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

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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 ₃ S ₅	C ₃₂ H ₄₃ FNNiO ₆ S 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	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
<i>a</i> /Å	8.0251(4)	13.4658(6)
<i>b</i> /Å	10.0806(6)	19.0314(10)
<i>c</i> /Å	12.6959(7)	24.7402(10)
α ^o	89.8210(17)	77.941(6)
β ^o	81.4586(15)	77.593(6)
γ ^o	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 [<i>R</i> (int) = 0.0247]	27358 [<i>R</i> (int) = 0.0441]
Goodness-of-fit on <i>F</i> ₂	1.158	1.060
Final <i>R</i> indices [<i>I</i> >2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0415, <i>wR</i> ₂ = 0.1039	<i>R</i> ₁ = 0.0744, <i>wR</i> ₂ = 0.2437
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0448, <i>wR</i> ₂ = 0.1090	<i>R</i> ₁ = 0.1214, <i>wR</i> 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)

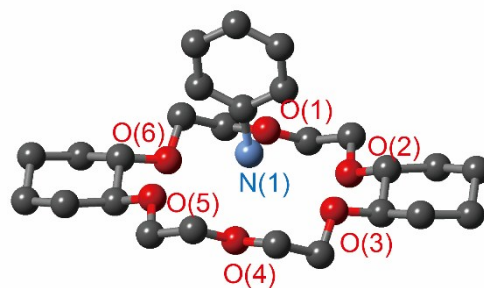


Figure S1. Distances between nitrogen atoms of the cation and oxygen atoms of the crown ether in **1** at 173 K

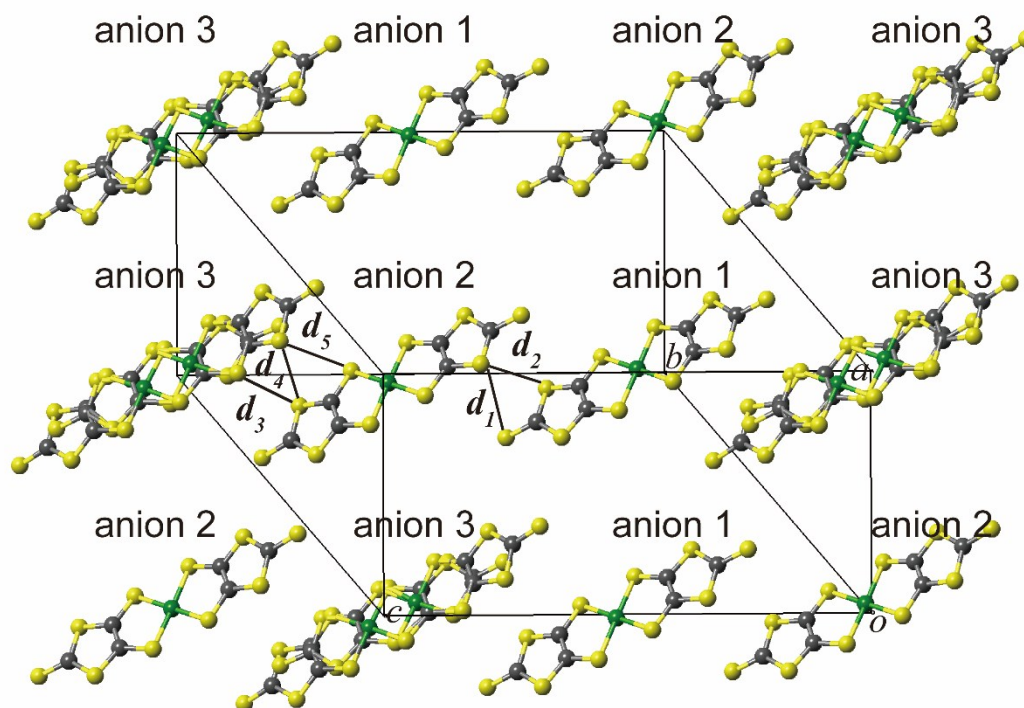


Figure S2. The $[\text{Ni}(\text{dmit})_2]^-$ arrangement in **2** ($d_1 = 3.627(3)$ Å, $d_2 = 3.302(2)$ Å, $d_3 = 3.26(2)$ Å, $d_4 = 3.315(2)$ Å, $d_5 = 3.619(3)$ Å,)

		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)

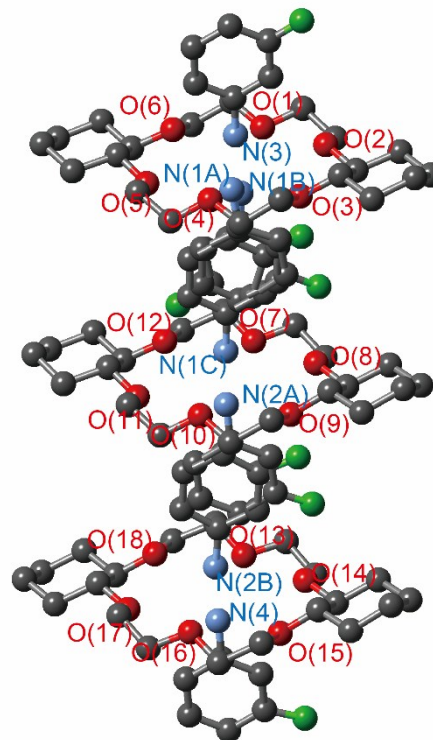
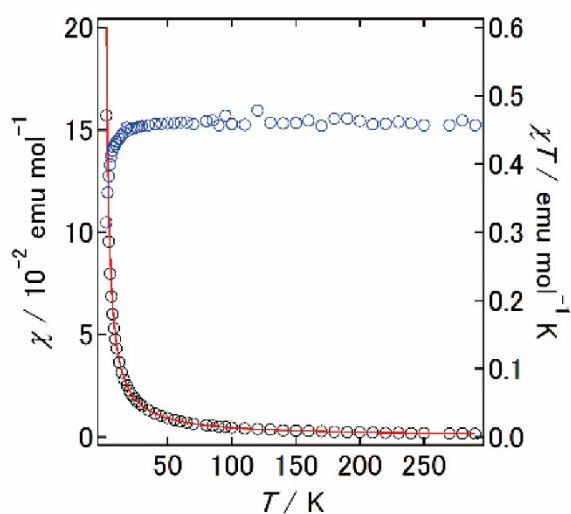


Figure S3. Distances between nitrogen atoms of the cations and oxygen atoms of the crown ethers in **2** at 173 K

(a)



(b)

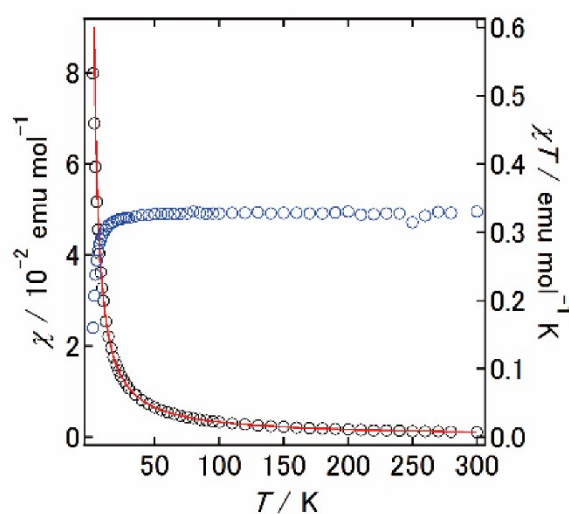


Figure S4 Magnetic properties of crystals (a) **1** and (b) **2**, black circle = χ vs T , blue circle = χT vs T , red line = fitting

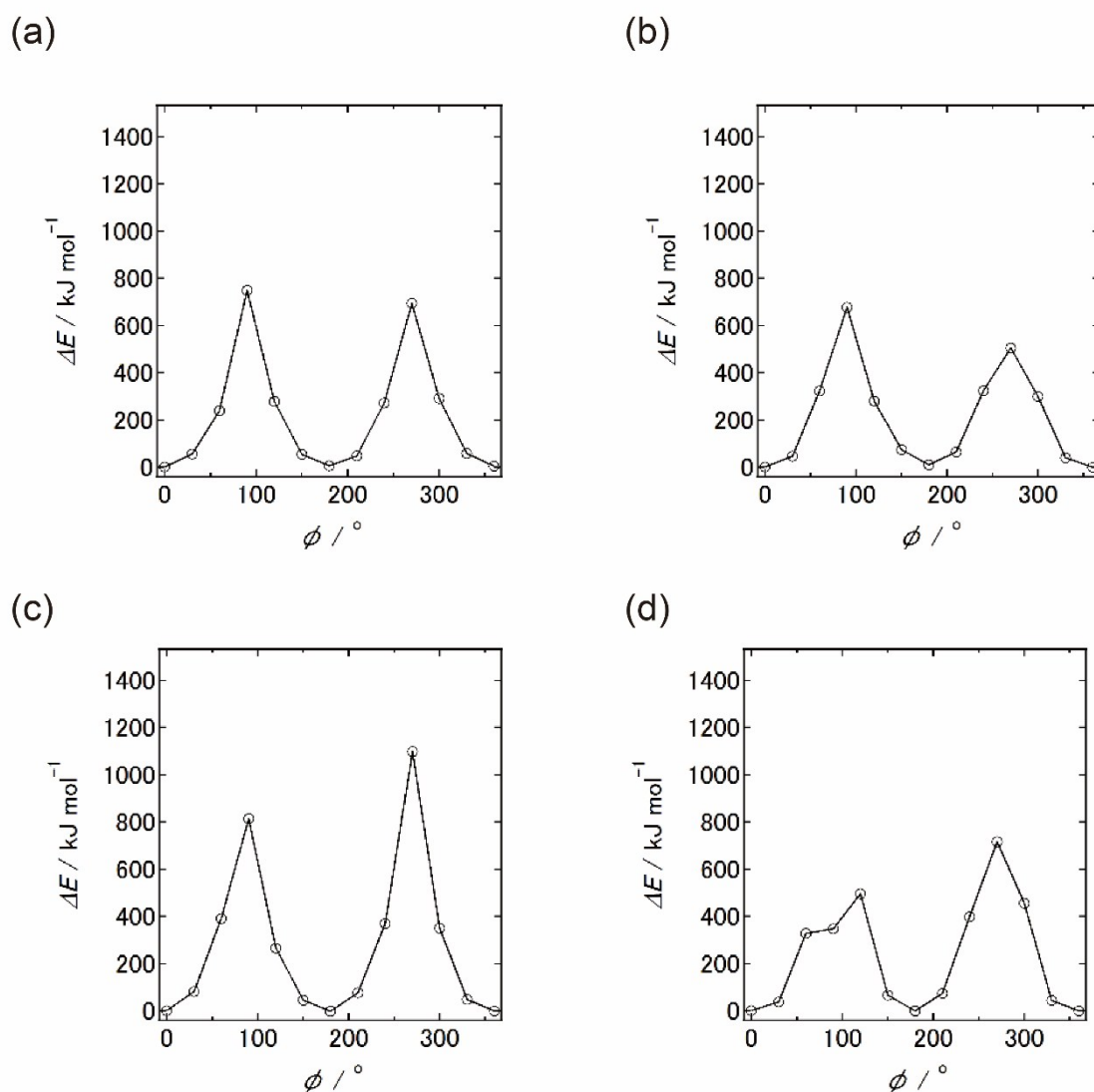


Figure S5 Potential energy curves for the rotation of *m*-FAni cations (a) 1A, (b) 2A, (c) 3 and (d) 4 in **2**. The energy for the rotation is overestimated because we are using fixed molecular coordinates. In the case of (*m*-FAni⁺)(DB[18]crown-6)[Ni(dmit)₂]⁻, in which the molecular rotation of *m*-FAni⁺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