Title:	Tunable Strategies Involving Flexibility and Angularity of Dual Linkers for a 3D Metal-Organic Framework Capable of Multimedia Iodine Capture
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Abstract:	The widespread use of nuclear power poses severe health and environmental risks owing to the nonregulated release and disposal of radioactive wastes in the environment. Among these wastes, the capture and removal of radioactive iodine poses a big challenge. To develop a novel material for capturing molecular iodine, we have strategically synthesized a nitrogen-rich three-dimensional (3D) metal-organic framework (MOF), {[Mn2(oxdz)2(tpbn)(H2O)2]·2C2H5OH}n (1), utilizing a bent heterocyclic dicarboxylate linker (H2oxdz: (4,4'-(1,3,4-oxadiazole-2,5-diyl)dibenzoic acid)) and a flexible bis(tridentate) ligand (tpbn: N, N', N″, N‴-tetrakis(2-pyridylmethyl)-1,4-diaminobutane). Based on its single-crystal structure, 1 is an eightfold interpenetrated 3D framework, consisting of a unique 4-connected {Mn2(tpbn)} subunit, in which the pores line up with the nitrogen atoms of the oxadiazole moiety. This can be considered as a big leap for the development of 3D MOFs using flexible bis(tridentate) ligands. To emphasize the role of the flexible methylene chain length in such ligand in the dimensionality of the resultant framework, the tphn (N, N', N″, N‴-tetrakis(2-pyridylmethyl)-1,6-diaminohexane) ligand with two additional methylene groups provides a one-dimensional (1D) CP {[Mn2(oxdz)2(tphn)(H2O)]·CH3OH}n (2). This spacer chain lengthening has a profound effect on the coordination of such ligand with Mn(II), further affecting the binding of oxdz. The inherent polarizable nature of the oxadiazole moiety and the presence of permanent pore of dimensions (19.122 × 19.253 Å2) in 1 have been exploited for the capture/removal of iodine not only from vapor and an organic solution but also from an aqueous media. It exhibits competent 100% reversible sorption of iodine with an uptake capacity of (1.1 ± 0.05) g/g of 1. The uptake value has been corroborated by both gravimetric and titrimetric analyses. The interaction of iodine with 1 has been notably studied with molecular simulations, kinetic models of sorption, field emission scanning electron microscopy (FESEM), and energy-dispersive X-ray spectroscopy (EDX) analysis. Moreover, 1 is highly stable and is recyclable without much loss of sorption capability up to five cycles.
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