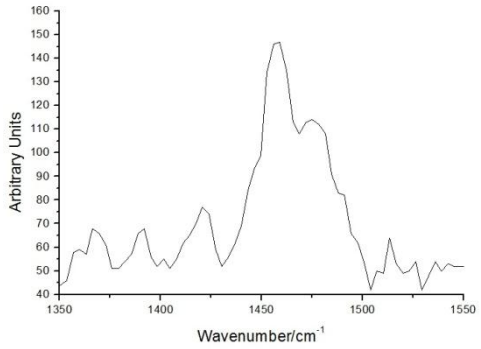
Electronic Supplementary Material (ESI) for Dalton Transactions

Supplementary Material for:

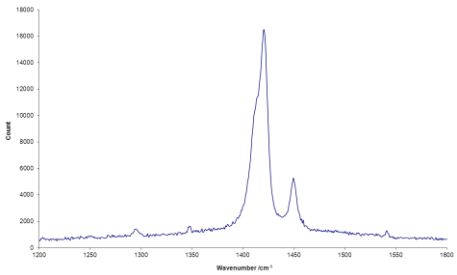
Hydrogen Bonded Anion Ribbons, Networks and Clusters and Sulfur-Anion Interactions in Novel Radical Cation Salts of BEDT-TTF with Sulfamate, Pentaborate and Bromide.

Andrew C. Brooks, Lee Martin, Peter Day, Elsa B. Lopes, Manuel Almeida, Koichi Kikuchi, Wataru Fujita, Kota Sasamori, Hiroki Aktusu, John D. Wallis*

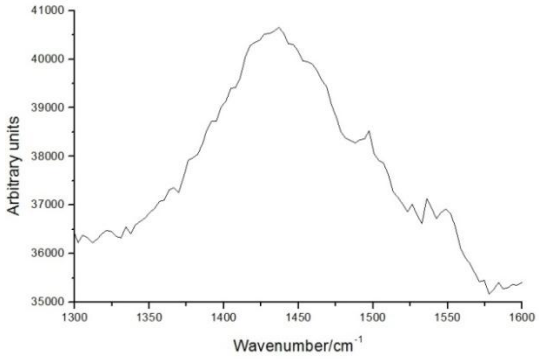
RAMAN IMAGES FOR RADICAL CATION SALTS.



$(BEDT\text{-}TTF)_3(SO_3NH_2)_2(H_2O)_2$



BEDT.Br



$ET_5[Br_4(H_5O_2)]$

CRYSTAL STRUCTURE OF $(BEDT\text{-}TTF)_3(SO_3NH_2)_2(H_2O)_2$ AT ROOM TEMPERATURE.

Crystal data: $3C_{10}H_8S_8.2SO_2NH_2.2H_2O$, M_r = 1382.14, triclinic, a = 6.761(8), b = 11.861(14), c = 16.726(16) Å, α = 90.86(4), β = 91.18(5), γ = 100.95(5)°, V = 1316(3) Å^3, Z = 1, P-1, D_c = 1.743 g cm^{-3}, μ(MoKα) = 1.101 mm^{-1}, T = 300(2) K, R_{int} 0.080, 5701 unique reflections, 1505 with F > 4σ(F), R = 0.125, wR = 0.358.

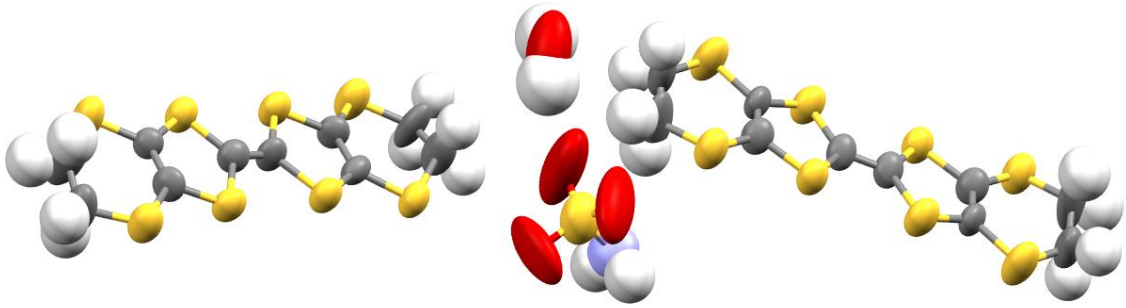


Figure A. Molecular structure of $(BEDT\text{-}TTF)_3(SO_3NH_2)_2(H_2O)_2$ at 300 K with anisotropic displacement parameters drawn at the 50% level.

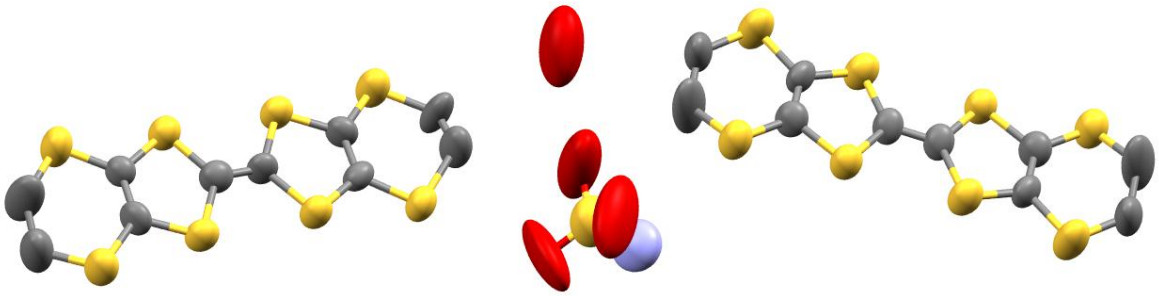


Figure B. Molecular structure of $(BEDT\text{-}TTF)_3(SO_3NH_2)_2(H_2O)_2$ at 300 K with anisotropic displacement parameters drawn at the 50% level with H atoms omitted.

CRYSTAL STRUCTURE OF (BEDT-TTF).Br AT ROOM TEMPERATURE.

Crystal data: $C_{10}H_8S_8.Br$, M_r = 464.55, monoclinic, a = 12.8238(16), b = 11.0175(10) c = 11.2402(11) Å, β = 103.712(11)°, V = 1542.8(3) Å^3, Z = 4, C2/c, D_c = 2.00 g/cm^3, μ(MoKα) = 3.73 mm^{-1}, T = 294(2) K, 1770 unique reflections, 1527 with F > 4σ(F), R = 0.060, wR = 0.104.

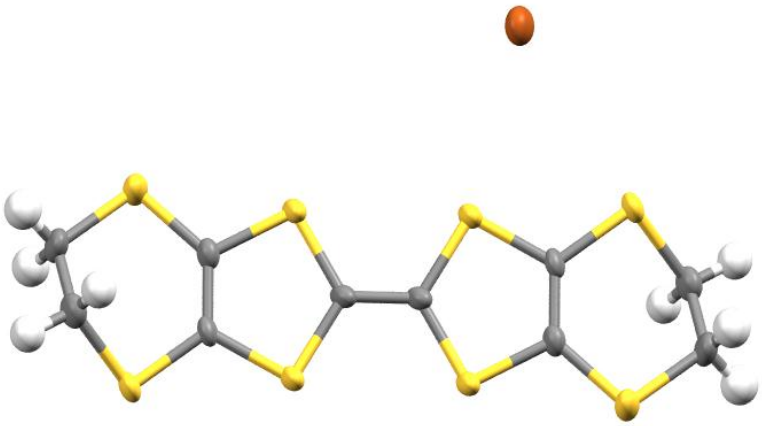


Figure C. Molecular structure of BEDT-TTF.Br at 294 K with anisotropic displacement parameters drawn at the 50% level.