

## Supporting information for ic0617700

### **Antiferromagnetic or Canted Antiferromagnetic Orderings of Fe(III) *d* Spins of FeX<sub>4</sub><sup>−</sup> Ions in BEDT-TTFVO(S)•FeX<sub>4</sub> (X = Cl, Br) [BEDT-TTFVO(S) = bis(ethylenedithio)tetrathiafulvaleno-quinone(-thioquinone)-1,3-dithiolemethide]**

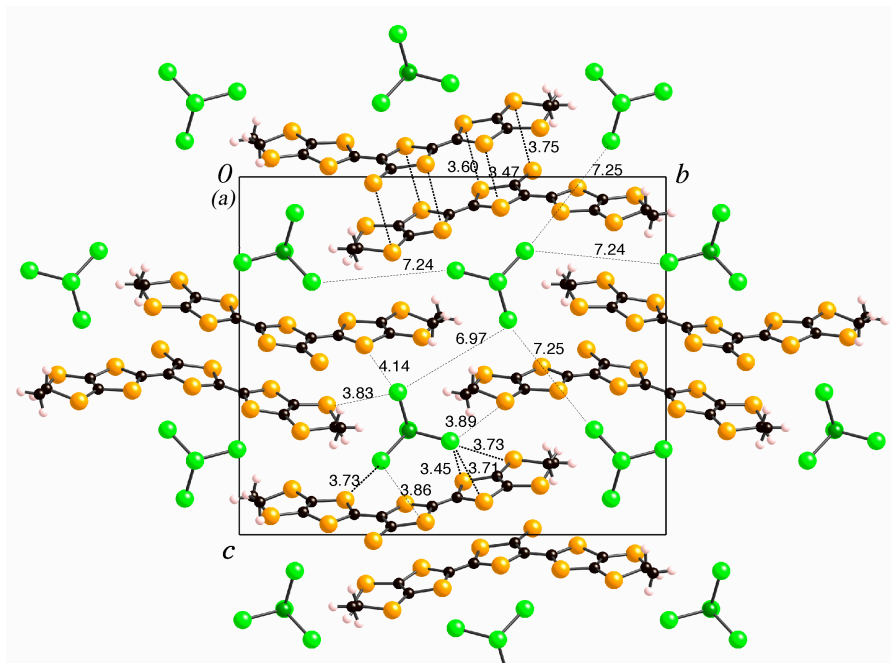
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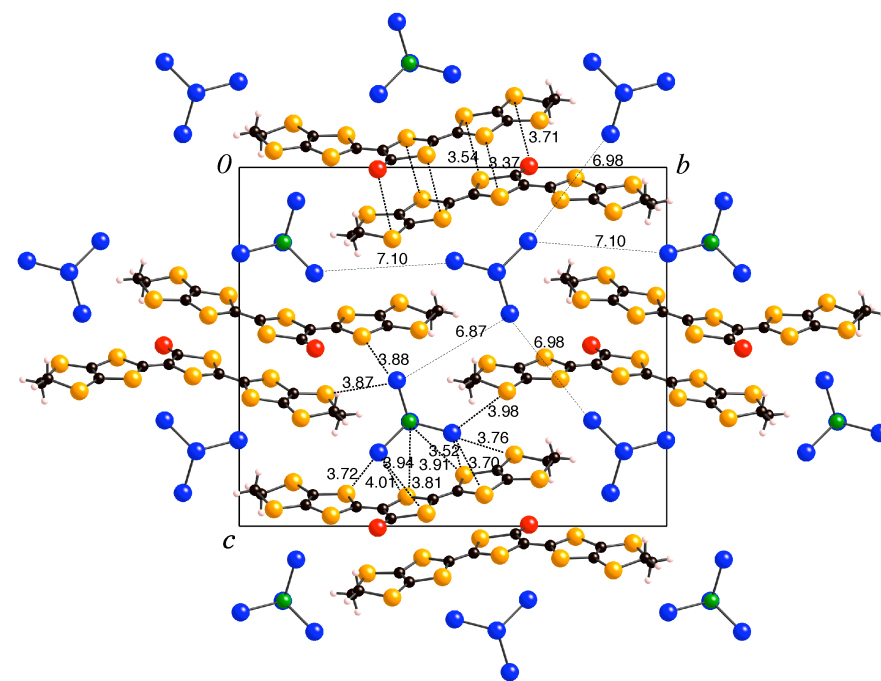
- (1) Projections of crystal structures of (a) **2•FeCl<sub>4</sub>**, (b) **1•FeBr<sub>4</sub>** and (c) **2•FeBr<sub>4</sub>** to *bc*-plane
- (2) Temperature dependence of ESR signal intensities for **2•GaBr<sub>4</sub>**
- (3) Field (*H*) dependences of magnetizations (*M*) and *dM/dH* (inset) (a) in the *H* region of ±6 kOe at different temperatures of 0.5 to 1.1 K for **2•FeCl<sub>4</sub>** and (b) in the *H* region of +4 to −6 kOe at different temperatures of 0.5 to 1.0 K for **1•FeBr<sub>4</sub>** (b)

(1) Projections of crystal structures of (a)  $2 \cdot \text{FeCl}_4$ , (b)  $1 \cdot \text{FeBr}_4$  and (c)  $2 \cdot \text{FeBr}_4$  to  $bc$ -plane

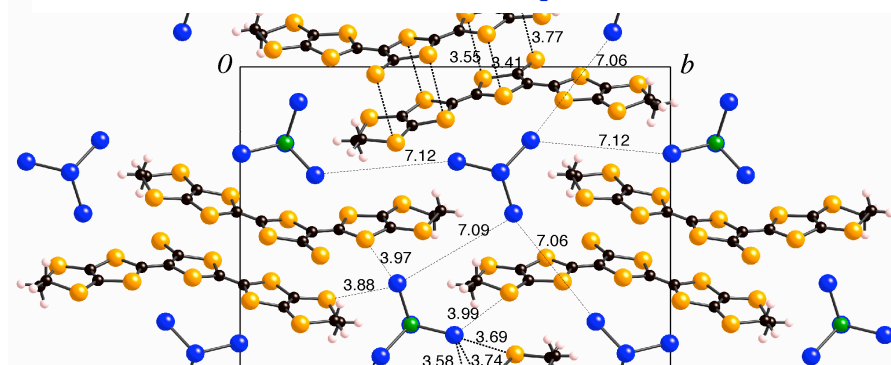
(a)



(b)

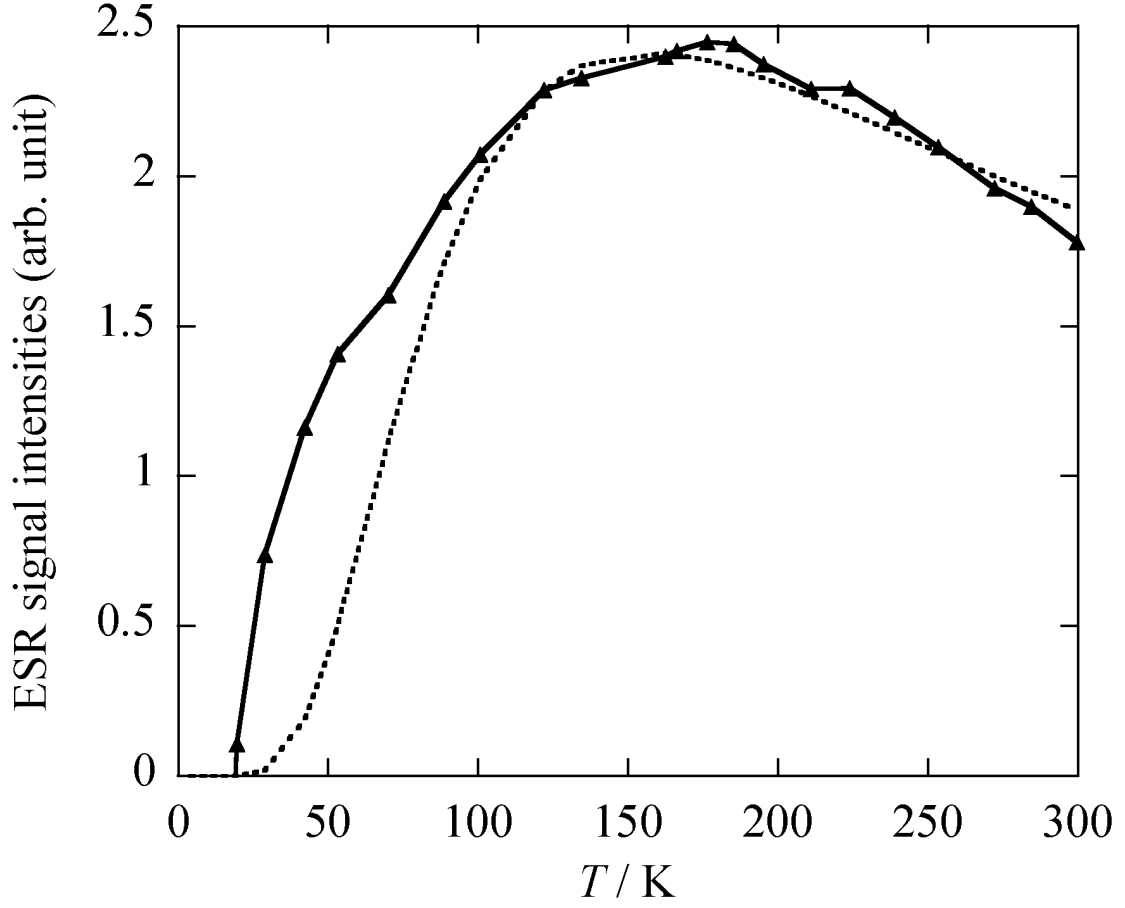


(c)





(2) Temperature dependence of ESR signal intensities for  $2\bullet\text{GaBr}_4$  (closed triangles). A dotted line indicates a fitting curve calculated for a S-T model;  $\chi = 2N_{\text{A}}g^2\mu_{\text{B}}^2/\{k_{\text{B}}T[3+\exp(-J/k_{\text{B}}T)]\}$  with  $J/k_{\text{B}} = -250$  K.



(3) Field ( $H$ ) dependences of magnetizations ( $M$ ) and  $dM/dH$  (inset) (a) in the  $H$  region of  $\pm 6$  kOe at different temperatures of 0.5 to 1.1 K for  $2\bullet\text{FeCl}_4$  and (b) in the  $H$  region of +4 to  $-6$  kOe at different temperatures of 0.5 to 1.0 K for  $1\bullet\text{FeBr}_4$

