Crystal Structure and Catalytic Properties of $(C_6H_8N)_3[PMo_{12}O_{40}]$

Tie-Jun Cai, Shu-Zi Lü, Chuan-Lei Zhang, Yi-lan Huang, Ren-yuan Liu, and Qian Deng

College of Chemistry and Chemical Engineering, Hunan University of Science and Technology, Xiangtan 411201, P. R. China

Reprint requests to Prof. Tie-Jun Cai. Fax: +86-731-58291379. E-mail: tjcai53@163.com

Z. Naturforsch. **2011**, *66b,* 1231 – 1236; received October 14. 2011

The 4-picolinium salt $(C_6H_8N)_3[PMo_{12}O_{40}]$ was synthesized hydrothermally and characterized by IR spectroscopy, TG-DTA data and single-crystal X-ray diffraction. The results indicate that the compound consists of a $[PMo_{12}O_{40}]^{3-}$ heteropolyoxoanion and 4-picolinium cations $[C_6H_8N]^+$. A supramolecular structure is formed *via* intermolecular hydrogen-bonding between the different structural units. Crystal data: monoclinic, space group $P2_1/c$, a = 19.7004(3), b = 14.0785(2), c = 33.0209(5) Å, β = 91.3590(10)°, V = 9155.8(2) Å^3, Z = 8, $wR2$ = 0.0730. $(C_6H_8N)_3[PMo_{12}O_{40}]$ has a high catalytic activity for the oxidative elimination of acetone from gases as tested in a continuous-flow fixed-bed micro-reactor. When the initial concentration is 5.2 g m^{-3} in air, and the flow rate is 3.3 mL min^{-1}, 93 % of the acetone is eliminated at 70 °C.

Key words: Heteropolyoxoanion, 4-Picoline, Hydrothermal Method, Crystal Structure, Oxidative Elimination