Supplementary Material (ESI) for Journal of Materials Chemistry

Supplementary Information

A novel paramagnetic molecular superconductor formed by bis(ethylenedithio)tetrathiafulvalene, tris(oxalato)ferrate(III) anions and bromobenzene as guest molecule: $ET_4[(H_3O)Fe(C_2O_4)_3]\cdot C_6H_5Br$

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Table 1S. Crystal data and structure refinement for $ET_4[(H_3O)Fe(C_2O_4)_3]\cdot C_6H_5Br$ (**1**).

Empirical formula	C52 H40 Br Fe O13 S32	
Formula weight	2034.52	
Temperature	292(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 10.2875(3) Å	α= 90°.
	b = 20.0546(15) Å	β= 93.238(5)°.
	c = 35.513(2) Å	γ = 90°.
Volume	7315.0(7) $Å^3$	
Z	4	
Density (calculated)	1.847 Mg/m^3	
Absorption coefficient	1.726 mm^{-1}	
F(000)	4116	
Crystal size	0.40 x 0.20 x 0.15 mm^3	
Theta range for data collection	2.03 to 27.48°.	
Index ranges	-13<=h<=13, -26<=k<=26, -46<=l<=45	
Reflections collected	38333	
Independent reflections	8228 [R(int) = 0.0741]	
Completeness to theta = 27.48°	97.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.774 and 0.672	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8228 / 0 / 487	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0487, wR2 = 0.1089	
R indices (all data)	R1 = 0.1086, wR2 = 0.1333	
Largest diff. peak and hole	0.746 and -0.931 $e.Å^{-3}$	

Table 2S.Intermolecular S···S distances shorter than 3.60 Å (the sum of the van der Waals radii).

ET molecules	Distances
A-B	S(2)-S(13) 3.3739(16)
	S(5)-S(15)^{i} 3.5926(16) (×2)
	S(6)-S(13) 3.3265(14)
	S(8)-S(11) 3.5392(16)
	S(8)-S(15) 3.5810(16)
B-B	S(10)-S(16)^{ii} 3.5131(15)
	S(16)-S(14)^{ii} 3.4391(14) (×2)

Symmetry codes: (i) –x+1/2, –y+1/2, –z;
(ii) -x+2, –y, –z.

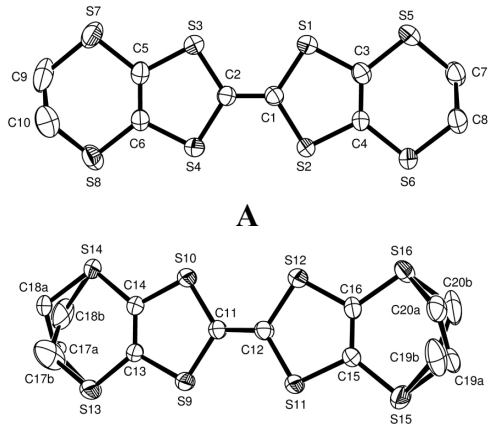

Figure 1S. Molecular geometry and labelling of the two independent ET molecules (A and B) in **1**.

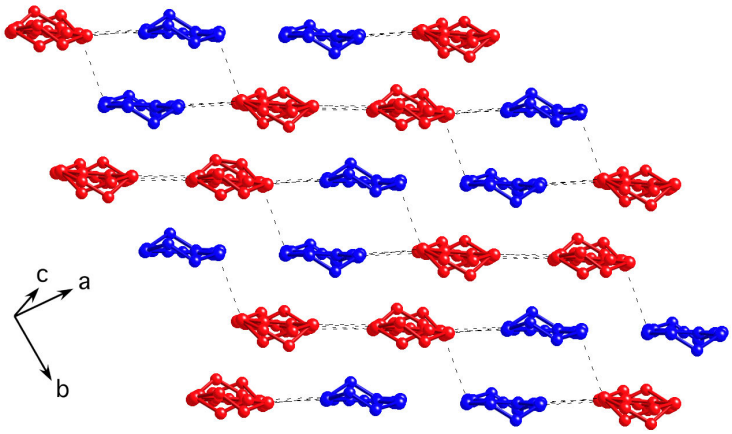

Figure 2S. View of the organic layer of **1** showing the β'' type of packing and the intermolecular S…S contacts shorter than 3.60 Å (the distances are listed in Table 1S). Molecules depicted in red have their ethylene groups disordered (B type molecule in Fig. 1S). Molecules depicted in blue have their ethylene groups ordered (A-type molecule in Fig. 1S).

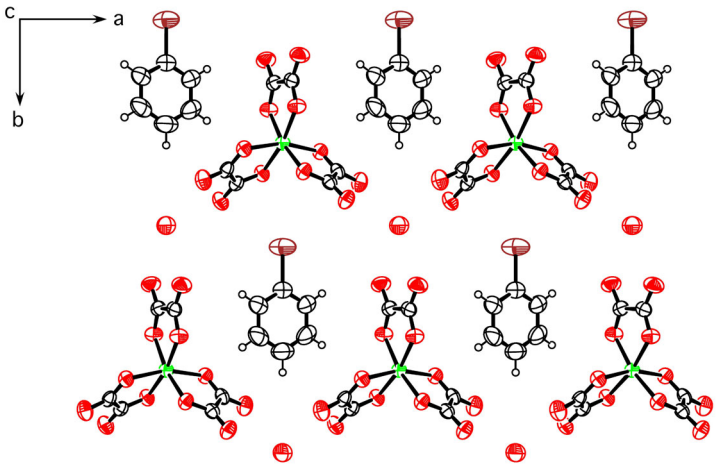

Figure 3S. View of the anion and solvent layer in **1** showing the bromobenzene molecules located in the pseudohexagonal cavity formed by the tris(oxalato)ferrate(III) anions and H_3O^+ cations.