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Decavanadates decorated with $[Cu(en)_2]^{2+}$: convenient synthetic route, crystal structures and analysis of vibrational spectra.

Autorzy

Mariia V. Pavliuk

Valeriya G. Makhankova

Oleksiy V. Khavryuchenko

Vladimir N. Kokozay

Irina V. Omelchenko

Oleg V. Shishkin

Julia Jezierska

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A novel synthetic route was elaborated to obtain $Cu/V_{10}O_{28}$ compounds in a one-pot procedure based on a “direct synthesis” approach using water or dmf as a solvent and ethylenediamine as a ligand. The crystalline compounds $(H_2en)_2[Cu(en)_2(H_2O)_2][V_{10}O_{28}]\cdot 4H_2O$ (**1**), $(H_3O)_2[\{Cu(en)_2(H_2O)\}_2V_{10}O_{28}]\cdot 3H_2O$ (**2**), $[\{Cu(en)_2\}_3(V_{10}O_{28})]\cdot 6H_2O$ (**3**) and $(H_2en)_3[V_{10}O_{28}]\cdot 2H_2O$ (**4**), with copper-to-vanadium ratios of 1:10, 2:10, 3:10 and 0:10, respectively, were isolated and characterized by single-crystal X-ray analysis, FTIR, magnetic measurements and EPR spectroscopy. As proven by EPR measurements on the reaction solutions, the reactions pass through the formation of V(IV) species. However, from BVS analysis of the crystal structures, it is clear that all V atoms in the final products have the +5 oxidation state. A probable mechanism of the reactions taking place during the synthesis was proposed based on additional synthetic experiments and EPR data. The vibrational spectra of the $V_{10}O_{28}^{6-}$ adducts with water, ammonia, H_2en^{2+} and copper complex species, as well as differently protonated decavanadates, were simulated based on quantum-chemical calculations, allowing the assignment of additional bands in the 990–970 cm^{-1} region to the δ(VOH) vibrations and modes arising due to strong H-bonding of protic molecules to the decavanadate moiety.

Słowa kluczowe

Polyoxometallates, Copper, Vanadium, X-band EPR, DFT

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