Crystal structure and dynamic properties of a bimetallic cyano complex Cd(C₄H₈O₂)Cu(CN)₃ with an interpenetrating 3D framework containing a 1,4-dioxane bridging ligand as a rotor

Electronic Supplementary Information (ESI)

Figure 1. IR spectra of Cd(C₄H₈O₂)Cu(CN)₃ (A) and Cd(C₄D₈O₂)Cu(CN)₃ (B) measured by Nujol mull method.

Figure 2. Powder X-ray diffraction patterns of Cd(C₄H₈O₂)Cu(CN)₃ (A) and Cd(C₄D₈O₂)Cu(CN)₃ (B) measured with Cu Kα radiation(λ = 1.5418 Å). The crystallinity of the duretared sample seemed to be inferior to that of the normal one, though the agreement between diffraction peaks of both samples was very well.
Figure 3. Motional Model for the 1,4-dioxane Rotor which is undergoing ring inversion and rotational motion simultaneously. (a) Ring inversion of the 1,4-dioxane is described as an interchange of two mirror images. (b) Rotational motion is modeled as a successive 60° jump about the z axis. The geometrical data of the chair form 1,4-dioxane molecule were cited from ref. 13.