

1A3a Synthesis and Structural Characterization of New Preyssler-type Phosphotungstate with Sodium-Ion in the Central Cavity

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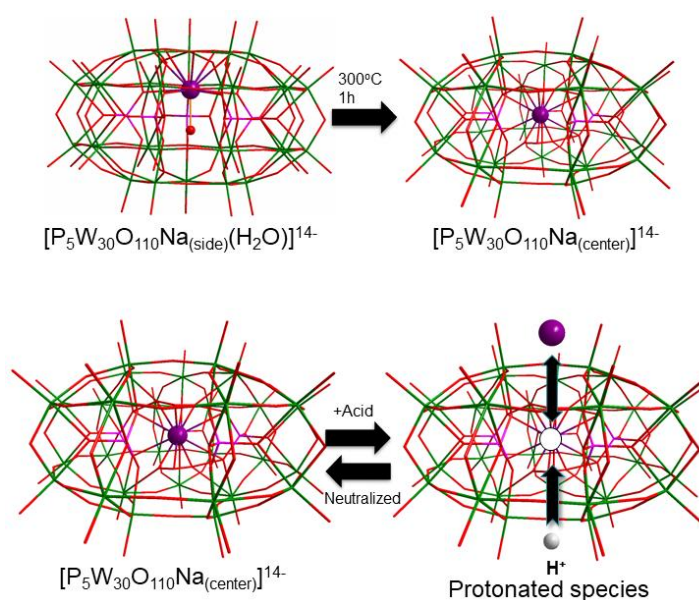
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A new Preyssler-type phosphotungstate with a sodium cation encapsulated in the central cavity, $[\text{P}_5\text{W}_{30}\text{O}_{110}\text{Na}(\text{center})]^{14-}$ is reported here. This new compound was prepared by heating treatment of the well-known Preyssler-type compound, $[\text{P}_5\text{W}_{30}\text{O}_{110}\text{Na}(\text{side})(\text{H}_2\text{O})]^{14-}$ in which a sodium cation occupies one of the two side cavities, at 300 °C produces a new compound $[\text{P}_5\text{W}_{30}\text{O}_{110}\text{Na}(\text{center})]^{14-}$ in which the sodium cation is encapsulated in the central cavity (scheme 1). The structure of the new compound confirmed by single crystal X-ray analysis, NMR techniques, ESI-MS, elemental analysis, and IR spectroscopy. In strong acid solution ($\text{H}^+ = 1.0 \text{ M}$), this sodium possibly vibrates in the central cavity.



Scheme 1. (Top) Migration of the encapsulated sodium from the side cavity to the central position in the Preyssler-type phosphotungstate under heat treatment and its behavior in acid condition (bottom). Green, pink, and red wires and violet and brown balls represent tungsten, phosphorus, oxygen, encapsulated sodium, and encapsulated water coordinated to sodium, respectively.