Incommensurate Structure of the Organic Superconductor (MDT-TS)I_{0.85}Br_{0.41}

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**Introduction**

In organic superconductors, the ratios of the donor molecules to anions are represented by an integer (typically 2:1) \([1]\). By contrast, the MDT-TS or (methylenedithio-tetraselenafulvalene) series salts are incommensurate ambient pressure organic superconductors and the charge transfer degrees deviate from 0.5 \([2]\). Moreover, (MDT-TSF)(AuI\(_2\))\(_{0.436}\) has shown the characteristic Fermi surface reconstruction by an incommensurate anion potential \([3]\). (MDT-TS)(I\(_3\))\(_{0.441}\), where MDT-TS is 5H-2-(1,3-diselenol-2-ylidene)-1,3,4,6-tetrathiapentalene, shows a metal-insulator transition at \(T_{MI} = 50\) K in spite of the basically same crystal structure as those of the MDT-TSF superconductors \([4]\). The ground state of this salt changes from an “incommensurate antiferromagnetic insulating state” with \(T_N = 50\) K to a superconducting phase at 3.2 K under 10.5 kbar \([5]\). We have discovered new organic conductor based on MDT-TS and I\(_x\)Br\(_y\). The new conductor shows superconducting phase transition under high pressure. The present paper reports the incommensurate lattice structure of (MDT-TS)I\(_{0.85}\)Br\(_{0.41}\).

**Results and Discussion**

Figure 1 shows the synchrotron radiation x-ray oscillation photograph at room temperature. This photograph clearly displays incommensurate layer lines. We distinguish the donor lattice and the anion lattice by indices \(h\) and \(h'\), respectively. In Fig. 1, there are several spots around \(h = 0\) line. These spots are originated in the convolution between \(h = 1\) and \(h' = 3\) lines. Although there is no clear spot at \(h = 1\) line which comes from the length of I\(_3\) or IBr\(_2\), the Raman spectra show that the anion has a unit of I\(_3\). Therefore, the anions exist as trihalide anion chains composed by I and Br. The ratio between the length of the \(a\)-axes (\(a/a'\)) is 1.2612(2) from Fig. 1, and the composition is estimated as (MDT-TS)I\(_{0.85}\)Br\(_{0.41}\) from the x-ray oscillation photograph and the energy dispersion spectroscopy. This composition means that the MDT-TS molecule does not make a simple IBr or IBr\(_2\) salt. We can speculate that the charge transfer degree is 0.420 under assuming tri-halide anions. This value lies in between (MDT-TS)(AuI\(_2\))\(_{0.441}\) and (MDT-TS)(I\(_3\))\(_{0.407}\). This result indicates that we can control the charge transfer degree (band-filling) in organic conductors based on MDT-TS with linear anions by changing the length of the anion.

**Figure 1**: X-ray oscillation photograph. The vertical direction is along the donor stacking direction.

**References**


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