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

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

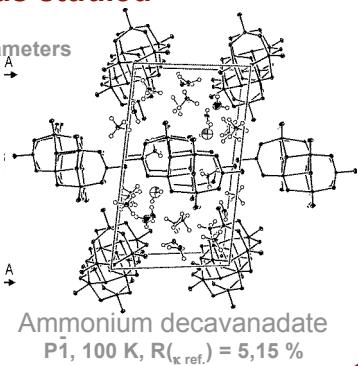
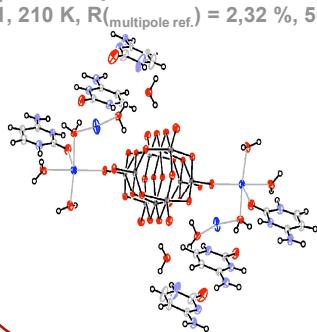
- Versatile activity (enzyme inhibitor or activator)
- Inhibition of Ca^{2+} ATP-ase, cAMP dependent protein kinase, phosphorylase, ...
- Inhibition of skeletal muscle myosin
- Activation of 5'-nucleotidase
- ...

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.

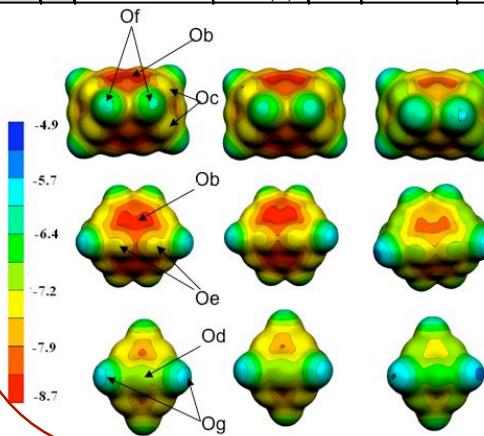
Compounds studied

Cytosine decavanadate
 $P\bar{1}$, 210 K, $R_{(multipole \text{ ref.})} = 2,32 \%$, 505 parameters

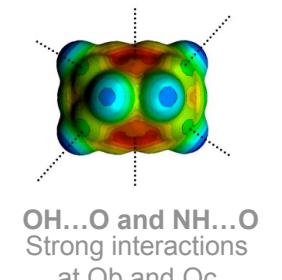


Net atomic charges (e) and electrostatic properties ($e \cdot \text{\AA}^{-1}$)

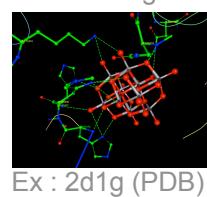
Experimental						Theoretical I					
$\text{Na}_5[V_{10}O_{28}] \cdot (\text{C}_4\text{N}_3\text{OH}_5)_3 \cdot (\text{C}_4\text{N}_3\text{OH}_6)_3 \cdot 10\text{H}_2\text{O}$ This work			$(\text{NH}_4)_6\text{V}_{10}\text{O}_{28} \cdot 6\text{H}_2\text{O}$ This work			$[\text{V}_{10}\text{O}_{28}]^{6-}$ (Henry, 2002)			$[\text{V}_{10}\text{O}_{28}]^{6-}$ (Kempf, 1992)		
Multipole refinement	k refinement	EP	charge e	EP	charge e	EP	charge e	EP	Mulliken	Ab initio SCF	
O6 1	a	-0.88(5)	-0.724	-0.7(1)	-0.861	-1.27					
O31	b	-0.97(5)	-0.873	-0.9(1)	-0.726	-8.2					
O32		-1.08(5)	-0.918	-0.6(1)	-0.713						
O24	c	-0.90(5)	-0.857	-1.2(1)	-0.666						
O25		-0.84(5)	-0.799	-0.6(1)	-7.1	-6.1	-0.93	-6.8			
O20		-0.81(5)	-0.808	-1.0(1)	-7.1						
O23		-0.91(5)	-0.900	-0.7(1)							
O22	d	-6.9	-0.93(5)	-6.6	-0.797	-6.8	-1.0(1)	-6.9	-0.686	-5.8	-0.94
O21	e	-7.4	-0.87(5)	-7.1	-0.783	-7.4	-0.8(1)	-7.2	-0.635	-6.4	-0.82
O27		-0.92(5)	-0.733	-0.5(1)	-0.5(1)						-7.0
O13	f	-6.2	-0.63(5)	-5.9	-0.573	-6.2	-1.1(1)	-6.4	-0.555	-5.3	-0.63
O12		-0.81(5)	-0.668	-0.7(1)	-0.7(1)						-5.9
O11	g	-5.8	-0.84(5)	-5.6	-0.717	-5.8	-0.5(1)	-5.7	-0.560	-4.9	-0.66
O10		-0.65(5)	-0.620	-1.2(1)							-5.5



Prediction of preferential non-covalent interactions



OH...O and NH...O
Strong interactions at Ob and Oc



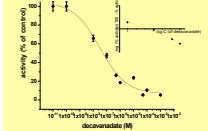
Conclusions

- EP of the $[V_{10}\text{O}_{28}]^{6-}$ is transferable (independent of the crystalline environment).
- In case of two cations the highest positive cation is surrounded by H_2O , the second cation is linked to the $[V_{10}\text{O}_{28}]^{6-}$.
- The main protonation site is Ob and Oc.
- Non-covalent predictions are tested and verified on 150 structures retrieved in CSD

Influence of decavanadate on rat synaptic plasma membrane ATPases activity

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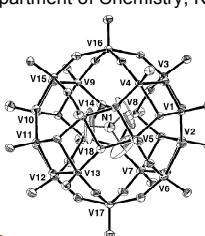


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Charge density on V18 polyoxovanadate

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Experiment realized on Crystal@Soleil in february 2009