

Crystal structure and dynamic properties of a bimetallic cyano complex $\text{Cd}(\text{C}_4\text{H}_8\text{O}_2)\text{Cu}(\text{CN})_3$ with an interpenetrating 3D framework containing a 1,4-dioxane bridging ligand as a rotor

Electronic Supplementary Information (ESI)

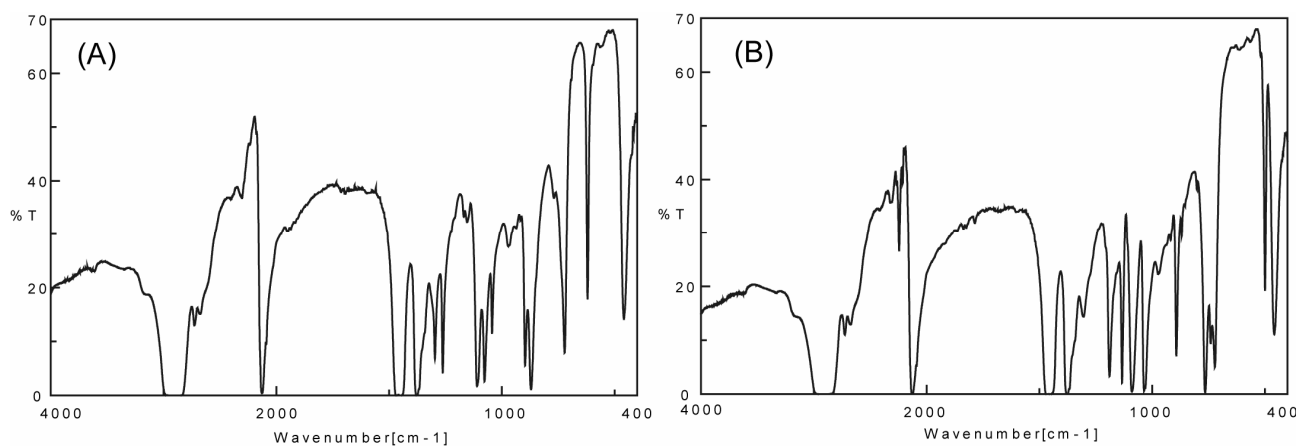


Figure 1. IR spectra of $\text{Cd}(\text{C}_4\text{H}_8\text{O}_2)\text{Cu}(\text{CN})_3$ (A) and $\text{Cd}(\text{C}_4\text{D}_8\text{O}_2)\text{Cu}(\text{CN})_3$ (B) measured by Nujol mull method.

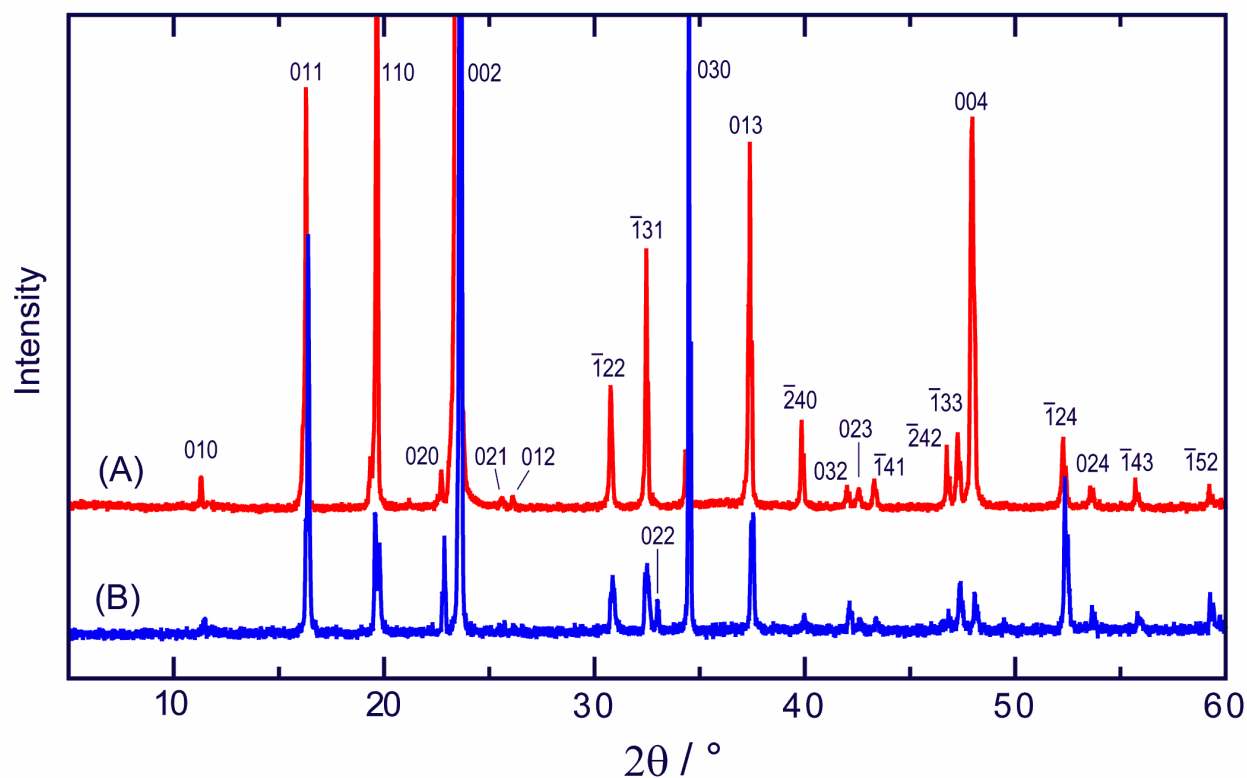
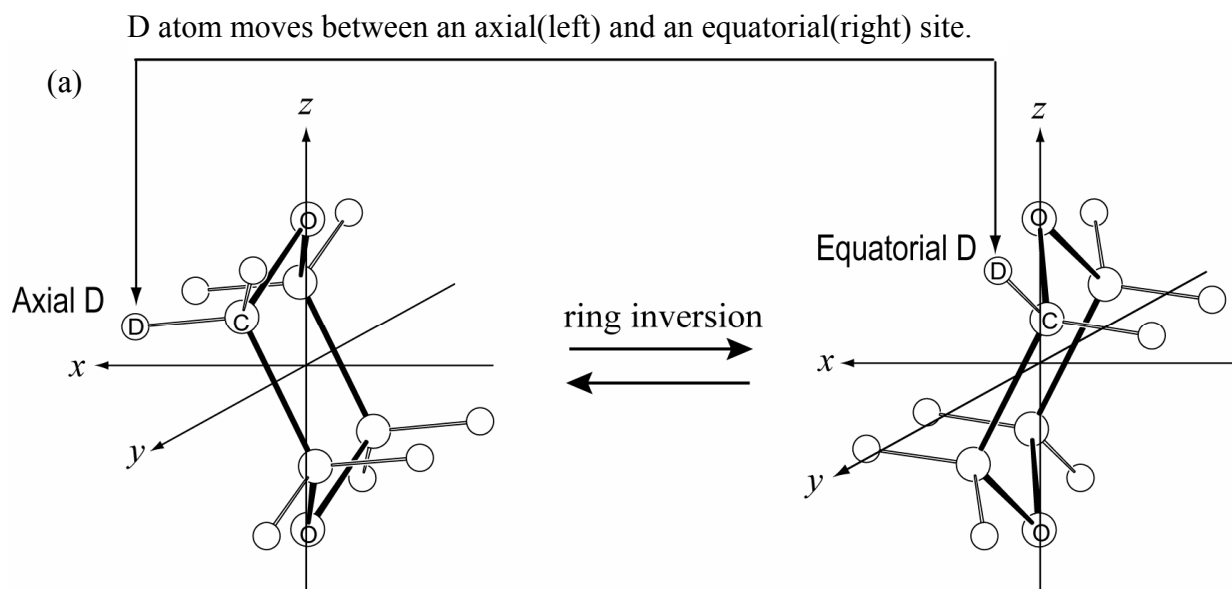


Figure 2. Powder X-ray diffraction patterns of $\text{Cd}(\text{C}_4\text{H}_8\text{O}_2)\text{Cu}(\text{CN})_3$ (A) and $\text{Cd}(\text{C}_4\text{D}_8\text{O}_2)\text{Cu}(\text{CN})_3$ (B) measured with $\text{Cu K}\alpha$ radiation ($\lambda = 1.5418 \text{ \AA}$). The crystallinity of the deuterated sample seemed to be inferior to that of the normal one, though the agreement between diffraction peaks of both samples was very well.



Euler angles for the D-C orientation for the axial and equatorial D in this coordinate system.

Axial D(left) $\alpha = 2.57^\circ$, $\beta = 96.70^\circ$, $\gamma = 0^\circ$

Equatorial D(right) $\alpha = 69.85^\circ$, $\beta = 56.35^\circ$, $\gamma = 0^\circ$

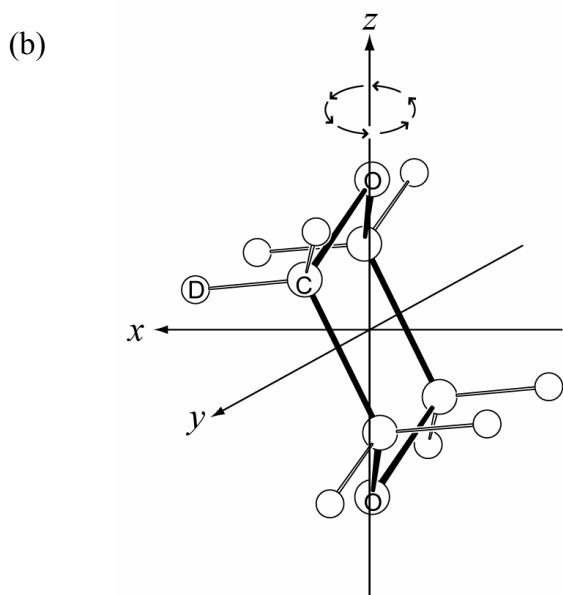


Figure3. Motional Model for the 1,4-dioxane Rotor which is undergoing ring inversion and rotational motion simultaneously. (a)Ring inversion of the 1,4-dioxane is described as an interchange of two mirror images. (b)Rotational motion is modeled as a successive 60° jump about the z axis. The geometrical data of the chair form 1,4-dioxane molecule were cited from ref. 13.