

**Related literature.** Platinum(II) complexes with imidazole, thiazole and other N-donor heterocyclic ligands have shown significant biological activity (Dehand & Jordanov, 1976; Van Kralingen & Reedijk, 1978; Van Kralingen, Reedijk & De Ridder, 1979) and are of interest as potential antitumor agents (Hacker, Douple & Krakoff, 1984). Thiazole is a potentially ambidentate ligand with either the N or S atom available for coordination. Although coordination by the soft S might be predicted (Pearson, 1963), the thiazole ring in tzbim is coordinated through the N atom. This behavior has been observed in Pd<sup>II</sup> and Rh<sup>III</sup> benzothiazole complexes (Churchill, Wasserman & Young, 1980; Muir, Rong & Muir, 1989), and in several Pt<sup>II</sup> styrylbenzothiazole complexes (Muir, Gómez, Muir, Cox & Cádiz, 1987; Gómez, Muir & Muir, 1988; Muir, Gómez, Muir, Cádiz, Cox & Barnes, 1988; Muir, Gómez, Muir & Cádiz, 1990). The average C—N, C—S and C—C distances and bond angles are similar to those found in the other complexes.

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## Potassium 4-(4-Nitrophenyl)phenolate Monohydrate

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**Abstract.** K<sup>+</sup>.C<sub>12</sub>H<sub>8</sub>NO<sub>3</sub><sup>-</sup>.H<sub>2</sub>O, *M<sub>r</sub>* = 271.32, monoclinic, *P*2<sub>1</sub>/*c*, *a* = 14.388 (2), *b* = 7.362 (1), *c* = 11.280 (2) Å, β = 107.79 (2)°, *V* = 1137.7 (3) Å<sup>3</sup>, *Z* = 4, *D<sub>x</sub>* = 1.58 g cm<sup>-3</sup>, λ(Mo *K*α) = 0.71069 Å, μ = 4.66 cm<sup>-1</sup>, *F*(000) = 560, *T* = 298 K, *R* = 0.0362 for 1710 unique reflections. The dihedral angle between the phenyl rings is 4° and the dihedral angle between one phenyl group and the adjacent NO<sub>2</sub> group is 4°. The anion shows a partial quinoid character and is stacked antiparallel. The potassium cation is eight-

fold coordinated through oxygen atoms in the range up to 3.1 Å. Hydrogen bridges between water and phenolate oxygens O—H···O with distances of 2.783 (3) and 2.784 (3) Å are indicated.

**Experimental.** 4-(4'-Nitrophenyl)phenol was prepared as described by Jones & Chapman (1952). The final product was obtained by reaction with potassium hydroxide dissolved in water. For recrystallization, water-containing ethanol was used. After evaporation blue-red plate-like crystals resulted. Size of the crystal 0.28 × 0.12 × 0.37 mm. Stoe Stadi-4 four-circle diffractometer, graphite-monochromated Mo *K*α radiation, lattice parameters from a least-

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Table 1. Positional and thermal parameters  $\{U_{eq} = (10^3/3)[\sum_i \sum_j U_{ij} a_i^* a_j^* (\mathbf{a}_i \cdot \mathbf{a}_j)]\}$  with e.s.d.'s in parentheses (not for  $U_{eq}$ )

|       | x          | y          | z          | $U_{eq}(\text{\AA}^2)$ |
|-------|------------|------------|------------|------------------------|
| K(1)  | 0.0330 (1) | 0.5045 (1) | 0.1993 (1) | 37                     |
| O(1)  | 0.0896 (1) | 0.1525 (2) | 0.1698 (1) | 34                     |
| O(2)  | 0.8473 (1) | 0.2358 (2) | 0.6322 (2) | 56                     |
| O(3)  | 0.8564 (1) | 0.0477 (2) | 0.4891 (2) | 54                     |
| O(W)  | 0.0078 (1) | 0.3278 (2) | 0.4123 (2) | 48                     |
| N(1)  | 0.8090 (1) | 0.1453 (3) | 0.5380 (2) | 40                     |
| C(1)  | 0.1848 (1) | 0.1551 (3) | 0.2188 (2) | 29                     |
| C(2)  | 0.2315 (1) | 0.2430 (3) | 0.3324 (2) | 32                     |
| C(3)  | 0.3316 (1) | 0.2440 (3) | 0.3832 (2) | 31                     |
| C(4)  | 0.3936 (1) | 0.1579 (3) | 0.3258 (2) | 27                     |
| C(5)  | 0.3467 (1) | 0.0698 (3) | 0.2130 (2) | 33                     |
| C(6)  | 0.2474 (1) | 0.0681 (3) | 0.1607 (2) | 35                     |
| C(7)  | 0.5004 (1) | 0.1571 (3) | 0.3810 (2) | 27                     |
| C(8)  | 0.5480 (1) | 0.2516 (3) | 0.4908 (2) | 34                     |
| C(9)  | 0.6486 (1) | 0.2495 (3) | 0.5428 (2) | 35                     |
| C(10) | 0.7037 (1) | 0.1519 (3) | 0.4834 (2) | 32                     |
| C(11) | 0.6605 (1) | 0.0558 (3) | 0.3757 (2) | 37                     |
| C(12) | 0.5604 (1) | 0.0600 (3) | 0.3256 (2) | 36                     |
| H(1W) | -0.031 (2) | 0.410 (3)  | 0.3945 (2) | 50*                    |
| H(2W) | 0.034 (2)  | 0.325 (3)  | 0.488 (2)  | 50*                    |

\*  $U_{iso}$  (fixed).

Table 2. Bond distances ( $\text{\AA}$ ) and selected bond angles ( $^\circ$ )

|             |           |                  |           |
|-------------|-----------|------------------|-----------|
| O(1)—C(1)   | 1.310 (1) | C(8)—C(9)        | 1.386 (3) |
| C(1)—C(2)   | 1.410 (3) | C(9)—C(10)       | 1.385 (3) |
| C(2)—C(3)   | 1.379 (3) | C(10)—C(11)      | 1.380 (3) |
| C(3)—C(4)   | 1.403 (3) | C(11)—C(12)      | 1.377 (3) |
| C(4)—C(5)   | 1.403 (3) | C(12)—C(7)       | 1.405 (3) |
| C(5)—C(6)   | 1.369 (3) | C(10)—N          | 1.451 (3) |
| C(6)—C(1)   | 1.418 (3) | N—O(2)           | 1.232 (2) |
| C(4)—C(7)   | 1.471 (3) | N—O(3)           | 1.231 (2) |
| C(7)—C(8)   | 1.403 (3) |                  |           |
| O(2)—N—O(3) | 122.5 (2) | H(1W)—O(W)—H(2W) | 109.8 (3) |

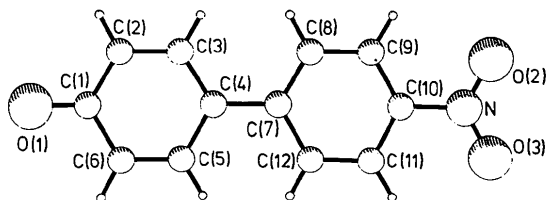


Fig. 1. Molecule with labelling scheme.

squares fit of 48 reflections with  $14 < \theta < 18^\circ$ . Scan  $2\theta/\omega = 1/1$ . For data collection 1925 reflections up to  $2\theta_{max} = 50^\circ$  in the range  $-16 \leq h \leq 16$ ,  $0 \leq k \leq 8$ ,  $0 \leq l \leq 13$  were measured; three standards showed no significant change in intensity. Standard deviations derived from counting statistics. 1710 reflections with  $|F_o| \geq 2\sigma(F_c)$  were used for refinements. Lp corrections were applied. The structure was solved by direct methods using the program package *SHELX76* (Sheldrick, 1976). Scattering factors and anomalous-dispersion coefficients for K<sup>+</sup> from *International Tables for X-ray Crystallography* (1974, Vol. IV), others from *SHELX76*. Full-matrix least-squares refinement of 170 parameters was performed with all non-hydrogen atoms having anisotropic thermal parameters. Non-water hydrogens were geometrically fixed at C—H 1.08  $\text{\AA}$  using *SHELX76* and were not refined. Water hydrogens were located by difference Fourier synthesis and refined with fixed temperature parameters. The function minimized was  $\sum w(|F_o| - |F_c|)^2$ . The refinement converged at  $R = 0.0362$ ,  $wR = 0.0295$ ,  $w = 1/\sigma^2(F_o)$ . Final difference Fourier density maxima  $\pm 0.3 \text{ e \AA}^{-3}$  and  $\Delta/\sigma_{max} = 0.034$ .

Table 1 lists the final atomic coordinates and Table 2 gives bond lengths and selected angles.\* Fig. 1 shows the molecular structure and Fig. 2 shows a projection along the monoclinic axis. The figures have been drawn with *PLUTO* (Motherwell & Clegg, 1978).

\* 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 53888 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

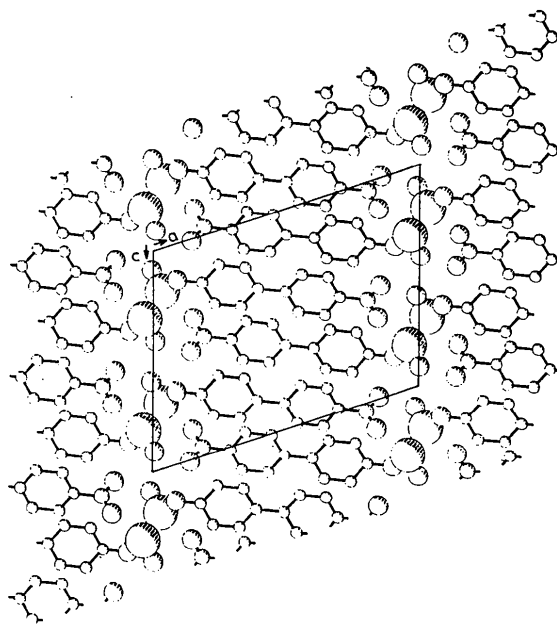


Fig. 2. Crystal structure projection along [010].

**Related literature.** The compound was prepared by Jones & Chapman (1952). The investigations were carried out to find possible candidates for non-linear optical effects and to learn about the packing of the biphenyl group in the solid state.

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