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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 ongoing 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···N head-to-tail interactions resulting in a ribbon packing motif, and an exceptionally close intermolecular N···N separation. This latter feature, we believe, explains the n-type semiconductor properties of the compound.

![Structure of 1](image1)

In collaboration with Prof. Takehiko Yamato’s group at Saga Univ., Japan, we have investigated a variety of photocative 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.

Keywords: organic materials, electronic materials, photoemission.

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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 polymorphism 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.


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

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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...
derivatives seem to be good candidates to obtain new materials because of the versatile behaviour of this metal[2]. For this reason, our research has been focused in the synthesis and characterization of hybrid vanadates with aromatic and aliphatic amines[3]. In this work we present the comparative study of a hybrid vanadate, Co(pym)(VO$_3$)$_2$ (pym = pyrimidine) and an inorganic one Co(H$_2$O)$_2$(VO$_3$)$_2$.2H$_2$O with closely related structures. The three-dimensional Co(pym)(VO$_3$)$_2$, 1, has been synthesized under mild hydrothermal conditions. The crystal structure of 1 was solved using single-crystal X-ray diffraction data, taking into account that the crystals are twins of two components. Compound 1 crystallizes in the monoclinic system, space group C2/c, a= 12.899(5) Å, b= 9.899(2) Å, c= 7.051(1) Å, β = 111.41(3)°, Z= 4. The crystal structure is built up from edge sharing VO$_3$ trigonal bipyramidal double chains and [CoO$_4$pym], chains. This resembles to the structure of the Co(H$_2$O)$_2$(VO$_3$)$_2$.2H$_2$O compound[4]. 2. For this reason a comparative study of their properties was carried out.

Magnetic measurements of 1 reveal the existence of a ferromagnetic transition. This fact was confirmed with magnetization measurements. The ferromagnetic transition was also studied by specific heat measurements. However, 2 shows an antiferromagnetic behaviour with a metamagnetic transition at low temperature. The comparative study of the magneto-structural correlations reveals that the magnetic interactions in 1 are propagated via pyrimidine molecules, while in 2 the unique magnetic exchange pathway is the one extended by the vanadate groups.

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The structure of oil-continuous products, such as margarine or emulsions, Non-triglyceride structuring of edible oils and emulsions. Ruud den Adela, Arjen Botb, Eli Roijersa, Echard Flötterc, Unilever Research & Development Vlaardingen, The Netherlands E-mail: ruud-den.adel@unilever.com

The structure of oil-continuous products, such as margarine or butter, is based on a network of small crystallites of triglycerides (also known as triacylglycerols or TAGs). Low molecular weight structuring agents that can serve as an alternative to crystallising triglycerides in edible oils have raised considerable interest in recent years. The requirement that potential structurants should at least hold the promise to be allowed in food applications is a severe limitation. Nevertheless, several systems have been identified [1], amongst which the class of γ-oryzanol + sterol organogelators is the most intriguing representative [2].