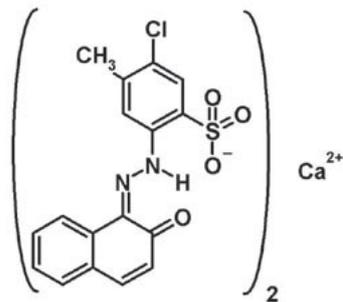


colours. All polymorphs were characterised by X-ray powder diffraction, DSC and DTA/TG. Additionally, temperature-dependent X-ray powder diffraction was used to determine the phase transitions, which occur upon heating.

[1] W. Herbst, K. Hunger, *Industrial Organic Pigments*, 3rd ed., Wiley-VCH, Weinheim, 269-270 (2004).



Keywords: polymorphism, organic compound, X-ray powder diffraction

## P06.07.58

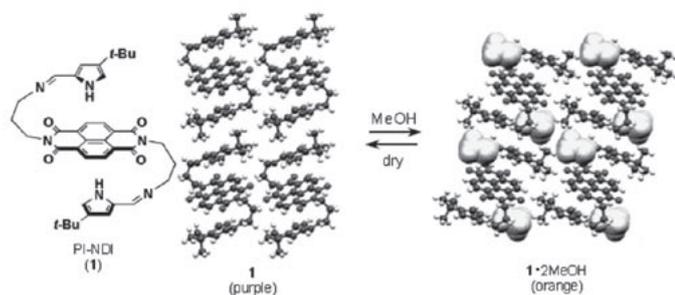
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### Development of Vapochromic Organic Crystals for Monitoring Systems of Sick-House Syndrome Gases

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Growing public awareness of the potential risk from exposure to volatile organic compounds (VOCs) in ordinary environment has prompted us to develop organic sensing materials by crystal engineering. Of particular interest are vapochromic materials that show reversible color change in visible spectral regions upon exposure to VOCs. Porous organic crystal of PI-NDI (**1**) was obtained by recrystallization from MeOH and subsequent removal of the solvent *in vacuo*. These purple crystals exhibit vapochromic behavior upon exposure to a variety of organic vapor such as MeOH (orange), acetone (orange), toluene (red) and triethylamine (yellow). It is noteworthy that sick-house gases such as formaldehyde can be also absorbed efficiently with irreversible color change to yellow. Powder structure analysis using synchrotron X-ray at SPring-8 (BL19B2) revealed that controlled intensity of D-A interaction between the PI and NDI units is a key for the vapochromism.



Keywords: solid-state gas-sensors, powder structure determination, inclusion complexes

## P09.05.54

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### Crystal engineering Intermolecular Hydrogen bond

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Crystal Engineering:

The rational design of supramolecular structure can be realized through crystal engineering based on relatively weak intermolecular forces. Among these forces, hydrogen bonding is the most common; however, other interactions including halogen-halogen or halogen-nitrogen have been used to organize molecules within the crystal. In particular, it is possible to define a supramolecular synthon as a structural unit within a supermolecule which can be formed and/or assembled by known or conceivable synthetic operations involving intermolecular interactions, by analogy with Corey's definition of a synthon in traditional organic synthesis. To understand the design of crystal packing of substituted benzene compounds, we look to different supramolecular synthons, to determine if there is a relationship between the role of substitution pattern and different types of intermolecular interactions.

Intermolecular:

Intermolecular forces are forces that act between stable molecules or between functional groups of macromolecules. Intermolecular forces include momentary attractions between molecules, diatomic free elements, and individual atoms. They differ from covalent and ionic bonding in that they are not stable, but are caused by momentary polarization of particles. Because electrons have no fixed position in the structure of an atom or molecule, but rather are distributed in a probabilistic fashion based on quantum probability, there is a positive chance that the electrons are not evenly distributed and thus their electrical charges are not evenly distributed.

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Keywords: Crystal engineering, Intermolecular, Hydrogen bond

## P10.01.56

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### Inorganic crystallography Geosciences

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Geosciences are the sciences of the earth, its stones, minerals and waterways. Geologists examine the history of minerals back to the origins of the planet, look at the development of the environment in recent decades, study the evolution of climate since the last Ice Age or deal with the question of why the dinosaurs died out. Geologists understand the process of sediment movement, how minerals are created, and the mineralogical constitution of the earth in the past, present and future. They are able to explain the origins of volcanoes and to forecast eruptions. Geosciences are a field study that deals with a great variety of topics. Geologists must understand the chemical composition of the waters, the physics of earthquakes and continental shifts, the evolution of life, the structures of precious stones but also the components of which the earth is made. Moreover, they must understand the impact of rain and snow on the mountains. In our society, the profession of geoscientist is a very important one,