Single-crystal-to-single-crystal transformation of flexible Co-MOF as catalyst for epoxidation reaction

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Abstract: Four novel metal–organic frameworks (MOFs) based on 1,4-phenylenediacetic acid (1,4-H$_2$phda), [Co(1,4-phda)(4,4’-bpa)] (1), [Co(1,4-phda)(4,4’-bpp)] (2), [Co(1,4-phda)(4,4’-bpa)(H$_2$O)$_2$] (3), and [Co(1,4-phda)(4,4’-bpa)] (3a) (4,4’-bpa = 1,2-bis(4-pyridyl)ethane and 4,4’-bpp = 1,3-bis(4-pyridyl)propane) with diverse structures were successfully by different synthetic methods. Compound 1 exhibits 3D framework, while 2, 3 and 3a form a 2D layer with different architectures. The irreversible SC-SC transformation from compound 3 to 3a was established owing to high stability of 3a via hydrogen bond, π···π and C—H···π interactions. Notably, the irreversible SC-SC transformation demonstrates the pore opening in 3 and closing in 3a as a result of the change in orientation and conformation of both 4,4’-bpa and 1,4-phda ligands. Furthermore, the functional properties as epoxidation of alkenes of 3a have been investigated. The heterogeneous catalytic properties of 3a exhibits high conversion (82%) and selectivity of epoxide products (57%) as well as good catalyst stability.

Keywords: Metal-organic framework; Epoxidation of alkenes; Single-crystal-to-single-crystal transformation; Cobalt(II); 1,4-Phenylenedicarboxylic acid