



Synthesis, Crystal Structure and Characterization of a new Polyoxovanadate $[(CH_3)_2CHCH_2NH_3]_4[H_2V_{10}O_{28}]$

Asha Siddikha¹, Muga Vithal^{2*} and Boodida Sathyanarayana¹

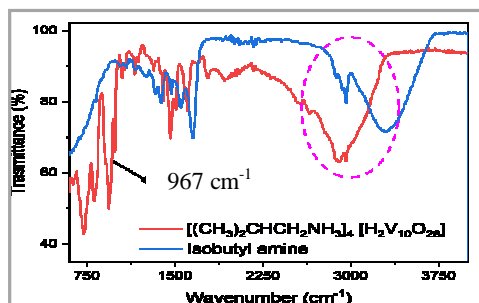
1. Department of Chemistry, JNTUH University College of Engineering, Science and Technology, Hyderabad-500 085, Telangana, **INDIA**
2. Department of Chemistry, Osmania University, Hyderabad-500 007, Telangana, **INDIA**
Email: mugavithal@gmail.com, muga_vithal@osmania.ac.in

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ABSTRACT

Polyoxovanadates (POVs), formed by vanadium and oxygen, possess a wide variety of applications in the field of chemical-, physical- and biological sciences as they are capable of exhibiting various structural motifs, like a baskets, cages, belts, barrels, etc., from different vanadium polyhedra. Among POVs, decavanadates $[H_nV_{10}O_{28}]^{(6-n)-}$ are extensively studied and structurally characterized because of its potential uses in materials chemistry, industrial chemistry and electrochemistry; moreover, it shows a vast biological activity. Here we report a structurally characterized decavanadate compound, $[(CH_3)_2CHCH_2NH_3]_4[H_2V_{10}O_{28}]$ (1). The title compound has been prepared by one-pot aqueous (acidic) synthesis involving V_2O_5 , HCl, isobutylamine, resulting in single crystals of compound 1. Compound 1 has been characterized by FTIR, TGA, Raman, FESEM-EDX microscopy and PXRD studies. It is unambiguously characterized by single-crystal X-ray diffraction analysis (Figure 1). The title compound $[(CH_3)_2CHCH_2NH_3]_4[H_2V_{10}O_{28}]$ crystallizes in the centrosymmetric monoclinic $P2(1)/c$ space group. In the crystal structure, the asymmetric unit consists of half of the cluster unit $[V_5O_{14}]^{3-}$ anion and two isobutylammonium cations, $[(CH_3)_2CHCH_2NH_3]^+$. Thus there are four $[(CH_3)_2CHCH_2NH_3]^+$ cations and one full decavanadate cluster anion present per formula unit. We have added two protons to the decavanadate cluster to counterbalance the charge of the cluster anion. The decavanadate anion is made up of ten edge-sharing $[VO_6]$ octahedra. The V-O bond length and O-V-O bond angles are in agreement with the reported data. In the crystal structure, the isobutyl ammonium cations are hydrogen bonded to the decavanadate cluster via $N-H\cdots O$ bonds.

Graphical Abstract:



FTIR spectra of compounds 1 and Isobutylamine

Keywords: Polyoxovanadates, Vanadium polyhedra, Decavanadate, Single-Crystal X-ray diffraction.