The Crystal Structure of Phenazine-5, 10-dioxides

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The authors have carried out an investigation of the crystal structure of phenazine-5, 10-dioxide in order to amplify the knowledge of the dative bond, N–O. In the course of the present investigation, the crystal structure of phenazine-*N*-oxide has been published[1].

Phenazine-5, 10-dioxide was prepared by oxidizing phenazine-*N*-oxide. It crystallizes out in needle-like crystals, deep red in color. They decompose at about 190°C. Oscillation and Weissenberg photographs taken with copper K_α radiation, showed that the crystal is monoclinic with the unit cell having the dimensions:

$$a=7.83,\quad b=3.95,\quad c=15.50\,\text{Å},\quad \beta=104°48'$$

and the space group $P2_1/c$. From the observed density, the unit cell was found to contain two molecules, implying that the molecules must be placed at special positions having centers of symmetry. The intensities of reflections, $(h0l)$ and $(0kl)$, obtained by the multiple-film technique were measured by the visual method, using standard scales, and no correction was made for absorption.

Since the dimension of the b-axis is short (3.95 Å), it was expected that there is no overlap of atoms in the projection to the b-plane. The optical transform methods[2] were employed to determine the orientation of the molecule in the unit cell, as well as to determine the signs of the structure factors of strong reflections[3]. The $h0l$ Fourier projection was refined in the usual way and the electron density map, $\rho(xz)$, is shown in Fig. 1. To determine the z-coordinates of atoms, we employed usual trial and error methods taking into account the plane structure of this molecule, followed by the least square methods. The atomic arrangement projected along the b and a axes are given in Figs. 2 and 3, respectively. This arrangement of molecules is quite similar to that reported for anthraquinone[4], whose unit cell dimensions are also similar to those of phenazine-5,10-dioxide. The configuration of this molecule is found to be

1) R. Curti et al., *Acta Cryst.*, **14**, 133 (1961).
2) C. A. Taylor, et al., ibid., **4**, 261 (1951).
3) C. A. Taylor and H. Lipson, *Nature*, **167**, 809 (1951); T. Watanabé and M. Otsuka, *Acta Cryst.*, **10**, 377 (1957).
4) S. N. Sen, *Indian J. Phys.*, **22**, 347 (1948).

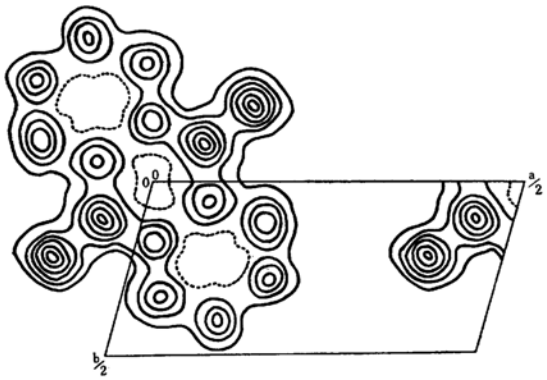

Fig. 1. Electron density map projected on the b plane.

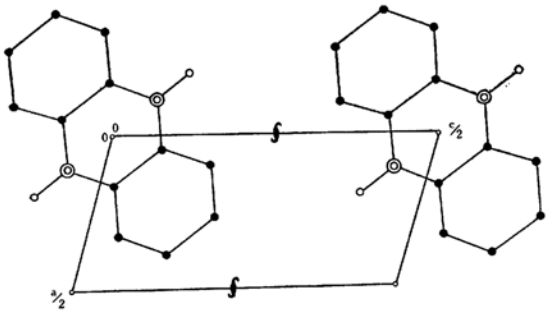

Fig. 2. Projection of the structure, on the b plane.
○ Oxygen, ◎ Nitrogen, ● Carbon.

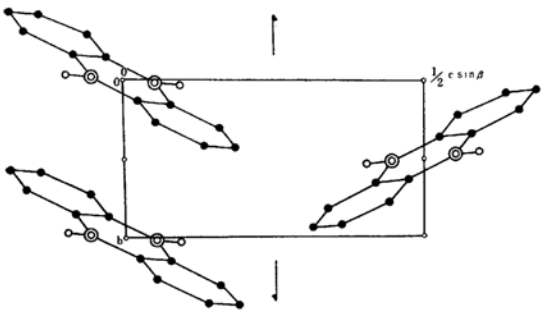

Fig. 3. The view of the structure along the a-axis.

almost planer with reasonable interatomic distances. In phenazine-*N*-oxide, a statistical arrangement of the oxygen atoms has been reported[1]. It is interesting to note that the average structure of phenazine-*N*-oxide is similar to the present structure.

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