Single-component Molecular Conductor Formed by Electron Transfer between d and ð Orbitals

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Recently, research on conducting systems that consist of a single-component molecule has attracted a lot of attention.[1] Herein, we report the crystal structure and electronic properties of novel linear chain rhodium(I,II) mixed-valence complex, $\{[Rh(3,6\text{-DBDiox-}4,5\text{-}Cl_2)(CO)_2]\}_\infty$ (**1**) where 3,6-DBDiox-4,5-Cl_2 is used to indicate the semiquinonate or catecholate form of 3,6-di-*tert*-butyl-4,5-dichloro-1,2-benzoquinone, formed by electron transfer between metal d and semiquinonate ð* orbitals.

X-ray crystal structure analysis of **1** was performed at 302 and 56 K using synchrotron radiation at BL02B1 beamline at the SPring-8 facility. Compound **1** only consists of linear chains of $[Rh(3,6\text{-DBDiox-}4,5\text{-}Cl_2)(CO)_2]$ molecules and these complex molecules form trimer units in the linear chain at 302 K. At 56 K, the trimer units in the linear chain dimerized and form hexamer units. Compound **1** shows a significantly large conductivity (17–34 S cm^{-1}) at room temperature regardless of the neutral molecule. The temperature dependence of the electrical conductivity shows a semiconducting behavior. The observed dimerization of trimers in the 1-D chain is considered to originate from Peierls distortion.

[1] Tanaka H., Okano Y., Kobayashi H., Suzuki W., Kobayashi A., *Science*, 2001, **291**, 285–287.

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