Structural Studies on [Au(tmdt)$_2$] and Metallization of [Ni(ptdt)$_2$] at High Pressure

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[Au(tmdt)$_2$] is a single-component molecular metal exhibiting a phase transition to antiferromagnetic (AF) metal state at 110 K (T_N) [1-3]. We have examined the crystal structure of [Au(tmdt)$_2$] at 9-300 K and up to 10.7 GPa (at room temperature). Both experiments were performed at Spring-8.

The crystal has a simple triclinic structure with only one molecule in the unit cell. Au(tmdt)$_2$ molecules are closely packed two-dimensionally in the (02$\bar{1}$) plane. The temperature dependences of the lattice constants and the intermolecular short S…S distances show anomalies at T_N. But no distinct anomaly was observed along the direction perpendicular to the (02$\bar{1}$) plane. The *ab initio* band structure calculation has predicted the development of very unique AF spin structure at T_N [3]: the up and down spins are distributed independently on the left and right tmdt ligands of one Au(tmdt)$_2$ molecule. The temperature dependence of Au-S bond length showed a sharp decrease at around 110 K; this may be a structural evidence for the proposed AF spin distribution model.

The crystal structure of [Au(tmdt)$_2$] was examined up to 10.7 GPa. The shortest intermolecular S···S distance at 10.7 GPa was found to be approximately 1 Å shorter than the S···S van der Waals distance.

The metallization of [Ni(ptdt)$_2$] at high pressure will be also reported [4].

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