or physical sensing devices. On-off switching of solid-state luminescence intensity have been achieved by adsorption and desorption of guest molecules or thermal stimuli. However, there has been few reports on the switching of luminescence mode. Here, we report the regulation of luminescence mode of organic salts of anthracene-2,6-disulfonic acid (ADS) with sec-butylamine by external stimuli. The organic salts yielded inclusion crystals with 1,4-dioxane, 1,4-thioxane or benzene. Whereas emission spectra of inclusion crystal with 1,4-thioxane or benzene have vibrational structure, that of inclusion crystal with 1,4-dioxane are broad and redshifted by 20 nm. This indicate that the latter exhibited excimer-like emission derived from the large π/π overlap of the anthracene moieties. Powder X-ray diffraction (PXRD) analyses indicated that the inclusion crystals with 1,4-dioxane showed supramolecular isomerization by chemical and physical stimuli. When the inclusion crystal with 1,4-dioxane was heated until 473 K, 1,4-dioxane was released completely from the crystal. The emission spectrum of the resulting crystal was similar to inclusion crystal with 1,4-thioxane or benzene. PXRD pattern and emission spectra suggest the rearrangement of ADS. By the exposure of the crystal to 1,4-dioxan, the PXRD peak shifted to the longer distance. After cooling of the crystal until 253 K, the peak in PXRD pattern and emission spectrum became similar to that of original crystal. These date confirm that the inclusion crystal with 1,4-dioxane changes the emission mode from monomer emission to excimer-like one through the reversible structure transition by external stimuli.

Keywords: solid-state dynamics, luminescence, organic crystals

P08.03.09

Acta Cryst. (2008). A**64**, C421

Computational studies of relationships between structure and lattice dynamics in organic crystals

Graeme M. Day[1], Ruoyu Li[2], Edward P. J. Parrott[2,3], J. Axel Zeitler[3], Lynn F. Gladden[3]

[1]University of Cambridge, Chemistry, Lensfield Road, Cambridge, Cambridgeshire, CB2 1EW, UK, [2]Cavendish Laboratory, University of Cambridge, J. J. Thomson Ave., Cambridge, CB3 0HE, UK, [3]Department of Chemical Engineering, University of Cambridge, Pembroke St., Cambridge, CB2 3RA, UK, E-mail：gmd27@cam.ac.uk

There is an increasing demand for accurate assignments of the vibrational modes in molecular organic crystals at terahertz frequencies (1 THz = 33 cm^{-1}), due to the rapidly growing number of experimental activities using terahertz time-domain spectroscopy (THz-TDS). The vibrational modes in this region are largely due to whole-molecule motions and are therefore dictated by the intermolecular interactions in the crystal. To date, a number of approaches have been developed to calculate vibrational spectra in the terahertz range, including lattice dynamics based on atom-atom model potentials [1] and on periodic electronic structure theory [2]. We have been applying the two methods to develop an understanding of relationships between structure and lattice dynamics in molecular organic crystals and to characterise observed THz-TDS spectra. Computational investigations of the vibrational modes in several series of small molecules with well-characterised crystal structures will be presented, along with the observed spectra. We find that the computational efficiency of the atom-atom approach can be exploited to rapidly investigate the effect of structural changes on lattice dynamics, while the more demanding electronic structure calculations must be used when the mixing of low-frequency molecular modes with the lattice modes becomes significant. Their combined use can be a successful approach to characterising observed spectra and is leading to an understanding of the influence of both molecular structure and intermolecular interactions on the dynamics in molecular crystals in the terahertz region.

[1] G.M.Day, J.A.Zeitler, W.Jones, T.Rades, and P.F.Taday, J.Phys. Chem. B, v.110, p.447, 2006.
[2] D.G. Allis, D.A. Prokhorova, and T.M. Korter, J. Phys. Chem. A, v.110, p.1951, 2006.

Keywords: dynamics, theoretical calculations, vibrational spectra

P08.03.10

Acta Cryst. (2008). A**64**, C421

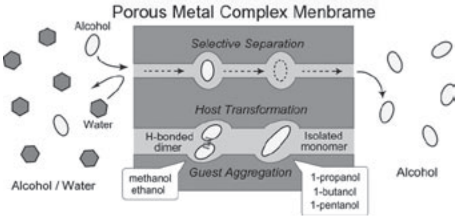
Alcohol vapor inclusion in transformable crystal hosts and application to separation membrane

Satoshi Takamizawa[1,2], Chihiro Kachi-Terajima[1], Takamasa Akatsuka[1], Masa-aki Kobara[1]

[1]Yokohama City University, International Graduate School of Arts and Sciences, 22-2 Seto, Kanazawa-ku, Yokohama, Kanagawa, 2360027, Japan, [2]PRESTO, Japan Science and Technology Agency (JST), Honcho, Kawaguchi, Saitama 332-0012, Japan, E-mail：staka@yokohama-cu.ac.jp

The vapor absorbency of series of alcohols from methanol to 1-pentanol was characterized on single crystal adsorbents, $[M^{II}_2(bza)_4(pyz)]_n$ (bza = benzoate; pyz = pyrazine; M = Rh (**1**), Cu (**2**)). The crystal structures for all alcohol-inclusions were determined by single-crystal X-ray crystallography at 90 K. The crystal phase transition induced by the guest adsorption occurred in the inclusion crystals except for the 1-propanol. A hydrogen-bonded dimer of adsorbed alcohol was found in the methanol and ethanol inclusion-crystals. In contrast, an isolated monomer existed in the channel for 1-propanol, 1-butanol, and 1-pentanol inclusions. Alcohol/water separation was characterized by a pervaporation (PV) technique using microcrystals of **2** dispersed in a poly(dimethylsiloxane) membrane [1].

[1] S. Takamizawa, C. Kachi-Terajima, T. Akatsuka, M. Kohbara, T. Jin, Chem. Asian J., 2(7), 837-848 (2007).



Keywords: gas-solid inclusion reaction, solid-state structural changes, single-crystal applications

P08.03.11

Acta Cryst. (2008). A**64**, C421–422

Gas-conforming ability of $[M^{III}(en)_3]Cl_3$ as transformable ionic-single crystal hosts

Ryosuke Miyake[1], Takamasa Akatsuka[2], Masa-aki Kohbara[3], Satoshi Takamizawa[4]

[1]Yokohama City University, International Graduate School of Arts and Sciences, 22-2 Seto, Kanazawa-ku, Yokohama, Kanagawa, 236-0027, Japan, [2]Yokohama City University, 22-2 Seto, Kanazawa-ku, Yokohama, Kanagawa, 236-0027, Japan, [3]Yokohama City University, 22-2 Seto, Kanazawa-ku, Yokohama, Kanagawa, 236-0027, Japan, [4]Yokohama City University, 22-2 Seto, Kanazawa-ku, Yokohama, Kanagawa, 236-0027, Japan, E-mail：ryosuke@yokohama-cu.ac.jp

Single crystal of $[Co(en)_3]Cl_3$ shows gas adsorbency for various gases