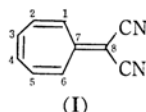


## The Crystal Structure of 8,8-Dicyanoheptafulvene

By Hirotaka SHIMANOUCHI,\* Tamaichi ASHIDA, Yoshio SASADA,  
Masao KAKUDO, Ichiro MURATA and Yoshio KITAHARA

(Received May 15, 1965)

8,8-Dicyanoheptafulvene (I) is a stable derivative of heptafulvene, which is a sort of the non-alternant hydrocarbon. This compound has been studied by several groups of workers in recent years.<sup>1-5)</sup>



The present investigation was undertaken in order to reveal its molecular parameters by X-ray analysis.

This compound crystallizes in a monoclinic unit cell with dimensions:  $a=7.84\text{ \AA}$ ,  $b=13.14\text{ \AA}$ ,  $c=3.99\text{ \AA}$ , and  $\beta=97.9^\circ$ . The space group is  $P2_1$  or  $P2_1/m$ . Since intensity statistics showed the existence of a center of symmetry, it was decided that the space group was the latter. There are two molecules in the unit cell, and the molecule should have a mirror plane in it.

Multiple-film equi-inclination Weissenberg photographs were taken for layers 0 to 3 about the  $c$  axis with  $\text{Cu-K}\alpha$  radiation, and the integrated intensities were estimated visually against a standard scale.

The structure was solved by the interpretation of Patterson projections along the  $c$  and  $b$  axes and Harker section  $P(u, 1/2, w)$ . The positional and thermal parameters of each atom

so obtained were refined by the least-squares method. The final electron density projection along the  $c$  axis is shown in Fig. 1. The molecule is planar and lies approximately parallel to the (101) plane; the interplanar spacing is  $3.4\text{ \AA}$ . A crystallographic mirror plane normal to the  $b$  axis passes through the atoms  $C_7$  and  $C_8$  and is perpendicular to the molecular plane.

A detailed account of this work will be presented in the near future.

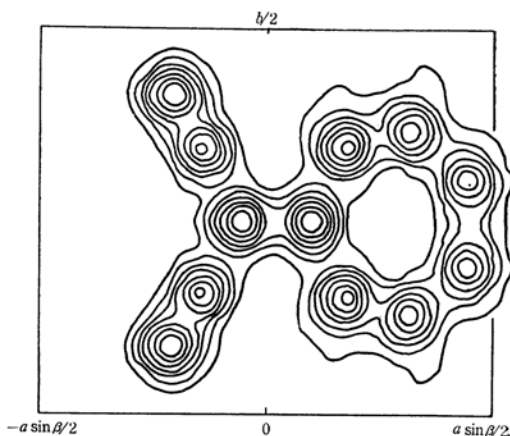


Fig. 1. The final electron density projection on the (001). Contours at intervals of  $1.0\text{ e. \AA}^{-2}$ , the lowest being at  $1.0\text{ e. \AA}^{-2}$ .

\* On leave from Department of Chemistry, Faculty of Science, Tohoku University.

1) T. Nozoe, T. Mukai, K. Osaka and N. Shishido, *This Bulletin*, **34**, 1384 (1961).

2) M. Yamakawa, H. Watanabe, T. Mukai, T. Nozoe and M. Kubo, *J. Am. Chem. Soc.*, **82**, 5665 (1960).

3) K. Hafner, H. W. Riedel and M. Danielisz, *Angew. Chem.*, **75**, 344 (1963); *Angew. Chem. internat. Edit.*, **2**, 215 (1963).

4) C. Jutz, *Chem. Ber.*, **97**, 2050 (1964).

5) D. J. Bertelli, C. Golino and D. L. Dreyer, *J. Am. Chem. Soc.*, **86**, 3329 (1964).

Institute for Protein Research  
Osaka University  
Kita-ku, Osaka  
(H. S., T. A., Y. S. & M. K.)  
Department of Chemistry  
Faculty of Science  
Tohoku University  
Ka'ahira-cho, Sendai  
(I. M. & Y. K.)