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Zeolite-Type Metal Oxalate Frameworks

Fei-Yan Yi, Huajun Yang, Xiang Zhao, Pingyun Feng, and Xianhui Bu**

Dedicated to Professor Jin-Shun Huang on the occasion of his 80th birthday

Abstract: *While many metal oxalate salts are known, few are known to form zeolite-type topologies. The construction of zeolite types, especially those with low framework density such as RHO, from linear ligands is generally perceived as less likely, because the 180° metal-ligand-metal geometry deviates too much from the established strategy of using ligands with bent coordination geometry (centered around 145°) to mimic the geometry in natural zeolites. We show the general feasibility of using linear ligands for the synthesis of zeolite types by reporting a family of indium oxalate salts with multiple zeolite topologies, including RHO, GIS, and ABW. Of particular interest is the synthesis of a zeolite RHO net with double 8-rings and large alpha cages, which are highly desirable zeolite features.*

Crystalline porous materials (CPM) have attracted considerable interest because they can be assembled into intriguing structures with novel topology.[1–6] In particular, zeolite topologies have been the target of numerous synthetic efforts for over half a century.[7,8] Natural zeolites are constructed from SiO_4 and AlO_4 tetrahedra. In classic aluminosilicates, the T-X-T angle (T = Si or Al, X = anionic crosslinker; for zeolites, $X = O^{2-}$) is centered around 145°, which is generally regarded as an important structural feature in zeolitic materials.[9] By mimicking this feature, a large family of metal–organic frameworks have been made from 4,5-imidazoledicarboxylic acid (H_3ImDC)[10] and various imidazolate ligands with different substituent groups.[11]

It has been recognized that in inorganic zeolites, the T-X-T angle generally decreases with increasing T–O bond length and that by tuning the T–O distance and corresponding T-O-T angle, new zeolite topologies can be made.[12] In the past two decades, great progress has been achieved at the lower end with T-X-T smaller than 145°, as shown by the synthesis of germanates and arsenates with a range of zeolite topologies.[12] The most dramatic example is that the T-X-T angle can be decreased to about 109° (same as X-T-X angles), as evidenced in zeolite-type metal chalcogenides such as M^{3+}/M^{4+} sulfides and selenides (M^{3+} = Ga, In, M^{4+} = Ge, Sn) with the zeolite RWY-type topology.[13]

In comparison, the progress in making zeolite-type nets at the higher end (the maximum T-X-T angle = 180°) has been limited. The common topology under such geometrical conditions is the diamond net or other relatively dense nets, usually with 6-membered rings (6 T-atoms).[14] An interesting strategy was reported that uses a ligand with a bite angle of 120° to assemble 3-rings and 180° ligand to crosslink 3-rings into the zeolite NPO topology.[15] So far, few zeolite nets are known that are constructed from only linear ligands with a T-X-T angle of 180° (the 180°bite angle for the X ligand) and zeolite types with low framework density (defined as the T-atom density which is the number of T-atoms in 1 nm^3) are even more difficult to access.[16]

Herein, we report a significant advance in the synthesis of zeolite-type MOFs by demonstrating the successful synthesis of a series of zeolite-type MOFs from a simple linear linker, oxalic acid (H_2ox). This is believed to be the first time that a zeolite RHO topology with double 8-rings (D8R) has been synthesized using a linear linker. It is also the first time that the RHO topology has been constructed using a ligand with only carboxylate functionality. A key synthetic strategy that led to this success is the exploration of the solvent system and different cationic structure-directing agents. In addition to zeolites RHO, GIS, ABW (denoted CPM-519-RHO, CPM-520-GIS, CPM-521-ABW), more common 4-connected nets such as diamond and quartz types have also been observed (Scheme 1, Table 1). These compounds are based on oxalate as a linear linker and In^{3+} as the four-connected nodes. The resulting anionic frameworks provide a unique opportunity for the use of the cation-templating strategy to develop new zeolite-type materials.

The novelty of this work can be easily seen from Figure 1, which shows the development of zeolite RHO in different compositions, from inorganic zeolites, ZIFs, and ZMOFs to this work. Comparisons among these four distinct types are made with respect to four aspects: linker types (X), T-X-T angle, unit-cell size, and large alpha cages.

CPM-519-RHO, which consists of only metal–O coordinate bonds, is unique compared to ZIF-RHO, which contains Zn–N bonds, and ZMOF-RHO, which contains mixed In–N and In–O bonds. In this sense, CPM-519-RHO is more like inorganic zeolites than ZIFs or ZMOFs.

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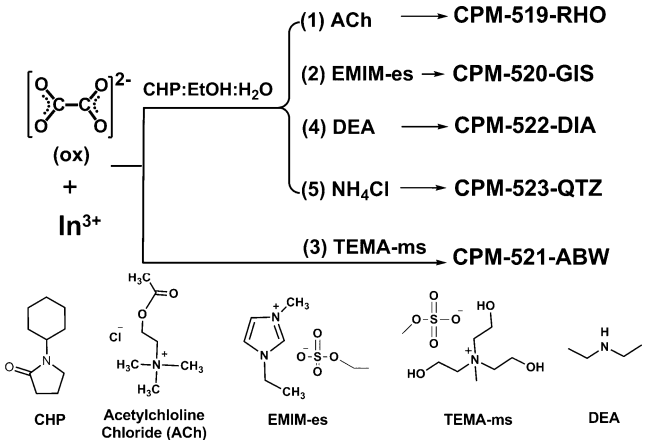
Table 1: Summary of crystal data and refinement results.[a]

Name	Templates	Net Type	Space group	R(F)	*a* [Å]	*b* [Å]	*c* [Å]	α [°]	β [°]	γ [°]
CPM-519-RHO	ACh	RHO	$Im\bar{3}m$	0.0228	28.315(9)	28.315(9)	28.315(9)	90	90	90
CPM-520-GIS	EMIM-es	GIS	$I4_1/amd$	0.0180	21.797(11)	21.797(11)	12.299(6)	90	90	90
CPM-521-ABW	TEMA-ms	ABW	*Pnma*	0.0609	11.060(5)	21.605(8)	10.642(4)	90	90	90
CPM-522-DIA-1	DEA	DIA	$P2_1/c$	0.0675	8.6289(14)	16.242(3)	8.4811(14)	90	100.141(3)	90
CPM-522-DIA-2	DMP	DIA	$C2/c$	0.0437	9.964(2)	17.055(4)	8.042(3)	90	127.32(1)	90
CPM-523-QTZ	NH_4Cl	QTZ	$P6_222$	0.0191	9.037(7)	9.037(7)	11.378(9)	90	90	120

[a] ACh = acetylcholine chloride; EMIM-es = 1-ethyl-3-(methylimidazolium) ethyl sulfate; TEMA-ms = Tris-(2-hydroxyethyl)-methyl-ammonium methylsulfate; DEA = diethylamine; DMP = N,N′-dimethylpropionamide.



Scheme 1. Synthetic conditions for compounds with the five topologies.

A main advance from this work is the synthesis of CPM-519 from the 180° ligand, H_2ox. Oxalate can be considered as in between inorganic anions and organic ligands. In earlier three types of RHO (i.e., silicates, ZIFs, and ZMOFs), the T-X-T angle is centered around 145° (between 137 to 154°)-(Figure 1), which seems to suggest a critical role for the T-X-T angle in the formation of the RHO topology. But the discovery of CPM-519 suggests that this geometric condition near 145° is not needed.

Different zeolite-type topologies have been achieved by using various structure-directing agents. CPM-519-RHO was synthesized by using acetylcholine chloride (ACh). CPM-520 with GIS topology was obtained by using 1-ethyl-3-methylimidazolium ethylsulfate (EMIM-es) as the organic template. When tris-(2-hydroxyethyl)-methyl-ammonium methylsulfate (TEMA-ms) was used, CPM-521 with ABW topology was successfully constructed. In addition, *dia* and *qtz* topologies were obtained by using diethylamine (DEA) and ammonium chloride (NH_4Cl) as templates, respectively.

In addition to the effects of various structure-directing agents, the solvent effect is another key factor. In this work, mixed solvents of 1-cyclohexyl-2-pyrrolidone (CHP), ethanol, and H_2O were adopted. With other solvents, such as N,N′-diethylformamide (DEF), tetramethylurea (T-murea), and

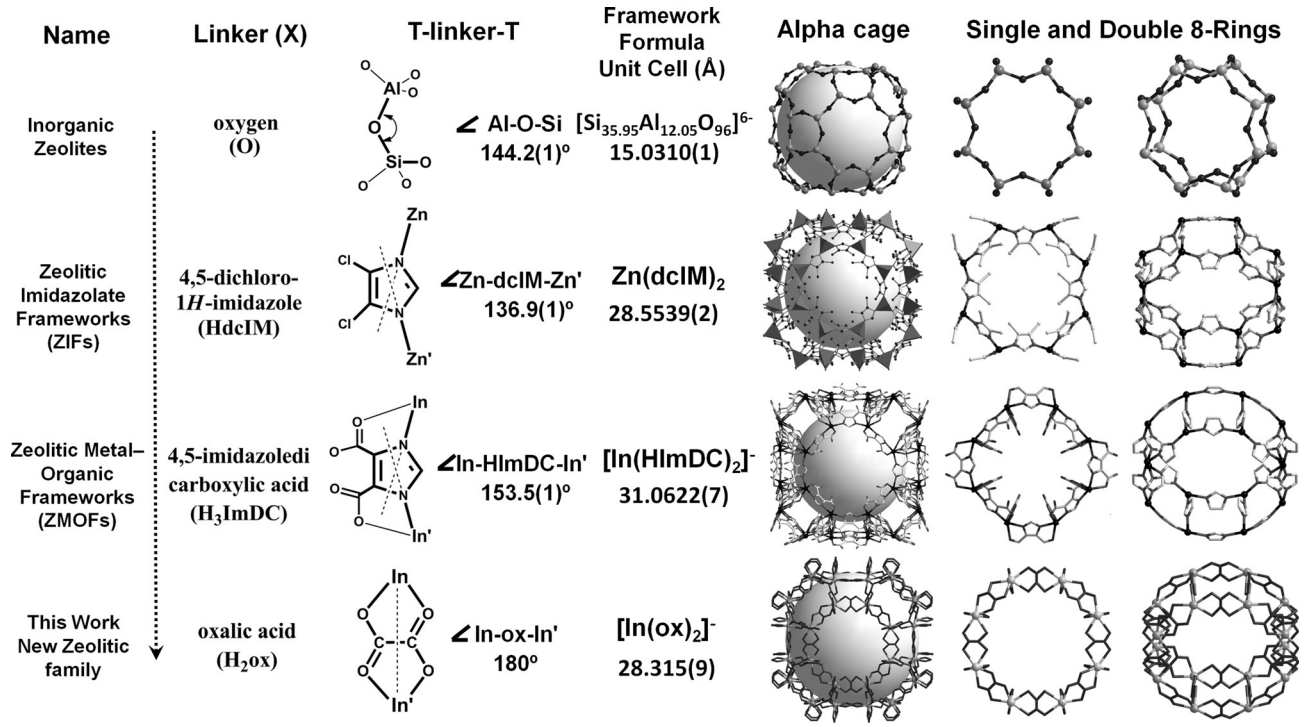


Figure 1. Evolutionary progress of RHO topology from inorganic zeolites[17] to ZIFs,[11a] ZMOFs,[10c] and this work.

N,N′-dimethylpropionamide (DMP), *dia* and *qtz* topologies can be easily synthesized, but not zeolite-type RHO, GIS, and ABW.

The different roles of ionic liquids are another interesting feature in this work. During the synthesis of CPM-520-GIS, a very small amount of an ionic liquid, EMIM-es, was added into the mixed solvent as a cationic template. This procedure is in contrast with the use of an ionic liquid as the solvent (i.e., ionothermal synthesis). Herein, the ionic liquid mainly serves as a cationic structure-directing agent. When another ionic liquid, tris-(2-hydroxyethyl)-methyl-ammonium methylsulfate (TEMA-ms), was used as the solvent, CPM-521-ABW was assembled.

The synthesis of this new zeolitic family, RHO in particular, from the linear ox-ligand may inspire the search for other zeolite types with large T-X-T angles. The key structural characteristics are as follows: the basic building unit {In(ox)$_4$} (Figure 2), anionic frameworks with an In–In distance of about 5.9 Å, In-ox-In angle of 180°, and a wide range of In-In-In angles from 78.2 to 141.7° (Scheme S1 in the Supporting Information).

A zeolite-type RHO with double-8-membered rings (D8R) and a large alpha cage is a quite desirable synthetic target. CPM-519 crystallizes in a highly symmetric cubic space group $Im\bar{3}m$. In this structure, a cage of approximately 26 Å can be observed and can be fit into the channels without touching the van der Waals surfaces of framework. Its potential guest-accessible void volume is 68.6% (15582.7 Å^3) of the crystal unit cell volume (22702.0 Å^3), as estimated using the PLATON program.[18] The location of organic cations could not be determined due to disorder.

In CPM-520-GIS, monomeric In^{3+} ions as 4-connected T-nodes are bridged into 4-rings and a 1D channel (Figure S2). Neighboring channels are connected by In$_4$(ox)$_4$ four-membered rings into 3D framework with 1D channels of 7.8 × 11.3 Å^2. Template cations of $TEMA^-$ are located in the channel.

In CPM-521-ABW, two different In-ox 1D chains are formed, (Figure S3). The 3D 4-connected uninodal ABW net is formed from interconnecting 1D chains. Three different channels can be observed, two ellipse channels A and B along the [100] and [010] directions, respectively, and a small tetragonal channel C along [001] direction. The diameters of the largest sphere are 4.0, 3.9, and 3.6 Å for channels A, B, and C, respectively.

In conclusion, this work shows effective use of the template effect to form new topologies in the metal oxalate system, as is typical in the synthesis of inorganic zeolites. The synthesis of zeolite RHO with oxalate ligand is an inspiring development that suggests the possibility of synthesizing other low-density zeolite types from oxalate or other ligands with large T-X-T angles. Such structures may provide new insight into the geometric and chemical factors that govern the formation of relatively low-density zeolite nets.

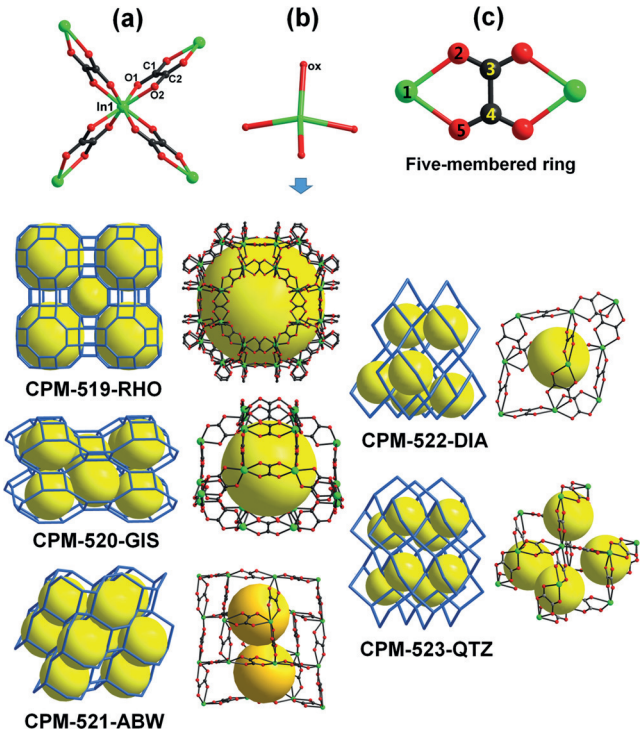


Figure 2. Five topologies and their frameworks composed of the following structural unit: a) the [In(ox)$_4$] building unit (crystal structure shown); b) a 4-connected In^{3+} node; and c) a 5-membered ring of -In-*O*-C–C-*O*-In-. In these topologies, In-ox-In bonds are simplified into blue lines, yellow spheres represent the largest sphere. C, O, and In atoms are shown in gray, red, and green in the crystal frameworks.

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Conflict of interest

The authors declare no conflict of interest.

Keywords: linear linkers · oxalates · RHO topology · template effects · zeolitic frameworks

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