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Structure-Stability-Relationship in [$CdBr_4$] series of Metal-Organic Materials

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ABSTRACT

To scrutinize the role of weak interactions in structure-stability of cadmium based metal-organic compounds a series of eighteen derivatives were analyzed through single crystal X-ray crystallographic data obtained from IUCr. The structural parameters obtained from the cif file were simulated for molecular dynamics to calculate the weak interactions in series of $CdBr_2$ based metal-organic composites. The structural frameworks depict that the metal halides are holding the organic moieties within the inorganic patterns through X-H…A, C-H…π, π…π, halogen-halogen and Metallophilic secondary interactions. The comprehensive structural statistics results that the average $CdBr_2$ = 2.762(1)Å and X-Cd-X bond angles lie in the range of 83.45 to 178.35^o in these compounds. The X-H…A hydrogen bond calculations result the average H…A bond length = $CdBr_2$ = 2.50Å and the average X-H…A bond angle = $CdBr_2$ = 137.5^o. This indicates that these hydrogen interactions are in the category of strong to moderate type of hydrogen bonds. The minimum value of H…π = 3.178(2)Å shows that such interactions are stabilizing the organic moieties within the metal-organic derivatives. It is observed that the minimum value of halogen…halogen weak interaction is 3.810(2)Å and the minimum value of metallophilic interaction distance is observed as 3.389Å which are linking the inorganic components of metal-organic derivatives. The IR and Raman spectra tensors indicates that IR, Raman and Hyper-Raman modes are dominant in $CdBr_2$ based derivatives as compared to other metal-organic compounds. The structural and spectroscopic parameters reveal that such weak interactions can be used to design the materials with spectroscopic applications.

Keywords: C-H…π, Raman tensors, structure stability, Weak X-H…A, π…π interactions.