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Article

Structures and properties of new organic conductors, BEDT-TTF, BEST and BETS salts of the $HOC_2H_4SO_3^-$ anion

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Supporting Information

GAMESS input options

ET^+ and $BETS^+$: ICHARG = 1, MULT = 2, SCFTYP = ROHF, RUNTYPE = ENERGY, DFTTYP = B3LYP, GBASIS = N31, and NGAUSS = 6.

I_3^-: ICHARG = -1, MULT = 1, SCFTYP = RHF, RUNTYPE = ENERGY, DFTTYP = B3LYP, and GBASIS = SBKJC.

$HOC_2H_4SO_3^-$: ICHARG = -1, MULT = 1, SCFTYP = RHF, RUNTYPE = ENERGY, DFTTYP = B3LYP, GBASIS = N31, and NGAUSS = 6.

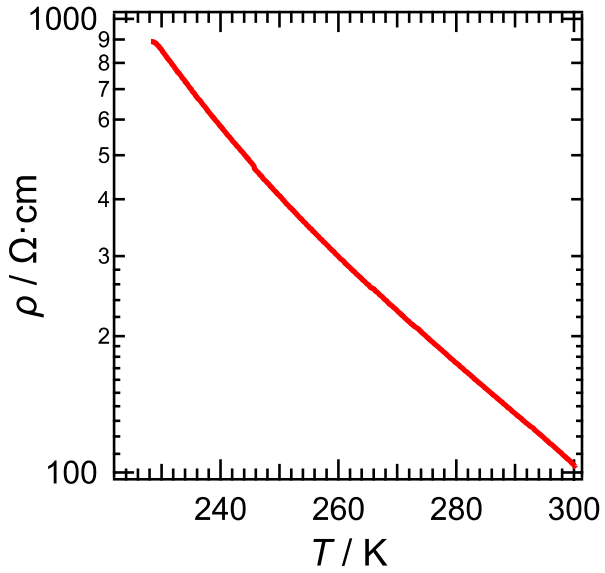

Figure S1. Temperature dependence of electrical resistivity of **1**.

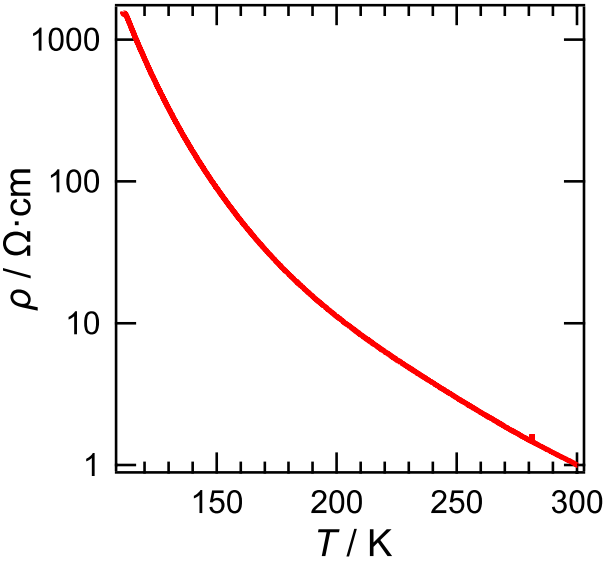

Figure S2. Temperature dependence of electrical resistivity of **2**.

Table S1. Madelung energies of **3** calculated excluding and including the point charges of tentatively oriented water molecules (W1 and W2 as shown in Figure 3d), where W1 and W1′ cannot coexist and W2 and W2′ also cannot coexist because the W1···W1′ and W2···W2′ distances are too short. Therefore, the point charges of W1 and W2′ are used for the calculation of (1) and (2) (see below).

3, α-$(BETS)_2(HOC_2H_4SO_3)\cdot H_2O$								Madelung E[*4]	
CO pattern[*1]	BETS charge				Configurations[*5] of anion/water			Excluding H_2O[*6]	Including H_2O
	A	A′	B	C		I	II		
(a) Non-CO	+0.5	+0.5	+0.5	+0.5	(1)	ρ/W1	ρ′/W2′	-304.3658	-294.3713
"	"	"	"	"	(2)	σ/W1	σ′/W2′	-303.8251	-296.8351
"	"	"	"	"	(3)	ρ/W1	σ′/W2′	-321.4955	-332.9706
"	"	"	"	"	(4)	σ/W2	ρ′/W1′	-321.4944	-332.9696
"	"	"	"	"			Average	-312.7952	-314.2867
(b) Horizontal[*2]	+1	0	+1	0	(1)	ρ/W1	ρ′/W2′	-444.3595	-434.9052
"	"	"	"	"	(2)	σ/W1	σ′/W2′	-441.4648	-435.0150
"	"	"	"	"	(3)	ρ/W1	σ′/W2′	-461.4680	-472.3274
"	"	"	"	"	(4)	σ/W2	ρ′/W1′	-459.1554	-470.2450
"	"	"	"	"			Average	-451.6119	-453.1232
(c) Horizontal	0	+1	0	+1	(1)	ρ/W1	ρ′/W2′	-446.8165	-436.2818
"	"	"	"	"	(2)	σ/W1	σ′/W2′	-448.6298	-441.0996
"	"	"	"	"	(3)	ρ/W1	σ′/W2′	-463.9675	-476.0583
"	"	"	"	"	(4)	σ/W2	ρ′/W1′	-466.2778	-478.1385
"	"	"	"	"			Average	-456.4229	-457.8946
(d) Vertical[*3]	+1	+1	0	0	(1)	ρ/W1	ρ′/W2′	-443.9287	-433.3586
"	"	"	"	"	(2)	σ/W1	σ′/W2′	-416.8843	-409.3188
"	"	"	"	"	(3)	ρ/W1	σ′/W2′	-447.8066	-458.7219
"	"	"	"	"	(4)	σ/W2	ρ′/W1′	-447.8055	-456.9075
"	"	"	"	"			Average	-439.1063	-439.5767
(e) Vertical	0	0	+1	+1	(1)	ρ/W1	ρ′/W2′	-416.4921	-407.0731
"	"	"	"	"	(2)	σ/W1	σ′/W2′	-442.4551	-436.0406
"	"	"	"	"	(3)	ρ/W1	σ′/W2′	-446.8737	-458.9086
"	"	"	"	"	(4)	σ/W2	ρ′/W1′	-446.8726	-458.9074
"	"	"	"	"			Average	-438.1734	-440.2324
(f) Horizontal	+1	0	0	+1	(1)	ρ/W1	ρ′/W2′	-446.8152	-438.7582
"	"	"	"	"	(2)	σ/W1	σ′/W2′	-448.6285	-443.5761
"	"	"	"	"	(3)	ρ/W1	σ′/W2′	-466.2777	-478.1385
"	"	"	"	"	(4)	σ/W2	ρ′/W1′	-463.9651	-476.0558
"	"	"	"	"			Average	-456.4216	-459.1322
(g) Horizontal	0	+1	+1	0	(1)	ρ/W1	ρ′/W2′	-444.3614	-432.4293
"	"	"	"	"	(2)	σ/W1	σ′/W2′	-441.4667	-432.5392
"	"	"	"	"	(3)	ρ/W1	σ′/W2′	-459.1583	-470.2478
"	"	"	"	"	(4)	σ/W2	ρ′/W1′	-461.4688	-472.3284
"	"	"	"	"			Average	-451.6138	-451.8862

[*1] CO patterns = charge ordering patterns shown in Figure 8, [*2] Horizontal = horizontal stripe, [*3] Vertical = vertical stripe, [*4] kJ mol^{-1} (unit cell), [*5] Configurations = Anion and water configurations at the I and II positions in the unit cell as shown in Figure 3d, [*6] The values are the same as Table 2.

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