Crystal Structure of Pyrazinamide

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The crystal structure of pyrazinamide*, $C_5H_5N_3O$, (a new potential medicine for tuberculosis[1]) has been examined by X-ray analysis. The crystal data obtained were:

$$a=23.07,\ b=6.72,\ c=3.72\text{Å},\ \beta=100.8°,$$

space group $P2_1/a$, four molecules per unit cell.

The analysis was carried on by two-dimensional procedures. By considering the molecular packings, all the atoms were roughly located in the projections onto (001) and (010). The atomic coordinates were refined by using structure factor maps and further by successive Fourier projections. At the present stage the discrepancy indices ($R=\sum||F_o|-|F_c||/\sum|F_o|$) are 0.17 for (*hk*0) and 0.20 for (*h*0*l*).

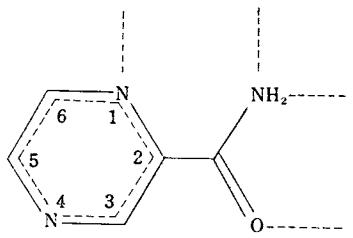

Fig. 1.

The molecule as shown in Fig. 1 is found to be approximately planar. Moreover the bond lengths C—C and C—N in the pyrazine ring show intermediate values between their single and double bonds. These suggest that there is a considerable amount of conjugation between the ring and the amide group.

Two amide groups are linked by a pair of NH—O hydrogen bonds forming a dimer molecule. These dimers are arranged in the direction (011), combining each other by NH—N'_1 hydrogen bonds. This structure explains the cleavage plane parallel to (100).

Further refinement is now going on by $(\rho_o-\rho_c)$ and least squares methods. The details of this work will be shortly published.

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* The sample used was supplied from Sankyo Co., Ltd.

1) S. Kushner et al., *J. Am. Chem. Soc.*, **74**, 3617 (1952).