

The β -N₂ structure Vegard (1932, 1934) assigned to the centrosymmetric space group $P\bar{3}m1$ with N atoms in Wyckoff positions 'd' with the molecular centers not coinciding with the space-group symmetry centers. Ruhemann (1932) implied preference for space-group $P6_3/mmc$ with N atoms in Wyckoff positions 'f' and molecular centers on symmetry centers. This solution appears to fit our, and indeed Vegard's own, data equally well. It has found wider acceptance in the literature (e.g. Wyckoff, 1951).

The $\alpha \rightarrow \beta$ transformation on warming is preceded by an anomaly in the specific-heat curve (Giauque &

Clayton, 1933) indicating the onset of restricted rotation. The molecular-volume data (Table 1) suggest that the molecules do not, however, attain free spherical rotation below the melting point. Models for the restricted rotation must conform to the observed axial ratio.

Helpful discussion with Dr Lipscomb and many colleagues is gratefully acknowledged.

References

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Table 1. *Molecular volume data* ($\times 10^{24}$ cm.⁻³)

	β Solid			Liquid	Freely rotating sphere
	α Solid	Molecular volume	c/a		
Present authors	44.5	48.1	1.627	57.5*	64.7†
Vegard	45.3	47.1	1.651	—	—
Ruhemann	45.6	46.4	1.633	—	—

* Calculated from density = 0.8084 g.cm.⁻³ (*Int. Crit. Tables*, Vol. III, p. 20. New York: McGraw-Hill 1928).

† Calculated from distance of approach of closest atoms in α -N₂ at 4.2° = 3.44 Å. This must be considered an upper limit.

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On the space group of 2-4-dinitroaniline. By A. K. M. SIDDIQ, JOYKUMAR SARAOGI and SHAMSHER ALI, *X-ray Crystallographic Laboratory, Dacca University, Dacca, East Pakistan*

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The crystals of 2-4-dinitroaniline, which are light yellowish, crystallize in well developed prismatic plates with forms {011}, {110}, {101}, and {010} dominating. Fig. 1 shows a typical crystal in a clinographic drawing.

The crystals, when examined under the polarizing

microscope, show oblique extinction on the *b*-face. The crystals therefore belong to the monoclinic system.

Oscillation and Weissenberg photographs taken with unfiltered Co *K* α radiation from crystal specimens oscillated about all the three principal axes gave (for $\lambda = 1.78$ Å) the following real and reciprocal cell dimensions.

$$\begin{array}{ll} a = 8.46 \text{ \AA} & a^* = 0.214 \\ b = 12.50 & b^* = 0.142 \\ c = 7.40 & c^* = 0.245 \\ \beta = 101^\circ 54' & \beta^* = 78^\circ 6' \end{array}$$

The density as measured by the method of flotation is 1.615 g.cm.⁻³. Thus there are four (calculated 4.007) molecules per unit cell.

Among the X-ray reflections, systematic absences occurred for reflections of the type (0*k*0) for $k = 2n+1$. The space group is therefore $P2_1/m$.

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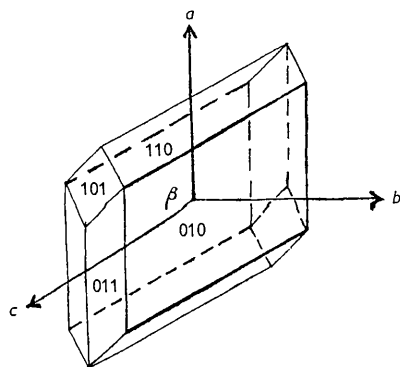


Fig. 1. Clinographic drawing of a crystal of 2-4-dinitroaniline.