Electronic Supplementary Material (ESI) for CrystEngComm.

One-dimensional supramolecular columnar structure of *trans-syn-trans*-dicyclohexano[18]crown-6 and organic ammonium cations

Yu Ohshima, Kazuya Kubo,* Takashi Matsumoto, Heng-Yun Ye, Shin-ichiro Noro, Tomoyuki Akutagawa, and Takayoshi Nakamura*

Graduate School of Environmental Science, Hokkaido University, N10W5, Kita-ku, Sapporo, Hokkaido 060-0810, Japan.

E-mail: kkubo@es.hokudai.ac.jp, E-mail: tnaka@es.hokudai.ac.jp; Fax: +81 11 706 9420; Tel: +81 11 706 9419

Supporting Information

Table S1. Crystallographic data for crystals **1** and **2**

	1	**2**
Empirical formula	$C_{16}H_{22}N_{0.5}Ni_{0.5}O_3S_5$	$C_{32}H_{43}FNNiO_6S_{10}$
Formula weight	917.99	935.99
Temperature/K	173(2)	173(2)
Wavelength/Å	0.71075	0.71075
Crystal system	triclinic	triclinic
Space group	$P\bar{1}$	$P\bar{1}$
a/Å	8.0251(4)	13.4658(6)
b/Å	10.0806(6)	19.0314(10)
c/Å	12.6959(7)	24.7402(10)
α/°	89.8210(17)	77.941(6)
β/°	81.4586(15)	77.593(6)
γ/°	79.9673(16)	81.569(6)
Volume/Å^3	999.88(10)	6021.1(5)
Z	2	2
Density/g cm^{-3} (calculated)	1.525	1.549
Absorption coefficient /mm^{-1}	1.050	1.051
F(000)	479	2922
Crystal size /mm^3	0.51 × 0.25 × 0.10	0.50 × 0.24 × 0.19
Reflections collected	9776	59294
Independent reflections	4494 [*R*(int) = 0.0247]	27358 [*R*(int) = 0.0441]
Goodness-of-fit on F_2	1.158	1.060
Final *R* indices [I>2sigma(I)]	R_1 = 0.0415, wR_2 = 0.1039	R_1 = 0.0744, wR_2 = 0.2437
R indices (all data)	R_1 = 0.0448, wR_2 = 0.1090	R_1 = 0.1214, wR_2 = 0.2437

		distance /Å
O(1)	N(1)	2.893(3)
O(2)	N(1)	2.998(3)
O(3)	N(1)	3.089(3)
O(4)	N(1)	2.893(3)
O(5)	N(1)	2.998(3)
O(6)	N(1)	3.089(3)

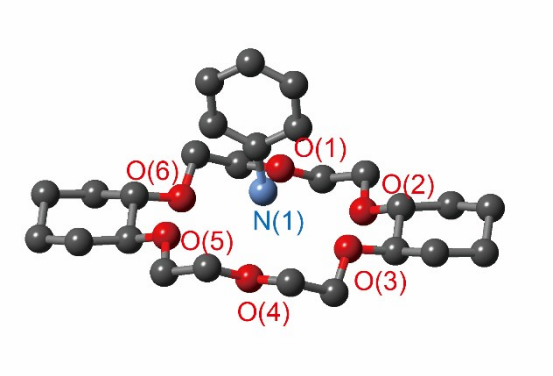

Figure S1. Distances between nitrogen atoms of the cation and oxygen atoms of the crown ether in **1** at 173 K

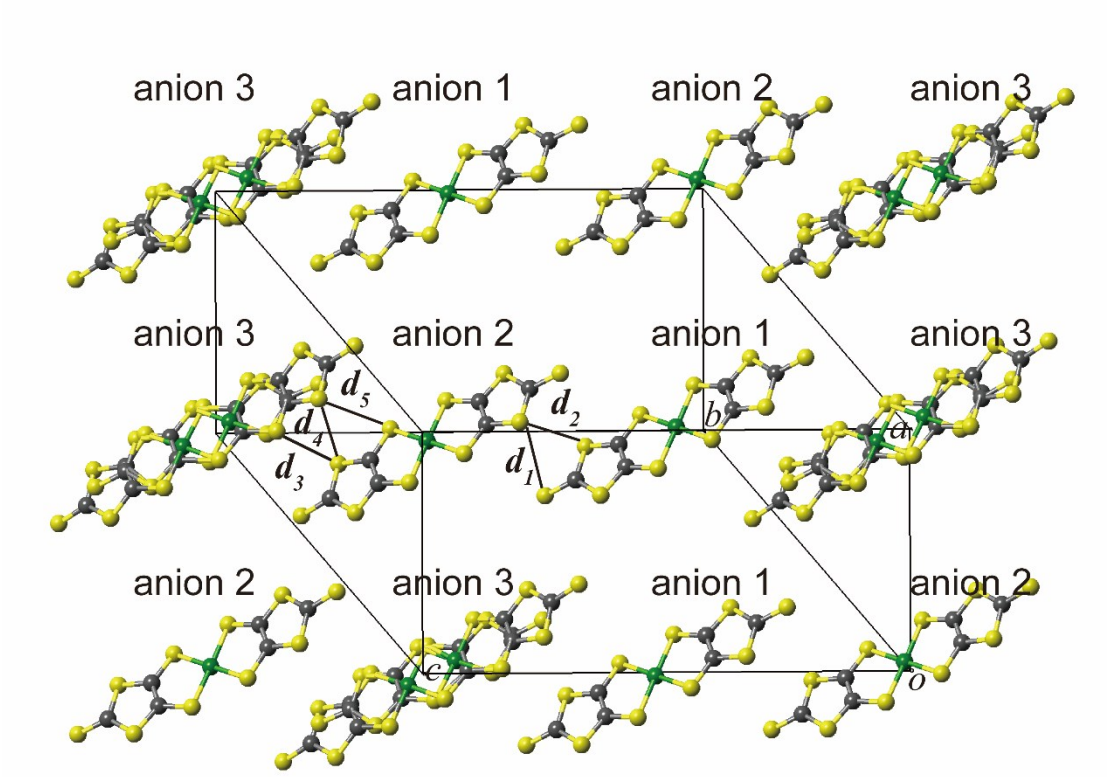

Figure S2. The $[Ni(dmit)_2]^-$ arrangement in **2** (d_1 = 3.627(3) Å, d_2 = 3.302(2) Å, d_3 = 3.26(2) Å, d_4 = 3.315(2) Å, d_5 = 3.619(3) Å,)

	distance /Å		distance /Å
N(1A) O(1)	2.81(2)	N(2A) O(10)	2.847(9)
N(1A) O(2)	3.34(1)	N(2A) O(11)	2.944(8)
N(1A) O(3)	3.12(2)	N(2A) O(12)	3.050(7)
N(1A) O(4)	2.82(2)	N(2B) O(13)	2.874(9)
N(1A) O(5)	2.83(1)	N(2B) O(14)	3.013(8)
N(1A) O(6)	2.94(1)	N(2B) O(15)	3.166(7)
N(1B) O(1)	2.80(2)	N(2B) O(16)	2.810(8)
N(1B) O(2)	3.13(2)	N(2B) O(17)	3.120(7)
N(1B) O(3)	2.93(2)	N(2B) O(18)	2.901(7)
N(1B) O(4)	2.91(2)	N(3) O(1)	2.868(7)
N(1B) O(5)	3.12(2)	N(3) O(2)	3.007(6)
N(1B) O(6)	3.19(2)	N(3) O(3)	3.087(6)
N(1C) O(7)	2.875(9)	N(3) O(4)	2.808(7)
N(1C) O(8)	3.017(8)	N(3) O(5)	3.251(6)
N(1C) O(9)	3.136(7)	N(3) O(6)	2.976(6)
N(1C) O(10)	2.802(8)	N(4) O(13)	2.810(8)
N(1C) O(11)	3.187(7)	N(4) O(14)	3.077(7)
N(1C) O(12)	2.912(7)	N(4) O(15)	2.949(8)
N(2A) O(7)	2.810(8)	N(4) O(16)	2.871(9)
N(2A) O(8)	3.153(7)	N(4) O(17)	3.001(8)
N(2A) O(9)	3.024(7)	N(4) O(18)	3.140(7)

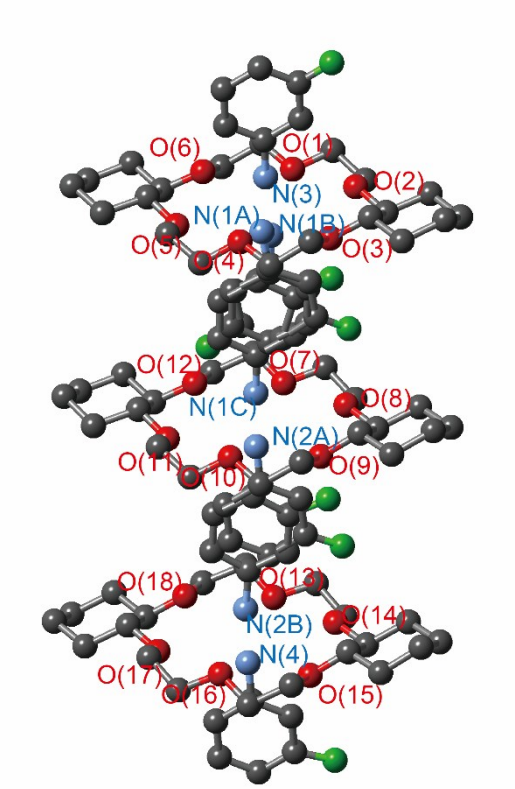

Figure S3. Distances between nitrogen atoms of the cations and oxygen atoms of the crown ethers in **2** at 173 K

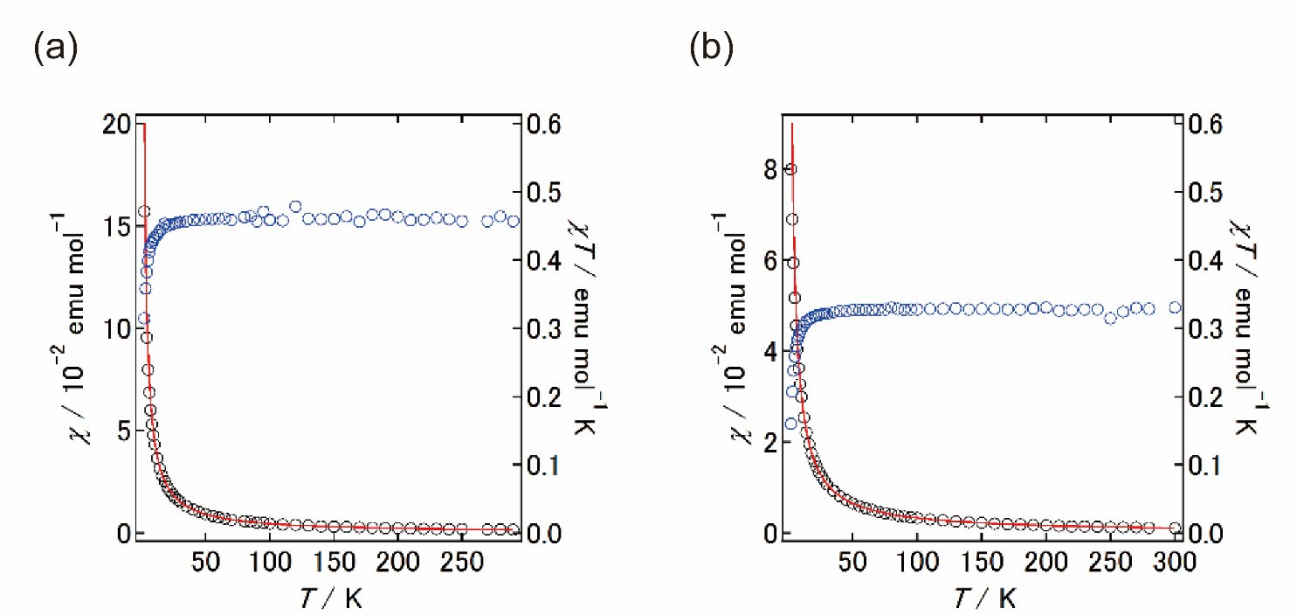

Figure S4 Magnetic properties of crystals (a) **1** and (b) **2**, black circle = χ vs T, blue circle = χT vs T, red line = fitting

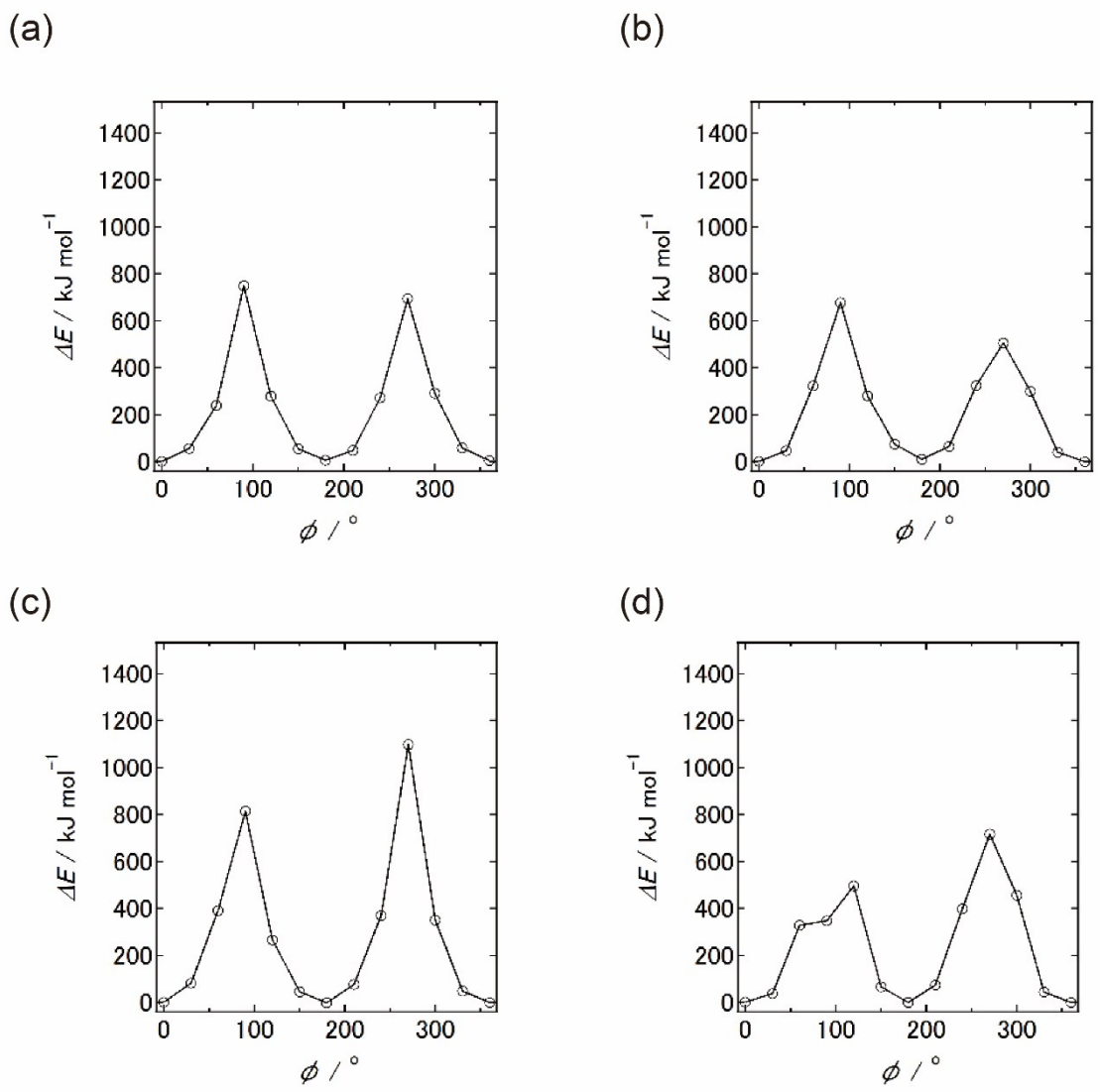

Figure S5 Potential energy curves for the rotation of *m*-FAni cations (a) 1A, (b) 2A, (c) 3 and (d) 4 in **2**. The energy for the rotation is overestimated because we are using fixed molecular coordinates. In the case of (*m*-FAni$^+$)(DB[18]crown-6)[Ni(dmit)$_2$]$^-$, in which the molecular rotation of *m*-FAni$^+$ was observed, the peak energy was 270 kJ/mol.