and min. height in final $\Delta\rho$ map 0·19 and $-0·15$ e Å^{-3} respectively. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974) were used. Atomic parameters are given in Table 1,* and selected bond distances and angles in Table 2. Fig. 1 shows a thermal ellipsoid plot with the atom numbering. Only the major orientation of the disordered methyl group is shown.

Related literature. The structure of 5-phenyl-2-[4-(5-phenyl-2-oxazolyl)phenyl]oxazole is reported by Ambats & Marsh (1965). In this compound all rings are virtually coplanar.

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52653 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of 2-Pyridyl 4-Nitrobenzoate

BY MAREK L. GŁÓWKA AND IWONA IWANICKA

Institute of General Chemistry, Technical University of Łódź, Zwirki 36, 90–924 *Łódź, Poland*

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Abstract. $C_{12}H_8N_2O_4$, $M_r = 244·2$, monoclinic, $P2_1/c$, $Z = 4$, $a = 3·866$ (1), $b = 26·913$ (3), $c = 10·638$ (1) Å, $\beta = 90·14$ (1)°, $V = 1106·9$ Å^3, $D_x = 1·46$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, Ni filter, $\mu = 0·85$ mm^{-1}, $F(000) = 504$, $T = 293$ K, $R = 0·046$ and $wR = 0·053$ for 1269 observed intensities. The molecules in the crystal show partial stacking with distances of 3·47 Å (pyridine) and 3·38 Å (benzene) between parallel aromatic rings.

Experimental. The compound crystallized from acetone yielded plate-like, badly shaped crystals. Data collections ($\theta_{\max} = 60°$ only, due to poor quality of the crystals) and accurate cell determination ($10 \leq \theta \leq 26°$, 25 reflections) were performed on a CAD-4 diffractometer. The crystal size was 0·26 × 0·08 × 0·07 mm, 1647 independent intensities [1269 considered observed with $I > 2\sigma(I)$] were measured with $\omega/2\theta$ scan technique ($0 \leq h \leq 4$, $0 \leq k \leq 30$, $-11 \leq l \leq 11$). Three standards monitored during data collection did not show any significant change in intensities. The data were corrected for Lorentz and polarization effects, and absorption correction according to Walker & Stuart (1983) was applied. Transmission factors 0·958–0·803.

The structure was solved by direct methods (Sheldrick, 1986) and refined by full-matrix least squares (Sheldrick, 1976) with anisotropic temperature factors for non-H atoms, isotropic temperature parameters for H atoms and an isotropic extinction parameter $g = 0·009$ (2) (Larson, 1967). The function minimized was $\sum w(|F_o| - |F_c|)^2$ where $w^{-1} = \sigma^2(F_o) + 0·0102F_o^2$. The refinement converged to a maximum shift/e.s.d. of 0·205, $R = 0·046$, $wR = 0·053$. The maximum peak in the final difference Fourier synthesis was 0·12 e Å^{-3}, 1·33 Å from O(8). All calculations were performed on an AMSTRAD 1512 microcomputer. Scattering factors were those incorporated in *SHELX*.

The molecular conformation and atomic labelling scheme are shown in Fig. 1. The atomic coordinates are given in Table 1 and selected bond distances and angles for non-H atoms are given in Table 2.*

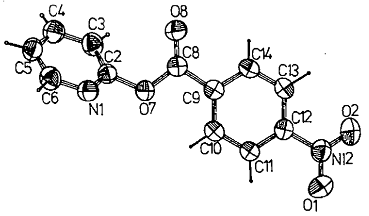

Fig. 1. A view of the molecule and labelling of the atoms in the structure of 2-pyridyl 4-nitrobenzoate (*ORTEP*: Johnson, 1976).

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* The anisotropic thermal parameters for non-H atoms, H-atom parameters and lists of structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52707 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Final atomic coordinates and equivalent isotropic temperature factors*

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq} (Å^2)
N(1)	−0·0823 (6)	0·6200 (1)	0·4468 (2)	3·99 (6)
C(2)	0·0653 (7)	0·6367 (1)	0·3446 (2)	3·45 (7)
C(3)	0·1409 (9)	0·6088 (1)	0·2392 (3)	4·49 (8)
C(4)	0·0471 (10)	0·5590 (1)	0·2421 (3)	5·16 (10)
C(5)	−0·1059 (9)	0·5406 (1)	0·3480 (3)	4·80 (9)
C(6)	−0·1656 (9)	0·5717 (1)	0·4464 (3)	4·72 (9)
O(7)	0·1719 (6)	0·6863 (1)	0·3554 (2)	4·16 (5)
C(8)	0·0839 (7)	0·7194 (1)	0·2655 (2)	3·19 (6)
O(8)	−0·0950 (6)	0·7093 (1)	0·1765 (2)	4·50 (6)
C(9)	0·2272 (6)	0·7695 (1)	0·2921 (2)	2·95 (6)
C(10)	0·3980 (7)	0·7804 (1)	0·4045 (2)	3·17 (6)
C(11)	0·5183 (7)	0·8279 (1)	0·4270 (2)	3·17 (6)
N(12)	0·5997 (7)	0·9140 (1)	0·3580 (2)	4·42 (7)
C(12)	0·4670 (7)	0·8636 (1)	0·3355 (2)	3·20 (6)
C(13)	0·3002 (7)	0·8536 (1)	0·2228 (2)	3·49 (7)
C(14)	0·1786 (7)	0·8062 (1)	0·2027 (2)	3·29 (6)
O(1)	0·7364 (9)	0·9229 (1)	0·4575 (2)	7·58 (9)
O(2)	0·5736 (9)	0·9443 (1)	0·2749 (2)	7·20 (9)

Table 2. *Selected bond lengths* (Å) *and valency and torsional angles* (°)

C(2)—O(7)	1·402 (3)	N(12)—O(1)	1·206 (3)
C(8)—O(7)	1·350 (3)	N(12)—O(2)	1·207 (3)
C(8)—O(8)	1·202 (3)	N(1)—C(2)	1·309 (3)
C(8)—C(9)	1·485 (4)	N(1)—C(6)	1·339 (4)
C(12)—N(12)	1·470 (4)		
C(2)—O(7)—C(8)	119·8 (2)	C(12)—N(12)—O(2)	118·4 (2)
O(7)—C(8)—O(8)	123·5 (3)	O(1)—N(12)—O(2)	123·0 (3)
O(7)—C(8)—C(9)	111·8 (2)	C(2)—N(1)—C(6)	115·9 (2)
O(8)—C(8)—C(9)	124·7 (2)	N(1)—C(2)—C(3)	125·5 (3)
C(12)—N(12)—O(1)	118·6 (2)		
N(1)—C(2)—O(7)—C(8)	−129·9 (3)	O(7)—C(8)—C(9)—C(10)	−6·4 (3)
C(3)—C(2)—O(7)—C(8)	55·3 (4)	O(8)—C(8)—C(9)—C(14)	−6·2 (4)
C(2)—O(7)—C(8)—O(8)	2·8 (4)	O(1)—N(12)—C(12)—C(11)	−2·9 (4)
C(2)—O(7)—C(8)—C(9)	−178·7 (2)	O(2)—N(12)—C(12)—C(13)	−3·6 (4)

Related literature. 2-Chloro-4,6-disubstituted-1,3,5-triazines have lately been proposed as a very efficient activator of the carboxylic group in the syntheses of esters, amides, carboxylic acid anhydrides and peptides (Kamiński, 1985, 1987). A comparison of an intermediate product, 2-(2,2-dimethylpropanoyloxy)-4,6-dimethoxy-1,3,5-triazine, with its benzene analog, the 4-nitrophenyl ester of 2,2-dimethylpropanoic acid, has shown that enhanced reactivity of the former substrate in the acylation reaction (Kamiński, Główka & Iwanicka, 1989) may result either from favourable electronic factors or from stabilization of a cyclic intermediate in the *s*-triazine derivative (Główka, Iwanicka & Kamiński, 1990). The present results are in agreement with this interpretation.

In the crystal, the molecules are packed almost perpendicular to the [100] direction. The angle between (100) and the pyridine least-squares plane is about 26° (29° for the benzene least-squares plane) and the distances between parallel rings are 3·47 Å (pyridine) and 3·38 Å (benzene).

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Structure of *p*-Chlorobenzenesulfonic Acid Monohydrate

By Tooru Taga and Tetsu Kobayashi

Faculty of Pharmaceutical Sciences, Kyoto University, Sakyo-ku, Kyoto 606, *Japan*

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Abstract. Oxonium *p*-chlorobenzenesulfonate, $C_6H_4ClO_3S^-.H_3O^+$, $M_r = 210·6$, monoclinic, $P2_1/c$, $a = 6·000\,(1)$, $b = 7·250\,(1)$, $c = 19·696\,(4)$ Å, $\beta = 98·17\,(2)°$, $V = 848·1\,(1)$ Å^3, $Z = 4$, $D_m = 1·65$, $D_x = 1·649$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 6·55$ cm^{-1}, $F(000) = 432$, $T = 296$ K, $R = 0·036$ for 2241 unique observed reflections. The average S—O, C—S—O and O—S—O values are 1·453 (2) Å,

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