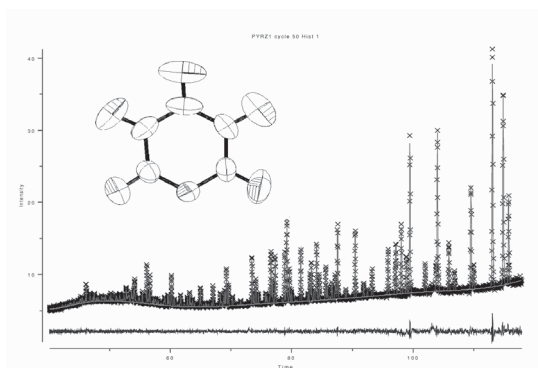


s7.m26.p2 **The effect of temperature on the crystal structure of pyridine.** S. Parsons, S. Crawford, *School of Chemistry, University of Edinburgh, Edinburgh, UK; W.I.F David, R.M. Ibberson, ISIS Facility, Rutherford-Appleton Laboratory, Didcot, UK. E-mail: stephen.crawford@ed.ac.uk*

A rich phase chemistry has been predicted for pyridine, with a computational study by Price et al. [1] revealing 12 energetically similar structures. This, coupled with the simple nature of the molecule makes pyridine a good candidate for detailed structural studies. As well as being interesting in itself, it is hoped that the structural behavior of pyridine may shed light on more fundamental trends in structure and bonding in molecular materials.

Previously only two crystal phases of pyridine have been identified by experiment. The  $Z'=4$  phase (pyridine-I) first found by Mootz *et al.* [2] is unexpectedly complicated and has been found to arise from a range of crystallisation conditions. The simpler  $Z'=1$  phase (pyridine-II) has previously only been grown for pyridine at high pressure [3], or for perdeuteropyridine from a pentane solution [4].

Using the HRPD instrument at the ISIS facility, we have performed a study of the crystallographic behaviour from 2K to melting of a pure perdeuteropyridine powder sample. Pyridine-I was found at lower temperatures, until a phase transition to pyridine-II was observed with increasing temperature. On further increase in temperature, a re-entry to the pyridine-II phase was seen.

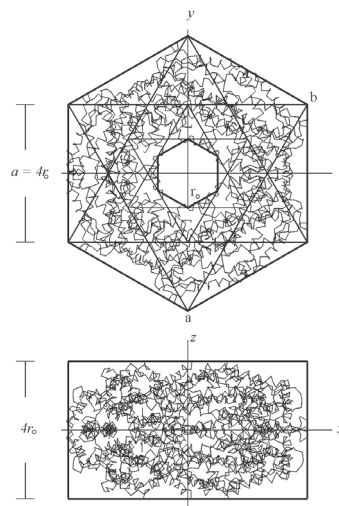


- [1] A.T Anghel, G.M. Day and S.L. Price, *Cryst. Eng. Comm.* (2002), **4**, 348  
 [2] D. Mootz, H-G Hussow. (1981). *J. Chem. Phys.* **75**, 1517.  
 [3] A. Dawson and S. Parsons. (2003). Unpublished Data  
 [4] R. Boese, M.T. Kirchner, A. Gehrke and D. Blaser (2003) Unpublished data.

s7.m26.p3 **Remarkable features in lattice parameter ratios of crystals.** R. de Gelder and A. Janner, *NSRIM Institute, Radboud University Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands. E-mail: alo@sci.kun.nl*

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The investigation of the lattice parameter ratios of tetragonal and hexagonal-rhombohedral inorganic compounds, as reported by Constant and Shlichta [1], has been extended to the structural data one finds for organic and organo-metallic compounds in the Cambridge Structural Database, CSD (294.400 entries), for the inorganic ones in the Inorganic Crystal Structure Database, ICSD (53.600 entries) and for the bio-macromolecules in the Protein Data Bank, PDB (18.800 entries). The results obtained confirm the general existence of sharp peaks as a function of ratios of lattice parameters and reveal additional exponential components, decaying for large and small values of these ratios. Most of the peaks correspond to lattices having a metric tensor with rational entries (integral lattices) [2]. The exponential component is interpreted as expressing a general statistical distribution valid for the generic crystal lattices, normally considered. The exponential fraction dominates in the organic and organo-metallic cases (CSD), is much less important for inorganic crystals (ICSD) and takes an intermediate character for bio-macromolecules (PDB). In particular, unexpected is the qualitative difference between the distributions of orthorhombic crystals (for  $a \leq b \leq c$ ) as a function of  $c/a$  and of  $c/b$ , respectively. For the hexagonal lattices, in the inorganic case (ICSD) the most important peak is at  $c=a$ . This corresponds to the isometric hexagonal lattice, first observed in the molecular form of the hexameric protein R-phycoerythrin [3] (Fig. 1). In the CSD and PDB crystal data hexagonal peaks also occur at  $c=a$  and  $c=a/2$  ( $00\frac{1}{2}$  centering). More peculiarities will be discussed in a future paper.



**Fig. 1.** Hexameric R-phycoerythrin: hexagonal form with  $c=a=4r_0$

- [1] B. Constant and P.J. Shlichta (2003). *Acta Cryst.* **A59**, 281-282.  
 [2] A. Janner (2004). *Acta Cryst.* **A60**, 198-200.  
 [3] A. Janner (2004). Submitted for publication.