(6) are alternately above and below their least-squares plane [distances: C(1) -0.28 , C(2) 0.29 , C(3) -0.27 , C(4) 0.24 , C(5) -0.22 , C(6) 0.24 Å], the ring has a chair conformation. The hydroxy and all but one of the carbonyl O atoms are on the same (+) side of the least-squares plane of the ring [distances: O(1) 1.01 , O(3) 1.70 , O(4) -2.42 , O(6) 1.10 , O(8) 0.93 , O(9) 1.13 Å]. However, all of the methoxy O atoms are on the opposite (–) side of the ring plane [distances: O(2) -0.93 , O(5) -1.55 , O(7) -0.85 , O(10) -0.43 Å]. These O-atom dispositions are also confirmed by examination of the values for the torsion angles in Table 2 and the view of the molecule shown in Fig. 1.

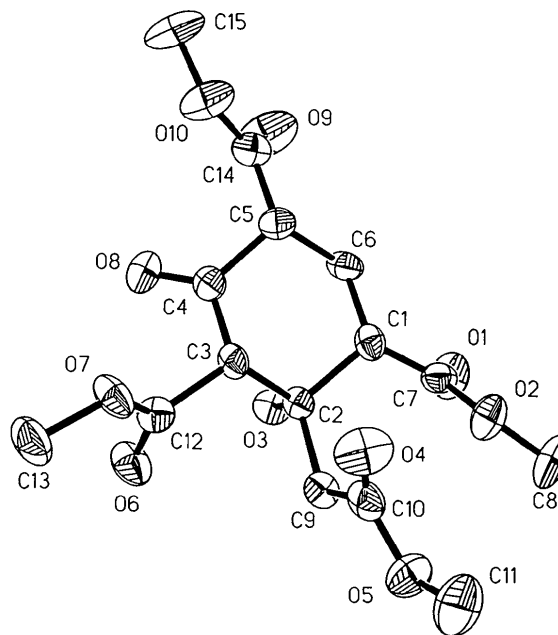


Fig. 1. Perspective view of the title compound showing 50% probability ellipsoids.

Experimental

Crystals of methyl 1-hydroxy-2,4,6-trimethoxycarbonyl-3-oxo-1-cyclohexaneacetate were recrystallized from methanol.

Crystal data

C ₁₅ H ₂₀ O ₁₀	Mo K α radiation
$M_r = 360.31$	$\lambda = 0.71073 \text{ \AA}$
Monoclinic	Cell parameters from 21 reflections
$P2_1/c$	$\theta = 3.8\text{--}7.8^\circ$
$a = 5.564 (2) \text{ \AA}$	$\mu = 0.121 \text{ mm}^{-1}$
$b = 17.816 (11) \text{ \AA}$	$T = 288 \text{ K}$
$c = 17.028 (9) \text{ \AA}$	Prism
$\beta = 92.10 (4)^\circ$	$0.46 \times 0.20 \times 0.050 \text{ mm}$
$V = 1687 (2) \text{ \AA}^3$	Colorless
$Z = 4$	
$D_x = 1.419 \text{ Mg m}^{-3}$	

Data collection

Siemens P3 diffractometer	$\theta_{\max} = 25^\circ$
$\theta/2\theta$ scans	$h = 0 \rightarrow 6$
Absorption correction: none	$k = 0 \rightarrow 19$
2498 measured reflections	$l = -18 \rightarrow 18$
2206 independent reflections	1 standard reflection monitored every 50 reflections
1059 observed reflections	intensity decay: 0.5%
$[I \geq 2\sigma(I)]$	
$R_{\text{int}} = 0.055$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 0.12P]$
$R(F) = 0.071$	where $P = [\max(F_o^2, 0) + 2F_c^2]/3$
$wR(F^2) = 0.127$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.027$	$\Delta\rho_{\max} = 0.240 \text{ e \AA}^{-3}$
1059 reflections	$\Delta\rho_{\min} = -0.225 \text{ e \AA}^{-3}$
226 parameters	Atomic scattering factors from SHELXL93 (Sheldrick, 1993)
H atoms refined as riding model	

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	U_{eq}
O(1)	1.2896 (9)	0.1256 (3)	0.4634 (3)	0.050 (1)
O(2)	1.0509 (8)	0.0422 (3)	0.4017 (3)	0.046 (1)
O(3)	1.1147 (7)	0.2550 (2)	0.3399 (2)	0.036 (1)
O(4)	0.6120 (9)	0.0791 (3)	0.2688 (3)	0.056 (2)
O(5)	0.9326 (9)	0.0287 (3)	0.2126 (3)	0.051 (1)
O(6)	0.8296 (8)	0.3101 (3)	0.1999 (3)	0.049 (1)
O(7)	0.4380 (8)	0.2893 (3)	0.2101 (2)	0.041 (1)
O(8)	0.6506 (9)	0.3706 (3)	0.3649 (3)	0.054 (2)
O(9)	0.7591 (10)	0.3502 (3)	0.5703 (3)	0.078 (2)
O(10)	0.3875 (9)	0.3559 (3)	0.5166 (3)	0.058 (2)
C(1)	0.8968 (11)	0.1634 (3)	0.4109 (3)	0.032 (2)
C(2)	0.9231 (11)	0.2026 (3)	0.3296 (3)	0.027 (2)
C(3)	0.6858 (11)	0.2458 (3)	0.3144 (3)	0.030 (2)
C(4)	0.6598 (11)	0.3045 (4)	0.3778 (4)	0.032 (2)
C(5)	0.6465 (12)	0.2705 (3)	0.4597 (3)	0.034 (2)
C(6)	0.8729 (11)	0.2221 (4)	0.4765 (3)	0.035 (2)
C(7)	1.1039 (14)	0.1111 (4)	0.4300 (4)	0.036 (2)
C(8)	1.2404 (14)	-0.0126 (4)	0.4070 (5)	0.066 (3)

C(9)	0.9848 (12)	0.1484 (3)	0.2635 (4)	0.032 (2)
C(10)	0.8165 (14)	0.0827 (4)	0.2509 (4)	0.039 (2)
C(11)	0.7970 (15)	-0.0379 (4)	0.1907 (5)	0.072 (3)
C(12)	0.6678 (12)	0.2850 (4)	0.2354 (4)	0.032 (2)
C(13)	0.3833 (13)	0.3269 (4)	0.1374 (4)	0.059 (2)
C(14)	0.6117 (14)	0.3298 (4)	0.5214 (4)	0.043 (2)
C(15)	0.3285 (15)	0.4159 (4)	0.5700 (5)	0.073 (3)

Table 2. Selected geometric parameters (\AA , $^\circ$)

O(1)—C(7)	1.189 (8)	O(10)—C(15)	1.449 (8)
O(2)—C(7)	1.347 (7)	C(1)—C(7)	1.507 (9)
O(2)—C(8)	1.437 (7)	C(1)—C(6)	1.538 (8)
O(3)—C(2)	1.423 (6)	C(1)—C(2)	1.564 (8)
O(4)—C(10)	1.190 (8)	C(2)—C(9)	1.531 (8)
O(5)—C(10)	1.342 (8)	C(2)—C(3)	1.543 (8)
O(5)—C(11)	1.448 (7)	C(3)—C(4)	1.513 (8)
O(6)—C(12)	1.190 (7)	C(3)—C(12)	1.516 (8)
O(7)—C(12)	1.336 (7)	C(4)—C(5)	1.525 (8)
O(7)—C(13)	1.432 (7)	C(5)—C(14)	1.508 (9)
O(8)—C(4)	1.198 (7)	C(5)—C(6)	1.545 (8)
O(9)—C(14)	1.203 (8)	C(9)—C(10)	1.508 (9)
O(10)—C(14)	1.331 (8)		
C(7)—O(2)—C(8)	116.5 (5)	C(3)—C(4)—C(5)	112.8 (5)
C(10)—O(5)—C(11)	117.2 (6)	C(14)—C(5)—C(4)	111.8 (5)
C(12)—O(7)—C(13)	118.4 (5)	C(14)—C(5)—C(6)	112.8 (6)
C(14)—O(10)—C(15)	116.9 (6)	C(4)—C(5)—C(6)	108.9 (5)
C(7)—C(1)—C(6)	110.4 (5)	C(1)—C(6)—C(5)	109.7 (5)
C(7)—C(1)—C(2)	111.8 (5)	O(1)—C(7)—O(2)	122.9 (7)
C(6)—C(1)—C(2)	110.6 (5)	O(1)—C(7)—C(1)	127.8 (6)
O(3)—C(2)—C(9)	108.5 (5)	O(2)—C(7)—C(1)	109.3 (6)
O(3)—C(2)—C(3)	109.0 (5)	C(10)—C(9)—C(2)	116.0 (6)
C(9)—C(2)—C(3)	114.0 (5)	O(4)—C(10)—O(5)	124.6 (7)
O(3)—C(2)—C(1)	106.1 (5)	O(4)—C(10)—C(9)	126.8 (7)
C(9)—C(2)—C(1)	113.6 (5)	O(5)—C(10)—C(9)	108.5 (6)
C(3)—C(2)—C(1)	105.3 (5)	O(6)—C(12)—O(7)	123.2 (6)
C(4)—C(3)—C(12)	108.1 (5)	O(6)—C(12)—C(3)	126.7 (6)
C(4)—C(3)—C(2)	109.2 (5)	O(7)—C(12)—C(3)	110.1 (6)
C(12)—C(3)—C(2)	114.0 (5)	O(9)—C(14)—O(10)	123.4 (7)
O(8)—C(4)—C(3)	123.5 (6)	O(9)—C(14)—C(5)	126.3 (7)
O(8)—C(4)—C(5)	123.8 (6)	O(10)—C(14)—C(5)	110.2 (6)
O(1)—C(7)—C(1)—C(2)	89.4 (9)		
O(1)—C(7)—C(1)—C(6)	-34.3 (10)		
O(3)—C(2)—C(3)—C(4)	-51.3 (6)		
O(3)—C(2)—C(1)—C(6)	52.3 (6)		
O(4)—C(10)—C(9)—C(2)	23.6 (11)		
O(6)—C(12)—C(3)—C(4)	90.8 (9)		
O(8)—C(4)—C(5)—C(6)	-123.3 (7)		
O(8)—C(4)—C(3)—C(2)	118.1 (7)		
O(9)—C(14)—C(5)—C(4)	-108.5 (8)		
C(10)—C(9)—C(2)—C(3)	-65.7 (7)		

The complete structural formula was initially unknown. Once subsequent refinement (SHELXL93; Sheldrick, 1993) and electron density map (SHELXTL/PC; Sheldrick, 1990) analysis yielded atoms with reasonable U_{iso} values, a comparison with spectral data confirmed the proposed structure. During refinement, H atoms were fixed at ideal positions riding on their associated non-H atom.

Data collection: P3/P4-PC Diffractometer Program (Siemens, 1991a). Cell refinement: P3/P4-PC Diffractometer Program. Data reduction: XDISK (Siemens, 1991b). Structure solution: XS (Siemens, 1990). Structure refinement: SHELXL93. Molecular graphics: SHELXTL/PC. Preparation of material for publication: SHELXTL/PC.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and 400 MHz ¹³C peak assignments have been deposited with the IUCr (Reference: SZ1017). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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3-Nitrobiphenyl

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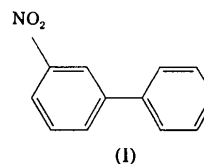
Abstract

The crystal structure of 3-nitrobiphenyl, $C_{12}H_9NO_2$, has been determined as a part of a systematic study of crystallization and crystal growth of biphenyl derivatives. It crystallizes with two similar molecules in the asymmetric unit. Unlike biphenyl itself, the torsion angles between the phenyl rings in each molecule are $-26(1)$ and $23(1)^\circ$. The nitro groups are parallel to the phenyl groups [$\tau = -6(1)$ and $-4(1)^\circ$].

Comment

The title biphenyl, (I), and its derivatives have been studied extensively in the past because of the differences found in the inter-ring torsion angle, φ , in the solid state (Hargreaves & Rizvi, 1962; Charbonneau & Delugeard,

1976, 1977; Brock, Blackburn & Haller, 1984; Brock & Haller, 1984b; Brock & Minton, 1989; Samdal, 1985) and the gas phase (Almenningen & Bastiansen, 1958; Bastiansen & Traetteberg, 1962). These systems have also been investigated because of the differences found in the dihedral angle between the phenyl rings (Cailleau & Baudour, 1979; Brock, 1980, and references therein; Sutherland & Rawas, 1983).



In continuation of our research on the systematic analysis of growth conditions and morphology modifiers for the preparation of substituted biphenyls from organic solvents (Rajnikant, Watkin & Tranter, 1995a,b), the crystal structure of the title compound, (I), was determined.

A perspective view of the molecule with atomic labelling is depicted in Fig. 1 and the unit-cell packing is shown in Fig. 2.

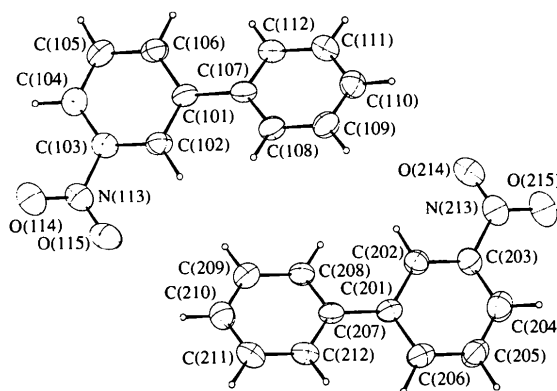


Fig. 1. View of the two independent molecules along the a axis. The molecules are separated in the view direction by approximately $a/2$. The ellipsoids are drawn at the 50% probability level.

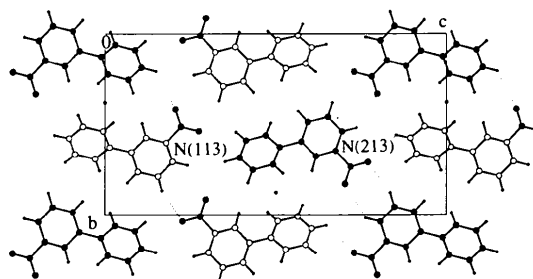


Fig. 2. The layer of molecules lying close to the plane perpendicular to the a axis at $x \approx \frac{1}{2}$. The molecules of types 1 and 2 are shown by open and filled circles, respectively. The pseudo-centres of symmetry at $\frac{9}{16}$, $\frac{3}{8}$, 0 and $\frac{7}{16}$, $\frac{7}{8}$, $\frac{1}{2}$ are shown. $O \cdots H$ contacts less than 3.0 Å are shown dotted.

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