

MS73.29.4

Acta Cryst. (2005). A61, C94**Dual-function Molecular Crystal with $[\text{Fe}^{\text{III}}(\text{C}_2\text{O}_4)\text{Cl}_2]^-$ Chain Anion**

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Looking for new dual-functional molecular crystal is an emergency task to molecular electronics. Two-dimensional honeycomb $\text{Cr}^{\text{III}}\text{Mn}^{\text{II}}(\text{C}_2\text{O}_4)^{3-}$ anion as a building block succeeded on built up ferromagnetic conductors, so as zero-dimensional FeCl_4^- anion to field-induced-organic superconductor with π -d interaction between donor and anion. It will be interesting to explore uniform one-dimensional anion with metal atom coordinated with $(\text{C}_2\text{O}_4)^{2-}$ and Cl^- . Several novel salts with one-dimensional $[\text{Fe}(\text{C}_2\text{O}_4)\text{Cl}_2]^-$ anion were synthesized, one iron atom bonds to two Cl atoms and four oxygen atoms of two oxalato groups in cis-mode. Depending on the counter-cation from A^+ , R_4N^+ and TTF series molecules, a uniform binding-arch or zigzag anion chain is found in the crystal. So dual-functional molecular crystal with magnetism property from paramagnetic, antiferromagnetic to ferromagnetic, conductivity from insulator, semiconductor, metal in charge-transfer complex and fast-ion conductor are constructed.

[1] Coronado E., Galan-Mascariros J.R., Gomez-Garcia C.J., Laukhin V.N., *Nature*, 2001, **408**, 447. [2] Uij S., Shinagawa H., Terashima T., Yakabe T., Terai Y., Tokumoto M., Kobayashi A., Tanaka H., Kobayashi H., *Nature*, 2001, **410**, 908.

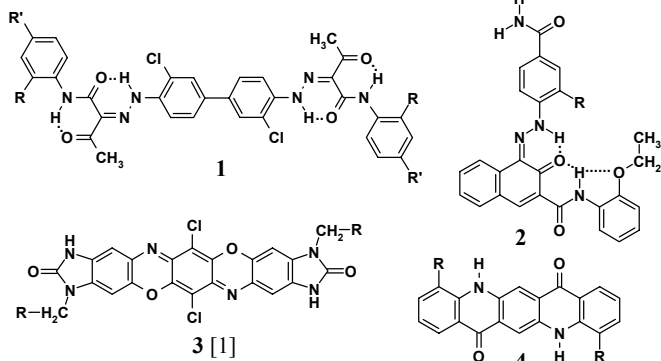
Keywords: crystal structure and properties, charge-transfer complex, iron compounds

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Acta Cryst. (2005). A61, C94**Crystal Engineering on Organic Pigments**

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The crystal structures of compounds **1-3** were determined from scratch by X-ray powder diffraction. Structure-property relationships were determined. Lattice energy calculations showed, how the crystal structures of **1-4** should be changed to improve the properties of the pigments (colour strength (**1**), weather fastness (**2**), density (**3**), and colour (**4**)). The corresponding new compounds or solid solutions were synthesized, and the improvements were proven experimentally. Some of the new pigments will be produced industrially.



R, R' = H, CH₃, OCH₃, F, Cl, Br, ...

[1] Schmidt M.U., Ermrlich M., Dinnebier R.E., *Acta Cryst.* 2005, **B61**, 37.

Keywords: crystal engineering, pigments, powder diffraction

MS74 TOTAL SCATTERING AND LOCAL ORDER

Chairpersons: Despina Louca, David Keen

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Acta Cryst. (2005). A61, C94**Static and Dynamic Pair Correlation Functions Determined by Neutron Scattering and Inelastic Correction to Total Scattering**

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The atomic pair-density function (PDF) is obtained as the Fourier-transform of the total scattering function. In case of x-ray scattering the PDF gives a snap-shot, a time averaged same-time correlation function, since the speed of light is so fast. However, the situation is more complex with neutrons, since the velocities of neutrons and atoms are comparable. On the other hand, it is easier to carry out inelastic scattering measurement with neutrons. The dynamic structure factor, $S(\mathbf{Q}, E)$, thus obtained, can be Fourier-transformed to give the dynamic PDF, or the frequency-resolved PDF. We show how the dynamic PDF helps to understand the nature of dielectric response of relaxor ferroelectric oxide, $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$, by direct observation of dynamic local ferroelectric polarization. The PDF obtained by powder diffraction without energy discrimination contains both static and dynamic information. For neutron scattering the dynamic part requires correction commonly known as the Placzek correction. We show how ineffective, or even damaging, this correction is, and show that the correct inelastic correction can be made within the Debye model of lattice vibration.

Keywords: total scattering, static and dynamic PDF, inelastic effects

MS74.29.2

Acta Cryst. (2005). A61, C94**The Local Structure of Ice VII Determined by Neutron Total Scattering**

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The structural characterization of the local geometry of the H-bond network in Ice VII has been a long-standing problem in ice physics. Rietveld refinements of neutron powder-diffraction data have revealed an apparently short molecular O-D bond-length [1,2] in the average structure. The assumption that the real bond-length is close to that found in the (ordered) ice VIII structure has led to the proposal of site disorder of the oxygen atom in ice VII. By converting the neutron-diffraction pattern of ice VII into a total structure factor, thereby retaining the information content of the diffuse scattering, we have been able to make a direct measurement of the molecular bond-length, demonstrating that it is indeed identical to that found in ice VIII. Additionally, we observe clear differences in the radial-distribution function from 1.5 - 2.0 Å, potentially indicating differences in the O...D separation between the two phases and, thus, H-bond geometry.

These results should have interesting implications for the interpretation of inelastic studies of the hydrogen-bond dynamics and may shed light onto the mechanism of bond centering at higher pressures.

[1] Kuhs W.F., et al., *J. Chem Phys.*, 1984, **81**, 3612. [2] Nelmes R.J., et al., *Phys. Rev. Lett.*, 1998, **81**, 2719.

Keywords: ice phases, neutron scattering, high pressure

MS74.29.3

Acta Cryst. (2005). A61, C94-C95**Medium Range Ordering of Local Polarizations in $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$**

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