Supporting Information

A New Organic Conductor of Tetramethyltetraselenafulvalene (TMTSF) with a Magnetic Dy(III) Complex

Qingyun Wan[1, 2] *, Masanori Wakizaka[1] *, Haitao Zhang[1], Yongbing Shen[3], Nobuto Funakoshi[1], Shinya Takaishi[1] *, Chi-Ming Che[2], and Masahiro Yamashita[1, 4] *

[1] Department of Chemistry, Graduate School of Science, Tohoku University, Aramaki-Aza-Aoba, Aoba-ku, Sendai 980-8578, Japan

[2] Department of Chemistry, State Key Laboratory of Synthetic Chemistry, HKU-CAS Joint Laboratory on New Materials, The University of Hong Kong, Pokfulam Road, Hong Kong, China.

[3] Frontier Institute of Science and Technology (FIST), State Key Laboratory for Mechanical Behavior of Materials, MOE Key Laboratory for Nonequilibrium Synthesis of Condensed Matter, Xi'an Jiaotong University, 99 Yanxiang Road, Xi'an, Shaanxi 710054, China.

[4] School of Materials Science and Engineering, Nankai University, Tianjin 300350, China.

* Correspondence: qywan@connect.hku.hk (W.Q.); masanori.wakizaka.a7@tohoku.ac.jp (M.W.); shinya.takaishi.d8@tohoku.ac.jp (S.T.); yamasita@agnus.chem.tohoku.ac.jp (M.Y.). Tel.: +81-22-765-6547

Table S1. Summary of the crystal data of compound **1**.

Formula	$C_{55}H_{49}N_6S_4Se_{20}DyO_6Cl_3$
Formula weight	2866.29 g/mol
Crystal size (mm^3)	0.1×0.03×0.02
Crystal system	orthorhombic
Space group	*Cmc2₁*
a (Å)	19.9823(6)
b (Å)	13.8784(5)
c (Å)	29.3863(9)
α (°)	90
β (°)	90
γ (°)	90
V ($Å^3$)	8149.5(5)
T (K)	120
Z	4
D_{calc} (g cm^{-3})	2.336
F (000)	5320.0
λ (Mo Kα) (Å)	0.71073
μ (mm^{-1})	10.098
Reflections collected	49327
Data/restraints/parameters	12224/1/480
GOF on F^2	1.029
R_{int}	0.0447
R_1[a]	0.0655
wR_2[b] (all data)	0.0964

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = \{[\Sigma w(F_o^2 - F_c^2)^2]/[\Sigma w(F_o^2)^2]\}^{1/2}$.

Table S2. A summary of C1-C2 distance in TMTSF-type molecules.

Ref	Chemical structure	Average charge of TMTSF	C1-C2 distance
Ref[1]	TMTSF	0	1.347 Å
Ref[2]	$(TMTSF)NO_3$	+1	1.360 Å
Ref[3]	$(TMTSF)_3(TFPB)_2$	+2/3	1.361/1.375/1.363/1.371 Å
Ref[4]	$(TMTSF)_2NbF_6$	+0.5	1.350 Å
Ref[5]	$(TMTSF)_2AsF_6$	+0.5	1.344 Å
Ref[6]	$(TMTSF)_2H_2F_3$	+0.5	1.357 Å
Ref[7]	$(TMTSF)_2NO_3$	+0.5	1.430 Å
Ref[8]	$(TMTSF)_3[Y(NO_3)_5]$	+2/3	1.356/1.316 Å

TFPB: tetrakis[3,5-bis(trifluoromethyl)phenyl]borate anions.

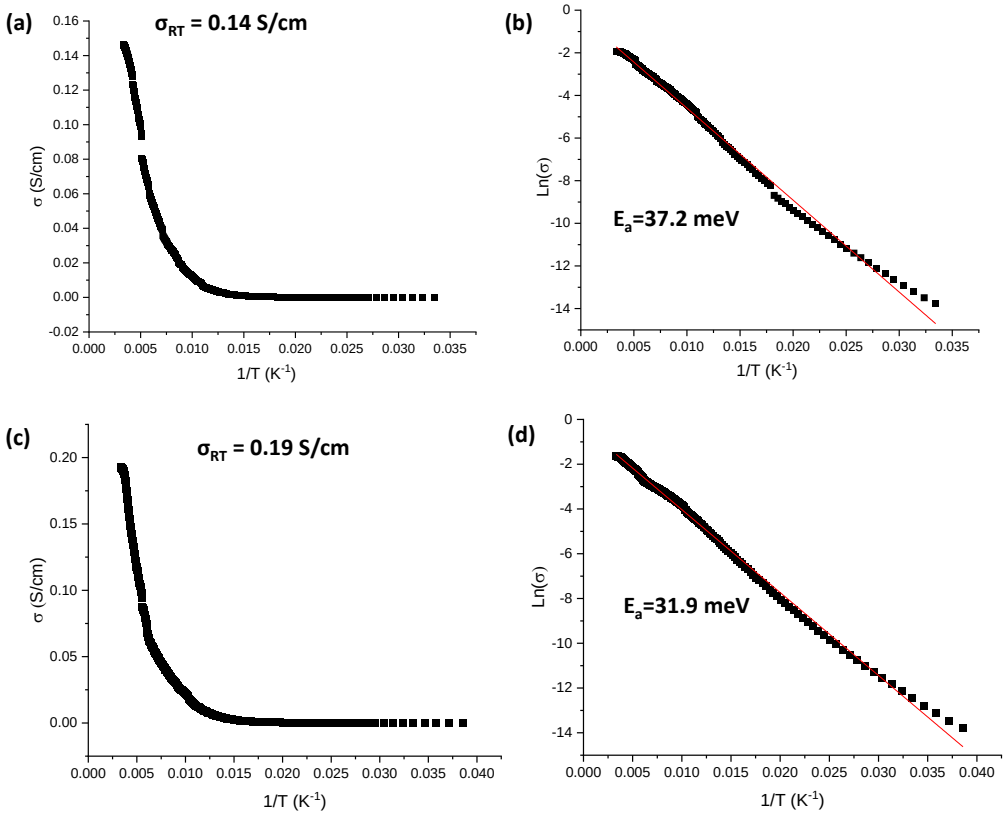


Figure S1. (a and c) Temperature dependence of σ (S·cm^{-1}) for two single crystals of **1**. (b and d) Ln(σ)-T^{-1} and its fitting curve to a linear function (red line) of panel a and c, respectively.

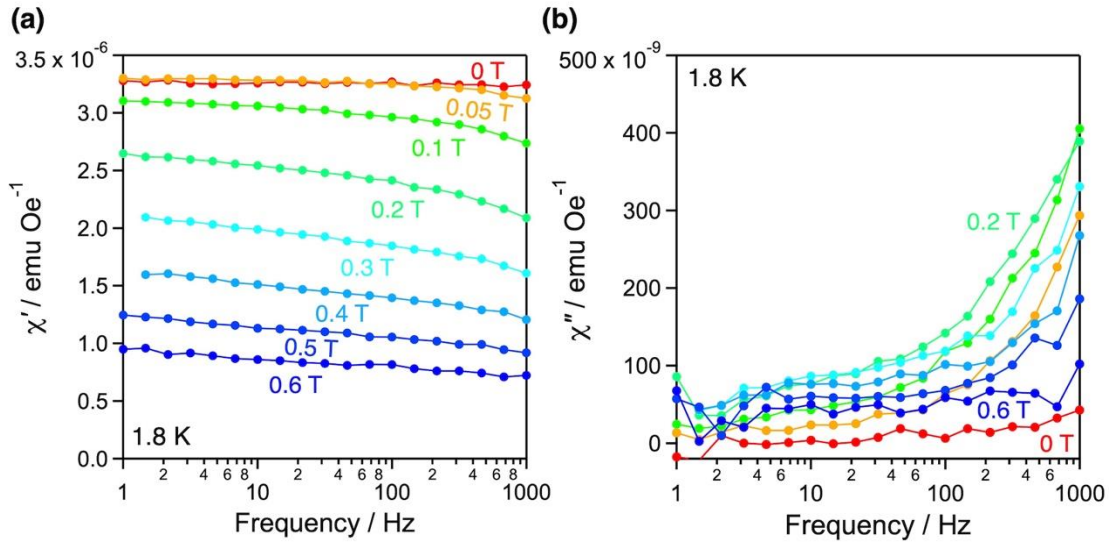
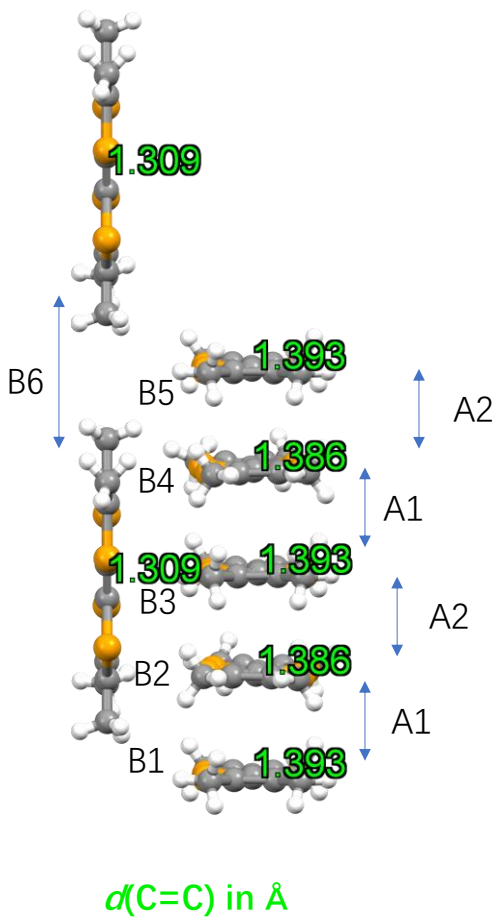
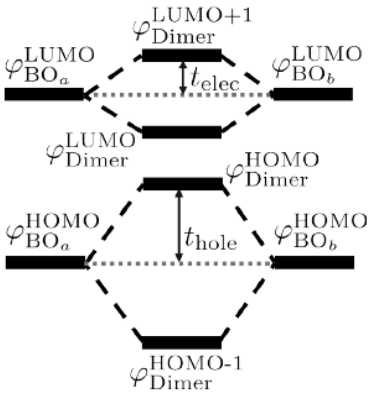


Figure S2. Frequency dependence of (a) the in-phase and (b) the out-of-phase magnetic susceptibility at 1.8 K as a function of the magnetic field of compound **1.**





	t(hole) (eV)	t(electron) (eV)
A1	0.2876	0.0258
A2	0.2914	0.0205
B1	0.0233	0.0649
B2	0.1739	0.1270
B3	0.2807	0.2235
B4	0.1351	0.0605
B5	0.0185	0.0695
B6	0.0020	0.0031

Figure S3. Calculation of charge transfer integral of *t(hole)* and *t(electron)* in the TMTSF dimers of compound **1**.

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