Furan-2,5-dicarboxylic acid, a promising platform molecule: polymer, monomer, and MOF

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Furan-2,5-dicarboxylic acid (FDCA), a small molecule discovered more than 100 years ago has been recently attracting attentions from both academic and industrial communities. Large-scale, economic production of FDCA has been accomplished, utilizing biomass fermentation residues, thanks to the breakthroughs in synthesis. [1] It has been ranked as one of the top platform molecules that are promising to produce functional materials via green chemistry. We report recent structural studies on three aspects of FDCA-based materials and their potential applications.

In the first case, crystal structure of a polymer, poly(ethylene furanoate) (PEF) which is a type of linear homopolymer of FDCA, is determined in a semi-quantitative way, using X-ray fiber diffraction method. Via 2D analysis of fiber diffraction pattern a monoclinic unit cell containing two staggered chains is proposed. [2] The chain staggering is attributed to the superior gas barrier properties of the solid-state PEF film. Secondly, co-crystallization of FDCA with polar aprotic solvents, namely, dimethyl sulfoxide (DMSO) and dimethylformamide (DMF) is investigated by using single-crystal crystallography. The two types co-crystals exhibit distinct hydrogen-bonding networks. Moreover, crystal structures of the FDCA-DMSO solvate provides a fingerprint of sulfur-oxygen interaction. [3] This weak specific interaction is further investigated by using X-ray pair distribution function (PDF) method and FTIR spectroscopy. Last but not least, 1D, 2D, and 3D metal organic frameworks synthesized by employing FDCA as linker and Zn(II) as central ion is reported. [4] We demonstrate that FDCA can be used as a versatile linker to produce coordinate polymers.

Reference

- [1] Jong, E. de, Dam *et al.* (2012). Biobased Monomers, Polymers, and Materials, edited by P. B. Smith & R. A. Gross, pp. 1–13. ACS Symposium Series. Washington, DC: American Chemical Society.
- [2] Mao, Y. et al. (2016). Polymer, 102, 308-314.
- [3] Mao, Y. & Zavalij, P. Y. (2018). Acta Cryst. C74, 986-990.
- [4] Mao, Y. & Zavalij, P. Y. (2019). Acta Cryst. C74, 1719-1724.