squares on a MicroVAX II computer with *SHELX*76 (Sheldrick, 1976). H atoms were located from a difference Fourier synthesis. All the H atoms were allowed to refine isotropically in final cycles. Final maximum $\Delta/\sigma = 0{\cdot}05$. Maximum and minimum heights in final difference Fourier synthesis 0·15 and $-0{\cdot}22$ e Å$^{-3}$ respectively. Refinement with weights given by $w = 1{\cdot}0000/[\sigma^2(F) + 0{\cdot}010894(F_o)^2]$ converged at $R = 0{\cdot}046$, $wR = 0{\cdot}050$. Atomic scattering factors were those of *SHELX*. Final positional and thermal parameters are listed in Table 1 and bond lengths and angles in Table 2.* A *PLUTO* (Motherwell & Clegg, 1978) drawing of the molecule showing the molecular geometry is presented in Fig. 1 and the molecular packing in the unit cell in Fig. 2.

**Related literature.** The 4-piperidone ring in this structure has a slightly distorted chair conformation; puckering is enhanced in the area of N(1) and decreased in the area of C(4). A similar conformational feature is also observed in the 4-piperidone rings of 3-methyl-2,6-diphenyl-4-piperidone (Sekar, Parthasarathy & Rajalingam, 1990) and 1,1′-di-(4-pyridyl)-2,2′,6,6′-bi(4-piperidone) dihydrochloride dihydrate (Cheer, Cosgrove & Vittimberga, 1984).

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# Structure of an Oxazoylphenyloxazole

BY HOLGER BECK AND GEORGE M. SHELDRICK

*Institut für Anorganische Chemie der Universität, Tammannstraße 4, D-3400 Göttingen,*
*Federal Republic of Germany*

AND JOACHIM HEGE AND WOLFGANG LÜTTKE

*Institut für Organische Chemie der Universität, Tammannstraße 2, D-3400 Göttingen,*
*Federal Republic of Germany*

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**Abstract.** 4-(3-Methylphenyl)-5-phenyl-2-[4-(5-phenyl-2-oxazolyl)phenyl]oxazole, $C_{31}H_{22}N_2O_2$, $M_r = 454{\cdot}53$, triclinic, $P\bar{1}$, $a = 7{\cdot}649\ (1)$, $b = 9{\cdot}824\ (1)$, $c = 15{\cdot}928\ (1)$ Å, $\alpha = 95{\cdot}36\ (1)$, $\beta = 100{\cdot}43\ (1)$, $\gamma = 94{\cdot}13\ (1)°$, $V = 1167{\cdot}12$ Å$^3$, $Z = 2$, $D_x = 1{\cdot}293$ Mg m$^{-3}$, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 0{\cdot}08$ mm$^{-1}$, $F(000) = 476$, $T = 298$ K, $R = 0{\cdot}043$ for 3498 observed reflections. The structure was determined to investigate the planarity of the ring system. The rings were found to be coplanar (torsional angles between rings 5° or less), except for the rings substituted in positions C(4) and C(5) where dihedral angles of 22·4 (2) and 34·1 (2)° were found.

**Experimental.** The synthetic compound was crystallized by liquid–vapor diffusion from a solution in a mixture of $CHCl_3$ and toluene with *n*-hexane. The crystal dimensions were $0{\cdot}3 \times 0{\cdot}7 \times 0{\cdot}75$ mm. Data were collected on a Stoe–Siemens four-circle diffractometer with monochromated Mo $K\alpha$ radiation using the profile-fitting mode involving variable scan

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

$U_{\mathrm{eq}}$ is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

| | $x$ | $y$ | $z$ | $U_{\mathrm{eq}}$(Å$^2$) |
|---|---|---|---|---|
| O(1) | 0·6647 (1) | 0·4226 (1) | 0·3477 (1) | 0·045 (1) |
| C(2) | 0·6329 (2) | 0·5567 (1) | 0·3511 (1) | 0·043 (1) |
| N(3) | 0·6678 (2) | 0·6201 (1) | 0·4286 (1) | 0·044 (1) |
| C(4) | 0·7266 (2) | 0·5211 (1) | 0·4812 (1) | 0·041 (1) |
| C(5) | 0·7228 (2) | 0·3998 (1) | 0·4322 (1) | 0·043 (1) |
| O(1′) | 0·3134 (1) | 0·9024 (1) | 0·0405 (1) | 0·052 (1) |
| C(2′) | 0·3622 (2) | 0·7722 (2) | 0·0376 (1) | 0·051 (1) |
| N(3′) | 0·3422 (2) | 0·7108 (1) | −0·0396 (1) | 0·067 (1) |
| C(4′) | 0·2754 (3) | 0·8072 (2) | −0·0910 (1) | 0·067 (1) |
| C(5′) | 0·2557 (2) | 0·9236 (2) | −0·0442 (1) | 0·053 (1) |
| C(21) | 0·5633 (2) | 0·6115 (1) | 0·2710 (1) | 0·043 (1) |
| C(22) | 0·5399 (2) | 0·5309 (2) | 0·1924 (1) | 0·054 (1) |
| C(23) | 0·4742 (2) | 0·5838 (2) | 0·1173 (1) | 0·057 (1) |
| C(24) | 0·4302 (2) | 0·7181 (2) | 0·1181 (1) | 0·047 (1) |
| C(25) | 0·4534 (2) | 0·7989 (2) | 0·1968 (1) | 0·053 (1) |
| C(26) | 0·5190 (2) | 0·7463 (1) | 0·2720 (1) | 0·050 (1) |
| C(41) | 0·7819 (2) | 0·5600 (1) | 0·5750 (1) | 0·043 (1) |
| C(42) | 0·7174 (2) | 0·6753 (2) | 0·6115 (1) | 0·047 (1) |
| C(43) | 0·7600 (2) | 0·7161 (2) | 0·6995 (1) | 0·056 (1) |
| C(44) | 0·8735 (3) | 0·6400 (2) | 0·7502 (1) | 0·065 (1) |
| C(45) | 0·9427 (2) | 0·5277 (2) | 0·7144 (1) | 0·065 (1) |
| C(46) | 0·8980 (2) | 0·4872 (2) | 0·6274 (1) | 0·052 (1) |
| C(43″) | 0·6816 (3) | 0·8388 (2) | 0·7374 (1) | 0·084 (1) |
| C(51) | 0·7508 (2) | 0·2568 (1) | 0·4448 (1) | 0·046 (1) |
| C(52) | 0·7028 (2) | 0·1988 (2) | 0·5147 (1) | 0·057 (1) |
| C(53) | 0·7193 (2) | 0·0623 (2) | 0·5232 (1) | 0·066 (1) |
| C(54) | 0·7826 (3) | −0·0192 (2) | 0·4621 (1) | 0·070 (1) |
| C(55) | 0·8307 (3) | 0·0369 (2) | 0·3931 (1) | 0·068 (1) |
| C(56) | 0·8160 (2) | 0·1742 (2) | 0·3842 (1) | 0·056 (1) |
| C(51′) | 0·1887 (2) | 1·0543 (2) | −0·0621 (1) | 0·053 (1) |
| C(52′) | 0·1149 (3) | 1·0753 (2) | −0·1459 (1) | 0·072 (1) |
| C(53′) | 0·0491 (3) | 1·1970 (2) | −0·1643 (1) | 0·084 (1) |
| C(54′) | 0·0536 (3) | 1·3014 (2) | −0·0997 (1) | 0·081 (1) |
| C(55′) | 0·1255 (3) | 1·2829 (2) | −0·0173 (1) | 0·083 (1) |
| C(56′) | 0·1932 (3) | 1·1603 (2) | 0·0018 (1) | 0·070 (1) |

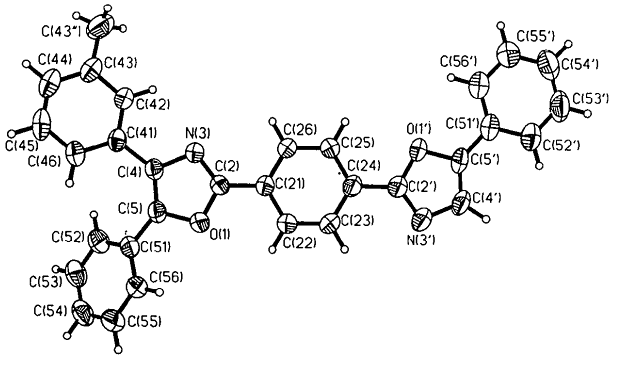

Fig. 1. 50% probability thermal ellipsoid plot with the atom numbering. Only the major orientation of the disordered methyl group is shown.

Table 2. *Bond lengths* (Å) *and bond angles* (°)

| | | | |
|---|---|---|---|
| O(1)—C(2) | 1·355 (2) | C(25)—C(26) | 1·374 (2) |
| O(1)—C(5) | 1·384 (2) | C(41)—C(42) | 1·388 (2) |
| C(2)—N(3) | 1·302 (2) | C(41)—C(46) | 1·390 (2) |
| C(2)—C(21) | 1·459 (2) | C(42)—C(43) | 1·393 (2) |
| N(3)—C(4) | 1·389 (2) | C(43)—C(44) | 1·385 (2) |
| C(4)—C(5) | 1·359 (2) | C(43)—C(43″) | 1·508 (3) |
| C(4)—C(41) | 1·482 (2) | C(44)—C(45) | 1·377 (3) |
| C(5)—C(51) | 1·462 (2) | C(45)—C(46) | 1·379 (2) |
| O(1′)—C(2′) | 1·357 (2) | C(51)—C(52) | 1·391 (2) |
| O(1′)—C(5′) | 1·382 (2) | C(51)—C(56) | 1·387 (2) |
| C(2′)—N(3′) | 1·295 (2) | C(52)—C(53) | 1·373 (2) |
| C(2′)—C(24) | 1·457 (2) | C(53)—C(54) | 1·380 (3) |
| N(3′)—C(4′) | 1·375 (2) | C(54)—C(55) | 1·370 (3) |
| C(4′)—C(5′) | 1·339 (2) | C(55)—C(56) | 1·380 (2) |
| C(5′)—C(51′) | 1·450 (2) | C(51′)—C(52′) | 1·391 (2) |
| C(21)—C(22) | 1·393 (2) | C(51′)—C(56′) | 1·381 (2) |
| C(21)—C(26) | 1·389 (2) | C(52′)—C(53′) | 1·366 (3) |
| C(22)—C(23) | 1·374 (2) | C(53′)—C(54′) | 1·378 (3) |
| C(23)—C(24) | 1·385 (2) | C(54′)—C(55′) | 1·361 (3) |
| C(24)—C(25) | 1·395 (2) | C(55′)—C(56′) | 1·383 (3) |

| | | | |
|---|---|---|---|
| C(2)—O(1)—C(5) | 105·0 (1) | C(24)—C(25)—C(26) | 120·7 (1) |
| O(1)—C(2)—N(3) | 113·6 (1) | C(21)—C(26)—C(25) | 120·5 (1) |
| O(1)—C(2)—C(21) | 118·1 (1) | C(4)—C(41)—C(42) | 118·5 (1) |
| N(3)—C(2)—C(21) | 128·3 (1) | C(4)—C(41)—C(46) | 122·7 (1) |
| C(2)—N(3)—C(4) | 105·0 (1) | C(42)—C(41)—C(46) | 118·8 (1) |
| N(3)—C(4)—C(5) | 109·1 (1) | C(41)—C(42)—C(43) | 121·7 (1) |
| N(3)—C(4)—C(41) | 119·3 (1) | C(42)—C(43)—C(44) | 118·1 (2) |
| C(5)—C(4)—C(41) | 131·5 (1) | C(42)—C(43)—C(43″) | 120·2 (1) |
| O(1)—C(5)—C(4) | 107·2 (1) | C(44)—C(43)—C(43″) | 121·7 (1) |
| O(1)—C(5)—C(51) | 114·6 (1) | C(43)—C(44)—C(45) | 120·8 (1) |
| C(4)—C(5)—C(51) | 138·1 (1) | C(44)—C(45)—C(46) | 120·7 (2) |
| C(2′)—O(1′)—C(5′) | 105·1 (1) | C(41)—C(46)—C(45) | 119·9 (1) |
| O(1′)—C(2′)—N(3′) | 113·7 (1) | C(5)—C(51)—C(52) | 120·9 (1) |
| O(1′)—C(2′)—C(24) | 118·5 (1) | C(5)—C(51)—C(56) | 120·3 (1) |
| N(3′)—C(2′)—C(24) | 127·8 (1) | C(52)—C(51)—C(56) | 118·7 (1) |
| C(2′)—N(3′)—C(4′) | 103·9 (1) | C(51)—C(52)—C(53) | 120·5 (2) |
| N(3′)—C(4′)—C(5′) | 111·4 (1) | C(52)—C(53)—C(54) | 120·3 (2) |
| O(1′)—C(5′)—C(4′) | 106·0 (1) | C(53)—C(54)—C(55) | 119·7 (2) |
| O(1′)—C(5′)—C(51′) | 118·2 (1) | C(54)—C(55)—C(56) | 120·5 (2) |
| C(4′)—C(5′)—C(51′) | 135·8 (1) | C(51)—C(56)—C(55) | 120·3 (2) |
| C(2)—C(21)—C(22) | 121·1 (1) | C(5′)—C(51′)—C(52′) | 120·0 (1) |
| C(2)—C(21)—C(26) | 120·1 (1) | C(5′)—C(51′)—C(56′) | 122·2 (1) |
| C(22)—C(21)—C(26) | 118·8 (1) | C(52′)—C(51′)—C(56′) | 117·9 (2) |
| C(21)—C(22)—C(23) | 120·5 (1) | C(51′)—C(52′)—C(53′) | 121·1 (2) |
| C(22)—C(23)—C(24) | 120·9 (1) | C(52′)—C(53′)—C(54′) | 120·3 (2) |
| C(2′)—C(24)—C(23) | 119·8 (1) | C(53′)—C(54′)—C(55′) | 119·5 (2) |
| C(2′)—C(24)—C(25) | 121·6 (1) | C(54′)—C(55′)—C(56′) | 120·6 (2) |
| C(23)—C(24)—C(25) | 118·6 (1) | C(51′)—C(56′)—C(55′) | 120·7 (2) |

width and speed (Clegg, 1981). 5022 reflections were measured, $2\theta_{\max} = 50°$, $-9 \le h \le 8$, $-11 \le k \le 11$, $0 \le l \le 18$. Three check reflections were used which showed no significant intensity change. The data were merged to give 4104 unique reflections ($R_{\mathrm{int}} = 0{\cdot}027$), of which 3498 with $F > 3\sigma(F)$ were used for all calculations (*SHELXS*86, Sheldrick 1990; *SHELX*76, Sheldrick 1976). Cell constants were refined from $\pm 2\theta$ values of 53 reflections with $20 < 2\theta < 25°$. Absorption correction was not necessary. An extinction correction was applied yielding a value of 0·0054 for the coefficient $x$, where $F_c^* = F_c(1 + 0{\cdot}002xF_c^2/\sin 2\theta)^{-0{\cdot}25}$. The structure was solved by direct methods and refined on $F$ to $R = 0{\cdot}043$, $wR = 0{\cdot}055$. All non-H atoms were refined anisotropically. Isotropic H atoms were included using a riding model (C—H = 0·96 Å). The methyl group was refined as two components, with restrained C—H and H—H distances and common $U$(H), such that the occupation factors [0·39 (2) and 0·61 (2)] summed to unity. 357 parameters were refined with the weighting scheme $w^{-1} = \sigma^2(F) + 0{\cdot}0003F^2$ which led to a featureless analysis of variance in terms of $\sin\theta$ and $F_o$ and gave $S = 2{\cdot}18$, max. $\Delta/\sigma = 0{\cdot}012$, max.

and min. height in final $\Delta\rho$ map 0·19 and $-0{\cdot}15$ 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.** $C_{12}H_8N_2O_4$, $M_r = 244{\cdot}2$, monoclinic, $P2_1/c$, $Z = 4$, $a = 3{\cdot}866\,(1)$, $b = 26{\cdot}913\,(3)$, $c = 10{\cdot}638\,(1)$ Å, $\beta = 90{\cdot}14\,(1)°$, $V = 1106{\cdot}9$ Å$^3$, $D_x = 1{\cdot}46$ Mg m$^{-3}$, $\lambda(\text{Cu } K\alpha) = 1{\cdot}54178$ Å, Ni filter, $\mu = 0{\cdot}85$ mm$^{-1}$, $F(000) = 504$, $T = 293$ K, $R = 0{\cdot}046$ and $wR = 0{\cdot}053$ 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 ($10 \le \theta \le 26°$, 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 ($0 \le h \le 4$, $0 \le k \le 30$, $-11 \le l \le 11$). 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 $g = 0{\cdot}009\,(2)$ (Larson, 1967). The function minimized was $\sum w(|F_o| - |F_c|)^2$ where $w^{-1} = \sigma^2(F_o) + 0{\cdot}0102F_o^2$. The refinement converged to a maximum shift/e.s.d. of 0·205, $R = 0{\cdot}046$, $wR = 0{\cdot}053$. 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.*

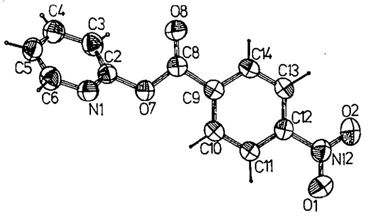

Fig. 1. A view of the molecule and labelling of the atoms in the structure of 2-pyridyl 4-nitrobenzoate (*ORTEP*: Johnson, 1976).

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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.