Supplementary Material for New Journal of Chemistry


# Supplementary data

| | **L1** | **2** | **3** | **4** | |
|---|---|---|---|---|---|
| | | | | **A molecule** | **B molecule** |
| C10 | -0.0217(26) | 0.0148(66) | 0.0367(118) | 0.0118(41) | 0.0271(42) |
| C11 | -0.0168(26) | 0.0113(64) | 0.0182(117) | -0.0002(42) | 0.0215(43) |
| S3 | 0.0442(10) | -0.0065(27) | -0.0155(49) | -0.0102(16) | -0.0099(16) |
| S4 | -0.0239(10) | -0.0072(27) | -0.0161(49) | 0.0019(16) | -0.0156(16) |
| S5 | -0.0247(10) | -0.0065(26) | -0.0121(46) | 0.0044(16) | -0.0146(17) |
| S6 | 0.0429(10) | -0.0059(27) | -0.0111(50) | -0.0076(16) | -0.0086(16) |
| S1 | -0.7168(23) | -0.0349 (68) | -0.0215 (123) | 0.6801(37) | 0.3728(37) |
| S2 | -0.8953(23) | 0.1873(71) | 0.1780(128) | 0.6976(37) | 0.3736(37) |
| O1 | -0.7773(35) | -0.0299(86) | -0.0198(148) | 1.1910(54) | 0.9290(59) |
| O2 | -0.6819(35) | -0.0061(102) | -0.0193(178) | 1.2123(51) | 0.8870(59) |

Figure S1. Deviation in Å of peripherical O from ethylenedioxy and S from 4-pyridylethylenedithio with respect to the TTF skeleton mean plane (S3 S4 C10 C11 S5 S6).

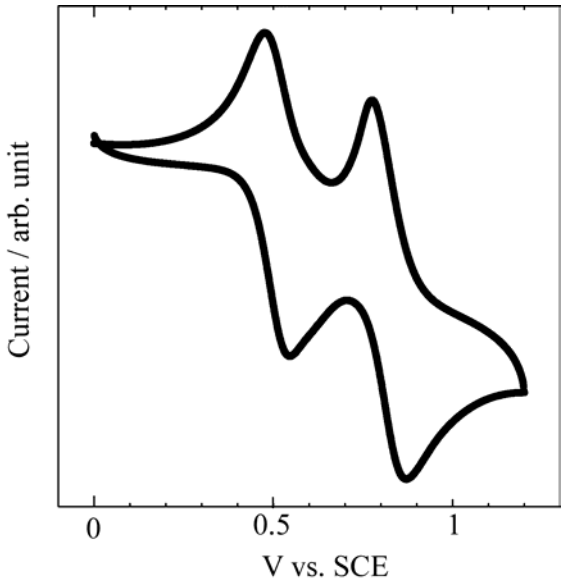
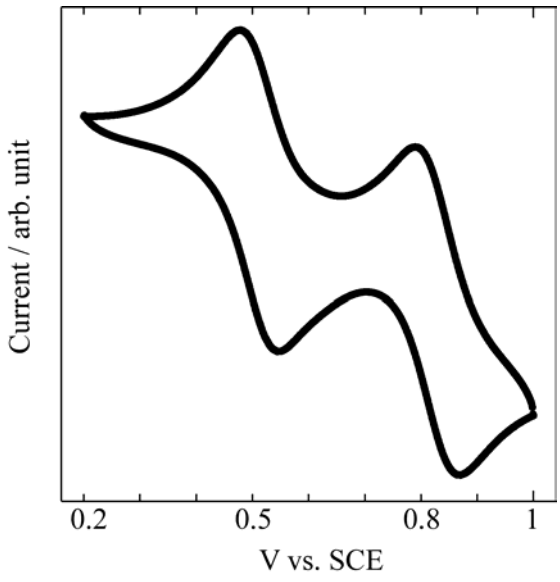
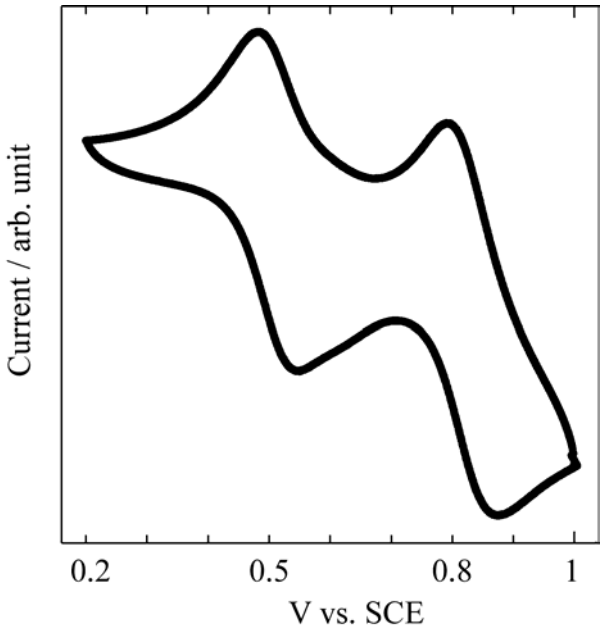



Figure S2. Chart of cyclic voltametry for **L1**.




- a -




- b -

Figure S3. Charts of cyclic voltametry for **2** (a) and **3** (b).

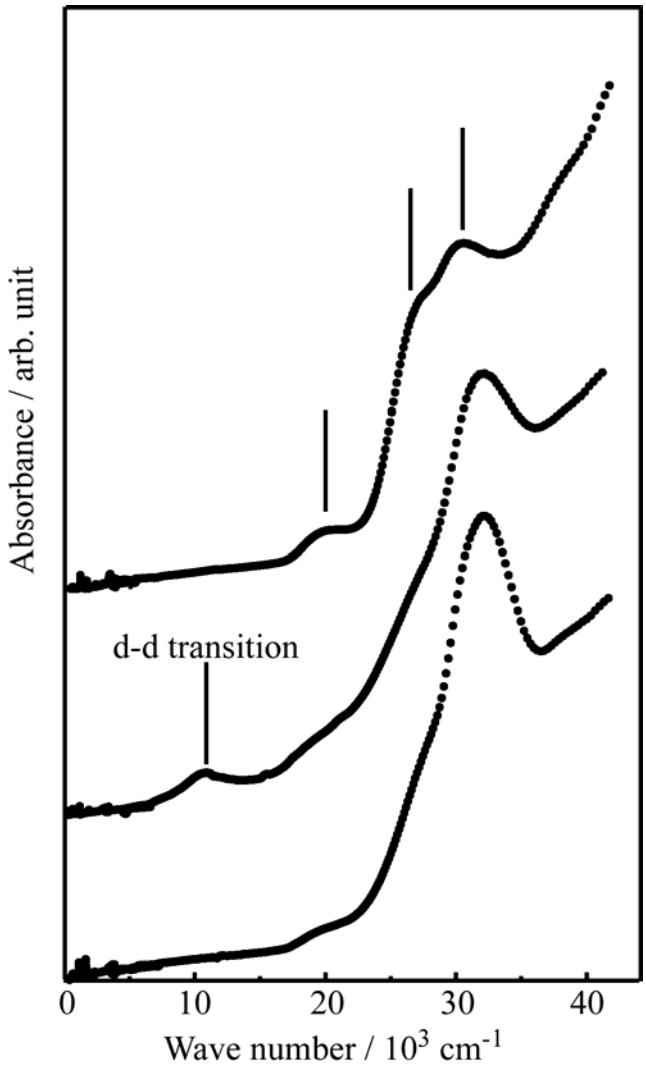



Figure S4. UV-vis-IR spectra of **L1** (up), **2** (middle), and **3** (down) in KBr disks. Bars indicate the absorption bands.

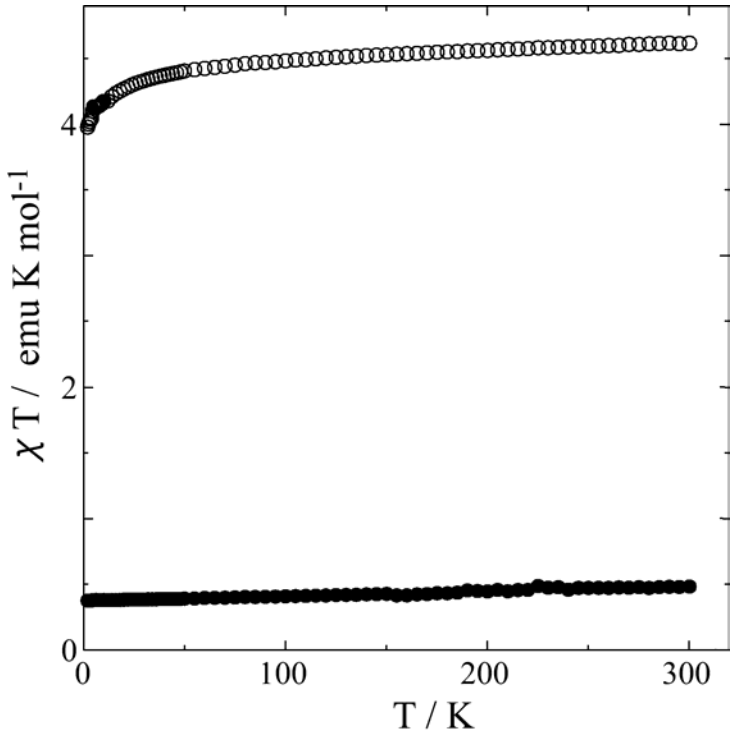
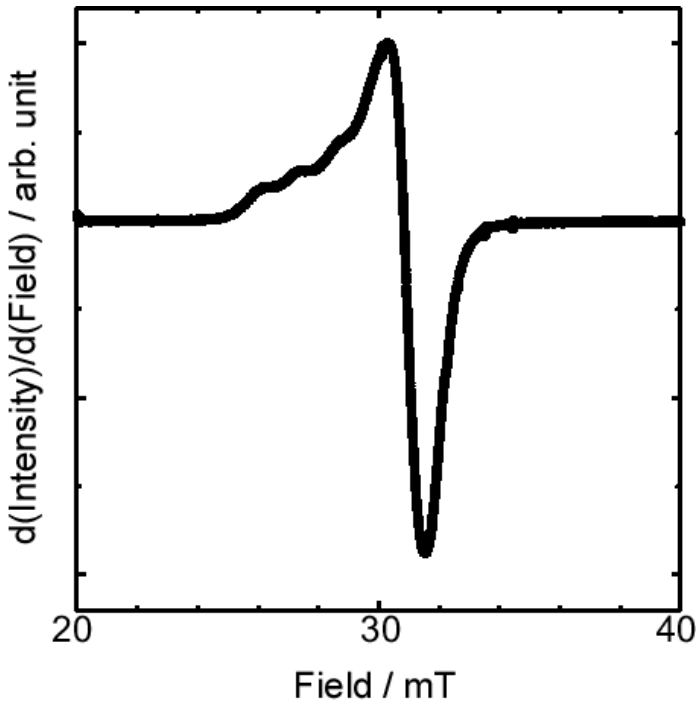
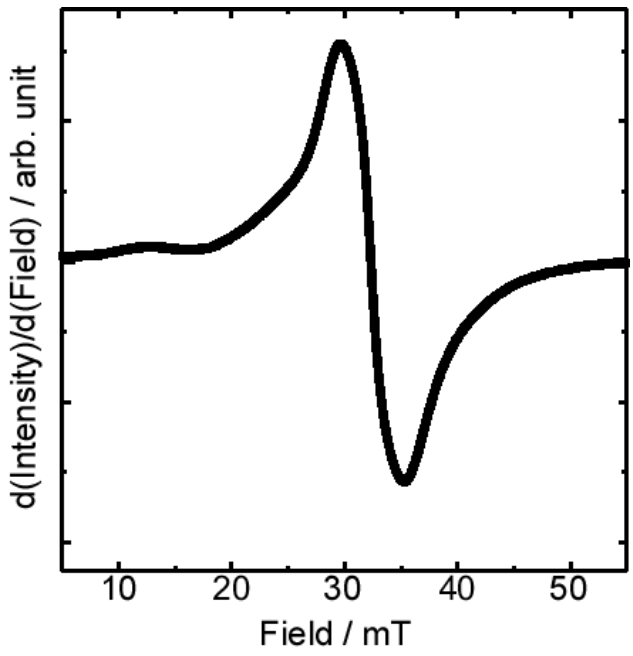



Figure S5. $\chi$T vs. T plots for **2** (closed circles) and **3** (open circles).




- a -




- b -

Figure S6. ESR spectra for (a) **2** and (b) **3** at room temperature.