The Structure Determination of Single-component Molecular-metal

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The single-component molecular metals, $Ni(tmdt)_2$[1] and related materials, have attracted much interests due to their characteristic properties. Many other related materials have been produced by changing the metal atom and extended-TTF ligands. The crystal structure determination of newly produced materials is often very difficult due to only small amount of powder sample being available.

In this study, we determined 5 crystal structures of $Ni(tmdt)_2$ related materials, which are $Ni(dt)_2$, $Pd(dt)_2$, $Au(tmdt)_2$, $Pd(tmdt)_2$, and $Pd(dmdt)_2$, by Genetic Algorithm combined with MEM/Rietevled method using synchrotron radiation X-ray powder diffraction data measured at SPring-8, BL02B2. The reliability factors, Rwp and RI, of Rietveld refinements are in the the range of 2~4% and 3~7%, respectively. It was found that the molecular stacking is different by the length of extended-TTF ligands. It is found that the positional relation of neighboring layers is closely related to the conductivity of materials.

[1] Tanaka H., et al., *Science,* 2001, **291**, 285-287.

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