

# International Conference and Expo on Chemistry and Chemical Science

October 19<sup>th</sup> 2022 | Webinar

## Halide induced single crystal - single crystal structural transformation

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### Abstract

Metal-organic frameworks (MOFs) have been recognized as an excellent platform for host-guest chemistry, which includes gas storage<sup>1</sup>, separation<sup>2</sup> and anion exchange<sup>3</sup> etc. The pore size of MOFs varies from a few angstroms to a few nanometres, making them ideal for incorporating species ranging from small gas molecules and organic molecules to large inorganic and organic species. Herein, we report the synthesis of novel metal-organic framework prepared by the solvothermal reaction between Cu(NO<sub>3</sub>)<sub>2</sub> and pyrazine molecules. In the framework Cu ions adapt to tetrahedral geometry with the oxidation number of +1. Assembly of these four-connected Cu nodes with pyrazine molecules resulted in the formation of 3D framework with 2D channel system which gives rise to diamondoid topology. Formation of the MOF was directed by anions which also compensate the charge in order to maintain the overall structural neutrality. The unusual feature of this MOF is that Cu(I) oxidizes to Cu(II) in the case of exchange the anions which in turn show a subtle flexibility of the framework. However, we assume that neither the coordination environment nor the geometry of the Cu ions of the framework changes due to this redox activity.

Initial adsorption studies showed the fully evacuated as-synthesized MOF (brown solid before undergoing oxidation) did not adsorb N<sub>2</sub> and Ar at 77 K and 87 K, respectively. This shows that channels are blocked by the template molecules which were anticipated from the analysis of the crystallographic structure. Therefore, anionic templates were exchanged with different type of anions (eg. F<sup>-</sup>, Cl<sup>-</sup>, Br<sup>-</sup>) in order to probe for adsorption. Accordingly, the permanent porosity of the MOF was confirmed by N<sub>2</sub> adsorption giving rise to different surface area and pore volume with varying anions depending on size and charge of the anions exchanged. Interestingly F<sup>-</sup>s, the smallest anion exchanged has the lowest surface area while Br<sup>-</sup> exchanged sample has the highest surface area. Moreover, the MOF reported here can be used as an anion exchanger in different applications.

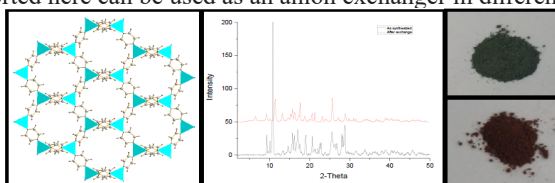


Figure 1: (a) structure of the MOF along the c-direction; (b) comparison of PXRD patterns of the as-synthesized MOF with the anion exchanged MOF; (c) As-synthesized compound (bottom) & anion exchanged compound (top).

### Biography

Dr. Mohamed Mohideen earned his PhD in Inorganic Chemistry from the University of St. Andrews, UK in 2011. He then held a postdoctoral researcher position at the King Abdullah University of Science & Technology, KSA. In 2014 he joined the Institute of Chemistry, Ceylon as a Senior Lecturer in Inorganic Chemistry. He held a Researcher position in the Department of Physical and Macromolecular Chemistry at the Charles University in Prague prior to joining Khalifa University as a Senior Lecturer in 2020. His research interests mainly aim to design and synthesize functional solid-state materials with a special focus on Metal Organic Frameworks and MXenes

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