Structural diversity in serine derived homochiral metal organic frameworks

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Abstract. Two new Zn(II) and Cd(II) based homochiral metal–organic frameworks (MOFs) [SerCdOAc and Zn(Ser)₂] have been synthesized using pyridyl functionalized amino acid, viz., serine, as an organic linker. The SerCdOAc structure is three dimensional, while that of the Zn(Ser)₂ is two dimensional. The polar voids of the corresponding MOFs are filled with solvent molecules (water in the case of SerCdOAc and methanol in the case of Zn(Ser)₂). In both cases, metal centres, i.e., Zn(II) and Cd(II), are hexacoordinated. However, with a change in the solvent for synthesis, ligand coordination mode and incorporation of additional coordinated anion resulted in a great change in the final MOF architecture. Herein, for the first time, we could achieve structural variety and synthesize MOFs composed of only metal ion and pyridyl functionalized amino acid linker.

Keywords. Amino acid; crystal engineering; hydrogen bonding; metal organic framework.

1. Introduction

Enantiopure amino acids and their derivatives have been a cynosure in the eyes of researchers as they serve as a backbone to the chemical processes of all flora and fauna. Extensive research on the property studies of the naturally occurring amino acids and their derivatives (e.g., peptides) as well as their synthetic analogues has been done over the last few decades for their biomimetic activities.¹ Yet, complete understanding of their structure and property relationships seem extremely complicated till date. For example, a small change in an amino acid within the peptide backbone results in an unexpected twist in the peptide conformers. Hence, comprehensive understanding of the basic interactions between amino acids and other analytes would reveal the key features of the amino acid functional properties, and ultimately serve as the basis to comprehend various chemical processes in vivo. In this respect, several attempts have been made in order to introduce amino acid moiety in organic polymers for high CO₂ affinity. On the other hand, organic-inorganic hybrid structures based on amino acids find their applications in enantioselective catalysis,² separation,³ and most importantly to understand complex biochemical processes and cycles.⁴ In this respect, metal-organic frameworks (MOFs) serve as a boon for application

in chiral separation and sensing, and nonlinear optics. MOFs are organic–inorganic hybrid porous material with potential applications like gas sorption,⁵ catalysis,⁶ magnetism,⁷ and conductivity.⁸ Hence, introduction of amino acid moiety in extended three dimensional backbone of MOF promises unique functionality and applicability owing to different side-arm residues of amino acids. Nevertheless, high binding and chelation ability of pure amino acids with transition metals often usher in zero/one dimensional complex formation instead of higher order porous MOFs.⁹ Not surprisingly, three dimensional MOFs with amino acid backbone are only a handful in number till date.¹⁰

Recently, our research group has attempted to use amino acid derived links (pyridyl functionalized valine, alanine, threonine, leusine, serine, etc.) to overcome the aforementioned problem.¹¹ We have rationally tuned these amino acid derived links in MOF backbone to afford extended homochiral MOFs with interesting topologies along with microporosity, which serve as porous platforms to understand the structure and property relationships.^{11a} These MOFs are water stable and undergo hydrolysis-mediated recrystallization at higher temperatures (> 90°C). The coordinated anions play a vital role in their differential recrystallization performances. Moreover, minute change in the constituting anion (from Cl[−] to Br[−], HCO₂[−] and CH₃CO₂[−]) manifests in a decrease in water sorption capability and proton conducting ability.^{11d} However, effect of a systematic change of the metal ion in amino acid–derived MOFs

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and the impact on structural integrity as well as property of the voids are still in infancy.

Herein, we report two new Zn(II) and Cd(II) based homochiral MOFs, i.e., CdSerOAc and Zn(Ser)₂. These MOFs have been synthesized using a pyridyl-functionalized amino acid, viz., serine, as an organic linker. The CdSerOAc MOF structure is three dimensional, having polar voids filled with solvent water molecules (three water molecules per asymmetric unit in case of SerCdOAc). The water molecules are hydrogen bonded to both MOF backbone as well as to themselves. These water molecules adopt complex hydrogen bonded helical chains running through the tetragonal polar voids of the SerCdOAc. However, in the case of Zn(Ser)₂, the resulting MOF adopts two dimensional sheet like structure, and the triangular voids are filled with solvent methanol molecules hydrogen bonded with the framework as well as the uncoordinated –CH₂OH groups protruding into the pore. In both cases, the metal centres [Zn(II) and Cd(II)] are hexacoordinated. However, with a change in the solvent for synthesis, ligand coordination mode and incorporation of additional coordinated anion resulted in dimensionality difference of the final MOF architecture. In this manuscript, for the first time, we could achieve structural variety as well as synthesize MOFs composed of only metal and pyridyl functionalized amino acid linker.

2. Experimental

2.1 Materials and methods

All reagents were commercially available and used as received. Powder x-ray diffraction (PXRD) patterns were recorded on a Phillips PANalytical diffractometer for Cu K α radiation ($\lambda = 1.5406 \text{ \AA}$) with a scan speed of 2° min^{-1} and a step size of 0.02° in 2θ . Fourier transform infrared (FT-IR) spectra were taken on a Bruker Optics ALPHA-E spectrometer with a universal Zn-Se ATR (attenuated total reflection) accessory in the 600–4000 cm^{-1} region or using a Diamond ATR (Golden Gate). Thermo-gravimetric analyses (TGA) were carried out on a TG50 analyzer (Mettler-Toledo) or a SDT Q600 TG-DTA analyzer under N₂ atmosphere at a heating rate of $10^\circ\text{C min}^{-1}$ within a temperature range of 20–900°C.

2.2 General data collection and refinement procedures

All single crystal data were collected on a Bruker SMART APEX^{12a} three circle diffractometer equipped

with a CCD area detector and operated at 1500 W power (50 kV, 30 mA) to generate Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$). The incident x-ray beam was focused and monochromated using Bruker Excalibur Gobel mirror optics. All crystals reported in this paper were mounted on nylon CryoLoops (Hampton Research) with Paratone-N (Hampton Research).

Initial scans of each crystal were performed to obtain preliminary unit cell parameters and to determine the mosaicity (breadth of spots between frames) of the crystal to select the required frame width for data collection. In every case frame widths of 0.5° were judged to be appropriate and full hemispheres of data were collected using the Bruker SMART software suite. Following data collection, reflections were sampled from all regions of the Ewald sphere to re-determine unit cell parameters for data integration and to check for rotational twinning using CELL_NOW.^{12c} Fortunately, no crystal decay was encountered during data collection. Following exhaustive review of the collected frames, the resolution of the dataset was judged. Data were integrated using Bruker SAINT Software^{12b} with a narrow frame algorithm and a 0.400 fractional lower limit of average intensity. Data were subsequently corrected for absorption by the program SADABS. The space group determinations and tests for merohedral twinning were carried out using XPREP. In all cases, the highest possible space group was chosen.

All structures were solved by direct methods and refined using the SHELXTL 97 software suite.^{12d} Atoms were located from iterative examination of difference F-maps following least squares refinements of the earlier models. Final models were refined anisotropically (if the number of data permitted) until full convergence was achieved. Hydrogen atoms were placed in calculated positions (C–H = 0.93 $\text{\AA}$) and included as riding atoms with isotropic displacement parameters 1.2–1.5 times U_{eq} of the attached C atoms. All structures were examined through the *Adsym* subroutine of PLATON^{12e} to ensure that no additional symmetry could be applied to the models. All ellipsoids in ORTEP diagrams are displayed at the 50% probability level unless stated otherwise. Crystallographic parameters are listed in tables 1 and 2.

2.3 Synthesis

2.3a (pPyridin-4-ylmethyl)-L-serine.NaOAc [SerOAc]: To an aqueous solution (10 mL) of L-serine (1.9 g, 17 mmol) and Na₂CO₃ (0.91 g, 8.5 mmol), 4-pyridine-carboxaldehyde (1.82 g, 17 mmol) in MeOH (10 mL) was added slowly under vigorous stirring. The solution was stirred for 1 h and cooled to 0–5°C in an ice bath.

NaBH₄ (0.76 g, 20.4 mmol) in 5 mL of H₂O was slowly added. The mixture was then stirred for another 3 h, and the pH was adjusted to 5–6 using 3 N AcOH. The clear solution was stirred further for 2 h and then evaporated to dryness. The solid was extracted in hot and dry MeOH (150 mL × 3), and the filtrate was evaporated in a rotavapor to get the ligand as a sodium acetate salt in the form of a white powder. Yield: 2.6 g, 60%. Figure 7b displays the IR spectrum.

2.3b $[\{Cd(Ser)(OAc)\}(H_2O)_3]_{\infty}[SerCdOAc]$: To an aqueous solution (1 mL) of SerOAc (0.05 g, 0.2 mmol), Cd(CH₃COO)₂·2H₂O (0.022 g, 0.1 mmol) in 5 mL MeOH was added and sonicated for 10 min to produce a clear solution, which was left for evaporation for 48–72 h to produce rod-shaped transparent crystals. Yield: 0.025 g, 65%. Elemental analysis: calcd C (31.40%), H (4.79%), N (6.66%); found C (31.20%), H (4.18%), N (6.55%). Figure 7b displays the IR spectrum. CCDC No. 1021364.

2.3c $[\{Zn(Ser)_2\}(CH_3OH)]_{\infty}[Zn(Ser)_2]$: To a methanolic solution (5 mL) of SerOAc (0.05 g, 0.2 mmol), Zn(CH₃COO)₂·2H₂O (0.022 g, 0.1 mmol) in 5 mL MeOH was added and sonicated for 10 min to produce a clear solution. The solution was left for evaporation for 24–48 h to produce rod-shaped transparent crystals. Yield: 0.025 g, 65%. Elemental analysis: calcd C (46.20%), H (5.81%), N (10.77%); found C (45.82%), H (5.58%), N (10.65%). Figure 7d displays the IR spectrum. CCDC No. 1021363.

3. Results and Discussion

Among all the 20 amino acids variants, serine serves as an important proteogenic amino acid with an extra hydroxymethyl functional group apart from the amino and the carboxy moieties. As a result, serine based materials possesses further opportunity for functionalization at the sidearm. Numerous synthetic methodologies have been developed for functionalized serine based biopolymers and soft materials. However, serine derived organic-inorganic hybrid materials are few in number. Nonetheless, a handful of them have utility in functional applications. For example, pyridyl functionalized serine linker has been utilized to prepare Cu based coordination polymer, which was used as a solid state catalyst for Biginelli catalytic reaction of benzaldehyde, urea and ethyl acetoacetate.¹³ However, the resulting framework is one dimensional. 1D materials suffer from the problem of unwanted leaching, poor structural ordering and lower thermal stability

than higher dimensional materials. As a result, higher dimensional serine based materials with empty void inside the structure can be envisaged as a suitable solution for the current problems. In this regard, our group has developed a pyridyl serine based porous MOF using Cd(II) as metal node. Moreover, the SerCdCl MOF^{11b} possesses 3D architecture with tetragonal polar voids and coordinated chlorine atoms as well as coordinated hydroxymethyl groups apart from the imino and carboxylate moieties, which exposed towards the pore aperture. The polar atoms are responsible for the highly hydrophilic nature of the resulting structure. The SerCdCl MOF exhibited high hydrophilicity and can selectively adsorb water molecules over nitrogen and hydrogen molecules. These findings open up a new avenue for the systematic exploration of the serine derived linker as an efficient platform to create functional porous MOFs. In this work, we have further synthesized two new MOFs based on the same linker but with two different metal ions [Zn(II) and Cd(II)] and they exhibit structural as well as property difference based on their constituents discussed vide supra.

3.1 Crystal structure of SerCdOAc

SerCdOAc crystallizes in the *P*2₁2₁ space group, comprising one Cd(II), one Ser ligand, one OAc[−] ion and three lattice H₂O molecules in the asymmetric unit (figure 2a). The Cd(II) centre adopts a slightly distorted square bipyramidal geometry, chelated by bidentate carboxylate [(Cd1–O1; 2.504(2) Å) and (Cd1–O2; 2.274(2) Å)], one amino functionality[(Cd1–N2; 2.331(1) Å)] and one pyridyl functionality [(Cd1–N1; 2.329(2) Å)] of the Ser linker coordinate to the axial and equatorial positions of the Cd(II), respectively (figures 1 and 2). Interestingly, the hydroxymethyl (–CH₂OH) group of the Ser linker coordinates with Cd(II) without losing its proton, which implies neutral binding mode of the same. One OAc[−] ion coordinates to the equatorial site in a bidentate fashion [(Cd1–O4; 2.481(2) Å) and (Cd1–O5; 2.322(2) Å)], which balances the overall negative charge of the Cd(II) atom. All adjacent Cd(II) nodes are connected by the pyridyl and carboxylate functionality to form a helical pitch along the crystallographic *a*-axis. The pyridyl moieties constitute tetragonal pore wall of the framework, which is hydrophobic in nature. The open channels along crystallographic *a*-axis are filled with solvent H₂O molecules, which are three in number per asymmetric unit of SerCdOAc (figure 3a). The water molecules are strongly hydrogen bonded by nearby carboxylate oxygen atoms [(O2···O7; 2.939(2) Å and O2···H7; 2.107(5) Å)]¹⁴ and the coordinated acetate

Figure 1. Schematic synthesis of the SerCdOAc MOF from the SerOAc ligand and $\text{Cd}(\text{OAc})_2$ in the water medium. The coordination environment along the Cd atom is depicted in the right hand side with atom numbering. Colour codes: Cd (dark green), N (blue), O (red), C (gray) and H (white).

anions [$\text{O4} \cdots \text{O6}$; 2.809(2) Å and $\text{O4} \cdots \text{H6}$; 2.030(2) Å] due to high hydrophilic intermolecular interactions between the coordinated hydroxymethyl ($-\text{CH}_2\text{OH}$) groups, carboxylate moieties and the Cd(II)-bound acetate anions (exposed towards the pore) with the water molecules (figure 3b). These channels have a cylindrical cross sectional area of 8.5×5.4 Å. A striking feature observed in this case is the hydrophilic interaction between ligand sidearm (i.e., coordinated hydroxymethyl ($-\text{CH}_2\text{OH}$) groups) and carboxylate moieties [$\text{O3} \cdots \text{O10}$, 3.321(7) Å], which is one of its kind in the field of amino acid based MOFs. There are further intermolecular $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds along the pore as well as between the neighbouring H_2O molecules due to short separation (ca. 2.7–2.8 Å). The homochiral framework constitutes a helical arrangement along crystallographic a axis. The water molecules are hydrogen bonded (figure 3c) with the carboxylate moieties of the linker and the coordinated acetate anions of the MOF that are exposed towards the pore cavity.

Comparing the molecular structure of the MOF viz., SerCdOAc with earlier structure of the same type of

constituent (SerCdCl) resulted in a huge difference, although both belong to the 3D category. The SerCdCl consists of pentacoordinated distorted square pyramidal Cd centre; while SerCdOAc has hexacoordinated slightly distorted square bipyramidal geometry. This is possible due to the bidentate mode of the acetate ion in SerCdOAc, while monodentate chloride anion coordinates to the Cd centre in SerCdCl. The increase in coordination number resulted in enhanced hydrophilicity of SerCdOAc over the CdserCl, which is evident from the increased number of water molecules per unit despite slight decrease in the pore size of the former. This aforementioned observation hints at future design of water adsorbent materials, where optimization of polar interactions should be the prime criteria over the pore size.

3.2 Crystal structure of $\text{Zn}(\text{Ser})_2$

$\text{Zn}(\text{Ser})_2$ crystallizes in the $C2$ space group, comprising one Zn(II), two Ser ligands and one lattice

Figure 3. (a) Ball and stick representation of the SerCdOAc MOF showing arrangement of the water molecules within the tetragonal polar voids viewed from the crystallographic *a* axis. (b) Hydrogen bonding interactions between the water molecules as well as the framework backbone (acetate and carboxylate moieties) depicted with the bonding distances. (c) Helical hydrogen bonded assembly of the solvent water molecules along the rectangular pore. (d) Space filling model of the SerCdOAc MOF featuring polar tetragonal voids. Water molecules have been removed for clarity. Colour codes: Cd (dark green), N (blue), O (red), C (gray) and H (white).

methanol molecule in the asymmetric unit (figure 5a). The Zn(II) centre adopts a slightly distorted square bipyramidal geometry (figure 4), chelated by monodentate carboxylate [(Zn1–O1; 2.018(1) Å), one amino functionality [(Zn1–N2; 2.212(3) Å)] and one pyridyl functionality [(Zn1–N1; 2.208(3) Å)] of the Ser linker

coordinate to the Zn(II). Interestingly, the hydroxymethyl (–CH₂OH) group of the Ser linker is free for both the linkers. All adjacent Zn(II) nodes are connected by the pyridyl, amino and carboxylate functionalities (figure 6a). The pyridyl rings constitute the triangular pore wall of the framework (figure 6b), which

Figure 4. Schematic representation of the linker SerOAc which react with Zn(OAc)₂ to produce corresponding Zn(Ser)₂ MOF architecture. Color codes: Zn (dark green), N (blue), O (red), C (gray) and H (white).

Figure 5. (a) Ligand (Ser) coordination mode in the Zn(Ser)₂ MOF. (b) ORTEP diagram of Zn(Ser)₂ MOF with all the atoms at 50% probability level.

Figure 6. (a) Arrangement of Ser ligands and their coordination modes across the Zn centre in Zn(Ser)₂. (b) Representation of a single pore of Zn(Ser)₂ with a view of the solvent methanol molecules from the crystallographic *c* axis. (c) 2D layer or sheet like architecture in Zn(Ser)₂ as viewed from crystallographic *b* axis. (d) Spacefill model representation of the Zn(Ser)₂ from crystallographic *c* axis showing the triangular voids. Methanol molecules have been removed for clarity. Color codes: Zn (dark green), N (blue), O (red), C (gray) and H (white).

is hydrophobic in nature. The open channels along crystallographic *c*-axis are filled with solvent methanol molecules. The methanol molecules are strongly hydrogen bonded by nearby oxygen atoms of the free hydroxymethyl ($-\text{CH}_2\text{OH}$) group of the Ser linker [$(\text{O}3 \cdots \text{O}4; 2.710(3) \text{ \AA}$ and $\text{O}4 \cdots \text{H}3; 1.900(3) \text{ \AA}$)] (figure 3). These channels have a cylindrical cross sectional area of $7.5 \times 5.5 \text{ \AA}$. The 2D layers are arranged in a sheet like fashion with a distance of ca. $6 \text{ \AA}$ in between the layers (figure 6c).

The structural comparison of the two MOFs, viz., SerCdOAc and $\text{Zn}(\text{Ser})_2$, shows that the former has a 3D architecture, while 2D sheet like structure prevail in the later case. Although in both the MOFs, the central Cd atom adopts hexacoordinated slightly distorted square bipyramidal geometry, the SerCdOAc consists of one Ser ligand utilizing six coordination modes (figure 2a) and a bidentate acetate anion, while the $\text{Zn}(\text{Ser})_2$ contains two Ser linker having three coordination mode (figure 5a). The Cd atom is oxygen rich in SerCdOAc and nitrogen rich in $\text{Zn}(\text{Ser})_2$. The hydroxymethyl groups are coordinated with Cd(II) in case of the SerCdOAc, while it is free and accessible

for post synthetic modification in the $\text{Zn}(\text{Ser})_2$. The SerCdOAc structure adopts tetragonal pore (figure 3d), while in case of $\text{Zn}(\text{Ser})_2$ the pore becomes trigonal with reduced dimensions (figure 6d). Moreover, the SerCdOAc prefers water molecules as a crystallizing solvent to fill the empty pore, while methanol molecules fit the role in $\text{Zn}(\text{Ser})_2$. These differences led to the structural diversity of the MOFs, which will help to design further MOFs with tunable structures and properties.

3.3 X-ray powder diffraction and thermogravimetric (TGA) analysis

Confirmation of the phase purity of the bulk material was carried out on both using powder x-ray diffraction (PXRD) experiments. Experimental and simulated PXRD patterns for SerCdOAc and $\text{Zn}(\text{Ser})_2$ are shown in figures 7a and 7c, respectively. All the major peaks of experimental PXRD match quite well with the simulated one, indicating reasonable crystalline phase purity in the bulk scale material.

Figure 7. (a) PXRD pattern of the SerCdOAc compared with the simulated pattern. (b) FT-IR spectra of the SerCdOAc compared with the ligand. (c) PXRD pattern of the $\text{Zn}(\text{Ser})_2$ compared with the simulated pattern. (d) FT-IR spectra of the $\text{Zn}(\text{Ser})_2$ compared with the ligand.

Figure 8. (a) TGA profile of the SerCdOAc under nitrogen environment in between 20–900°C. (b) TGA profile of the Zn(Ser)₂ under nitrogen environment in between 20–800°C.

Thermo-gravimetric analysis (TGA) performed on as-synthesized MOFs revealed that SerCdOAc has high thermal stability for all data regarding guest mobility and thermochemical stability. The TGA trace for SerCdOAc (figure 8a) showed a gradual weight-loss step of 12.5% [3 H₂O; calcd. 12.8%] (20–120°C), corresponding to the escape of all H₂O molecules trapped in the pores followed by a plateau (120–205°C) indicating its high thermal stability in absence of guest molecules (figure 8a). Further weightloss (~55%)

indicates the decomposition of the framework. Zn(Ser)₂ also exhibit high guest mobility and thermochemical stability, as evident from its TGA profile. The TGA trace for Zn(Ser)₂ showed a gradual weightloss step of 12.1% [2 MeOH; calcd. 12.3%] (20–70°C), corresponding to the escape of all H₂O molecules trapped in the pores followed by a plateau (70–195°C) indicating its high thermal stability in absence of guest molecules (figure 8b). Further weightloss (~45%) indicates the decomposition of the framework entity.

Table 1. Crystal data and structure refinement for SerCdOAc.

Identification code	SerCdOAc
Empirical formula	C ₁₁ H ₂₀ CdN ₂ O ₈
Formula weight	420.70
Temperature/K	100(2)
Crystal system	orthorhombic
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> /Å	6.1983(5)
<i>b</i> /Å	15.0070(15)
<i>c</i> /Å	16.5317(16)
α /°	90.00
β /°	90.00
γ /°	90.00
Volume/Å ³	1537.8(2)
<i>Z</i>	4
ρ_{calc} /mg/mm ³	1.817
<i>m</i> /mm ¹	1.461
<i>F</i> (000)	848
Crystal size/mm ³	0.50 × 0.20 × 0.20
Theta range for data collection	5.96 to 58.18°
Index ranges	−8 ≤ <i>h</i> ≤ 3, −19 ≤ <i>k</i> ≤ 16, −19 ≤ <i>l</i> ≤ 21
Reflections collected	4346
Independent reflections	3041[<i>R</i> (int) = 0.0706]
Data/restraints/parameters	3041/2/212
Goodness-of-fit on <i>F</i> ²	1.036
Final <i>R</i> indexes [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0442, <i>wR</i> ₂ = 0.1029
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0499, <i>wR</i> ₂ = 0.1142
Largest diff. peak/hole / e Å ^{−3}	1.077/−0.650

Table 2. Crystal data and structure refinement for Zn(Ser)₂.

Identification code	Zn(Ser) ₂
Empirical formula	C ₂₀ H ₃₀ N ₄ O ₈ Zn
Formula weight	519.87
Temperature/K	293(2)
Crystal system	monoclinic
Space group	C2
a/Å	13.3648(6)
b/Å	13.2781(3)
c/Å	8.7485(3)
α/°	90.00
β/°	124.168(6)
γ/°	90.00
Volume/Å³	1284.53(8)
Z	2
ρ_{calc}/mg/mm³	1.344
m/mm¹	1.004
F(000)	544
Crystal size/mm³	0.5 × 0.2 × 0.2
Theta range for data collection	6.14 to 58.44°
Index ranges	-17 ≤ h ≤ 17, -17 ≤ k ≤ 16, -11 ≤ l ≤ 11
Reflections collected	2939
Independent reflections	2202[R(int) = 0.0176]
Data/restraints/parameters	2202/1/153
Goodness-of-fit on F²	1.064
Final R indexes [I>2σ(I)]	R ₁ = 0.0275, wR ₂ = 0.0613
Final R indexes [all data]	R ₁ = 0.0287, wR ₂ = 0.0623
Largest diff. peak/hole / e Å⁻³	0.269/-0.204

4. Conclusion

Research on amino acid based MOFs are still in its early stage and sufficient understanding is needed on amino acid based MOFs for their structure and subsequent property change with respect to coordinate covalent bonding with metal ions. In this manuscript, we have systematically explored structural diversity using Cd(II) and Zn(II) as metal node, keeping the linker entity same. This resulted in the generation of a 3D MOF, i.e., SerCdOAc, and a 2D MOF viz., Zn(Ser)₂. In case of SerCdOAc one Ser ligand and one acetate anion bind to the Cd(II), while two Ser linker bind the Zn(II) in case of Zn(Ser)₂. Both the MOFs feature hydrophilic pore surface, and encapsulate helical water chain in case of SerCdOAc and methanol molecules in between the 2D layers of the Zn(Ser)₂. The rational synthesis of these MOFs open up new avenues towards realizing functionalized chiral MOFs with utility in industrially relevant chiral solvent sorption and separation.

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