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Concerted aryl interactions in zinc-imidazole – Oxovanadate hybrid organic-inorganic materialsSamroeng Krachodnok¹, Kenneth J. Haller¹, Ian D. Williams²¹Science, Suranaree University of Technology, Chemistry, 111 University Avenue, Muang, Nakhon Ratchasima, 30000, Thailand, ²Department of Chemistry, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China, E-mail: roengkra@hotmail.com

Noncovalent interactions involving aromatic sections of molecules are common and ubiquitous, and particularly when acting in concert, rival the robustness of hydrogen bonds. Herein, we report the ability of an imidazole and its derivatives capable of both hydrogen bonding and aromatic interactions in four zinc-imidazole – oxovanadate compounds, namely $[\text{ImH}]_2[\{\text{Zn}(\text{Im})_3\}_2\text{V}_{10}\text{O}_{28}] \cdot 2\text{H}_2\text{O}$ (1), $[\text{2-MeImH}]_2[\{\text{Zn}(2\text{-MeIm})_4\}_2\text{V}_{10}\text{O}_{28}]$ (2), $\text{Zn}(2\text{-MeIm})_3\text{V}_2\text{O}_6 \cdot \text{H}_2\text{O}$ (3), and $[\text{Zn}(\text{Im})_4]_2[\text{V}_4\text{O}_{12}]$ (4), to form extended concerted aryl interaction motifs. The tetrahedral zinc complexes in 1 to form two edge-to-face (EF) C – H ··· pi hydrogen bond interactions in 1D herringbone fashion along the a axis and interact with organic cations acting as guest molecules to construct concerted (OFF)₂ embraces as well as in 2 to form 1D chains of $-\text{[Zn}(2\text{-MeIm})_4]-(\text{OFF})(\text{EF})_2-\text{[Zn}(2\text{-MeIm})_4]-(\text{EF})_4-$ along diagonal axis. In contrast the tetrahedral zinc complexes in 3 engage in concerted (EF)₆ embrace motifs and further bind through four tilted offset aryl rings to generate 2D nets perpendicular to the a axis, and in 4 to form 1D chains of $-\text{[Zn}(\text{Im})_4]-(\text{EF})_6-\text{[Zn}_2\text{Im}_4]-(\text{EF})_2-\text{[Zn}_2\text{Im}_4]-(\text{EF})_6-\text{[Zn}(\text{Im})_4]-(\text{EF})_4-$ along the c axis with adjacent chains held together by two pairs of N – H ··· pi face-to-face (FF) hydrogen bond interactions to form 2D nets perpendicular to the a axis.

Keywords: concerted aryl interactions, zinc-imidazole-oxovanadate, hybrid organic-inorganic materials

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Assemblies of three mixed-ligands coordination polymers with novel 3D metal-organic frameworksChing-Chun Yang¹, Chih-Chieh Wang^{1,2}, Gene-Hsiang Lee³¹Soochow University, Chemistry, No 70, LinShih Rd., Shih-Lin., Taipei, Taiwan, 11102, Taiwan, ²E-mail: ccwang@scu.edu.tw, Tel: +886-2-28819471 ext 6824, ³Instrumentation Center, National Taiwan University, Taipei, Taiwan., E-mail: acvb.yang@msa.hinet.net

Three metal coordination polymers having formulas, $[\text{Co}(\text{dpe})(\text{BDC}) \cdot \text{H}_2\text{O}]_n$ (1), $[\text{Ni}(\text{dpe})(\text{BDC}) \cdot \text{H}_2\text{O}]_n$ (2) and $[\text{Zn}(\text{dpe})(\text{BDC}) \cdot 4\text{H}_2\text{O}]_n$ (3) (dpe=1,2-bis(4-pyridyl)ethane, BDC= terephthalic acid), have been synthesized and structurally characterized by using single-crystal X-ray diffraction, elemental analysis, infrared spectroscopy and thermogravimetry (TG). Compound (1) and (2) are isostructural and the metal centers (Co(II) and Ni(II)) are distorted octahedral geometric environment bonded to two nitrogen donors of two bridging dpe ligands with *anti*-conformation and four oxygen donors of two bridging BDC²⁻ ligands with bis-chelating coordination mode forming a three-dimensional (3D) interpenetrating diamond-like metal-organic framework (MOF), which exhibit high thermo-stability and keep their crystalline forms up to about 390 °C. In compound (3), the Zn(II) ions is tetrahedral geometric environment bonded with two nitrogen donors of two bridging dpe ligands with *gauche*-conformation and two oxygen donors of two BDC²⁻ ligands with bis-monodentate coordination mode forming a novel extended 3D architecture. The 1D helical chains are constructed through the

connectivity between the Zn(II) ions and *gauche*-dpe ligands, which are intercalated guest water molecules. Adjacent chains are then linked via the bridges of BDC²⁻ ligands adopting a zigzag pattern to complete the 3D MOF. The TG measurement of (3) reveals that the 3D networks exhibit high thermo-stability and keep their crystalline forms up to about 300 °C. The cyclic de- and ab-sorption procedures of water molecules are observed.

Keywords: metal-organic framework, coordination polymer, pi-pi interactions

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Structural characterization and thermal stability of three coordination polymers with 2D MOFsChuan-Yien Liu¹, Gene-Hsiang Lee², Hsin-Ta Wang¹¹National Taipei University of Technology, Department of Molecular Science and Engineering & Institute of Organic and Polymeric Materials, 1, Sec. 3, Chung-hsiao E. Rd., Taipei, Nil, 10608, Taiwan, ²Instrumentation Center, National Taiwan University, Roosevelt Road, Section 4, Taipei, 106, Taiwan, E-mail: cyliu0123@ntu.edu.tw

Three coordination polymers with 2D metal-organic frameworks (MOFs), $\{[\text{Cd}(3\text{-bpd})_2(\text{NCS})_2\text{C}_2\text{H}_5\text{OH}]\}_n$ (1), $\{[\text{Cd}(3\text{-bpd})(\text{dpe})(\text{NO}_3)_2]\cdot(3\text{-bpd})\}_n$ (2), $\{[\text{Cd}(\text{dpe})_2(\text{NCS})_2]\cdot 3\text{-bpd} \cdot \text{H}_2\text{O}\}_n$ (3) (3-bpd = 1,4-bis(3-pyridyl)-2,3-diaza-1,3-butadiene), were prepared and fully characterized by infrared spectroscopy, elemental analysis, thermogravimetric analysis, and single-crystal X-ray diffraction. In compound 1, each Cd(II) ion is six-coordinate bonded to six nitrogen donors of four 3-bpd with bis-monodentate coordination mode and two NCS⁻ ligands. The distorted square building blocks connect to each other to generate a 2D non-interpenetrating MOF. Each square unit consists of four Cd(II) atoms and 3-bpd ligands, which form a 4⁴-membered ring structure. In 2, the Cd(II) ion is six-coordinate bonded to six nitrogen donors of two 3-bpd, two dpe and two NO₃⁻ ligands. Both the 3-bpd and dpe ligands adopt bis-monodentate coordination mode to connect the Cd(II) ions forming a 2D, non-interpenetrating parallelogram MOF. Each parallelogram unit consists of four Cd(II) atoms and two 3-bpd ligands, two dpe, which also form a 4⁴-membered ring structure. In 3, the Cd(II) ions is coordinated by four pyridine nitrogen donors of dpe ligands in the basal plane and two NCS⁻ nitrogen donors in the axial sites. The dpe acts as a bridging ligand to connect the Cd(II) ions forming a 2D interpenetrating MOFs by using a square-planar node as the basic unit, which also form a 4⁴-membered ring structure. The free 3-bpd ligands shown in 2 and 3 play an important role on the construction of their 3D supramolecular architecture.

Keywords: framework structures, X-ray structure, coordination polymers

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Investigation structure and phase transitions of hybrids inorganic-organic metal vanadatesKittipong Chainok¹, Kenneth J. Haller¹, A. David Rae², Anthony C. Willis², Ian D. Williams³¹Suranaree University of Technology, Chemistry, 111 University Avenue, Muang, Nakhon Ratchasima, 30000, Thailand, ²Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia, ³Department of Chemistry, Hong Kong University of Science