



# Structure-Stability-Relationship in [CdBr<sub>4</sub>] 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<sub>2</sub> 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... $\pi$ ,  $\pi$ ... $\pi$ , halogen-halogen and Metallophilic secondary interactions. The comprehensive structural statistics results that the average CdBr<sub>2</sub> = 2.762(1)Å and X-Cd-X bond angles lie in the range of 83.45 to 178.35° in these compounds. The X-H...A hydrogen bond calculations result the average H...A bond length = CdBr<sub>2</sub> = 2.50Å and the average X-H...A bond angle = CdBr<sub>2</sub> = 137.5°. This indicates that these hydrogen interactions are in the category of strong to moderate type of hydrogen bonds. The minimum value of H... $\pi$  = 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<sub>2</sub> 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... $\pi$ , Raman tensors, structure stability, Weak X-H...A,  $\pi$ ... $\pi$  interactions.

## I INTRODUCTION

The hybrid materials can be defined in many different ways. Essentially there are two classes of hybrid materials class I and class II and here we will only consider materials with a covalent link between organic and inorganic moieties, i.e. 'class II' hybrid materials. Class I materials are merely a physical mixture of organic and inorganic components [1, 2]. In general, the benefit of hybrid materials relies in the combination of a closely interacting

organic phase with an inorganic phase, inducing new properties that cannot be achieved with only one of these phases separately. Organic materials typically allow for much larger diversity of functional properties than inorganic materials due to the wide variety of organic moieties. This permits fine-tuning of interactions with the surrounding environment. Most inorganic materials only interact with the environment via the surface OH-groups (even though often present with different bond strengths) [3, 4] and the M-O-M groups (in which M is a metal), limiting their versatility. On the other hand, organic materials are characterized by a low stability (chemically, thermally and mechanically) in various operating conditions. For instance, polymers are often only stable in a narrow range of solvents, as they tend to dissolve, swell or tear locally. Similarly, sealing of e.g. polymer membranes is often inadequate due to lack of stability in a wide diversity of solvents or in harsh conditions (e.g. high temperatures, acids) [5]. Inorganic materials are often very stable under these conditions. In contrast to polymers, they show no swelling and allow for high temperature treatments, e.g. to induce crystallization to further enhance the chemical and mechanical stability, or to attach layers or highly inert glass or ceramic sealings. However, ceramic materials may have stability issues under hydrothermal, acid or basic conditions. For example, amorphous silicates, especially pure silica, are known to have a low hydrothermal stability, giving rise to limited applicability in contact with water. Many metal oxides are unstable in either acids or bases. It is generally accepted that amorphous metal oxides materials are chemically less stable than crystalline ones, although transition metal oxides are often more stable than silica. The crystallization processes itself however can also have drawbacks as uncontrolled crystallization may give rise to structural collapse. While methods exist to control this process for large pores, crystallization can affect the integrity of thin-film microporous and mesoporous structures. This limits the availability of inorganic membranes with subnanometer pores and makes the production of nanofiltration membranes expensive. Although silica materials are less chemically stable, their structure is much easier to shape as uncontrolled crystallization does not occur (with the exception of zeolite membranes that are a separate class of materials). Another important factor is that a rigid pore structure can be more easily introduced in inorganic materials than in organic materials, making them better suited for sieving based on molecular size. These benefits and drawbacks allow both inorganic and organic materials to be utilized in various applications, but limit their applicability as the result of their respective restrictions in adjusting their performance to specific applications. For this reason, hybrid materials are being developed that combine the benefits of both types of materials or even introduce new unique properties.

## **II SIMULATION AND COMPUTATIONAL MOLECULAR DYNAMICS**

Motivated by the industrial applications of metal-organic materials, as they are the future of nanotechnology of materials science due to combination of two different branches of solid state sciences such as organic and inorganic, in which the properties of two different materials can be clubbed together into single composite, a series of eighteen cadmium based metal-organic molecules were selected from international union of crystallography, U.K. to analyze the role of secondary interactions in the structure-stability and structure-property relationship. The crystallographic open data base (COD), of international union of crystallography, U.K. was used to gather the available cadmium

based metal-organic molecules structural data in the crystallographic information file format. The crystal structure data with IUPAC name for selected series of hybrid derivatives has been deposited in supplementary data with codes CdBr-1[6], CdBr-2[7], CdBr-3[8], CdBr-4[9], CdBr-5[10], CdBr-6[11], CdBr-7[12], CdBr-8[13], CdBr-9[14], CdBr-10[15], CdBr-11[16], CdBr-12[17], CdBr-13[18], CdBr-14[19], CdBr-15[20], CdBr-16[21], CdBr-17[22], CdBr-18[23]. The molecular dynamics simulations for studying the physical evolutions of weak interactions were performed with DIAMOND-Crystal and molecular structure visualization and functions program [24].

### III RESULTS AND DISCUSSION

The structural parameters were calculated by Crystal and molecular structure visualization and function programs which were further used to analyze the role of weak interactions in molecular frameworks of selected series of cadmium based metal-organic derivatives. With the crystallographic information file data, a wide range of structural functions were generated and the weak interactions were calculated and constructed by diamond software [24]. The crystallographic data obtained from the computational simulations for cadmium-centered bond distances and angles are presented in supplementary data Table 1. The calculated values of metallophilic and halogen interactions with Cd...Cd, X...X, distance and X-Cd...Cd-X torsion angles at respective symmetry positions are presented in Table 1.

**Table 1:** Crystallographic data for Cd-centered bond distances (Å) and range of bond angles (°) in [CdBr].

Code	Cd-X bond distance (Å)	X-Cd-X (°) range
CdBr1	Cd-Br1 = 2.583(2) Cd-Br2 = 2.640(1)	105.86
CdBr2	Cd-Br = 2.708(1) Cd-Br = 2.790(1)	86.14-178.35
CdBr3	Cd-Br2 = 2.576(3) Cd-Br1 = 2.582(3) Cd-Br3 = 2.587(4)	108.00-112.10
CdBr4	Cd-Br3 = 2.581(1) Cd-Br1 = 2.584(1)	103.70-117.20
CdBr5	Cd-Br2 = 2.636(2) Cd-Br1 = 2.674(4)	102.48
CdBr6	Cd-Br3 = 2.582(2) Cd-Br2 = 2.592(1)	104.24
CdBr7	Cd1-Br2 = 2.585(1) Cd1-Br1 = 2.628(2) Cd2-Br3 = 2.785(1)	86.79-180

	Cd3-Br3 = 2.784(1)	
CdBr8	Cd-Br1 = 2.687(1) Cd-Br2 = 2.722(1) Cd-Br2 = 2.760(1) Cd-Br3 = 2.773(1) Cd-Br3 = 2.854(1) Cd-Br3 = 2.924(1)	83.45-174.12
CdBr9	Cd-Br = 2.591(1)	114.77
CdBr10	Cd1-Br2 = 2.590(4)	108.83-109.79
CdBr11	Cd1-Br1 = 2.785(1)	89.57-180
CdBr12	Cd1-Br1 = 2.681(1) Cd1-Br1 = 2.900(1)	87.15-176.93
CdBr13	Cd1-Br1 = 2.686(1)	180
CdBr14	Cd1-Br1 = 2.574(3)	114.68
CdBr15	Cd1-Br2 = 2.589(1) Cd1-Br1 = 2.635(1) Cd1-Br1 = 3.019(1)	89.13-109.31
CdBr16	Cd1-Br1 = 2.718(4)	180
CdBr17	Cd1-Br2 = 2.562(1) Cd1-Br1 = 2.605(1)	121.01
CdBr18	Cd1-Br2 = 2.505(1) Cd1-Br1 = 2.512(1)	113.59

### 3.1. HYDROGEN BONDING

The hydrogen bond geometry for CdBr<sub>2</sub> derivatives indicates that the acceptor bond length lies in the range of 1.91 Å to 3.09 Å and the donar-acceptor length exist in between 2.712(7) Å to 3.824(1) Å and H-centered D-A angle has values from 100° to 175°.

The d-θ scatter plot for hydrogen bonding interactions shows that most of the data points exist in H...A distance range of 3.5 to 3.8 Å and X-H...A angle ranges from 75° to 120° in the selected series of metal-organic compounds which indicate these interactions are moderate type of hydrogen bonds as shown in Fig. 1.

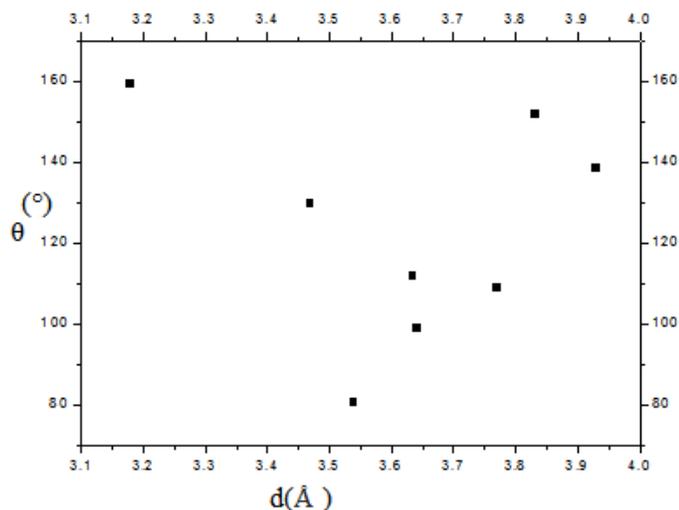


Figure 1. d (H...A) and  $\theta$  (X-H...A) scatter plot for cadmium based metal-organic derivatives.

### 3.2 $\pi$ -INTERACTIONS

The  $\pi$ -interactions were constructed by selecting the center of two phenyl rings and their corresponding distances and torsion angles were calculating, which shows that the minimum value of  $\pi \dots \pi$  interactions in cadmium bromide is 3.633(2) Å for compound CdBr18 with torsion angle 61.66(3)° having symmetry position 1-x,2-y,1-z,1-x,1-y,1-z and x,1+y,z and the maximum  $\pi \dots \pi$  interaction is 3.924(7) Å for compound CdBr11 with torsion angle 118.62(2)° having symmetry position 0.5-x,0.5+y,-z as shown in Table 2.

Table 2:  $\pi \dots \pi$  interactions in selected series of metal-organic compounds.

Code	$\pi \dots \pi$ interaction	$\pi \dots \pi$ (Å) Distance	Max. torsion angle (°) $\pi \dots \pi$
CdBr9	$\pi \dots \pi^{iv}$	3.888(7)	$C2^x - \pi \dots \pi - C4^{xi} = 66.83(3)$
CdBr11	$\pi \dots \pi$	3.924(7)	$C2^{xii} - \pi \dots \pi - C2 = 118.62(2)$
CdBr18	$\pi \dots \pi^v$	3.633(2)	$C6^{ii} - \pi \dots \pi - C2^{xiii} = 61.66(3)$

Symmetry Codes: (ii) 1-x, 1-y, 1-z (iv) 0.25+x, 0.75-y, -0.25+z (v) 1-x, 2-y, 1-z (vi) 2-x, 2-y, z (x) 0.5-x, 0.5-y, -1+z (xi) 0.25-x, 0.25+y, -0.75+z (xii) 0.5-x, 0.5+y, -z (xiii) x, 1+y, z

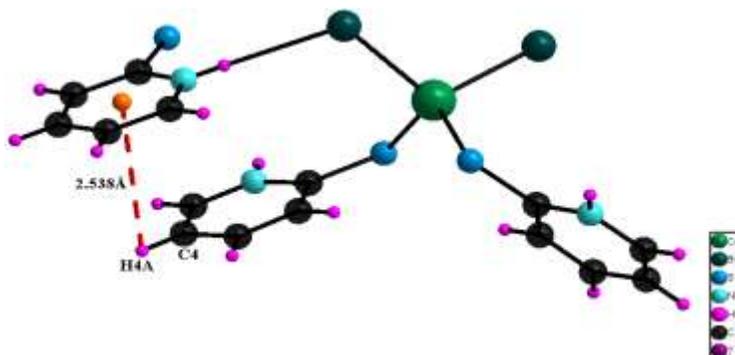
The minimum value of H... $\pi$  interactions bond distance for cadmium bromide is 3.178(2) Å in CdBr10 compound and maximum is 3.930(3) Å for CdBr13 compound where as the minimum C-H... $\pi$  bond angle is 80.49(3)° for CdBr9 compound and 159.41(3)° is the maximum bond angle for CdBr10 as calculated in Table 3.

**Table 3: C-H... $\pi$  interactions in selected series of metal-organic compounds.**

Code	C-H... $\pi$ interaction	H... $\pi$ (Å) Distance	C-H... $\pi$ (°)
CdBr4	C9-H9 <sup>xx</sup> ... $\pi$	3.634(4)	111.84(3)
CdBr9	C4-H4A <sup>xxi</sup> ... $\pi$	3.539(7)	80.49(3)
CdBr10	C8-H8C <sup>xxii</sup> ... $\pi$	3.178(2)	159.41(3)
CdBr12	C1-H1 <sup>xxiii</sup> ... $\pi$	3.769(2)	108.72(3)
CdBr13	C1-H1 <sup>iv</sup> ... $\pi$	3.930(3)	138.34(2)
CdBr16	C3-H3B <sup>xxiv</sup> ... $\pi$	3.469(3)	129.72(2)
CdBr17	C6-H6B <sup>xxv</sup> ... $\pi$	3.831(5)	151.72(3)
CdBr18	C2-H2 <sup>iii</sup> ... $\pi$	3.642(2)	98.71(3)

Symmetry Codes: (iii) 1-x, 1-y, 1-z (iv) x, -1+y, z (xx) 1-x, -y, -z (xxi) 0.25-x, 0.25+y, -0.75+z (xxii) 1-y, x, 1-z (xxiii) 0.5+x, 0.5-y, 0.5+z (xxv) 0.5+x, 0.5-y, 1-z

Different structural motifs were obtained within the organic moiety through  $\pi$ -interactions such as a bifurcated C-H... $\pi$  interaction in CdBr9 with H4A atom at symmetry position 0.5-x, 1-y, -0.5+z in which  $\pi$  acts as acceptor of H4A atom of organic moiety of the metal-organic derivatives linking the organic components in 1D chain of C-H... $\pi$  interactions as shown in Fig. 2.



**Figure 2. C-H...  $\pi$  interaction in CdBr9 with H4A atom at symmetry position 0.5-x, 1-y, -0.5+z.**

### 3.3. HALOGEN-HALOGEN INTERACTIONS

The bond lengths of Cd-Br contact lies in an average range of 2.509Å to 2.791Å. The bond distances for these derivatives illustrate that most of the data points lie in between 2.55 to 2.65Å whereas the data points for CdBr2, CdBr8, CdBr11, CdBr12, CdBr13, CdBr16 and CdBr18 shows the deviation from this range and it could be due to variety of X-H...A interactions. The Br-Cd-Br bond angles have wide variety with minimum range of 108.83 to 109.79° for CdBr8 and maximum range of 86.79 to 180° for the derivatives CdBr7. The Cd...Cd distance in

Compound CdBr<sub>2</sub> is calculated as 3.962(1)Å which shows that the structure is stabilized by metallophilic interactions apart from X-H...A and Br...Br secondary interactions and it is seen in this compound [CdBr<sub>2</sub>] that the minimum value of Br...Br bond distances comes out to be 3.810(2)Å and 3.962(3)Å. In CdBr<sub>7</sub> derivative of the selected series, one of the Cd atom having symmetry position (x, y, 1+z) establishes a close contact of 3.389(3)Å with another Cd atom.

The Cd...Cd bond distance in compound CdBr<sub>7</sub> is calculated as 3.389 Å which shows that the structure is stabilized by metallophilic interactions apart from X-H...A and Br...Br secondary interactions. The minimum value of Br...Br bond distances are shown by the derivatives coded as CdBr<sub>2</sub>, CdBr<sub>7</sub>, CdBr<sub>8</sub>, CdBr<sub>11</sub>, CdBr<sub>12</sub> and CdBr<sub>15</sub> having values 3.810(2), 3.827(1), 3.944(1), 3.924(1), 3.850(1) and 3.978(2)Å respectively which shows that the crystal structures are stabilized by secondary interactions. The minimum value of torsion angle [Br-Cd...Cd-Br] is 22.43(4)<sup>o</sup> for the compound CdBr<sub>17</sub> having -x, 0.5+y, 0.5-z symmetry positions and maximum torsion angle for the compound CdBr<sub>12</sub> is 178.08(5)<sup>o</sup> having 1-x, 1-y, -z symmetry positions.

### 3.4. METALLOPHILIC INTERACTIONS

The secondary interactions in CdBr<sub>7</sub> shows the minimum value between Cd...Cd atoms in these compounds comes out to be 3.389(3)Å with symmetry position of x, y, 1+z respectively.

## IV IR AND RAMAN TENSORS

IR and Raman spectra tensors have been calculated by using fractional co-ordinates obtained from single crystal XRD data as presented in Table 4. In which the lattice parameters and the fractional coordinates were used to study spectral active modes of IR and Raman spectra tensors in the SAM structural utility tool of Bilbao crystallographic server [11-12]. The quantitative comparison of the crystal structures of the selected series of metal-organic compounds through theoretically structural models shows that these compounds have the promising results for spectroscopic applications.

**Table 4. IR, Raman and Hyper-Raman Tensors in selected series of metal-organic compounds.**

Compound	Active Mode Equation	Wykoff Positions	Infra-Red	Raman	Hyper-Raman
CdBr 2,9	( $\Gamma_{\text{acoustic}} = A_1 + B_1 + B_2$ )	WP2=[8a,16b]	A <sub>1</sub> =2 B <sub>1</sub> =2 B <sub>2</sub> =2	A <sub>1</sub> =2 A <sub>2</sub> =2 B <sub>1</sub> =2 B <sub>2</sub> =2	A <sub>1</sub> =2 A <sub>2</sub> =2 B <sub>1</sub> =2 B <sub>2</sub> =2
CdBr 3	( $\Gamma_{\text{acoustic}} = B_2 + E$ )	WP4=[2b,2c,4e,8f]	B <sub>2</sub> =4 E=4	A <sub>1</sub> =3 B <sub>1</sub> =3	A <sub>1</sub> =3 A <sub>2</sub> =2

				$B_2=4$ $E=4$	$B_1=3$ $B_2=4$ $E=4$
CdBr 4,6,	$(\Gamma_{\text{acoustic}} = 3A_u)$	WP1=[2i]	$A_u=1$	$A_g=1$	$A_u=1$
CdBr 7	$(\Gamma_{\text{acoustic}} = A_u + {}^1E_u + {}^2E_u)$	WP4=[1a,1b,2d,6g ]	$A_u=4$ ${}^1E_u=4$ ${}^2E_u=4$	$A_g=2$ ${}^1E_g=2$ ${}^2E_g=2$	$A_u=4$ ${}^1E_u=4$ ${}^2E_u=4$
CdBr 8	$(\Gamma_{\text{acoustic}} = B_1 + B_2 + B_3)$	WP3=[2a,2b,4c]	$B_1=3$ $B_2=3$ $B_3=3$	$A=3$ $B_1=3$ $B_2=3$ $B_3=3$	$A=3$ $B_1=3$ $B_2=3$ $B_3=3$
CdBr 10	$(\Gamma_{\text{acoustic}} = B_2 + E)$	WP3=[4a,8d,16e]	$B_2=3$ $E=3$	$A_1=2$ $B_1=3$ $B_2=3$ $E=3$	$A_1=2$ $A_2=2$ $B_1=3$ $B_2=3$ $E=3$
CdBr 11	$(\Gamma_{\text{acoustic}} = B_{1u} + B_{2u} + B_{3u})$	WP4=[2a,4g,4j,8p]	$B_{1u}=4$ $B_{2u}=4$ $B_{3u}=4$	$A_g=3$ $B_{1g}=3$ $B_{2g}=2$ $B_{3g}=2$	$A_u=1$ $B_{1u}=4$ $B_{2u}=4$ $B_{3u}=4$
CdBr 12,14	$(\Gamma_{\text{acoustic}} = A_u + 2B_u)$	WP2=[4e,8f]	$A_u=2$ $B_u=2$	$A_g=2$ $B_g=2$	$A_u=2$ $B_u=2$
CdBr 13	$(\Gamma_{\text{acoustic}} = A_u + 2B_u)$	WP2=[4a,8f]	$A_u=2$ $B_u=2$	$A_g=1$ $B_g=1$	$A_u=2$ $B_u=2$
CdBr 16	$(\Gamma_{\text{acoustic}} = A_u + 2B_u)$	WP2=[2a,4e]	$A_u=2$ $B_u=2$	$A_g=1$ $B_g=1$	$A_u=2$ $B_u=2$
CdBr 17	$(\Gamma_{\text{acoustic}} = B_1 + B_2 + B_3)$	WP1=[4a]	$B_1=1$ $B_2=1$ $B_3=1$	$A=1$ $B_1=1$ $B_2=1$ $B_3=1$	$A=1$ $B_1=1$ $B_2=1$ $B_3=1$
CdBr 18	$(\Gamma_{\text{acoustic}} = A_u + 2B_u)$	WP1=[4e]	$A_u=1$ $B_u=1$	$A_g=1$ $B_g=1$	$A_u=1$ $B_u=1$

## V CONCLUSION

The analysis of weak interactions such as X-H...A, C-H... $\pi$ ,  $\pi$ ... $\pi$ , halogen...halogen and Cd...Cd in cadmium based metal-organic derivatives results that these interactions are responsible for holding the inorganic and organic moieties in single composite. The  $\pi$ ... $\pi$  interactions are binding the organic moieties into dimmer patterns whereas the halogen-halogen and metallophilic interactions are holding the inorganic constituents into 1D chain and 2D layer patterns. The metallic constituents of these derivatives provide the mechanical strength to the composite whereas the organic moiety is responsible for its optical as well as spectroscopic properties. The spectroscopic studies for IR, Raman and Hyper-Raman tensors show that these materials can be used in junction diodes of hybrid solar cells in which the stability of the hybrid structure is maintained by these weak interactions. Looking upon the industrial applications of hybrid material, they are the future of nanotechnology due to combination of two different branches of solid state sciences such as organic and inorganic in which the properties of two different scientific worlds were clubbed together into single composite material.

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