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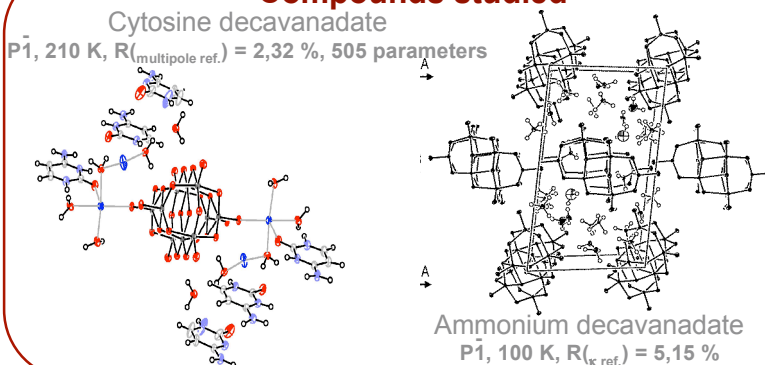
## Biological properties of $[V_{10}O_{28}]^{6-}$

- 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

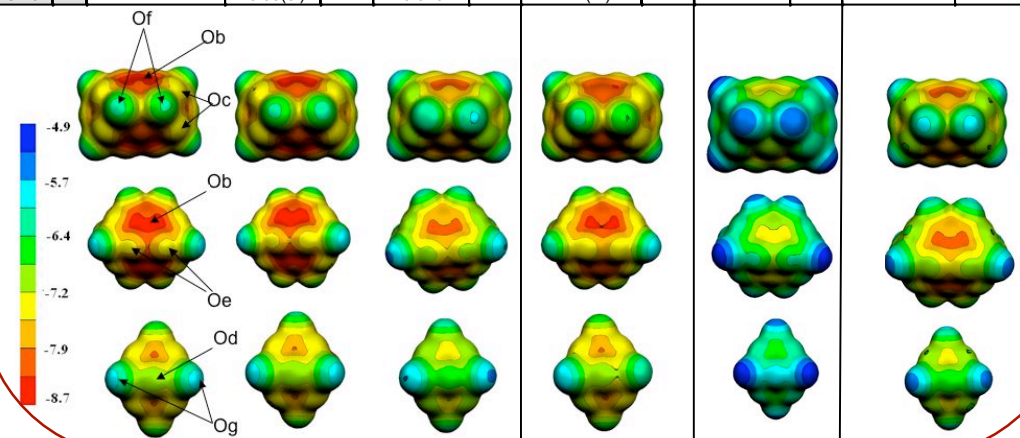
- To contribute to a better understanding of the reactivity *via* an accurate description of the experimental electron density and electrostatic properties of a two decavanadate compounds

## Compounds studied

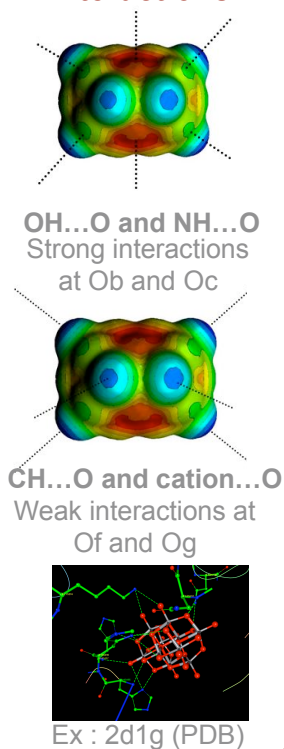


## Net atomic charges (e) and electrostatic properties ( $e \cdot \text{\AA}^{-1}$ )

		Experimental						Theoretical			
		Na <sub>3</sub> [V <sub>10</sub> O <sub>28</sub> ] (C <sub>4</sub> N <sub>2</sub> OH <sub>5</sub> ) <sub>3</sub> (C <sub>2</sub> N <sub>2</sub> OH <sub>5</sub> ) <sub>3</sub> · 10H <sub>2</sub> O			(NH <sub>4</sub> ) <sub>6</sub> V <sub>10</sub> O <sub>28</sub> · 6H <sub>2</sub> O			[V <sub>10</sub> O <sub>28</sub> ] <sup>6-</sup> (Henry, 2002)		[V <sub>10</sub> O <sub>28</sub> ] <sup>6-</sup> (Kempf, 1992)	
		Multipole refinement t	k refinement t	AIM	Multipole refinement t	k refinement t	PACHA	Mulliken n	Ab initio SCF		
		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)	-8.2	-0.873		-0.9(1)		-0.726		-7.4
O32			-1.08(5)		-0.918	-8.7	-0.6(1)	-8.5	-0.713	-7.4	-1.04
O24			-0.90(5)		-0.857		-1.2(1)		-0.666	-6.1	-0.93
O25	c	-7.2	-0.84(5)	-6.9	-0.799	-7.1	-0.6(1)	-7.1	-0.666	-6.1	-0.93
O20			-0.81(5)		-0.808		-1.0(1)		-0.666	-6.1	-0.93
O23			-0.91(5)		-0.900		-0.7(1)		-0.666	-6.1	-0.93
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			-0.87(5)		-0.783		-0.8(1)		-0.635	-6.4	-0.82
O27	e	-7.4	-0.92(5)	-7.1	-0.733	-7.4	-0.5(1)	-7.2	-0.635	-6.4	-0.82
O13			-0.63(5)		-0.573		-1.1(1)		-0.555	-5.3	-0.63
O12	f	-6.2	-0.81(5)	-5.9	-0.668	-6.2	-0.7(1)	-6.4	-0.555	-5.3	-0.63
O11			-0.84(5)		-0.717		-0.5(1)		-0.560	-4.9	-0.66
O10	g	-5.8	-0.65(5)	-5.6	-0.620	-5.8	-1.2(1)	-5.7	-0.560	-4.9	-0.66



## Prediction of preferential non-covalent interactions



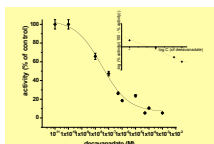
## Conclusions

- 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 H<sub>2</sub>O, 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

Krstić D.<sup>6</sup>, Čolović M.<sup>7</sup>, Bosnjaković-Pavlović N.<sup>1,2</sup>, Spasojević-de Biré A.<sup>2</sup>, Vasić V.<sup>7</sup>

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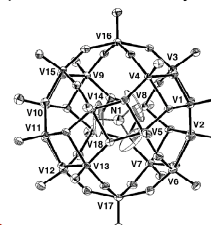


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## Charge density on V18 polyoxovanadate

Spasojević – de Biré<sup>2</sup>, Giot, M<sup>2</sup>, Guiblin N.<sup>2</sup>, Hayashi Y.<sup>8</sup>, Bosnjakovic - Pavlovic N.<sup>1,2</sup>,

<sup>8</sup> Department of Chemistry, Kanazawa University, Japan



Experiment realized on Crystal@Soleil in february 2009