

A Series of Guest-Defined Metal-Complex/Disulfonate Frameworks of Hydrogen-Bonded $[\text{Co}(\text{en})_2(\text{ox})]^+$ and 2,6-Naphthalenedisulfonate

Xin-Yi Wang and Slavi C. Sevov*

Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, Indiana 46556

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ABSTRACT: A new series of soft-host frameworks assembled by charge-assisted hydrogen bonds between a cationic metal complex (MC) and an anionic disulfonate specifically $[\text{Co}(\text{en})_2(\text{ox})]^+$ and 2,6-naphthalenedisulfonate (NDS), is synthesized and structurally characterized. The five new compounds have a general formula $(\text{MC})_2(\text{NDS}) \cdot n(\text{guest})$ where guests are H_2O , dimethylformamide (DMF), dimethyl sulfoxide (DMSO), *p*-nitrophenol (pnp), and 4-dimethylaminopyridine (dmapy). All five structures are of the pillared-layer type where the layers are constructed of MC cations held together by a multitude of hydrogen bonds, both direct and indirect via sulfonate groups. The organic residues of the disulfonate serve as pillars. The structures of the layers and the orientations of the pillars adjust to the specifics of the guest molecules, and, as a result, four different patterns are observed. Compared to the recently reported analogous compounds with $[\text{Co}(\text{NH}_3)_6]^{3+}$, these compounds have larger interpillar galleries because of the lower charge of the complex. The same effect was observed in a similar series with $[\text{Co}(\text{en})_2(\text{ox})]^+$ complexes but linked with 4,4'-biphenyldisulfonate. The factors that influence the frameworks such as the charge of the metal complex and the guest molecules are discussed.

Introduction

Considerable research efforts have been devoted to searching for new and better inclusion compounds. One of the main reasons is their potential for eventual applications in a variety of technologically useful processes.¹ These compounds typically have three-dimensional (3D) frameworks made of building blocks held together by a range of interactions. Various guest molecules often occupy the cavities in the frameworks and are usually very weakly bonded to them by either van der Waals forces or a handful of hydrogen bonds.² The bonding within the frameworks, on the other hand, can vary from strong interactions such as covalent and coordination bonding to relatively weak forces such as hydrogen-bonding and π -interactions.^{3–10} The strength of the interactions puts such self-assembled frameworks roughly into two different types: rigid and soft. Although the known rigid frameworks are by far more numerous than the soft ones,¹¹ the latter exhibit a number of unique and beneficial features. Among them are their great flexibility and overall durability; that is, the structures readily adjust to different guest molecules during formation while preserving the same overall topology and connectivity.⁴

Among the hydrogen-bonded frameworks, those with charge-assisted hydrogen bonds between cations and anions are of special interest because of the additional strength brought by the electrostatic attractions.^{4,7,8} Two very good examples of such frameworks are the guanidinium sulfonates (GS)^{4,9,10} and the metal-complex sulfonates (MCS)^{12–16} schematically shown in Figure 1. The GS system includes a series of pillared-layer compounds with layers made of hydrogen bonded guanidinium cations and disulfonate anions pillared by the organic residues of the disulfonates. One of the typical structures is the bilayer structure depicted in Figure 1a. As shown by Ward et al., these frameworks are very durable and yet flexible in their ability to adjust to very different guest molecules.^{4,9,10} The large number of available GS compounds makes possible their further exploration for various applications and for better understanding of the factors that control formation of such frameworks. The

MCS frameworks, on the other hand, are an emerging class, and the few known examples can be viewed as related to the GS compounds by replacing two guanidinium cations from two layers with a cationic metal complex with ligands that can provide protons for hydrogen bonding such as ammonia,^{12,15–18} water,^{19–21} and various amines.^{13,14,19,22–24} As a result, two neighboring layers of guanidinium are “sewed” together by the metal centers between them; that is, the metal complexes provide two layers of ligands capable of hydrogen bonding (Figure 1b,c). Within the layers, the metal-complexes are held together primarily by hydrogen bonds to the $-\text{SO}_3^-$ terminals of the disulfonate. The layers are connected into a 3D framework by the organic pillars of the disulfonate groups. Besides the ability to generate 3D structurally flexible frameworks, such MCS systems provide additional flexibilities; namely, the overall charge of the metal complex and the nature of the ligands can be varied as well. As demonstrated in previous papers by us and Shimizu et al.,^{13,14} the charge of the metal complex is one of the important factors that define the size of the interpillar galleries and, therefore, the size and number of the guest molecules that can be accommodated. Lower charges correspond to a lower number of charge-balancing pillars per metal complex and, thus, to larger cavities. The overall effective charge of the metal complex has been reduced by (1) including a noncoordinating anion such as chloride in the structure,¹⁵ (2) using a metal complex with a metal center of a lower charge such as Ni^{2+} ,^{14,19} and (3) using a complex with coordinated anionic ligand(s) such as the oxalate in $[\text{Co}(\text{en})_2(\text{ox})]^+$.¹³ The first two approaches have been utilized by Shimizu’s group and have produced several MCS compounds with interesting gas absorption properties.^{14,15,19}

We have already reported two series of MCS compounds with 4,4'-biphenyldisulfonate (BPDS),^{12,13} one of them with the trication $[\text{Co}(\text{NH}_3)_6]^{3+}$ and the second one with the monocation $[\text{Co}(\text{en})_2(\text{ox})]^+$. The compounds exhibit pillared-layer structures with different organic guest molecules as shown in Figure 1, panels b and c, for the tri- and monocations, respectively. We have continued these investigations by changing the disulfonate and reported here is yet another series of pillared-layer

* To whom correspondence should be addressed. E-mail: ssevov@nd.edu.

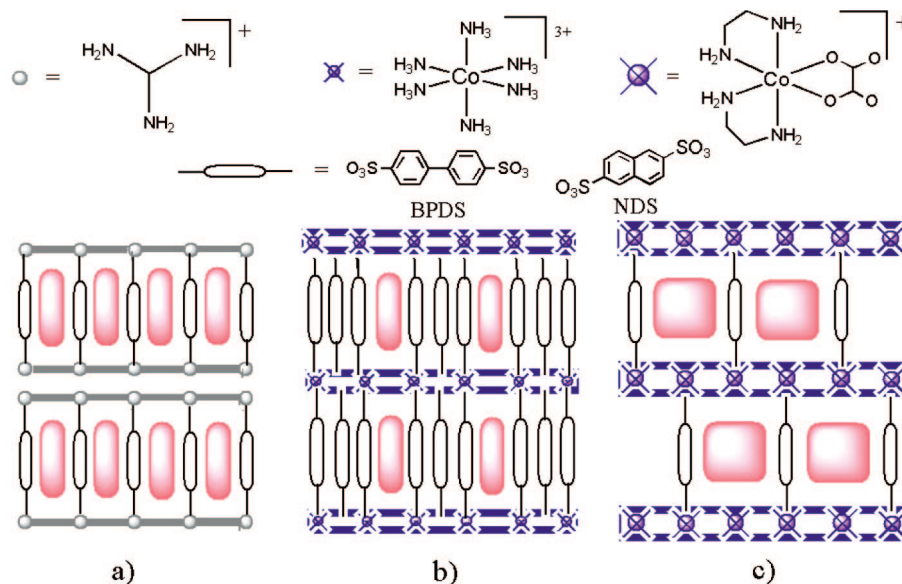
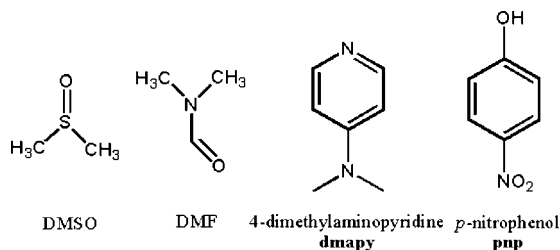


Figure 1. (a) A typical guanidinium disulfonate bilayer structure with layers made of hydrogen-bonded guanidinium and sulfonate groups and pillars of the organic residue of the disulfonate. The ratio of the disulfonate to guanidinium is 0.5. (b) A proposed and later observed metal complex disulfonate structure with layers made of hydrogen-bonded $[\text{Co}(\text{NH}_3)_6]^{3+}$ and sulfonate groups. The ratio of disulfonate to metal complex is 1.5. (c) A proposed framework made of $[\text{Co}(\text{en})_2(\text{ox})]^+$ and disulfonate. The ratio of disulfonate to metal complex is 0.5.

Chart 1. The Guest Molecules Used in This Work



compounds with frameworks made of $[\text{Co}(\text{en})_2(\text{ox})]^+$ and 2,6-naphthalenedisulfonate (NDS). The general formula of the compounds is $(\text{MC})_2(\text{NDS}) \cdot n(\text{guest})$ with guest molecules of H_2O , dimethylformamide (DMF), dimethyl sulfoxide (DMSO), *p*-nitrophenol (pnp), and 4-dimethylaminopyridine (dmapy) shown in Chart 1. The structures have the basic features envisioned in Figure 1c, but the use of different guest molecules leads to different structural variations, which, in turn, testify to the high flexibility of these soft molecular frameworks.

Experimental Section

The complex $[\text{Co}(\text{en})_2(\text{ox})]\text{Br} \cdot \text{H}_2\text{O}$ was synthesized according to the literature.²⁵ The 2,6-naphthalenedisulfonic acid disodium salt (Na_2NDS , 98%, TCI America), solvents, and guest molecules (>98%, all from Acros Organics) were used as purchased.

Synthesis of $[\text{Co}(\text{en})_2(\text{ox})]_2(\text{NDS}) \cdot 4\text{H}_2\text{O}$ (1). A solution of $[\text{Co}(\text{en})_2(\text{ox})]\text{Br} \cdot \text{H}_2\text{O}$ (0.2 mmol) in 4 mL of hot H_2O was mixed with 4 mL of aqueous solution of Na_2NDS (0.1 mmol). The resulting clear solution was stirred for 10 min, filtered, and left undisturbed at room temperature to allow for slow evaporation. Red-colored block crystals of **1** were obtained in 10 days as a single phase (moderate yield).

Synthesis of $[\text{Co}(\text{en})_2(\text{ox})]_2(\text{NDS}) \cdot 2(\text{DMSO})$ (2). A solution of $[\text{Co}(\text{en})_2(\text{ox})]\text{Br} \cdot \text{H}_2\text{O}$ (0.3 mmol) in 5 mL of hot H_2O was mixed with 3 mL of aqueous solution of Na_2NDS (0.15 mmol). Two milliliters of DMSO were added and the solution was stirred for 10 min, filtered, and left undisturbed at room temperature to allow for slow evaporation. Red platelike crystals of **2** were obtained in 10 days together with some starting materials (moderate yield).

Synthesis of $[\text{Co}(\text{en})_2(\text{ox})]_2(\text{NDS}) \cdot 2(\text{pnp})$ (3). A solution of $[\text{Co}(\text{en})_2(\text{ox})]\text{Br} \cdot \text{H}_2\text{O}$ (0.2 mmol) in 6 mL of hot H_2O was mixed with

6 mL of aqueous solution of Na_2NDS (0.1 mmol). Five milliliters of methanol solution of pnp (90 mg) were added and the solution was stirred for 10 min, filtered, and left undisturbed at room temperature to allow for slow evaporation. Orange plate-shaped crystals of **4** were obtained in 10 days (single phase, moderate yield).

Synthesis of $[\text{Co}(\text{en})_2(\text{ox})]_2(\text{NDS}) \cdot 3(\text{DMF})(\text{H}_2\text{O})$ (4). A solution of $[\text{Co}(\text{en})_2(\text{ox})]\text{Br} \cdot \text{H}_2\text{O}$ (0.3 mmol) in 5 mL of hot H_2O was mixed with 3 mL of aqueous solution of Na_2NDS (0.15 mmol). Three milliliters of DMF were added and the solution was stirred for 10 min, filtered, and left undisturbed at room temperature to allow for slow evaporation. Red-colored column-shaped crystals of **3** were obtained in 1 week (single phase, moderate yield).

Synthesis of $[\text{Co}(\text{en})_2(\text{ox})]_2(\text{BPDS}) \cdot 2(\text{dmapy})$ (5). A solution of $[\text{Co}(\text{en})_2(\text{ox})]\text{Br} \cdot \text{H}_2\text{O}$ (0.2 mmol), Na_2NDS (0.10 mmol) in 8 mL of hot H_2O was mixed with 5 mL of acetonitrile solution of 4-dimethylaminopyridine (1 mmol). The solution was stirred for 5 min, filtered and left undisturbed at room temperature. Red column-shaped crystals of **5** were obtained in 1 week (single phase, moderate yield).

Structure Determination. Single-crystal X-ray diffraction data sets were collected on a Bruker APEX-II diffractometer with a CCD area detector at 100 K ($\text{Mo K}\alpha$, $\lambda = 0.71073 \text{ \AA}$). The crystals were taken from the mother liquid and were immediately covered with Paratone-N oil in order to prevent eventual loss of guest molecules. The structures were solved by direct methods and refined by a full-matrix least-squares technique based on F^2 using the SHELXL97 program.²⁶ The hydrogen atoms in the cobalt complex and the NDS ligand were refined as riding on the corresponding non-hydrogen atoms while they were fixed to the ideal geometry for the water molecules. Half of the DMF molecules in **3** and the dmapy molecules in **5** are disordered and have high U_{eq} values. More details of the data collection and structure refinements are presented in Table 1.

Results and Discussion

All five new compounds have pillared-layer type frameworks made of metal complex cations $[\text{Co}(\text{en})_2(\text{ox})]^+$ and disulfonate anionic linkers of 2,6-naphthalenedisulfonate. These building blocks are assembled and held together by a multitude of charge-assisted hydrogen bonds. Topologically, the five structures are very similar to the reported series of compounds with the same metal complex but with biphenyldisulfonate as the linker. The metal complex $[\text{Co}(\text{en})_2(\text{ox})]^+$ used in both series is capable of hydrogen bonding as both a hydrogen-donating and hydrogen-accepting unit via its ethylenediamine and oxalate ligands,

Table 1. Crystallographic Data for Compounds 1–5

compound	1 (H ₂ O)	2 (DMSO)	3 (pnp)	4 (DMF)	5 (dmapy)
formula	C ₁₁ H ₂₃ N ₄ O ₉ SCo	C ₁₃ H ₂₅ N ₄ O ₈ S ₂ Co	C ₁₇ H ₂₄ N ₅ O ₁₀ SCo	C ₃₁ H ₆₃ N ₁₁ O ₁₉ S ₂ Co ₂	C ₃₆ H ₅₈ N ₁₂ O ₁₄ S ₂ Co ₂
<i>M_r</i> [g mol ⁻¹]	446.32	488.42	549.40	1075.90	1064.92
crystal system	triclinic	monoclinic	triclinic	monoclinic	monoclinic
space group	<i>P</i> $\bar{1}$	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> $\bar{1}$	<i>C</i> 2/ <i>c</i>	<i>C</i> 2/ <i>c</i>
<i>a</i> [Å]	7.7554(3)	6.3976(3)	6.9070(2)	29.3244(13)	29.1670(13)
<i>b</i> [Å]	8.4738(3)	11.8749(6)	12.5690(3)	11.8856(5)	11.8769(6)
<i>c</i> [Å]	13.5889(5)	25.1729(12)	12.8507(3)	12.8941(6)	13.0194(6)
α [°]	74.1360(10)		82.113(2)		
β [°]	87.0490(10)	93.088(3)	85.852(2)	106.036(2)	106.560(2)
γ [°]	85.9300(10)		88.226(2)		
<i>V</i> [Å ³]	856.37(5)	1909.63(16)	1101.92(5)	4319.2(3)	4323.0(4)
<i>Z</i>	2	4	2	4	4
ρ_{calcd} [g cm ⁻³]	1.731	1.699	1.656	1.655	1.636
μ (Mo, K α) [mm ⁻¹]	1.180	1.168	0.939	0.955	0.946
R1/wR2 ^a (<i>I</i> > 2 σ (<i>I</i>))	0.0320/0.0842	0.0342/0.0758	0.0267/0.0742	0.0454/0.1163	0.0359/0.0926
R1/wR2 ^a (all data)	0.0355/0.0862	0.0488/0.0826	0.0300/0.0762	0.0605/0.1304	0.0436/0.0969

^a R1 = $[\sum \Delta F_o] / \sum |F_o|$; wR2 = $\{[\sum w[(F_o)^2 - (F_c)^2]^2] / [\sum w(F_o)^2]\}^{1/2}$; $w = [\sigma(F_o)^2 + (AP)^2 + BP]^{-1}$ where $P = [(F_o)^2 + 2(F_c)^2]/3$.

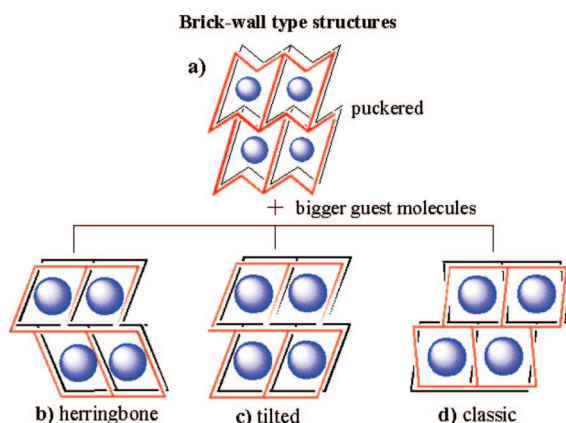


Figure 2. Versions of the brick-wall structure observed for the three-dimensional MCS frameworks: (a) puckered, (b) herringbone, (c) tilted, and (d) classical.

respectively. This allows for direct hydrogen bonding between the metal complexes in addition to those between the complex and the disulfonate. Such direct hydrogen bonding is absent in the guanidinium/disulfonate systems and in the more typical metal-complex/disulfonate compounds where guanidinium and the metal complex are only capable of proton-donating from the terminal -NH₂ groups of guanidinium or amine ligands of the metal complexes.

Overall, the hydrogen bonding in all guanidinium/disulfonate and metal-complex/disulfonate structures results in the formation of layers made of either guanidinium or metal complex cations that are grafted by the terminal sulfonate groups of the disulfonate. The organic residues of the disulfonates play the role of the pillars while the guest molecules occupy the galleries between the pillars and influence the structure specifics. The five different guest molecules used in the present study produced four different framework types: puckered, herringbone, tilted, and classical brick-wall structures (Figure 2).

Structure of 1. This compound, $[\text{Co}(\text{en})_2(\text{ox})]_2 \cdot 4\text{H}_2\text{O}$, forms when no organic guest molecules are available. Although the structure is of a pillared-layer type, the layers in this case are puckered, and the size of the interpillar galleries is effectively reduced by this puckering (Figures 2a and 3). The layers are parallel to the *ab* plane and are made of one crystallographic unique cobalt complex. The complexes are hydrogen-bonded to each other both by direct hydrogen bonds involving the oxalate and ethylenediamine ligands and by indirect hydrogen bonding via the -SO₃ groups above and below the layers. The

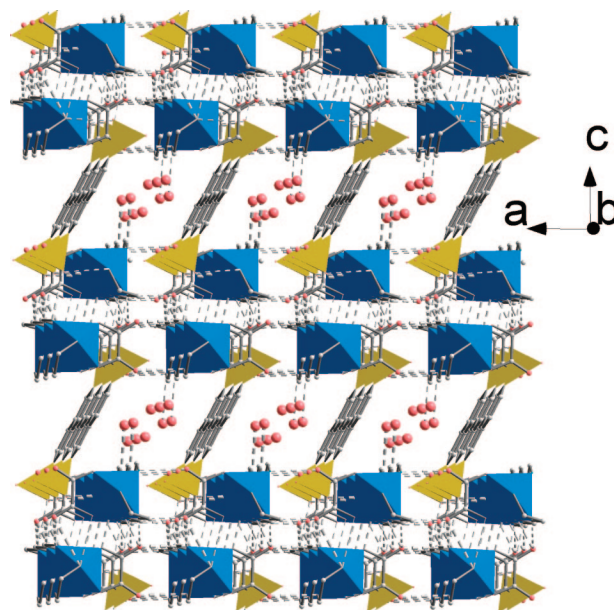


Figure 3. The three-dimensional puckered brick-wall framework of **1** without H₂O as guest molecules.

layers are pillared by the naphthalene residue along the *c* axis forming infinite galleries along *b*. The galleries are filled with water molecules that are hydrogen-bonded between themselves and some to the ethylenediamine ligands of the complexes. At a first glance, the structure resembles very closely the prototypical GS structure as depicted in Figure 1a, that is, a bilayer-type structure where the pillars are positioned at only one side of a layer. However, unlike the GS structures, the cobalt complexes and the sulfonate groups in the “bilayer” of **1** are all connected to each other and, therefore, the structure is more properly described as containing puckered single layers with pillars between, that is, a puckered brick-wall structure. The puckering effectively reduces both the distances between the layers as well as those between the cobalt centers within the layers, and this yields small galleries. The underlying reason for this is, of course, the absence of large organic guest molecules to occupy large galleries. The same effect was observed in the corresponding compound with biphenyldisulfonate (BPDS) where the absence of large guest molecules similarly led to the relatively close-packed structure of the resulting compound $[\text{Co}(\text{en})_2(\text{ox})]_2(\text{BPDS}) \cdot 3.5\text{H}_2\text{O}$.¹³ Thus, these two compounds without large organic guest molecules demonstrate the impor-

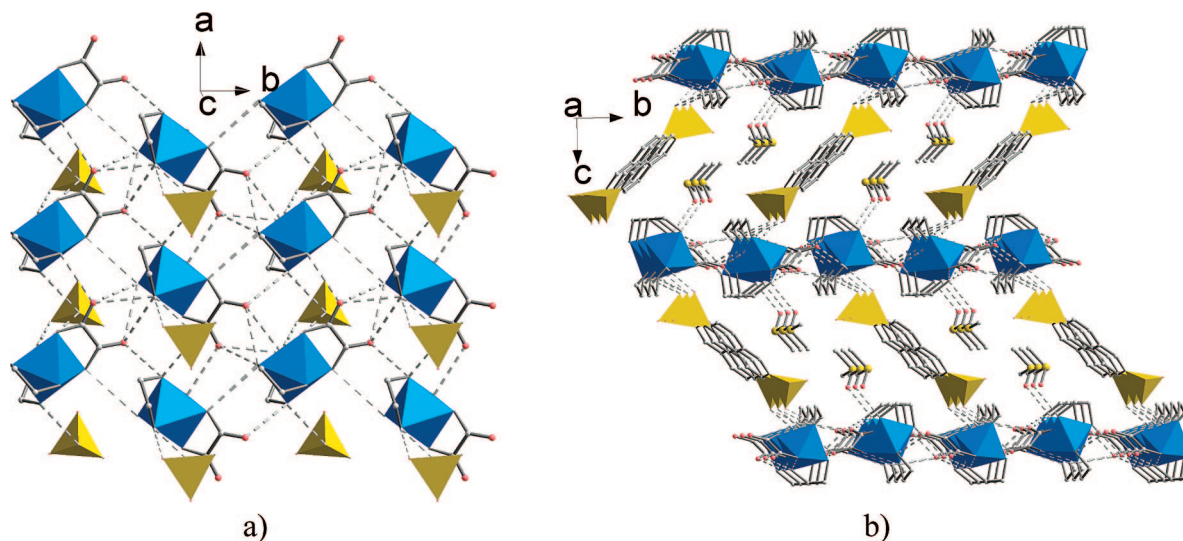


Figure 4. (a) The hydrogen-bonded layers of $[\text{Co}(\text{en})_2(\text{ox})]^+$ (blue octahedra) in **2** with the sulfonate groups of the pillars (yellow tetrahedra) alternating above and below the layers. (b) The pillared-layer “herringbone” type framework of **2** viewed along *a* with DMSO molecules shown in the infinite galleries.

tance of the latter for the openness of the structures. To some extent, the guest molecules act as neutral templates in the formation of the open frameworks.

Structure of 2. The structure of $[\text{Co}(\text{en})_2(\text{ox})]_2(\text{NDS}) \cdot 2(\text{DMSO})$ is dramatically different from **1** and has large galleries occupied by the DMSO molecules. Clearly, the presence of DMSO in the synthetic mixture influences the way the building blocks are assembled. These are the same building blocks and in the same ratio as in compound **1**, but the resulting structure is quite different with its wide galleries (Figures 2b and 4). The size, shape, overall electronic structure, and hydrogen-bonding capabilities of the DMSO guest molecule affect the galleries and the overall structural details. For example, the DMSO molecules form hydrogen bonds with the ethylenediamine in $[\text{Co}(\text{en})_2(\text{ox})]^+$. The layers, built of one unique cobalt complex in two different orientations, are now flat with no obvious puckering (Figure 4a). Numerous direct intercomplex hydrogen bonds and indirect ones via sulfonate groups covering both sides of the layers are responsible for the bonding within the layers.

The naphthalene pillars alternate on the sides of the layer, and this arrangement places them relatively far from each other, at a distance of ca. 8.4 Å (perpendicular to the pillars). At the same time they are tilted along *c* at about 45° with respect to the layers and the tilting directions alternate from one interlayer space to another (Figure 4b). This results in a “herringbone” pattern (Figure 2b) with infinite galleries along the *b* axis. This structural pattern and even the unit cell parameters are very similar with a DMF-filled structure with BPDS linkers, namely, $[\text{Co}(\text{en})_2(\text{ox})]_2(\text{BPDS}) \cdot 2(\text{DMF})$.¹³ This demonstrates the universality of the structure type in the metal-complex/disulfonate systems even when different pillars and guests are used. The interlayer distance in **2** is about 12.6 Å, which corresponds to calculated potential void space of 25.0%,²⁷ and these numbers are comparable to those observed in $[\text{Co}(\text{en})_2(\text{ox})]_2(\text{BPDS}) \cdot 2(\text{DMF})$, 13.2 Å and 25.8%, respectively.

Structure of 3. This compound, $[\text{Co}(\text{en})_2(\text{ox})]_2(\text{BPDS}) \cdot 2(\text{pnp})$, forms when guest molecules of *p*-nitrophenol are present during the synthesis. Like **2**, the structure of **3** has all the expected features for a MCS structure with a monocationic metal complex. However, instead of the herringbone structure of **2** with tilted linkers alternating tilting direction, the linkers in

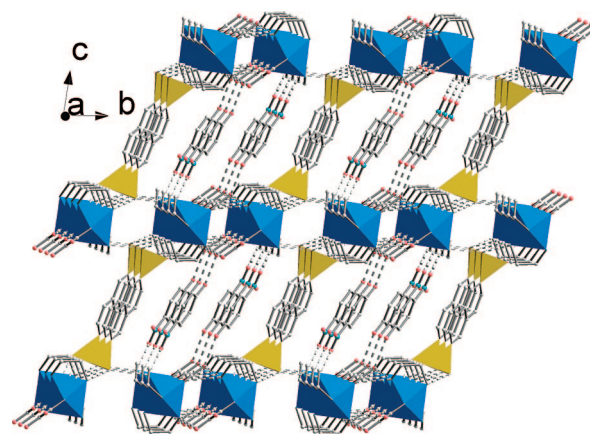


Figure 5. The tilted brick-wall framework of **3** with *p*-nitrophenol guest molecules.

compound **3** are all tilted in the same direction (Figures 2c and 5). The layers of hydrogen-bonded metal complexes and sulfonate groups are parallel to the *ab* plane. Large infinite galleries along the *a* axis are efficiently occupied by the pnp guest molecules. Like the DMSO in **2**, the pnp molecules form hydrogen bonds with the cobalt complexes and define the overall structure. Eventual π -interactions between the guest molecules as well as between them and the pillars were expected but none was found. The calculated space available for guests is 32.7%.

Structures of 4 and 5. These two compounds, $[\text{Co}(\text{en})_2(\text{ox})]_2(\text{NDS}) \cdot 3(\text{DMF})(\text{H}_2\text{O})$ and $[\text{Co}(\text{en})_2(\text{ox})]_2(\text{NDS}) \cdot 2(\text{dmapy})$, form with DMF and 4-dimethylaminopyridine, respectively, as guest molecules. They crystallize in the same space group with very similar cell parameters and, except for the guests, their structures are virtually the same (Figure 6). The pillared-layer framework exhibits the classical brick-wall structure with pillars that are slightly tilted and alternate their positions on the two sides of each layer. The pillars also alternate their tilting directions and thus stagger within the rows that they form along *c*. The galleries between these rows of pillars are occupied by three DMF and one water molecules in **4**, and two dmapy molecules in **5** per formula. They are all hydrogen-bonded to the cobalt complexes. The interlayer distances are

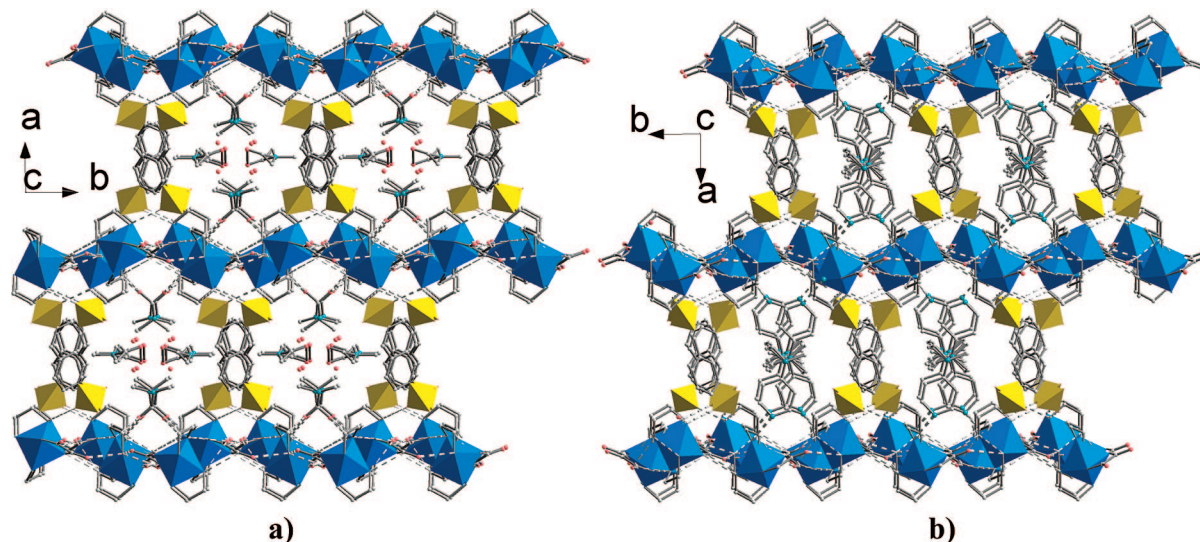


Figure 6. The classical brick-wall structures of (a) **4** with DMF and (b) **5** with 4-dimethylaminopyridine in the galleries of the framework. Some of the guest molecules in them are disordered.

about 14 Å for both **4** and **5**, and the calculated space available for guest molecules of the frameworks is 34.0%.

The emerging class of soft open frameworks constructed by charge-assisted hydrogen bonding between metal-complex cations and disulfonate anions has already shown structural diversity and abundance of compounds despite the limited number of metal complexes, disulfonates, and guest molecules that have been used so far.^{10–14} As in the extensively studied GS systems most of the MCS compounds have well-defined pillared-layer frameworks. The layers are always formed by the metal complexes as the core and sulfonate groups on the two sides of the layers where they form hydrogen bonds with the complexes. Complexes such as $[\text{Co}(\text{en})_2(\text{ox})]^+$ with hydrogen-bond donating and accepting ligands exhibit direct hydrogen bonds as well. Remarkable infinite galleries occupied by different guest molecules are found between the organic pillars in many of these structures.

Several important factors influence the overall structure of the frameworks. Some of these are (a) the number of protons capable of hydrogen-bonding at the metal complex, (b) the charge of the complex, and (c) the size, shape, electronic structure, and hydrogen-bonding capabilities of the guest molecule. Generally, more hydrogen-bonding protons and higher positive charge of the complex as in $\text{Co}(\text{NH}_3)_6^{3+}$ and $\text{Co}(\text{en})_3^{3+}$ leads to more and stronger interactions with the disulfonate pillars and, therefore, to better bonded overall structure.^{12,14–16} However, the high positive charge requires more charge-balancing disulfonate pillars per metal complex and leads to more packed structures and less guest-accessible space in the framework. The monocationic metal complex $[\text{Co}(\text{en})_2(\text{ox})]^+$, on the other hand, is charge balanced by only a half-pillar and generates much more open structures but with fewer charge-assisted hydrogen bonds to the pillars. The latter “shortcoming”, however, is balanced with the capability of these particular complexes to hydrogen-bond directly to each other because of the two types of ligands they have. Thus, the compounds constructed by $[\text{Co}(\text{en})_2(\text{ox})]^+$ and either BPDS or NDS have larger galleries and accommodate larger guest molecules.¹³ Finally, the role of the guest molecules is to “define” the specifics and fine-tune the otherwise very similar structures, and this demonstrates very clearly great flexibility that these soft frameworks have. The guest molecules seem to “guide” the final

orientation and connectivity of the building blocks to fit snugly around the molecules.

In conclusion, five new hydrogen-bonded MCS compounds were designed by considering the roles of the charge of the metal complex and the influence of the guest molecules. These series of compounds show typical pillared-layer frameworks and extend the diversity of the MCS system. The guest molecules tune the compounds into several different structure types. The rich structures and flexibility of the MCS compounds mimic the rich GS systems. Since the charge and overall geometry of the complex can be readily modified by the choice of metal and ligands and also the disulfonate can also be easily modified, the resulting frameworks can be designed to various desired specifications. Although it is difficult to predict structures based on the starting materials, the series of metal-complex/disulfonate compounds presented here and in previous publications bring us very close to this capability for this particular system. The structures fit into very few general types with very similar topologies and it becomes easier to envisage the framework that a particular combination of metal complex, disulfonate, and guest molecule may produce. The presence of the metal in these compounds presents one more variable and may also bring some additional physical properties based on unpaired electrons and redox capabilities.

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Supporting Information Available: X-ray crystallographic CIF files for the five compounds are available free of charge via the Internet at <http://pubs.acs.org>.

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