Poster

Investigation of A Novel Organocobalt Complex of B12 Model Catalyst

J.Liu[1]*, Xiaofan Yang [2] and David Hadlleton[2]

[1] *Department of Physics, University of Warwick, Coventry CV4 7AL, UK,*

[2]*Department of Chemistry, University of Warwick, Coventry CV4 7AL, UK*

jie.liu.3@warwick.ac.uk

We investigated the organocobalt complexes of B_{12} models as cobalt based catalysts, which are extensively used in radical polymerization[1]. The complexes of obidoximes possessing an O-BF_2-O moiety were prepared (Figure 1a). During crystallization experiments, apart from the crystals of (H_2O)Co-(dimethylglyoximeBF$_2$)$_2$ (**1**, Figure 1b) were obtained, a new one-dimensional cobalt- based coordination polymer [Co-(dimethylglyoximeBF2)$_2$]n (**2**, Figure 1c) was discovered for the first time. Detailed characterizations via crystal structure determination from single crystal X-ray diffraction data at 100 K have been discussed . The crystal structure of **2** reveals that cobalt atoms are bridged by oxygen atoms to lead to an unusual co-ordination polymer **2**. The ligand units of O-BF_2-O moiety in complex **2** orient above and down the main equatorial plane, adopting an extended chair conformation[2], and face the adjacent molecular neighbour's dimethylglyoxime (dmg) moiety planes. The shorter bond length of Co-O in **2** (1.942~1.963Å) result in the enhancement of the intramolecular interactions between two closest molecular group of O-Co-(dmgBF_2)$_2$ compared with the bond length of Co-O (2.275 Å) in **1**, consequently **2** displays a better thermostability than **1**. The application of this cobalt based coordination polymer on the free radical polymerization was investigated.

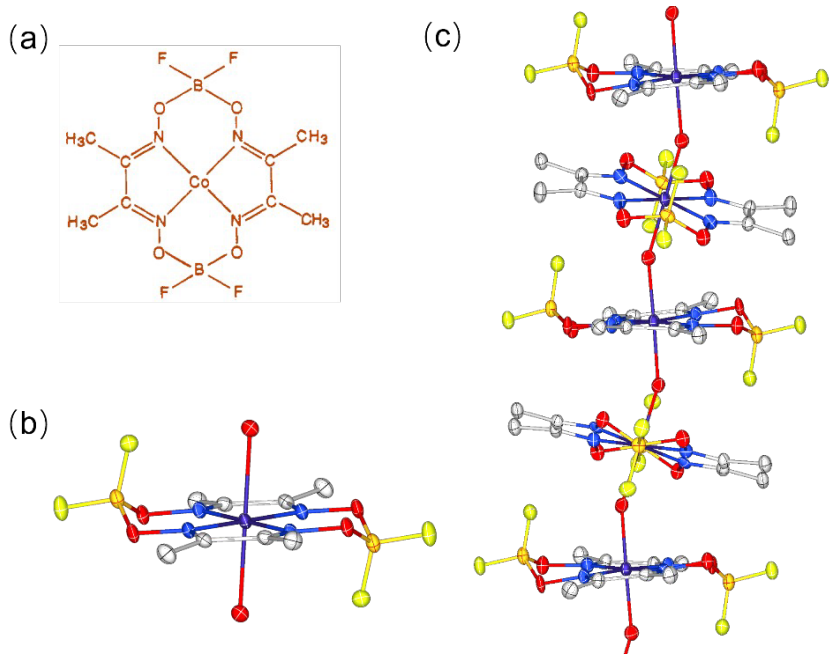

Figure 1. (a) Chemical structure of Co-(dmgBF_2)$_2$; (b) Crystal structure of complex **1**. The hydrogen atoms are not included in the ORTEP drawing for clarity, thermal ellipsoids are drawn at 50% probability. (c) Crystal structure of complex **2**, The hydrogen atoms are not included in the ORTEP drawing for clarity, thermal ellipsoids are drawn at 50% probability.

[1] Liebman J.F., Rappoport Z. (2023) The Chemistry of Organocobalt Compounds. John Wiley & Sons; Andreja Bakac A., Brynildson M. E. , and Espenson J H. (1986), *Inorg. Chem*. **25**, 4108; Nurdin L., Piers W. E., Lin J.B., and . Gelfand B. S. (2020) *Organometallics*, **39**, 2269.

[2] Moore S. J., Kutikov A., Lachicotte R. J., Marzilli and L. G., (1999), *Inorg. Chem*. **38**, 4, 768.