

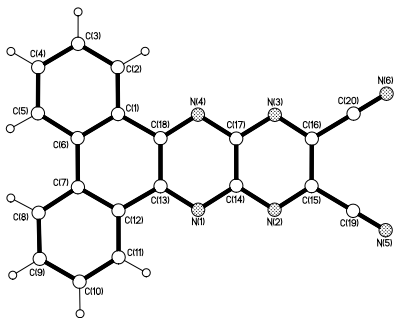
FA4-MS33-P01

Structure-property relationships in acenes and pyrenes for organic electronics. Mark R.J. Elsegood.

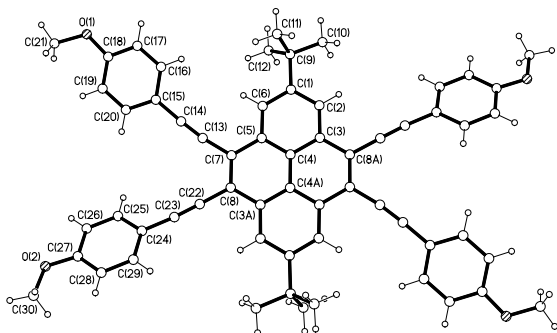
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Compounds incorporating several fused, aromatic rings offer considerable promise in organic electronics. In the actual electronic devices the compounds are spun out as thin films. However, a knowledge of their structure from X-ray crystallography is vital in the on-going work to improve device performance. In collaboration with Dr. Jonathan Hill's MANA group at NIMS, Tsukuba, Japan, we are engaged in the synthesis and self-assembly of soluble oligoazaacenes [1,2]. One successfully targeted compound is 2,3-dicyanotetraazabenzotriphenylene, **1**. The crystal structure exhibits π - π stacking, C-H \cdots N head-to-tail interactions resulting in a ribbon packing motif, and an exceptionally close intermolecular N \cdots N separation. This latter feature, we believe, explains the *n*-type semiconductor properties of the compound.

**1**

In collaboration with Prof. Takehiko Yamato's group at Saga Univ., Japan, we have investigated a variety of photoactive compounds, for example, the pyrene-based, cruciform-shaped compound, **2**. In this compound, the key feature is that the aromatic decks are **not** very closely stacked and it is this that is believed to be important in the light being emitted at the valuable blue end of the visible spectrum [3]. Diffraction data have been obtained for several other examples, some collected at the ALS synchrotron source, Berkeley, CA.

**2**

[1] Richards G.J., Hill J.P., Okamoto K., Shundo M., Elsegood M.R.J., Mori T., Ariga K., *Langmuir*, 2009, 25, 8408. [2] Richards G.J., Hill J.P., Subbaiyan N.K., D'Souza F., Karr P.A., Elsegood M.R.J., Teat S.J., Mori T., Ariga K., *J. Org. Chem.*, 2009, 74, 8914. [3] Hu, J.-Y. Era, M.; Elsegood, M.R.J., Yamato, T., *Eur. J. Org. Chem.*, 2010, 72.

Keywords: organic materials, electronic materials, photoemission.

FA4-MS33-P02

Possible polyamorphic relationship between liquid and crystalline phases in SnI₄ Kazuhiro Fuchizaki,

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From in situ synchrotron x-ray diffraction measurements on liquid tin tetraiodide, which consists of SnI₄ molecules at ambient pressure, we have established that the liquid forms existing above and below a break point pressure, 1.5 GPa, where the slope of the melting curve of the crystalline phase changes abruptly, have different structures [1]. This discovery offers evidence of thermodynamically stable polyamorphism in general compounds as well as in elements such as phosphorus. The vertex-to-face orientation between the nearest molecules plays a key role in the transition from the low-pressure to the high-pressure liquid phase [1].

The liquid-liquid critical point (LLCP) scenario, which presumes the existence of a critical point associated with the liquid-liquid phase transition, seems to be naturally applicable to describe the aspect observed in SnI₄. Indeed, the LLCP scenario can consistently explain all our findings, including the stability limits of the two amorphous states. Our recent experimental investigation suggests that the LLCP is, if it exists, located close to the break point on the melting curve. Mean field treatments for the scenario allows us to estimate the differences in the molar entropy and volume, respectively, between the two liquid phases. Although the former is about 5 times larger than the corresponding value between the two amorphous states in ice, the latter is quite comparable with that found in ice, implying that the value represents a specific volume contraction upon collapsing a tetrahedral open network structure. Moreover, we infer that the vertex-to-face orientation correlation in the high-pressure liquid structure reflects a molecular arrangement in the high-pressure crystalline phase whose structure still remains unresolved.

[1] Fuchizaki K., *J. Chem. Phys.* 2009, 130, 121101. [2] Stokely, K.; Mazza, M. G.; Stanley, H. E.; Franzese, G. *Proc. Natl. Acad. Sci.* 2010, 107, 1301.

Keywords: liquid state, high pressure, synchrotron X-ray diffraction

FA4-MS33-P03

Co(pym)(VO₃)₂ and Co(H₂O)₂(VO₃)₂·2H₂O: structure, magnetic properties and relationships.

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The use of organic molecules for the design of new inorganic materials has allowed the preparation of compounds with major technological applications[1]. In this context, vanadium