Short Communications

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Crystal study of quinaldic acid at low temperature.

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The lattice dimensions of quinaldic acid, which is a monoclinic crystal, were determined at 25 °C and −150 °C. The dimer formation and hence hydrogen bonding in this acid was indicated by a study of infrared absorption. From extinction rules as well as statistical test, the space group $P2/c \times (C_{2h}^4)$ was assigned.

The infrared spectroscopic study of the compounds containing groups X(:O)OH by Braunholtz, Hall, Sheppard & Mann (1959) showed a possibility of the shift of the OH stretching peak from 3600 cm^{-1}. Therefore infrared spectroscopic measurements at different concentrations as well as dielectric measurements were made for quinoline-2-carboxylic acid, $C_{10}H_7O_2N$. These results indicated the presence of dimers. The present paper gives the crystal data of this acid at 25 °C and −150 °C.

The unit cell is monoclinic. Measurements were made by using Cu $K\alpha$ radiation and by employing oscillation and Weissenberg techniques. The axial parameters of the unit cell from zero layer Weissenberg photographs were refined by the method of least squares using high angle spots (Huges, Yakel & Freeman, 1961).

Room temperature (25 °C)	Low temperature (−150 °C)	Coefficient of expansion $\times 10^6$
$a = 9{\cdot}77 \pm 0{\cdot}01$ Å	$a = 9{\cdot}52 \pm 0{\cdot}01$ Å	$\alpha_a = 150{\cdot}0\ C^{\circ -1}$
$b = 5{\cdot}97 \pm 0{\cdot}01$	$b = 5{\cdot}86 \pm 0{\cdot}01$	$\alpha_b = 107{\cdot}3\ C^{\circ -1}$
$c = 28{\cdot}00 \pm 0{\cdot}02$	$c = 27{\cdot}36 \pm 0{\cdot}02$	$\alpha_c = 133{\cdot}7\ C^{\circ -1}$
$\beta = 90° 30' \pm 5'$	$\beta = 90° \pm 5'$	

The observed density 1·42 g.cm^{-3}, determined by the flotation method with potassium iodide solution, agrees with the value 1·41 g.cm^{-3} calculated for eight molecules per unit cell.

The space group assigned to this crystal on the basis of the extinction rule and statistical test is $P2/c$. Although two forbidden spots 105 and $10\bar{5}$ were found on low temperature Weissenberg photographs, at room temperature their intensities became so weak that they were visible only on heavily exposed photographs. These two spots have been interpreted as being due to the Renninger effect (Khan, 1967). Hence the above space group for quinaldic acid is established beyond doubt.

Because the molecule contains light atoms only and there is no other information such as magnetic susceptibility data, the authors are not at present undertaking any further study of the structure determination of this substance.

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The unit-cell dimensions and space group of 2-(benzylthio)imidazoline and 2-(benzylthio)tetrahydropyrimidine hydrochlorides.

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Correction to *Acta Cryst.* **22**, 926 (1967).

The c value of the unit cell of 2-benzylthioimidazoline reported in the Abstract of a recent paper (Del Pra, 1967) should be read 10·04 Å, instead of 11·25 Å.

Reference

DEL PRA, A. (1967). *Acta Cryst.* **22**, 926.