# The Crystal Structure of Carbazole

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The analysis has been performed to make clear whether hydrogen bonds N–H···N are formed in carbazole crystal and whether the molecule is planar. Single crystals in colorless plates were obtained by keeping the melted substance slightly below its melting point, 237°C. The crystals are orthorhombic with four molecules in a unit cell of dimensions $a=7.76$, $b=19.15$ and $c=5.74$ Å. The density measured by floatation in sulfuric acid was 1.29 g./cm$^3$ and the calculated value is 1.31 g./cm$^3$. The space group was found to be $Pn2_1a$ or $Pnma$. Since Wilson statistics showed the existence of a center of symmetry, it was decided that the corresponding space group was the latter.

Using the multiple-film technique, intensity data were obtained from zeroth-layer Weissenberg photographs around the main axes $a$, $b$ and $c$, taken with filtered Cu$K\alpha$ radiation. The intensities of reflexions were estimated visually with a calibrated scale.

The approximate co-ordinates of nitrogen and carbon atoms were obtained by the trial method considering packing. The structure thus obtained was refined initially by electron density projections on (001) and (100) and finally by the least-squares method.

The discrepancy index $R$ calculated with the final least-squares co-ordinates is respectively 0.14 for $hk0$, 0.15 for $0kl$ and 0.14 for $h0l$ if non-observed reflexions were omitted. The final electron density projection along the $c$-axis and the crystal structure projected on (010) are shown in Fig. 1 and Fig. 2 respectively.

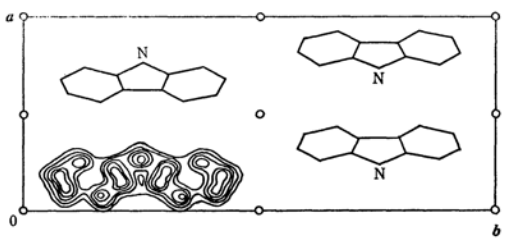


Fig. 1. Crystal structure projected on (001).

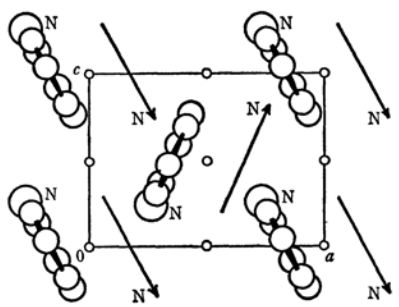


Fig. 2. Crystal structure projected on (010).

Carbazole molecule is planar, and a crystallographic mirror plane normal to the $b$-axis passes through the N atom and is perpendicular to the molecular plane. The N···N distance is 3.89 Å, and this shows that the hydrogen bond is not formed in the crystal as expected by Aihara[1] (1953) from the measurement of the vapor pressure.

Fluorene[2] crystal takes the same space group as carbazole and resembles closely to that of carbazole in both cell dimensions and atomic parameters. A full paper will be published in the near future.

1) A. Aihara, *J. Chem. Soc. Japan, Pure Chem. Sect. (Nippon Kagaku Zassi)*, **76**, 492 (1955).
2) D. M. Burns and J. Iball, *Proc. Roy. Soc.*, **A227**, 200 (1955).