# Supplementary Material

**First nanoparticles of a conductor based on the organic donor molecule BETS: κ-$(BETS)_2FeCl_4$**

Kane Jacob, Christophe Faulmann, Dominique de Caro and Lydie Valade (LCC-CNRS, Toulouse, France)

1) Refined cell and indexed peaks for κ-$(BETS)_2FeCl_4$ nanoparticles grown in the presence of OATM (10 molar eq. *vs.* BETS)

| | |
|---|---|
| Bibliographic data: | |
| Audit creation date: | 1996-08-14 |
| Audit creation method: | CSD-ConQuest-V1 |
| Author name: | H.Kobayashi, H.Tomita, T.Naito, A.Kobayashi, F.Sakai, T.Watanabe, P.Cassoux |
| Chemical name systematic: | bis(bis(Ethylenedithio)tetraselenafulvalene) tetrachloro-iron |
| Formula sum: | $C_{20}H_{16}Cl_4Fe_1S_8Se_8$ |
| Journal name: | J.Amer.Chem.Soc. |
| Journal volume: | 118 |
| Page first: | 368 |
| Structure and profile data: | |
| Formula sum: | $Fe_4Cl_{24}Se_{32}S_{32}C_{80}$ |
| Formula mass/ g/mol: | 5587.7800 |
| Density (calculated)/ g/cm$^3$ | 2.6044 |
| F(000): | 2592,0000 |
| Mass Absorption Coefficient/ cm^2/g: | 82.6906 |
| Space group (No.): | P n m a (62) |
| Lattice parameters: | |
| a/ Å: | 11.680(4) |
| b/ Å: | 35.92(2) |
| c/ Å: | 8.491(3) |
| alpha/ °: | 90 |
| beta/ °: | 90 |
| gamma/ °: | 90 |
| V/ $10^6$ pm$^3$ | 3562.2200 |

**Non-indexed peaks**

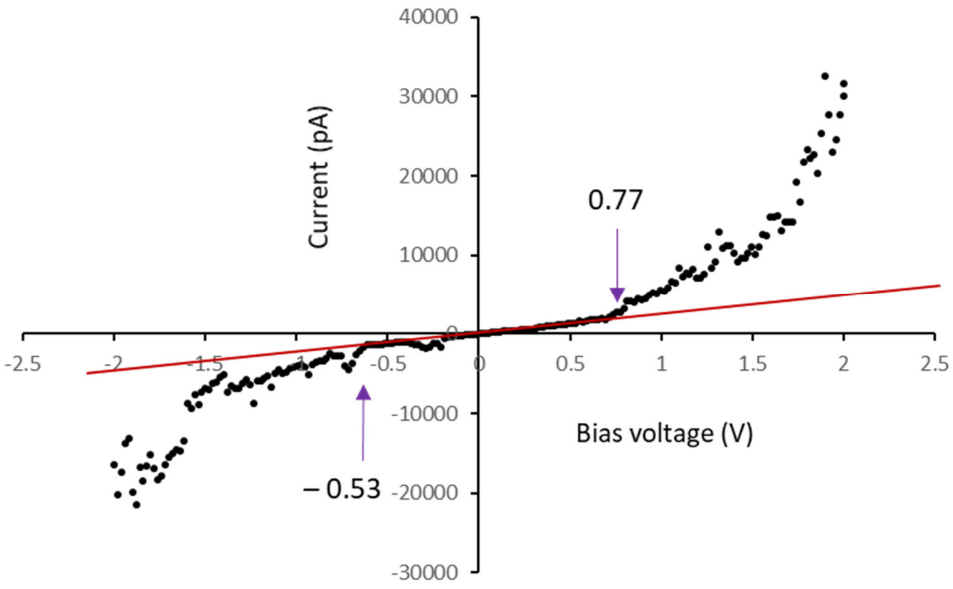
| No. | Th. (o) [°] | d-sp. (o) [Å] | Rel. Int. [%] | Height [cts] | Sin2 (o) |
|---|---|---|---|---|---|
| 1 | 4.6790 | 18.870510 | 3.32 | 9948.6450 | 167 |

**Indexed peaks**

| No. | h | k | l | 2Θ (c) [°] | 2Θ (o) [°] | 2Θ (d) [°] | d-sp. (c) [Å] | d-sp. (o) [Å] | d-sp. (d) [Å] |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 2 | 0 | 4.9251 | 4.9249 | 0.0002 | 17.928120 | 17.928700 | -0.000582 |
| 2 | 0 | 4 | 0 | 9.8592 | 9.9326 | -0.0733 | 8.964062 | 8.898049 | 0.066012 |
| 3 | 0 | 3 | 1 | 12.7915 | 12.6421 | 0.1494 | 6.915005 | 6.996370 | -0.081365 |
| 4 | 1 | 0 | 1 | 12.8874 | 12.9014 | -0.0140 | 6.863772 | 6.856346 | 0.007426 |
| 5 | 0 | 6 | 0 | 14.8118 | 14.5743 | 0.2375 | 5.976040 | 6.072887 | -0.096846 |
| 6 | 1 | 3 | 1 | 14.8717 | 14.8794 | -0.0077 | 5.952113 | 5.949033 | 0.003080 |
| 7 | 0 | 5 | 1 | 16.1754 | 16.1322 | 0.0432 | 5.475216 | 5.489779 | -0.014563 |
| 8 | 2 | 2 | 1 | 19.0769 | 19.2390 | -0.1620 | 4.648482 | 4.609694 | 0.038787 |
| 9 | 1 | 1 | 2 | 22.4286 | 22.3939 | 0.0347 | 3.960833 | 3.966892 | -0.006059 |
| 10 | 1 | 4 | 2 | 24.4240 | 24.3144 | 0.1096 | 3.641562 | 3.657730 | -0.016169 |
| 11 | 0 | 10 | 0 | 24.8111 | 24.7688 | 0.0423 | 3.585625 | 3.591647 | -0.006022 |
| 12 | 2 | 1 | 2 | 26.0621 | 26.0029 | 0.0592 | 3.416274 | 3.423919 | -0.007645 |
| 13 | 2 | 9 | 0 | 27.0617 | 27.1027 | -0.0410 | 3.292314 | 3.287432 | 0.004883 |
| 14 | 0 | 11 | 1 | 29.3313 | 29.4326 | -0.1014 | 3.042522 | 3.032273 | 0.010249 |
| 15 | 0 | 12 | 0 | 29.8786 | 29.8933 | -0.0146 | 2.988020 | 2.986590 | 0.001430 |
| 16 | 1 | 11 | 1 | 30.3310 | 30.4082 | -0.0773 | 2.944482 | 2.937173 | 0.007309 |
| 17 | 0 | 1 | 3 | 31.7358 | 31.7744 | -0.0386 | 2.817270 | 2.813932 | 0.003337 |
| 18 | 4 | 3 | 1 | 33.2470 | 33.2214 | 0.0256 | 2.692586 | 2.694606 | -0.002020 |
| 19 | 3 | 9 | 1 | 33.8385 | 33.7772 | 0.0613 | 2.646862 | 2.651525 | -0.004663 |
| 20 | 0 | 13 | 1 | 34.1576 | 34.2230 | -0.0654 | 2.622860 | 2.618001 | 0.004859 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 21 | 3 | 6 | 2 | 34.6525 | 34.6113 | 0.0412 | 2.586526 | 2.589509 | -0.002983 |
| 22 | 0 | 14 | 0 | 35.0067 | 35.0107 | -0.0040 | 2.561160 | 2.560875 | 0.000285 |
| 23 | 2 | 2 | 3 | 35.6102 | 35.6226 | -0.0124 | 2.519124 | 2.518278 | 0.000846 |
| 24 | 2 | 3 | 3 | 36.0619 | 36.0701 | -0.0082 | 2.488602 | 2.488059 | 0.000544 |
| 25 | 4 | 7 | 1 | 36.9278 | 36.8612 | 0.0666 | 2.432213 | 2.436453 | -0.004240 |
| 26 | 4 | 2 | 2 | 37.6836 | 37.6433 | 0.0403 | 2.385150 | 2.387612 | -0.002462 |
| 27 | 2 | 14 | 0 | 38.3377 | 38.3177 | 0.0201 | 2.345944 | 2.347127 | -0.001183 |
| 28 | 4 | 4 | 2 | 38.7099 | 38.8123 | -0.1024 | 2.324241 | 2.318344 | 0.005897 |
| 29 | 1 | 9 | 3 | 39.8289 | 39.7924 | 0.0365 | 2.261483 | 2.263475 | -0.001993 |
| 30 | 0 | 16 | 0 | 40.2083 | 40.2002 | 0.0081 | 2.241015 | 2.241447 | -0.000431 |
| 31 | 0 | 14 | 2 | 41.1454 | 41.1607 | -0.0153 | 2.192116 | 2.191334 | 0.000781 |
| 32 | 1 | 11 | 3 | 43.0264 | 43.0129 | 0.0136 | 2.100534 | 2.101165 | -0.000631 |
| 33 | 1 | 0 | 4 | 43.3518 | 43.3140 | 0.0378 | 2.085522 | 2.087254 | -0.001732 |
| 34 | 4 | 12 | 1 | 44.6262 | 44.6040 | 0.0222 | 2.028877 | 2.029836 | -0.000960 |
| 35 | 1 | 17 | 1 | 44.9233 | 44.9218 | 0.0015 | 2.016146 | 2.016211 | -0.000065 |
| 36 | 2 | 0 | 4 | 45.4834 | 45.4794 | 0.0040 | 1.992611 | 1.992779 | -0.000168 |
| 37 | 3 | 3 | 4 | 49.5027 | 49.5363 | -0.0336 | 1.839822 | 1.838653 | 0.001169 |
| 38 | 6 | 10 | 0 | 53.4699 | 53.4762 | -0.0063 | 1.712293 | 1.712105 | 0.000188 |
| 39 | 2 | 12 | 4 | 55.3753 | 55.3957 | -0.0203 | 1.657800 | 1.657239 | 0.000560 |
| 40 | 7 | 1 | 1 | 56.1317 | 56.1246 | 0.0072 | 1.637240 | 1.637432 | -0.000192 |
| 41 | 4 | 19 | 0 | 58.1352 | 58.1254 | 0.0098 | 1.585495 | 1.585739 | -0.000244 |
| 42 | 2 | 18 | 3 | 58.8269 | 58.8270 | 0.0000 | 1.568490 | 1.568490 | 0.000001 |
| 43 | 3 | 20 | 2 | 60.8807 | 60.8801 | 0.0006 | 1.520405 | 1.520418 | -0.000014 |
| 44 | 4 | 16 | 3 | 61.5598 | 61.5449 | 0.0149 | 1.505250 | 1.505578 | -0.000329 |
| 45 | 8 | 1 | 0 | 63.6657 | 63.6817 | -0.0159 | 1.460440 | 1.460113 | 0.000327 |
| 46 | 4 | 4 | 5 | 64.3036 | 64.3085 | -0.0049 | 1.447483 | 1.447385 | 0.000098 |
| 47 | 7 | 13 | 1 | 66.2833 | 66.2850 | -0.0017 | 1.408970 | 1.408938 | 0.000032 |

2) *I-V* curve for a κ-$(BETS)_2FeCl_4$ nanoparticle aggregate grown in the presence of OATM (10 molar eq. *vs.* BETS)




From the linear part of the curve around the origin of the coordinate system, we determine ΔV = 0.77 – (–0.53) = 1.30 V, *i.e.*, an energy gap of $E_g$ = 1.30 eV.