

### Melting-point Variation in Isomeric Dibromobenzenes

Kamil F. Dziubek, Andrzej Katrusiak, *Faculty of Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznań, Poland*. E-mail: rumianek@amu.edu.pl

Single crystals of 1,2- and 1,3-dibromobenzenes have been *in situ* pressure crystallized in diamond anvil cells and studied by X-ray diffraction. Both structures are orthorhombic: 1,2-dibromobenzene (0.3 GPa), space group *Pbca*,  $Z = 8$ ,  $a = 7.831(1) \text{ \AA}$ ,  $b = 15.256(1) \text{ \AA}$ ,  $c = 11.701(2) \text{ \AA}$ ; 1,3-dibromobenzene (0.2 GPa), space group  $P2_12_12_1$ ,  $Z = 8$ ,  $a = 4.105(1) \text{ \AA}$ ,  $b = 12.899(5) \text{ \AA}$ ,  $c = 25.987(28) \text{ \AA}$ . The relationship between the molecular symmetry and the melting point of the dibromobenzene isomers has been discussed. According to the empirical Carnelley's rule high molecular symmetry is related with high melting point [1], [2]. This effect however can be justified in various ways. The melting points are: 278-280 K for 1,2-, 266 K for 1,3-, and 356-360 K for 1,4-dibromobenzene. The Br...Br intermolecular interactions are distinct in both these structures, and they can be considered to be the main factor responsible for the molecular rearrangements in these crystals.

[1] Carnelley T., *Philos Mag. 5th series*, 1985, **13**, 112-130. [2] Brown R. J. C., Brown R. F. C., *J. Chem. Educ.*, 2000, **77**, 724-731.

**Keywords:** high-pressure structure determination, halogens, structure-property relationships in solids