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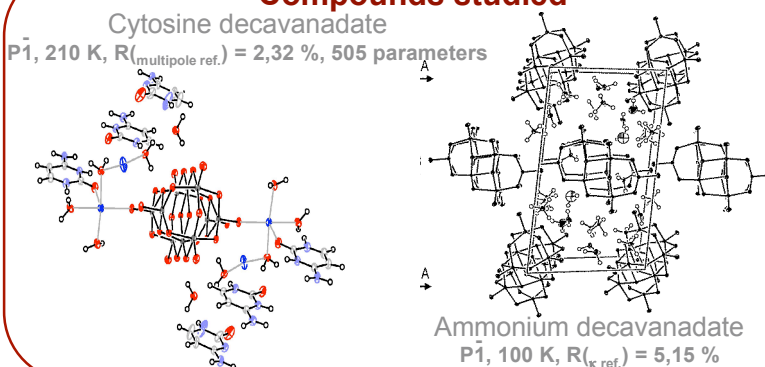
Biological properties of $[V_{10}O_{28}]^{6-}$

- 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

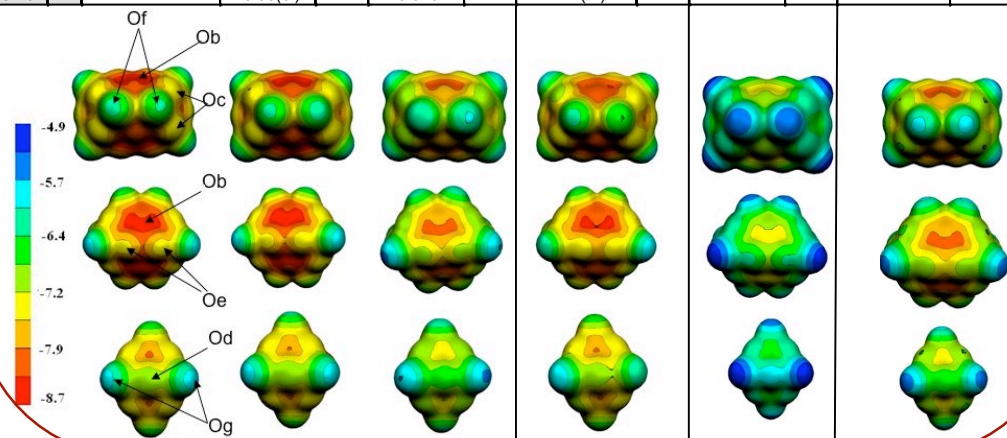
- To contribute to a better understanding of the reactivity via an accurate description of the experimental electron density and electrostatic properties of a two decavanadate compounds

Compounds studied

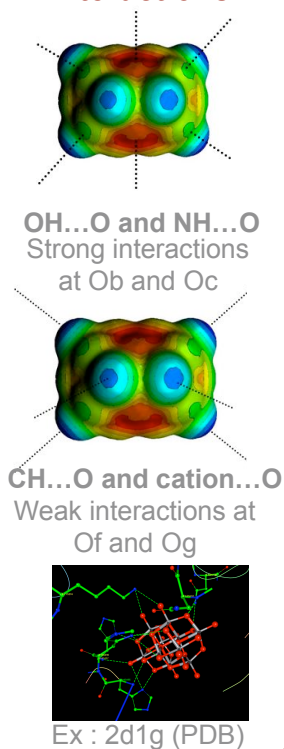


Net atomic charges (e) and electrostatic properties ($e \cdot \text{Å}^{-1}$)

		Experimental						Theoretical			
		Na ₃ [V ₁₀ O ₂₈] (C ₄ N ₂ OH ₅) ₃ (C ₄ N ₂ OH ₅) ₃ · 10H ₂ O			(NH ₄) ₆ V ₁₀ O ₂₈ · 6H ₂ O			[V ₁₀ O ₂₈] ⁶⁻ (Henry, 2002)		[V ₁₀ O ₂₈] ⁶⁻ (Kempf, 1992)	
		Multipole refinement t	k refinement t	AIM	Multipole refinement t	k refinement t	AIM	PACHA	Mulliken n	Ab initio SCF	
EP	charge	EP	charge	EP	charge	EP	charge	EP	charge	EP	
O61	a	-0.88(5)	-0.724	-0.7(1)	-0.861	-1.27					
O31	b	-8.7	-0.97(5)	-0.873	-0.9(1)	-7.4	-0.726	-7.4	-1.04	-8.2	
O32			-1.08(5)	-0.918	-0.6(1)	-8.5	-0.713	-7.4	-1.04	-8.2	
O24			-0.90(5)	-0.857	-1.2(1)						
O25	c	-7.2	-0.84(5)	-0.799	-0.6(1)	-7.1	-0.666	-6.1	-0.93	-6.8	
O20			-0.81(5)	-0.808	-1.0(1)						
O23			-0.91(5)	-0.900	-0.7(1)						
O22	d	-6.9	-0.93(5)	-0.797	-1.0(1)	-6.9	-0.686	-5.8	-0.94	-6.5	
O21			-0.87(5)	-0.783	-0.8(1)						
O27	e	-7.4	-0.92(5)	-0.733	-0.5(1)	-7.2	-0.635	-6.4	-0.82	-7.0	
O13			-0.63(5)	-0.573	-1.1(1)						
O12	f	-6.2	-0.81(5)	-0.668	-0.7(1)	-6.4	-0.555	-5.3	-0.63	-5.9	
O11			-0.84(5)	-0.717	-0.5(1)						
O10	g	-5.8	-0.65(5)	-0.620	-1.2(1)	-5.7	-0.560	-4.9	-0.66	-5.5	



Prediction of preferential non-covalent interactions



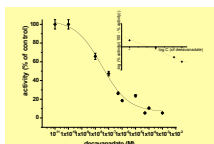
Conclusions

- EP of the $[V_{10}O_{28}]^{6-}$ is transferable (independent of the crystalline environment).
- In case of two cations the highest positive cation is surrounded by H₂O, the second cation is linked to the $[V_{10}O_{28}]^{6-}$
- 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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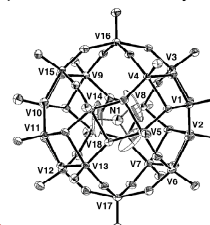


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Charge density on V18 polyoxovanadate

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Experiment realized on Crystal@Soleil in february 2009