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Direct observation of Au-Au interaction in the Au complex with Reversible Mechanochromic Luminescence properties.

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1 Introduction

The Au complex **1** shows unique optical property. The Complex **1** shows blue color luminescence in a crystalline form when black light (365 nm) is illuminated. On the other hand the luminescence color changed to yellow after the grinding. When the ground powder is treated with a dichloromethane droplets, the blue luminescence is recovered.[1] Hypothesis of the origin of the color change is the reversible formation of intermolecular Au-Au bond at aurophilic bonding length region (2.7-3.3 Å). We had tried to detect this Au-Au distance by EXAFS but failed to observe it clearly, probably due to the thermal disorder. Actually the complex **2** with Au-Au distance at 3.32 Å shows little peak at 100 K as shown in Fig.1. We decided to carry out much lower temperature studies in order to reduce the thermal vibration. We have used a He cryostat to obtain XAFS data measured at 4 K where we can obtain the Au-Au peak clearly.

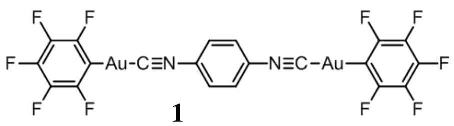
2 Experiment

Fig.2 shows the He Cryostat (JANIS STVP-100) modified to X-ray absorption spectroscopy.

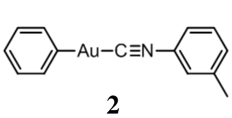
The sample was cooled to 4 K within 1 hour. The temperature can be controlled by a heater and liquid He flow rate within the precision of less than 1 K.

3 Results and Discussion

Fig.3 shows Fourier transform of Au complex **2** measured at 4 K. The peak corresponding to the Au-Au clearly appeared at 3.2 Å. The curve fitting analysis showed that the Au-Au distance = 3.38 Å well corresponding to the crystal data of Au-Au = 3.31 Å. We can conclude that the low temperature measurement tremendously decreases the thermal vibration and observe the weak Au-Au interaction. We are now challenging to elucidate Au-Au interaction in compound **1**.



1



2

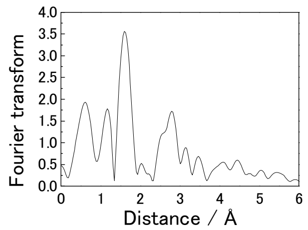


Fig.1 Fourier transform for complex **2** at 100 K.

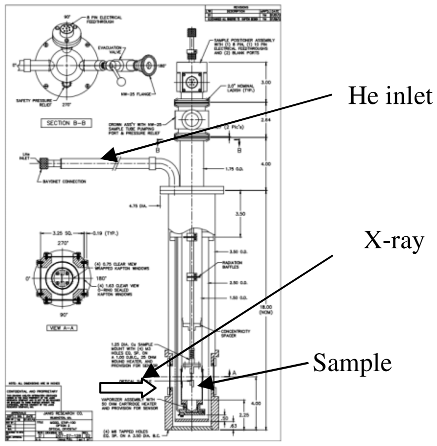


Fig. 2 He Cryostat for the XAFS measurement

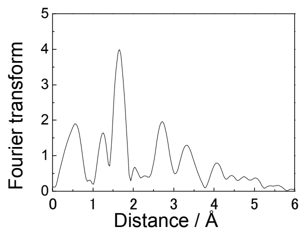


Fig.3 Fourier transform for **2** at 4 K

1. H. Ito, T. Saito, N. Oshima, N. Kitamura, S. Ishizaka, Y. Hinatsu, M. Wakeshima, M. Kato, K. TsugeM. Sawamura, *J. Am. Chem. Soc.* **2008**, *130*, 10044.

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