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Title:	Conformational isomerism involving the carboxylate groups of a linker in metal organic frameworks and its distinctive influence on the detection of ketones
Authors:	Kumar, Sandeep (/jspui/browse?type=author&value=Kumar%2C+Sandeep) Bhambri, Himanshi (/jspui/browse?type=author&value=Bhambri%2C+Himanshi) Mandal, Sanjay K. (/jspui/browse?type=author&value=Mandal%2C+Sanjay+K.)
Keywords:	carboxylate isomerism
Issue Date:	2021
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Citation:	New Journal of Chemistry, 45(43), 20219–20226.
Abstract:	In this work, the influence of solvent and reaction conditions (solvothermal vs. room temperature) on the product formation is analyzed using two Zn(II) MOFs, {[Zn(bpaipa)]·DMF·2H ₂ O} _n (1) and {[Zn(bpaipa)]·5H ₂ O} _n (2), where H ₂ bpaipa = 5-(bis(pyridin-2-ylmethyl)amino)isophthalic acid. Both 1 and 2 are isolated in >80% yields from the reaction of Zn(OAc) ₂ ·2H ₂ O and H ₂ bpaipa under solvothermal and ambient conditions, respectively. With a difference in lattice solvent accommodation inside their pores, 1 and 2 are rare examples of conformational isomerism involving the carboxylate groups of bpaipa as determined by their single crystal X-ray structures. Using N ₂ adsorption experiments at 77 K, the difference in their pores was also verified. Their bulk phase purity and crystallinity were established by powder X-ray diffraction. Both 1 and 2 are thermally stable but 1 is more stable than 2 as demonstrated by the thermogravimetric analysis. Interestingly, their luminescence properties in different solvents are also influenced by such a structural difference. Utilizing the luminescence behavior of 1 and 2, the selective and sensitive detection of various ketones, including acetone and cyclohexanone (for an indirect sensing of RDX), is explored in three different solvents.
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