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Physical parameters of organic molecular crystals by micro-indentation

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Abstract : Vicker's hardness studies were performed on single crystal cleavages of anthracene, phenanthrene and anthraquinone and the hardness values so obtained were used to find the surface energy and solubility of these organic compounds. In is observed that the variation of these parameters is linear with hardness. Also, the heat of sublimation, melting point of the solid and the latent heat of fusion show a linear behaviour.

Keywords : Vicker's indentation, microhardness, single crystals

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1. Introduction

Correlation between the hardness and lattice energy of a variety of crystals is reported [1,2]. Hardness and the energy needed for the formation of Schottky defects in alkali halides has been shown [3]. The existence of a relationship between the Vicker's hardness and the surface energy of cleavable crystals has been reported [4]. This paper presents the results of the various physical parameters obtained from hardness studies and their relation.

2. Experimental techniques

Crystal growth :

Single crystals of anthracene, phenanthrene and anthraquinone were grown from the melt by the Bridgman method. The starting material was column chromatographed, twice vacuum sublimed and zone refined. The material was transferred to the crystal growth tubes without exposure to the atmosphere [5]. The crystals were cleaved in the usual manner using a sharp blade. Smooth (001) cleavages were selected after optical examination.

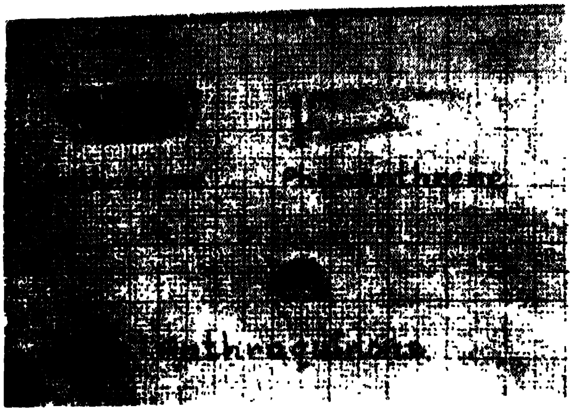

Plate I.

Microhardness

The crystals were indented on a Carl Zeiss NU 2 Universal Research Microscope. The indents were made with a pyramidal diamond indentor. Loads (P) varied from 5 gm to 100 gm in small steps. A number of indents were made at each load at random on the surface. The mean diagonal length was used in calculating the Vicker's hardness number (VHN) using the formula

$$\mathrm{VHN} = 1.854 \times P/d^2, \tag{1}$$

where P is the applied load in kg and d, the mean diagonal length in mm. The indentation time of 10 s was kept constant as this time was adequate to minimize the vibration effects on the results. The crystal size was much larger than the indentation size, thus eliminating the boundary effects on the results. The distance between the indents was five times the size of the largest indentation mark. The crystal thickness was relatively large such that the indenter did not sense the lower surface [6]. A number of crystals were indented.

3. Results and discussion

Table 1 gives the Vicker's hardness values obtained for the three aromatic hydrocarbons studied. In solubility, the bonds existing between the molecules in a lattice are ruptured. Hardness and cleavage surface energy of crystals also involve the rupturing of bonds between the molecules Hence, a relation should exist between these quantities.

Sangwal [4] has given a relation between the Vicker's hardness and the cleavage surface energy as

$$H_\gamma = 10^{-3}\gamma_s^2, \tag{2}$$

where H_γ is in kgf/mm^2 and γ_s in dyne/cm.

He has also given the relation between the solubility and hardness as

$$C_0 = \left(316\, H_\gamma^{1/2}/B\right)^n, \tag{3}$$

where *B* and *n* are constants. *B* has the value of 170 which is characteristic of the monoclinic structure and *n* has the value of 14 for this structure.

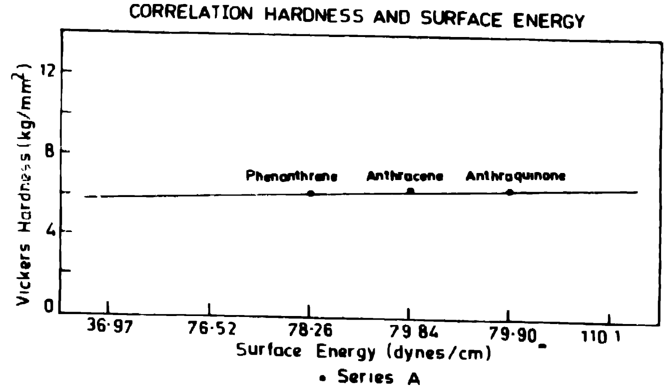

Figure 1. Correlation hardness and surface energy.

Figures 1 and 2 give the correlation between the hardness *versus* surface energy and solubility for the compounds studied.

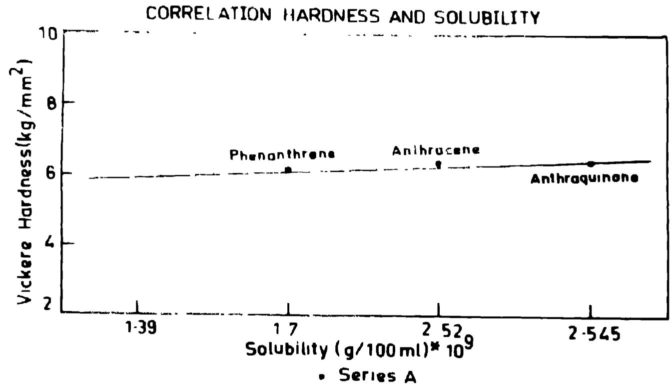

Figure 2. Correlation hardness and solubility.

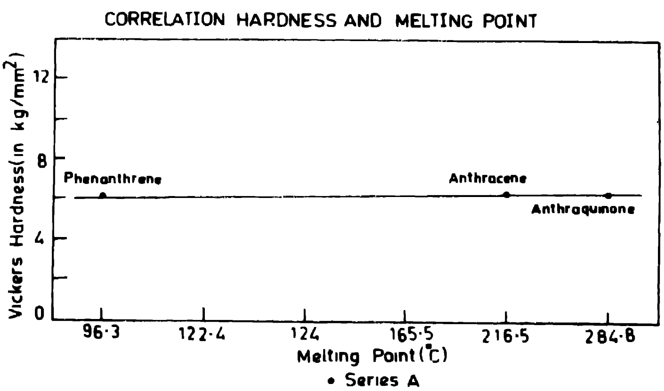

Figure 3. Correlation hardness and melting point.

To see what type of behaviour other physical properties exhibit, the melting point, heat of sublimation and latent heat of fusion are also plotted *versus* the hardness. These also exhibit a linear behaviour (Figures 3–5).

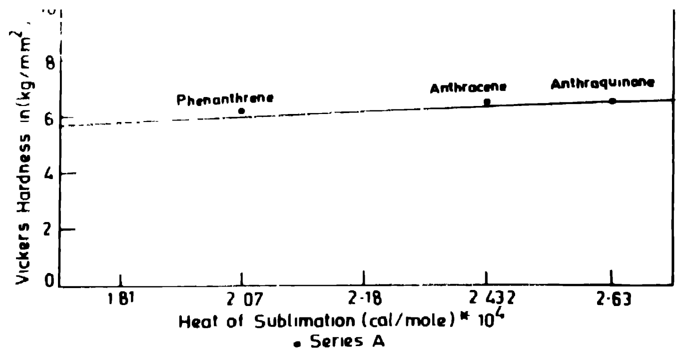

Figure 4. Correlation hardness and heat of sublimation.

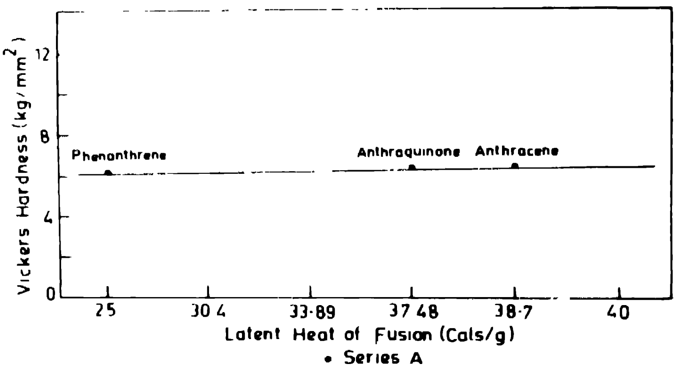

Figure 5. Correlation hardness and latent heat of fusion

4. Conclusions

1. The hardness of crystals show a linear behaviour with respect to the empirically found cleavage surface energy of crystals and the solubility.
2. Other physical properties such as melting point, heat of sublimation and latent heat of fusion show a similar behaviour.

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