Poster Presentation

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Vapochromism of Organic Cocrystal Induced by Crystalline Solvent Exchange

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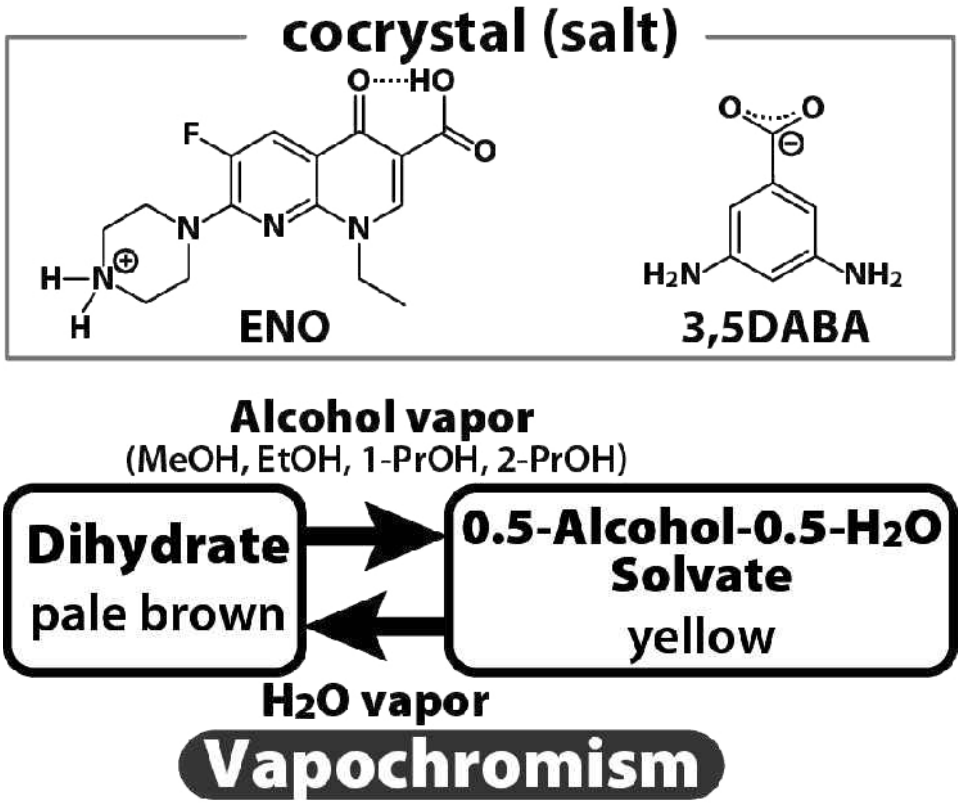
Vapochromic materials, which show color change induced by vapors, are expected to be applied to the sensing of volatile organic compounds or humidity. As for the metal complex crystals, many vapochromic crystals are reported, however, vapochromic organic crystals are not common. Therefore, it is important to find vapochromic organic crystals and to reveal the mechanistic aspects of structure transformations and color change based on the crystal structures. Pale brown Enoxacin-3,5-Diaminobenzoic Acid (ENO-3,5DABA) dihydrate cocrystal changed to yellow on exposure to four kinds of alcohol solvent vapors (methanol, ethanol, 1-propanol, 2-propanol), and these yellow crystals returned to pale brown dihydrate crystal by humidity, which is called vapochromism. The single crystals recrystallized from water (pale brown) and methanol (yellow) are equal to the dihydrate and the methanol vapor applied forms, respectively, and their crystal structure determination revealed that the cocrystals are 1:1 salt of ENO and 3,5DABA. Surprisingly, in the methanol vapor applied from, the crystalline solvent was changed to 0.5-methanol-0.5-water solvate (composition is ENO:3,5DABA:MeOH:H2O=2:2:1:1). Thus the dihydrate cocrystal undergoes solvent exchange transformation on exposure to methanol vapor and the color changes from pale brown to yellow. Because the XRD patterns of the yellow 0.5-methanol-0.5-water solvate cocrystal and the forms exposed to other alcohol solvent vapors shows high similarity, they are isostructure crystals. The color change is caused by the π…π interaction formation between the ENO molecule and 3,5DABA molecule in alcohol solvate form via solvent exchange transformations.



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