



Prediction of non-covalent interactions generated by a decavanadate anion. The use of two experimental electrostatic studies

Nada Bošnjaković-Pavlović, Anne Spasojevic - de Biré, Nouhza Bouhmaida, João Costa Pessoa, U. Mioc, Nour-Eddine Ghermani

► To cite this version:

Nada Bošnjaković-Pavlović, Anne Spasojevic - de Biré, Nouhza Bouhmaida, João Costa Pessoa, U. Mioc, et al.. Prediction of non-covalent interactions generated by a decavanadate anion. The use of two experimental electrostatic studies. Open day CPOS, Mar 2009, London, United Kingdom. hal-02304875

HAL Id: hal-02304875

<https://hal.science/hal-02304875>

Submitted on 23 Sep 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Prediction of non-covalent interactions generated by a decavanadate anion. The use of two experimental electrostatic studies.

N. Bosnjakovic-Pavlovic^{1,2}, A. Spasojevic-de Biré², N. Bouhaida³, J. Pessoa⁴, U. Mioc¹, N. E. Ghermani^{2,5}

¹ Faculty of Physical–Chemistry, University of Belgrade, 11000 Belgrade, Serbia

² Laboratoire SPMS, UMR 8580 du CNRS, Ecole Centrale Paris, 92295 Châtenay-Malabry Cedex, France

³ Laboratoire Sciences des Matériaux, Faculté des sciences Marrakech-Semlalia, Maroc

⁴ Centro de Quimica Estrutural, Instituto Superior Tecnico, Universidade Tecnica de Lisboa, P-1049-001 Lisboa, Portugal

⁵ Laboratoire PCB, UMR 8612 du CNRS, Faculté de Pharmacie, Université Paris-Sud, 92296 Châtenay-Malabry Cedex, France



Biological properties of $[V_{10}O_{28}]^{6-}$

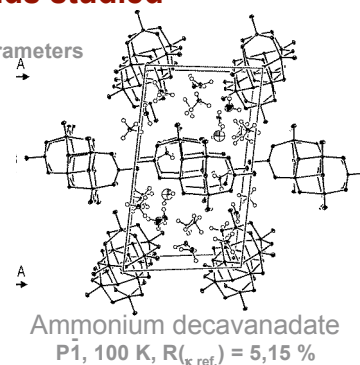
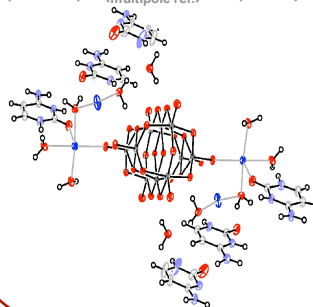
- Versatile activity (enzyme inhibitor or activator)
- Inhibition of Ca^{2+} ATP-ase, cAMP dependent protein kinase, phosphorylase, ...
- Inhibition of skeletal muscle myosin
- Activation of 5'-nucleotidase
- ...

Goal of the study

- To contribute to a better understanding of the reactivity *via* an accurate description of the experimental electron density and electrostatic properties of a two decavanadate compounds.

Compounds studied

Cytosine decavanadate
 $P1$, 210 K, $R_{\text{(multipole ref.)}} = 2,32 \%$, 505 parameters



Net atomic charges (e) and electrostatic properties ($e \cdot \text{\AA}^{-1}$)

		Experimental						Theoretical			
		$Na_3[V_{10}O_{28}](C_4N_5OH_6)_3 \cdot (C_4N_5OH_6)_3 \cdot 10H_2O$						$(NH_4)_6V_{10}O_{28} \cdot 6H_2O$		$[V_{10}O_{28}]^{6-}$	
		This work						This work		(Henry, 2002)	
		Multipole refinement		k refinement		AIM		k refinement		PACHA	