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# Four cadmium(II) polymeric frameworks constructed by 2-methyl or 2-ethyl imidazole dicarboxylates

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ABSTRACT

Four polymeric frameworks, $\{[Cd(HMIDC)(phen)]\cdot H_2O\}_n$ (**1**), $\{[Cd_4(HMIDC)_4]\cdot 8H_2O\}_n$ (**2**), Cd(HMIDC)(2,2′-bipy)]$_n$ (**3**), and $\{[Cd(HEIDC)(2,2'\text{-bipy})]_2\}_n$ (**4**) ($H_3$MIDC = 2-methyl-1*H*-imidazole-4,5-dicarboxylic acid, $H_3$EIDC = 2-ethyl-1*H*-imidazole-4,5-dicarboxylic acid, phen = 1,10-phenanthroline, 2,2′-bipy = 2,2′-bipyridine) have been hydro(solvo)thermally synthesized and structurally characterized by single-crystal X-ray diffraction. Compounds **1**, **3** and **4** are one-dimensional (1D) infinite chains, in which the $HMIDC^{2-}$ or $HEIDC^{2-}$ units as $\mu_2$-mode link the Cd(II) atoms with phen or 2,2′-bipy chelating the central ions. Compound **2** shows a three-dimensional (3D) structure constructed from 2D layer motifs joined by $\mu_2$-$HMIDC^{2-}$ or $\mu_3$-$MIDC^{3-}$ ligands. The thermal and solid-state photoluminescence properties of complexes **1**–**4** have been determined as well.

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## 1. Introduction

Recently, the metal–organic frameworks (MOFs) constructed from the *N*-heterocyclic carboxylate ligands have attracted great interest due to their intriguing architectures and topologies, and potential applications as functional materials [1–9]. By these studies, people found that it is very important to design and synthesize various organic ligands to prepare interesting MOFs. In this context, much attention has been put into this kind of organic compound, imidazole 4,5-dicarboxylic acid ($H_3$IDC), considering its abundant coordination fashions and results in the formation of the structures of higher dimensions [10–59]. Prompted by these interesting findings, people have synthesized two analog ligands of $H_3$IDC, 2-methyl-1*H*-imidazole-4,5-dicarboxylic acid ($H_3$MIDC) [60–64] and 2-ethyl-1*H*-imidazole-4,5-dicarboxylic acid ($H_3$EIDC) [17,61,65], to build up desired complexes. But the reported polymeric frameworks bearing $H_3$MIDC or $H_3$EIDC are limited (the $H_3$IDC-based, $H_3$MIDC-based or $H_3$EIDC-based coordination polymers are listed in Table 1) [10–65]. Also, up date, the reports concerning the structural factors of $H_3$MIDC and $H_3$EIDC for dominating the self-assembly are rare. Indeed, only we have given the primary prediction about the ethyl substituent effect in the ligand $H_3$EIDC [65].

In this paper, we still chose the two ligands, $H_3$MIDC and $H_3$EIDC to prepare more MOFs. We hope to continuously explore more useful information of the methyl or ethyl substituent effect in such ligands by quantum-chemical calculation.

Herein, we report the hydro(solvo)thermal syntheses, structural determinations of four coordination polymers, namely $\{[Cd(HMIDC)(phen)]\cdot H_2O\}_n$ (**1**), $\{[Cd_4(HMIDC)_4]\cdot 8H_2O\}_n$ (**2**), [Cd(HMIDC)(2,2′-bipy)]$_n$ (**3**), and $\{[Cd(HEIDC)(2,2'\text{-bipy})]_2\}_n$ (**4**) (phen = 1,10-phenanthroline, 2,2′-bipy = 2,2′-bipyridine). Single crystal X-ray diffractions reveal that one to three hydrogen atoms can be removed from ligand $H_3L$ (L = MIDC or EIDC), forming $H_2L^-$, $HL^{2-}$ and $L^{3-}$ anions and the deprotonated $H_{3-n}L^{n-}$ ($n$ = 1, 2 or 3) could coordinate to metal ions in $\mu_2$, $\mu_3$ or $\mu_4$ modes (Scheme 1). The thermal and solid-state photoluminescence properties of complexes **1**–**4** have been determined as well.

## 2. Results and discussion

### 2.1. Synthesis and characterization

As is discussed in our recent publication [61,65], the introduction of ethyl group into $H_3$EIDC has some effect on the NBO charge distributions of oxygen and nitrogen atoms. The NBO charge distributions of O and N atoms in $H_3$EIDC all increase slightly, which shows that the coordination abilities of these atoms may be enhanced, especially of carboxylate oxygen atoms. Here, we have calculated the NBO charge distributions of O and N atoms in the free ligand $H_3$MIDC, and found that $H_3$MIDC shows similar calculation result as $H_3$EIDC (Supporting information). That is to say, the N and O atoms in both $H_3$EIDC and $H_3$MIDC all still indicate strong coordination abilities, compared with the free ligand $H_3$DIC. So

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**Table 1**
$H_3$IDC-based, $H_3$MIDC-based or $H_3$EIDC-based coordination polymers.

| Imidazole dicarboxylato ligand | Polymer | Structural feature | Refs. |
|---|---|---|---|
| $H_3$IDC | $[Ag(H_2IDC)]_n$ | 2D layer | [10] |
| | $[Ag_5(HIDC)_2(CN)]_n$ | 3D framework | [11] |
| | $\{[Ba(H_2IDC)_2(H_2O)_4]\cdot 2H_2O\}_n$ | 2D sheet | [12,13] |
| | $[Ca(HIDC)(H_2O)_2\cdot H_2O]_n$ | 2D network | [14] |
| | $[Cd(HIDC)(H_2O)]_n$ | 2D sheet | [11,15] |
| | $[Cd(H_2IDC)_2(H_2O)_2]$ | 1D chain | [11] |
| | $[Cd(HIDC)(H_2O)_2]_n$ | 3D framework | [16] |
| | $[Cd(H_2IDC)_2(H_2O)_2]\cdot 2H_2O$ | 1D chain | [11] |
| | $[Cd_3(H_2O)_2(IDC)_2\cdot H_2O]$ | 3D framework | [17] |
| | $[Cd_5(HIDC)_2(IDC)_2(H_2O)]\cdot H_2O$ | 3D framework | [11] |
| | $[Cd_{27}(IDC)_{16}](SO_4)_3\cdot 22DMF$ | 3D framework | [18] |
| | $[Cd_2(HIDC)(C_2O_4)]$ | 3D framework | [11] |
| | $[Cd_5(HIDC)_2(IDC)_2(py)_2]_n$ (py = pyridine) | 3D porous framework | [19] |
| | $[Cd(HIDC)(py)]_n$ | 3D framework | [20] |
| | $\{[Cd_5(IDC)_2(HIDC)(4,4'\text{-bipy})_3(py)_2(H_2O)_3]\cdot 2NO_3\cdot 2H_2O\}_n$ (4,4′-bipy = 4,4′-bipyridine) | 3D porous framework | [19] |
| | $\{[Cd_5(IDC)_3(4,4'\text{-bipy})_2(H_2O)_2]\cdot NO_3\cdot 3.5H_2O\}_n$ | 3D porous framework | [19] |
| | $\{(4,4'\text{-}H_2bipy)[Cd_9(HIDC)_4(IDC)_4(4,4'\text{-bipy})_4]\cdot 8H_2O\}_n$ | 3D framework | [49] |
| | $[Cd(HIDC)(H_2O)(prz)_{0.5}]_n$ (prz = piperazine) | 2D achiral framework | [21] |
| | $[Cd(\mu_3\text{-HIDC})(bbi)_{0.5}]_n$ (bbi = 1,1′-(1,4-butanediyl)bis(imidazole)) | 3D framework | [22] |
| | $[Cd(HIDC)(pytpy)]_n$ (pytpy = 4′-(3-pyridyl)-2,2′:6′,2″-terpyridine) | 1D chain | [23] |
| | $[Cd(HIDC)(bix)]_n$ (bix = 1,4-bis(imidazol-1-ylmethyl)-benzene) | 3-fold-interpenetrated diamondoid network | [24] |
| | $[Cd(HIDC)(phen)]_n$ | 1D chain | [16] |
| | $[\{NaCd_4(IDC)_3(prz)\}\cdot 3H_2O]_n$ | 3D framework | [25] |
| | $\{Na_4[Cd_7(IDC)_6]\cdot 3(4,4'\text{-bipy})\cdot 7H_2O\}_n$ | 3D framework | [26] |
| | $\{[KCd_4(IDC)_{2.5}(4,4'\text{-bipy})_2(H_2O)_2]\cdot 1.5NO_3\cdot 3H_2O\}_n$ | 3D porous framework | [19] |
| | $\{(Bu_4N)K_3[Cd_7(IDC)_6]\cdot 6H_2O\}_n$ | 3D Metal-Organic Framework | [26] |
| | $Cd_8Na_8(HIDC)_9(IDC)_4(H_2pip)_2\cdot(EtOH)_5(H_2O)_{37}$ (pip = piperzine) | Zeolitic AST topology | [27] |
| | $[Co(HIDC)(H_2O)(pyz)_{0.5}]_n$ (pyz = pyrazine) | 2D achiral network | [21] |
| | $\{[Co_3(IDC)_2(4,4'\text{-bipy})(H_2O)_4]\cdot 2H_2O\}_n$ | 2-fold interpenetrated 3D architecture | [28] |
| | $\{[Co_3(IDC)_2(4,4'\text{-bipy})_3]\cdot 6H_2O\cdot DMF\}_n$ | 3D open framework with hexagonal channels | [28] |
| | $[Co(HIDC)(4,4'\text{-bipy})_{0.5}(H_2O)]_n$ | 2D layer | [29] |
| | $[Co_3(IDC)_2(4,4'\text{-bipy})_3]\cdot 4,4'\text{-bipy}\cdot 8H_2O$ | 3D framework | [30] |
| | $Co_3(IDC)_2(pyz)_3]\cdot 8H_2O$ (2,5-bptz = 2,5-bis(4-pyridyl)-1,3,4-thiadiazole) | 3D framework | [30] |
| | $[Co_3(IDC)_3(2,5\text{-bptz})_3]\cdot 2,5\text{-bptz}\cdot 9H_2O$ | 3D framework | [30] |
| | $Na_2[Co^{II}{}_2Co^{III}{}_2(IDC3\text{-})_4(2,2'\text{-bipy})_4]\cdot 12H_2O$ | 1D chain | [31] |
| | $[Fe(HIDC)(H_2O)]_n$ | 2D layer | [21] |
| | $[Fe(HIDC)(H_2O)(prz)_{0.5}]_n$ | 2D achiral | [21] |
| | $[In_5(HIDC)_{10}(1,2\text{-}H_2dach)_{2.5}(DMF)_3(CH_3CN)_2(H_2O)_{10}]_n$ (1,2-dach = 1,2-diaminocyclohexane) | Zeolite-like frameworks | [32] |
| | $[In_{48}(HIDC)_{96}(HPP)_{24}(DMF)_{36}(H_2O)_{192}]$ (HPP = 1,3,4,6,7,8-hexahydro-2H-pyrimido[1,2-a]pyrimidine) | Porous anionic zeolite-like framework | [33] |
| | $[In(HIDC)_2(imidazole)(DMF)_4(CH_3CN)(H_2O)_4]$ | Porous anionic zeolite-like framework | [33] |
| | $[Mg(HIDC)(H_2O)_2](H_2O)_{1.5}$ | 1D chain | [34] |
| | $\{[Mg(HIDC)(H_2O)_2]\cdot 1.5H_2O\}_n$ | 1D chain | [35] |
| | $[Mg(HIDC)(H_2O)]_n$ | 2D network | [35] |
| | $\{[Mg_3(IDC)_2(H_2O)_5]\cdot 2H_2O\}_n$ | 3D framework | [35] |
| | $[Mn(HIDC)(H_2O)]_n$ | 2D layer | [21] |
| | $[Mn_3(IDC)_2(H_2O)_4]$ | 3D framework | [36] |
| | $[Mn(HIDC)(H_2O)]_n$ | 2D layer | [37] |
| | $[MnHIDC)(H_2O)(prz)_{0.5}]_n$ | 2D achiral layer | [21] |
| | $[Mn(HIDC)(4,4'\text{-bipy})_{0.5}(H_2O)]_n$ | 2D sheet | [14] |
| | $Mn(phen)(HIDC)]_n$ | 1D zigzag chain | [38] |
| | $[KMn_4(IDC)_3(prz)\cdot 3H_2O]_n$ | 3D framework | [39] |
| | $Ni(cyclam)]_4[Ni(cyclam)(H_2O)_2]_2\{[Ni(cyclam)][Co_8(IDC)_{12}]\}\cdot 41H_2O$ (cyclam = 1,4,8,11-tetraazacyclotetradecane) | 3D framework | [40] |
| | $\{[Li_{11}(Ni_8IDC_{12})\,(H_2O)_{12}]Li_9(H_2O)_{20}\}_n$ | 3D framework | [41] |
| | $\{[Na_{20}(Ni_8IDC_{12})(H_2O)_{28}]\,(H_2O)_{13}(CH_3OH)_2\}_n$ | 3D framework | [41] |
| | $\{[Na_{16}(Ni_8IDC_{12})(H_2O)_{20}(H_3O)_4](MeCN)(H_2O)_{18.5}\}$ | 3D framework | [42] |
| | $[Pb_2(HIDC)_2]_n$ | 2D framework | [43] |
| | $[Pb(HIDC)(H_2O)]_n$ | 3D framework | [44] |
| | $[Pb(HIDC)]_n$ | 2D (3,3)-net framework | [45] |
| | $[Zn(HIDC)(bib)_{0.5}]_n$ (bib = 4-bis(imidazol-1-yl)-butane) | 2D sheet | [46] |
| | $[Zn_3(IDC)_2(\mu_2\text{-}H_2O)_2H_2O]_n$ | 3D porous framework | [47] |
| | $[Zn_5(IDC)_2(HIDC)_2(DMF)_4]_n$ | 3D framework | [48] |
| | $[Zn(HIDC)(4,4'\text{-bipy})0.5(H_2O)]_n$ | 2D layer | [29] |
| | $[Zn_3(IDC)_2(4,4'\text{-bipy})(H_2O)_2]_n$ | 3D framework | [49] |
| | $\{[Zn_3(IDC)_2(4,4'\text{-bipy})_3]\cdot(4,4'\text{-bipy})\cdot 8H_2O\}_n$ | 3D framework | [49] |
| | $[Zn(phen)(H_2IDC)_2]_n$ | 1D zig-zag chain | [50] |
| | $\{[Zn(HIDC)(pytpy)]\cdot H_2O\}_n$ | 1D chain | [23] |
| | $[Zn_{12}(guanidinium)_8(IDC)_8(HIDC)_4\cdot(DMF)_8(H_2O)_3]_n$ | Zeolite-like AST topology | [27] |
| | $[Zn_8K_8(HIDC)_{12}(DMF)_5(H_2O)_{16}]_n$ | Zeolite-like AST topology | [27] |

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