Charge Order-Disorder Phase Transition in α'-(BEDT-TTF)$_2$IBr$_2$

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Among a variety of BEDT-TTF charge-transfer salts, the α-type BEDT-TTF salts shows rich properties such as charge ordering, superconductivity, zero-gap semiconductor or Dirac fermion, persistent photoconduction, photoinduced phase transition, and non-linear optical response. α'-(BEDT-TTF)$_2$IBr$_2$ has a two-dimensional herringbone arrangement of BEDT-TTF molecules similar to the α-(BEDT-TTF)$_2$I$_3$, although it is not isomorphous to the α-type BEDT-TTF salts. The bandwidth of the calculated semi-metallic band of α'-(BEDT-TTF)$_2$IBr$_2$ is narrowest among the α-type BEDT-TTF salts.

We present the anomalies at ~200 K in electrical resistivity, transmittance and reflectance in the far-infrared region, and magnetic susceptibility of α'-(BEDT-TTF)$_2$IBr$_2$. This phase transition is investigated by means of infrared, Raman, and far-infrared spectroscopy. Through the spectroscopic investigation, we found that the positive charges on BEDT-TTF molecules are strongly localized due to strong Coulomb interaction both in low-temperature (LT) and high-temperature (HT) phases. We show the spectroscopic data which suggest the charge order in LT phase and charge disorder in HT phase. The phase transition at ~200 K in α'-(BEDT-TTF)$_2$IBr$_2$ is the charge order-disorder phase transition without being accompanied by structural change. Based on the localized picture, we qualitatively interpreted the experimental results above and below the phase transition.[1]

The effect of the hydrostatic pressure was investigated by electrical resistivity and Raman spectroscopy. The charge-ordered state is successively suppressed by hydrostatic pressure up to 1.2 GPa. The resistivity and Raman spectrum are qualitatively changed above 1.4 GPa. We speculate that the phase transition changes the character from charge order-disorder to metal-insulator.

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