

# SPECIATION ATLAS OF POLYOXOMETALATES IN AQUEOUS SOLUTIONS

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With the growing number of successful and promising applications of polyoxometalates (POMs) in various fields, such as biology, medicine, pharmacy, environmental science, material and energy science, and catalysis, understanding their speciation in solution is of paramount importance and is crucial for the successful application of POMs [1]. Factors such as pH, temperature, incubation time, type of buffer solution, presence of a reducing or chelating agent, and the effect of ionic strength must be considered to assign the activity of POMs to the species actually present in solution.

The study of complex polyatomic ion speciation has proven challenging due to numerous factors affecting stability and limited direct methods available. To address these challenges, we have developed a speciation atlas for polyoxometalates commonly used in catalytic and biological applications in aqueous solutions. Compiled for six different polyoxometalate archetypes with three types of addenda ions based on 1,309 NMR spectra under 54 different conditions, the atlas has revealed a previously unknown behavior of polyoxometalates that may account for their potency as biological agents and catalysts. This atlas provides a species distribution database and a predictive model for other polyoxometalates, which is fully accessible to interested readers. The speciation atlas aims to understand what happens in POM solution and encourage verification of compounds' stability under experimental conditions.

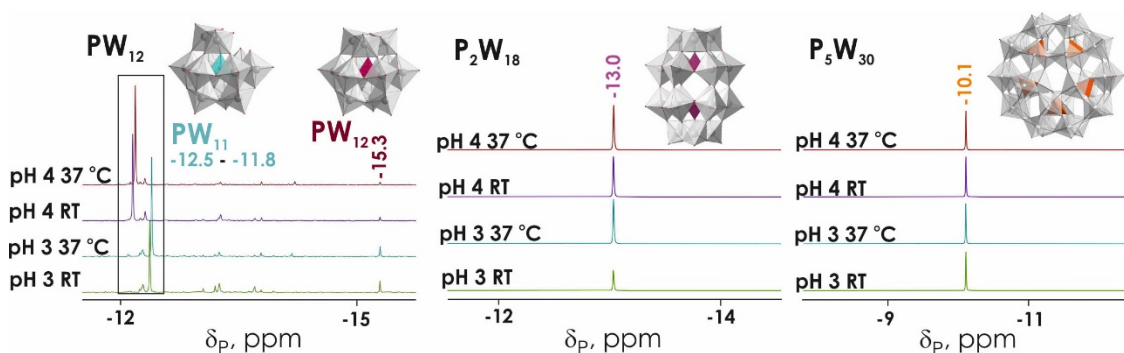


Figure 1.  $^{31}\text{P}$  NMR spectra of 10mM Keggin-type  $\text{Na}_3[\alpha\text{-PW}_{12}\text{O}_{40}]$ , Wells-Dawson type  $\text{K}_6[\alpha\text{-P}_2\text{W}_{18}\text{O}_{62}]$ , and Preyssler-type  $\text{K}_{12.5}\text{Na}_{1.5}[\text{NaP}_5\text{W}_{30}\text{O}_{114}]$  POMs solutions in 0.1 M sodium phosphate buffer at pH 3 and 4, recorded at room temperature (RT) and after 24 h incubation at 37 °C. Signals are attributed to the color of the central  $\{\text{PO}_4\}$  unit in POMs. Color code:  $\{\text{WO}_6\}$ , light grey;  $\{\text{PO}_4\}$ , blue, burgundy, pink or orange.

The research reported in this work was funded by the Austrian Science Fund (FWF) (P33089 (to A.R.); P33927 (to N.I.G.)), Austria's Agency for Education and Internationalization (OeAd) (HR 06/2020) and the University of Vienna.