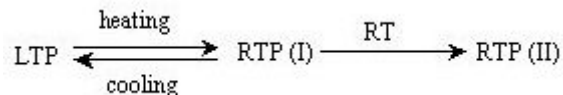


W0136

Three Polymorphs of Compound $[\text{Mn}^{\text{II}}(\text{15-crown-5})(\text{H}_2\text{O})_2](\text{NO}_3)_2$. Xiang Hao, Sean Parkin, Carolyn P. Brock, Dept. of Chemistry, Univ. of Kentucky, Lexington, KY 40506-0055, USA.

Single-crystal X-ray diffraction studies indicate that compound $[\text{Mn}^{\text{II}}(\text{15-crown-5})(\text{H}_2\text{O})_2](\text{NO}_3)_2$ has three crystalline polymorphs: LTP, RTP (I), and RTP (II). The scheme below shows their relationship.



The crystals came out of water near 295 K first as RTP (I), which transformed spontaneously to RTP (II) in a few months. The process is irreversible. On the other hand, RTP (I) can also undergo a reversible transformation to LTP upon slow cooling (not flash cooling). And LTP will transform to RTP (I) upon heating. The transformation takes place at *ca.* 278-283 K.

All three structures were solved and refined without problem. LTP, a modulated superstructure, crystallizes in $P2_1/c$ with $Z' = 3$. The modulations are three-fold along the c direction and two-fold along a . RTP (I) crystallizes in $P\bar{1}$ with $Z' = 2$. It is twinned about $[112]$. RTP (II) crystallizes in $P4_3$ with $Z' = 2$, and is twinned merohedrally.

LTP and RTP (I) have very similar packing, which explains why the transformation between them is reversible. However, the packing in RTP (I) and RTP (II) is very different, and the conformation of the cation $[\text{Mn}^{\text{II}}(\text{15-crown-5})(\text{H}_2\text{O})_2]^{2+}$ changed significantly after the transformation from RTP (I) to RTP (II).