Title:	Neutral Luminescent Metal-Organic Frameworks: Structural Diversification, Photophysical Properties, and Sensing Applications
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Keywords:	Metals Ligands Fluorescence Metal organic frameworks olvents
Issue Date:	2017
Publisher:	ACS Publications
Citation:	Inorganic Chemistry, 56 (23)
Abstract:	Utilizing flexible bis(tridentate)polypyridyl ligands, the two new luminescent 2D metal organic frameworks {Zn2(tpbn)(2,6-NDC)2}n (1) and {[Zn2(tphn)(2,6-NDC)2]·4H2O}n (2), where tpbn = N,N′,N″,N‴-tetrakis(2-pyridylmethyl)-1,4-diaminobutane, tphn = N,N′,N″,N‴-tetrakis(2-pyridylmethyl)-1,6-diaminohexane, and 2,6-H2NDC = 2,6-naphthalenedicarboxylic acid, have been isolated in good yields under solvothermal conditions. Their solid-state molecular structures have been determined by single-crystal X-ray diffractometry. Both 1 and 2 have pentacoordinated Zn(II) centers with an N3O2 environment from three nitrogen atoms of the tpbn or tphn ligand and two carboxylate oxygen atoms from two different 2,6-NDC linkers. However, the binding modes of the tridentate part of polypyridyl ligands to the Zn(II) center are different in 1 and 2—meridional (tpbn) vs facial (tphn) due to an increase (1.5 times) in the methylene chain length. Thus, the binding mode of 2,6-NDC to the Zn(II) center differs: bis(monodentate) syn-anti in 1 and bis(monodentate) syn-syn in 2. This difference in binding modes of the components has a profound effect on the conformation of the six-membered ring (metal centers are considered as the vertices in it) within the 2D framework: honeycomb vs chair form for 1 and 2, respectively. In addition to further characterization by elemental analysis and UV–vis and FT-IR spectroscopy, their framework stabilities in water and thermal properties have been studied by powder X-ray diffraction and thermogravimetric analysis, respectively. On the basis of thermodiffractometry, 1 and 2 retain their crystallinity and overall structure up to 350 and 325 °C, respectively. Their luminescent properties have been utilized to demonstrate sensing of various solvents as well as nitro-aromatic compounds in water, which correlate well with their structural differences. Through the spectral overlap, lifetime measurements, and nature of the Stern–Volmer plots, the fluorescence quenching pathway for the nitro-analytes, particularly 2,4,6-trinitrophenol (TNP), is established for 1 and 2. Their recyclability and stability after sensing experiments are found to be excellent.
URI:	https://pubs.acs.org/doi/abs/10.1021/acs.inorgchem.7b02264 (https://pubs.acs.org/doi/abs/10.1021/acs.inorgchem.7b02264) http://hdl.handle.net/123456789/1690 (http://hdl.handle.net/123456789/1690)
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