

# Mo18ポリオキサメタレート・テトラブチルアンモニウム塩単結晶の構造相転移

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## Structural Phase Transition Behavior Observed for Single Crystal of Tetrabutylammonium Salt of Mo18 Polyoxometalate

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複数拠点利用者  
との共同研究

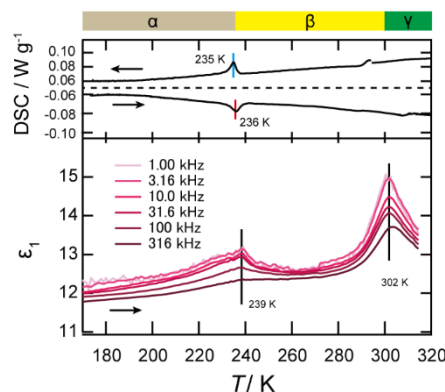


Figure 1. DSC traces and temperature dependence for the dielectric complex.

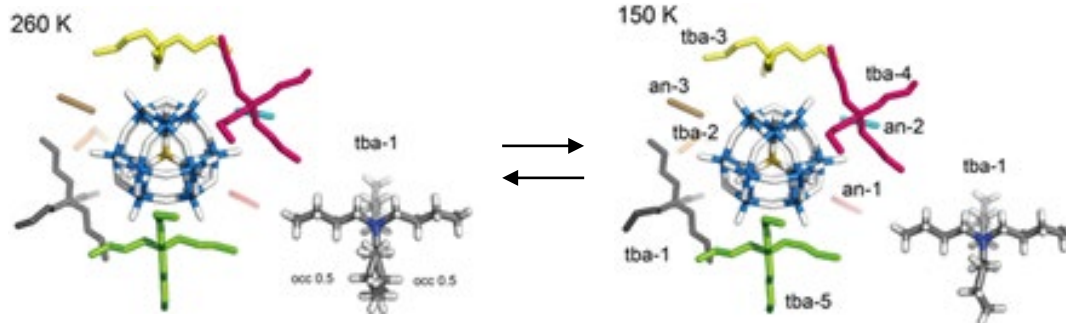


Figure 2. Structures of 1 at 150 K and 260 K. The POM clusters are represented by stick models. The tetrabutylammonium (tba) and acetonitrile (an) molecules are colored according to crystallographic equivalency. The structures on the right of the figure illustrate the orientational disorder in tba-1.

Ionic single crystals of the polyoxometalate  $[\text{MoV}_2\text{Mo}^{\text{VI}}_{16}\text{O}_{54}(\text{SO}_3)_2]^{6-}$  salted with tetrabutylammonium were found to exhibit dielectric anomalies at 235 and 302 K. The clear DSC peak at 235 K indicates the first - order nature of transition. The next transition at 302 K was concluded to be second - order in nature, demonstrating the existence of three different phases ( $\alpha$ ,  $\beta$ , and  $\gamma$ ). Temperature - dependent single - crystal X - ray diffraction analysis revealed that the structural phase transitions occur owing to orientational changes in the structures of the cation alkyl chains.

ポリオキサメタレート  $[\text{MoV}_2\text{Mo}^{\text{VI}}_{16}\text{O}_{54}(\text{SO}_3)_2]^{6-}$  のテトラブチルアンモニウム塩は、235と302 Kで相転移を示した。DSCから、低温側の相転移は一次転移であり、高温側の相転移は二次転移である事が明らかとなり、3種類の固相 $\alpha$ 、 $\beta$ および $\gamma$ 相が存在した。温度可変結晶構造解析から、有機カチオンの配向変化が相転移に重要な役割を果たしていることが明らかとなった。