The Redetermination of the Lattice Constants of Phenazine 5, 10-Dioxide

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In a previous paper,[1] we have reported on the crystal structure of phenazine 5, 10-dioxide. Quite independently, another paper on the same subject has been published by Curti et al.[2]

The atomic coordinates and the crystal structure derived therefrom agree in both papers in the main. However, there are small differences in the unit cell dimensions between the two investigations. Therefore, we have carried out a careful determination of the unit cell dimensions on two specimens, one prepared by us and another kindly sent to us by Professor Curti. It was not possible to get more accurate values for the spacings on the basis of powder diffractometry because of overlapping. A Weissenberg camera was used, and the Debye-Sherrer reflections from pure sodium chloride were superimposed on reflections from a single crystal of phenazine 5, 10-dioxide. There were no significant differences between the unit cell dimentions obtained from the two specimens. They are:

$$a=7.75\pm0.02\,\text{Å}, \qquad b=4.09\pm0.02\,\text{Å},$$

$$c=15.36\pm0.05\,\text{Å}, \text{ and } \beta=104°48'\pm10'.$$

The new data are closer to those of Curti et al. Fortunately, there are no serious changes necessary between the intramolecular atomic distances reported in the previous paper, except

1) Y. Namba, T. Oda and T. Watanabé, This Bulletin, **36**, 79 (1963).

2) R. Curti and V. Riganti, *Instituto Lombardo (Rend. Sc.)*, **A94**, 117 (1960).

that the value of 1.39 Å for the C_6–N bond should be revised to 1.36Å. There are slightly larger changes in the intermolecular atomic distances between molecules related by the unit translation along the b-axis, namely, +0.09Å on the average, the largest being between C_5 and O′ (Fig. 5), for which the reported value, 3.45Å, should be read as 3.59Å.

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