Investigation of the cytosine-decavanadate interaction from an experimental charge density: a supramolecular arrangement of $Na_3V_{10}O_{28}(C_4N_3OH_5)_3(C_4N_3OH_6)_3{\cdot}10H_2O$ in the solid state

N. Bosnjakovic-Pavlovic[a,b], N. Bouhmaida[a,c], A. Spasojevic-de Biré[a], I. Correia[d], I. Tomaz[d], F. Avecilla[e], J. Pessoa[d], U.B. Mioc[b], and N.E. Ghermani[a,f]

[a]Ecole Centrale Paris, SPMS UMR CNRS 8580 1 Grande Voie des Vignes 92295 Châtenay-Malabry, France; [b]Faculty of Physical Chemistry P.O. Box 137, 11001 Belgrade, Serbia-Montenegro; [c]LSM, Faculté des Sciences Semlalia, P.O. Box 2390, 40000 Marrakech, Morocco; [d]Centro de Quimica Estrutural, Instituto Superior Tecnico, Av. Rovisco Pais, P-1049-001 Lisboa, Portugal ; [e]Departamento de Química Fundamental, Facultad de Ciencias, Campus da Zapateira s/n, 15071 A Coruña, Spain; [f]PPB UMR CNRS 8612, Faculté de Pharmacie 5 Rue Jean-Baptiste Clément, 92296 Châtenay-Malabry, France.
nada@spms.ecp.fr, nadab@ffh.bg.ac.yu

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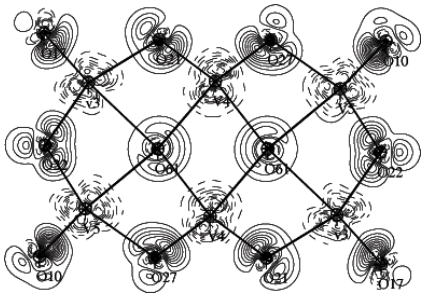
X-ray diffraction measurements were carried out on a Siemens SMART CCD diffractometer from room to 100 K using MoK_α radiation. The title complex crystallizes in the $P\bar{1}$ space group at room temperature. Below 200 K, we have observed substructure diffraction peaks which double the unit cell vanishing the centre of inversion. High resolution data collection was performed at 210 K to a resolution of 0.44 Å for an electron density study. The crystal packing shows a supramolecular network where the decavanadate anions are bridged by the sodium cations on the one hand and cytosine molecules through hydrogen bonds on the other. The pyrimidine bases are grouped in two kinds of dimers: a cytosine-cytosinium one and a shared-proton pair. The reversible dynamic cytosine-cytosinium conversion is probably responsible of the centrosymmetric loss at low temperature. The electron density ($P\bar{1}$ at 210 K) was refined using the Hansen-Coppens multipole model [1]. The best results were based on a vanadium $4s^0 3d^3$ configuration (V^{2+}) leading to the agreement factors R = 2.76%, R_w = 2.97% and gof = 1.16. The static electron density (figure) displays different V-O overlap and the oxygen polarizations in the decavandate anions.



The atomic charges and the electrostatic potential distribution will be presented and discussed.

[1] N. Hansen & P. Coppens Acta Cryst., 1978, A34, 909.