

## A novel hybrid decavanadate with a dicationic imidazolium ionic liquid

Lorena M. Braga<sup>1</sup>, Andressa V. Hilário<sup>2</sup>, Grazielli da Rocha<sup>1</sup>, Tatiana Zanette<sup>3</sup>, Pascual Oña-Burgos<sup>3</sup>, Katia B. Gusmão<sup>2</sup>, Christian W. Lopes<sup>1</sup>, Francine Bertella<sup>1</sup> and Giovana G. Nunes<sup>1</sup>

<sup>1</sup>Departamento de Química, Universidade Federal do Paraná, Curitiba, Brazil

<sup>2</sup>Instituto de Química, Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil

<sup>3</sup>Instituto de Tecnología Química, Universitat Politècnica de València-Consejo Superior de Investigaciones Científicas, València, Espanha

E-mail: lorena.moreira@ufpr.br

**Thematic Area:** Supramolecular Chemistry

**Keywords:** decavanadate, ionic liquid, dicationic imidazolium

Hybrid decavanadate ( $[\text{H}_x\text{V}_{10}\text{O}_{28}]^{(6-x)-}$  or  $\text{V}_{10}$ ) salts featuring organic cations are highly fascinating materials for diverse applications, such as gas adsorption and catalysis.<sup>1,2</sup> The direct reaction of the ionic liquid 1,1'-(1,4-phenylenebis(methylene))bis(3-methylimidazolium) bromide ( $\text{PhimBr}_2$ ) with  $\text{V}_{10}$  in aqueous solution produced yellow crystals of a new compound  $(\text{Phim})_2[\text{H}_4\text{V}_{10}\text{O}_{28}] \cdot 6\text{H}_2\text{O}$  (**PhimV<sub>10</sub>**, Figure 1). The product was characterized by infrared spectroscopy (IR), single-crystal and powder X-ray diffraction, elemental and thermogravimetric analysis (TGA). **PhimV<sub>10</sub>** crystallizes in a triclinic space group,  $P\bar{1}$  crystal system. The asymmetric unit contains half of tetra-protonated decavanadate, one **Phim**<sup>2+</sup> cation and 3 water molecules. The supramolecular network is defined by an extensive net of weak to moderate hydrogen bonding ( $\text{C}\cdots\text{H}-\text{O}$  and  $\text{O}\cdots\text{H}-\text{O}$ ) involving the  $\text{V}_{10}$ , water molecules and cations. **Phim**<sup>2+</sup> are organized in pairs through a single  $\pi\cdots\pi$  stacking interaction with a distance between centroids of 3.723 Å. The TGA showed a series of events corresponding to the loss of the 6 water molecules (Exp. 7.02%; Theor. 6.73%) up to 150 °C and the thermal decomposition of the two **Phim**<sup>2+</sup> cations (ca. 35% of weight loss) around 450 °C. Therefore, the sample was treated at 150 °C for 3 h prior the catalytic reaction to remove the water molecules. The IR spectrum of the reminiscent solid presented bands at 1556, 1153, 964 and 587  $\text{cm}^{-1}$ , assigned to the  $\nu(\text{C}-\text{C})$ ,  $\nu(\text{C}-\text{N})$ ,  $\nu(\text{V}=\text{O})$  and  $\nu(\text{V}-\text{O}-\text{V})$  and the absence of bands expected for the water molecules. The catalytic performance for carbon dioxide fixation was investigated using propylene oxide and  $\text{ZnBr}_2$  as co-catalyst. The preliminary catalytic results of **PhimV<sub>10</sub>** exhibited moderate yield towards propylene carbonate (58%), highlighting its potential as a catalyst for  $\text{CO}_2$  fixation into cyclic carbonates.

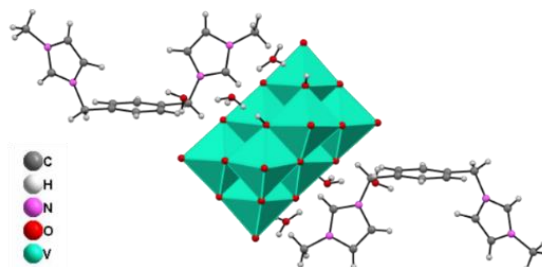


Figure 1: Polyhedral representation of  $(\text{C}_{16}\text{H}_{20}\text{N}_4)_2[\text{H}_4\text{V}_{10}\text{O}_{28}] \cdot 6\text{H}_2\text{O}$ .

**Acknowledgments:** UFPR/CAPES/CNPq/FUNDAÇÃO ARAUCÁRIA/PROEX

### References

- [1] A. García-García *et al.*, *Inorganics*, **9**, 67 (2021).
- [2] Y. Zhao *et al.*, *Crystal Growth & Design*, **21**, 1019-1027 (2021).