

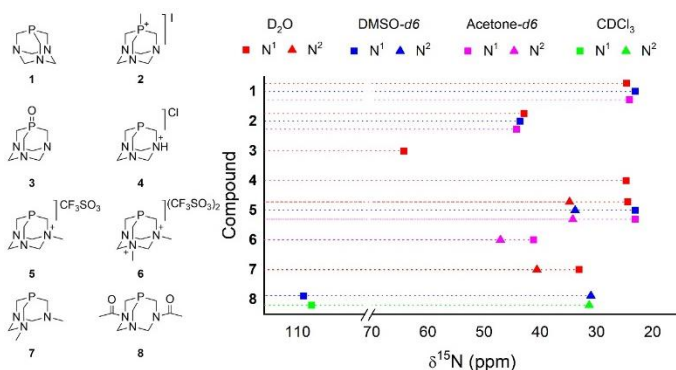
## New insight on the $\kappa$ -*P,N* coordination of 1,3,5-triaza-7-phosphaadamantane and derivatives and their complexes: new $\kappa$ -*P,N*-heterometal complexes and a $^{15}\text{N}$ NMR survey.

A. Alguacil<sup>1,2</sup>, F. Scalambra<sup>1,2</sup>, A. Romerosa<sup>1,2\*</sup>

<sup>1</sup> Department of Chemistry and Physics, University of Almería, Almería, 04120, Spain, aaa518@ual.es

<sup>2</sup> Inorganic Chemistry Lab-CIESOL, University of Almería, Almería, 04120, Spain

Nowadays hydrophilic phosphines are very common ligands in organometallic and coordination chemistry. Their scaffolds usually present polar substituents such as hydroxyl, carboxylate, sulfonate or amino groups, allowing to access fields as aqueous catalysis and biological applications. The PTA ligand (1,3,5-triaza-7-phosphaadamantane) contains a soft phosphorus atom and three hard nitrogen atoms, which can be functionalized providing a large variety of derivatives<sup>[1]</sup> that became of spread usage to obtain catalysts, bioactive agents, luminescent compounds, microgels and new materials.<sup>[2,3]</sup>



**Figure 1.**  $\delta^{15}\text{N}$  for compounds 1-8. The notations N<sup>1</sup> and N<sup>2</sup> correspond to N<sup>1</sup> = N(CH<sub>2</sub>)<sub>3</sub> for compounds 1-4, while for 5-8 N<sup>1</sup> = N-R (R = Me, AcO) and N<sup>2</sup> = N(CH<sub>2</sub>)<sub>3</sub>.

In the present study, the  $^{15}\text{N}$  detection through  $^1\text{H}$ - $^{15}\text{N}$  HMBC provided the construction of a small library of  $^{15}\text{N}$  chemical shifts that shed

light on important features regarding the  $\kappa\text{N}$ -coordination in PTA and derivatives. We investigated some non-coordinated PTA derivatives in solution, as well as some previously published representative Ru-half-sandwich complexes  $\kappa\text{P}$ - or  $\kappa\text{P,N}$ -coordination. Additionally, new mono- and polymetallic complexes containing dmoPTA and/or PTA were synthesised and characterized by single crystal X-ray diffraction.

### Acknowledgements

We acknowledge Junta de Andalucía for the FEDER project PY20\_00791 and PAI group FQM-317.

### References

- [1] J. Bravo, S. Bolaño, L. Gonsalvi, M. Peruzzini, *Coord. Chem. Rev.* **2010**, 254, 555–607
- [2] A. Guerriero, M. Peruzzini, L. Gonsalvi, *Coord. Chem. Rev.* **2018**, 355, 328–361
- [3] F. Scalambra, M. Serrano-Ruiz, A. Romerosa, *Dalt. Trans.* **2017**, 46, 5864–5871