

## Electronic Supplementary Information

for

### **Thermodynamic study of lanthanide(III) complexes with bifunctional monophosphinic acid analogues of H<sub>4</sub>dota and comparative kinetic study of yttrium(III) complexes with H<sub>4</sub>dota-like ligands**

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**Figure S1** Dependence of <sup>1</sup>H (A) and <sup>31</sup>P (B) NMR chemical shift on pH.

**Figure S2** An example of the data obtained for the formation of yttrium(III)-macrocycle complexes in the presence of Arsenazo III ( $c_Y = 7.8 \times 10^{-7} \text{ mol dm}^{-3}$ ,  $c_{\text{Lig}} = 1.7 \times 10^{-5} \text{ mol dm}^{-3}$ , pH 6.07).

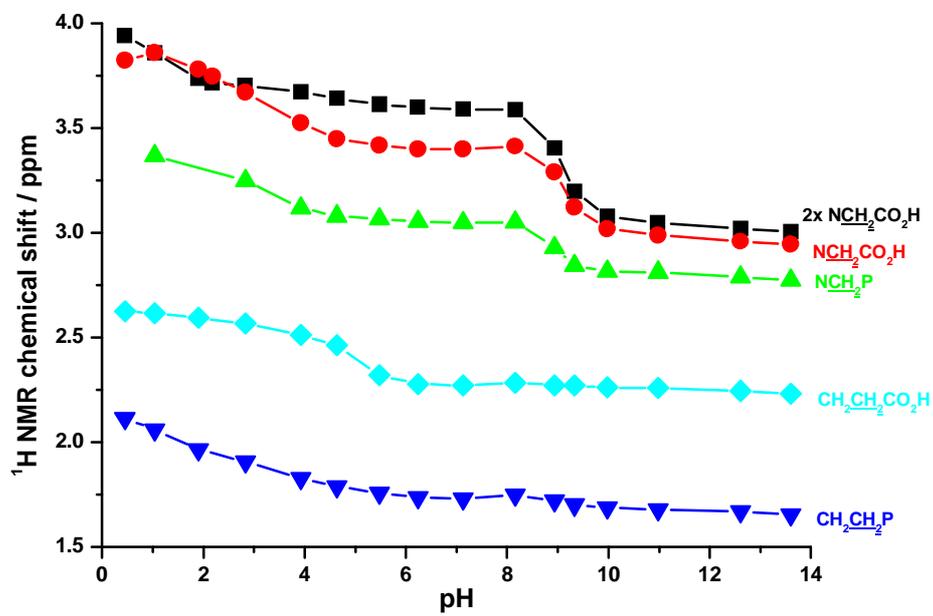
**Figure S3** An example of the experimental data obtained for the formation of the yttrium(III) complex of H<sub>5</sub>do3ap<sup>PrA</sup> in presence of Arsenazo III ( $c_Y = 7.8 \times 10^{-7} \text{ mol dm}^{-3}$ ,  $c_{\text{Lig}} = 1.7 \times 10^{-5} \text{ mol dm}^{-3}$ ) at different pH values.

**Figure S4** Correlation of rate constant  $k_H$  for dissociation of the yttrium(III) complexes with the first protonation constant of the ligands. The solid line was fitted for all the studied ligands and the dotted line was fitted only through three the most similar ligands (H<sub>4</sub>dota, H<sub>5</sub>do3ap<sup>PrA</sup> and H<sub>4</sub>do3ap<sup>ABn</sup>).

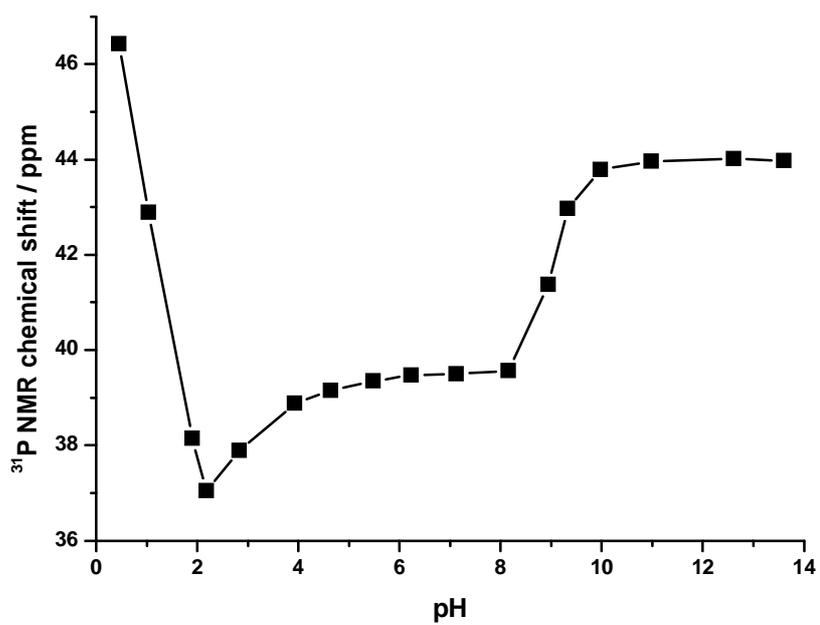
**Figure S1**

Dependence of  $^1\text{H}$  (A) and  $^{31}\text{P}$  (B) NMR chemical shift on pH.

**A**

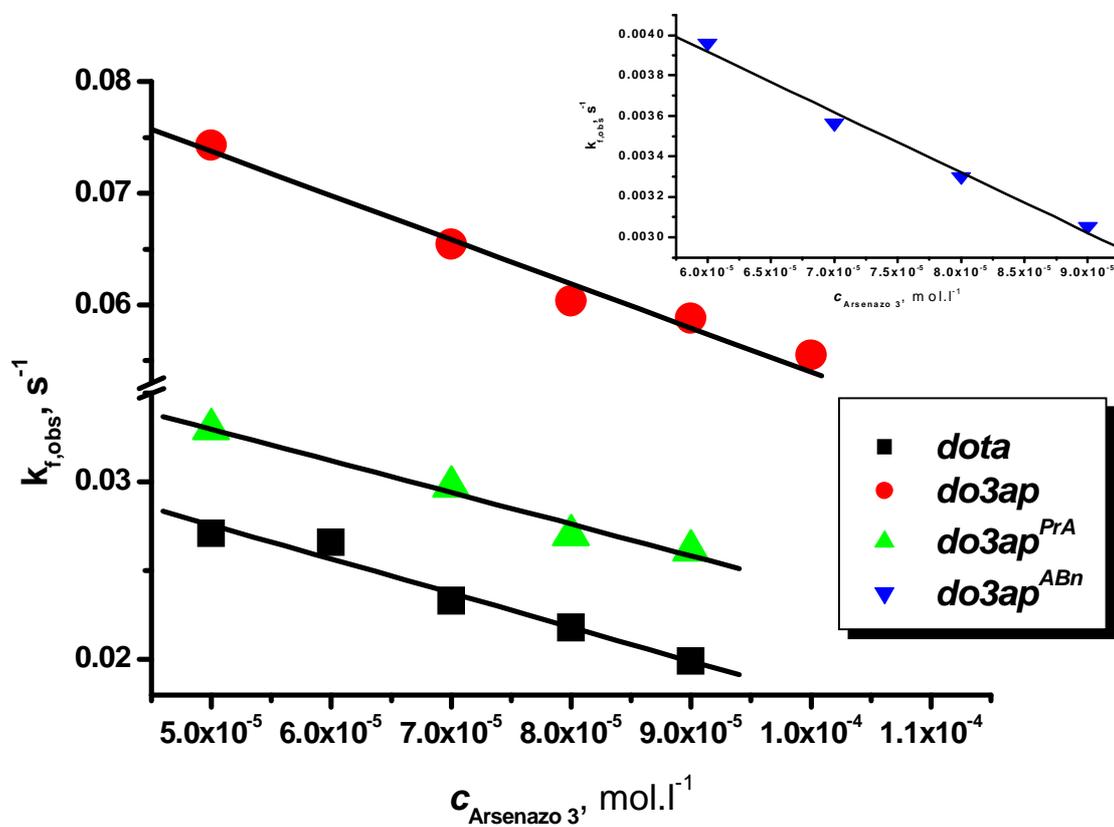


**B**



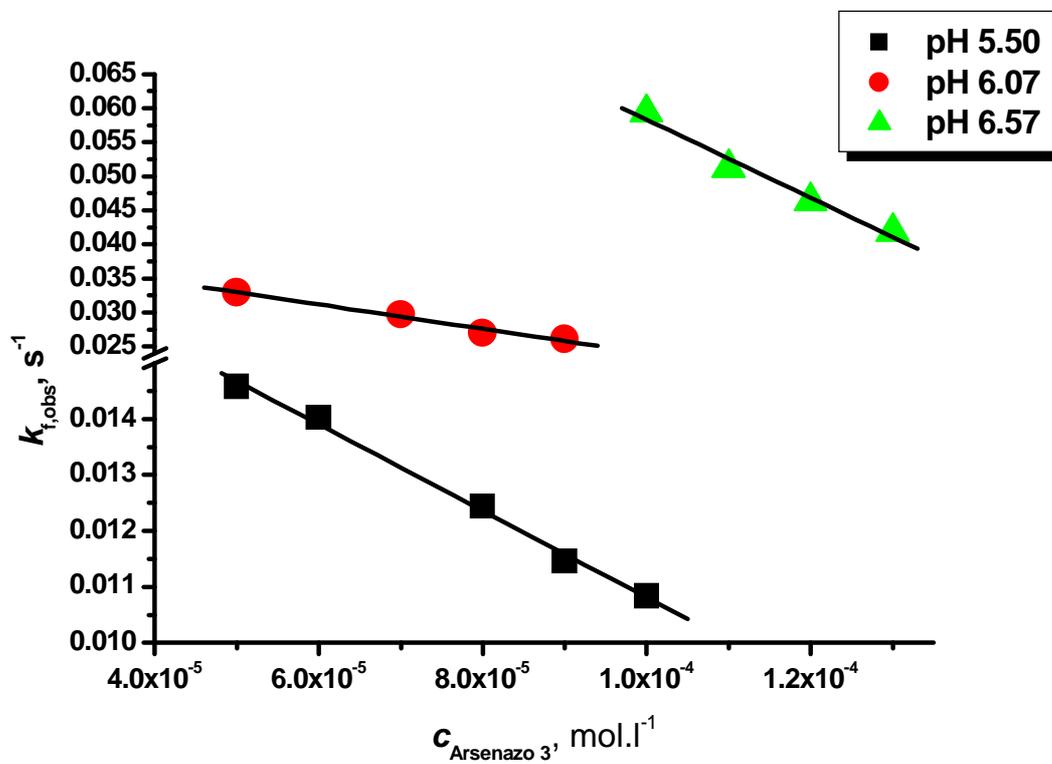
**Figure S2**

An example of the data obtained for the formation of yttrium(III)-macrocycle complexes in the presence of Arsenazo III ( $c_Y = 7.8 \times 10^{-7} \text{ mol dm}^{-3}$ ,  $c_{\text{Lig}} = 1.7 \times 10^{-5} \text{ mol dm}^{-3}$ , pH 6.07).



**Figure S3**

An example of the experimental data obtained for the formation of the yttrium(III) complex of  $\text{H}_5\text{do3ap}^{\text{PrA}}$  in presence of Arsenazo III ( $c_Y = 7.8 \times 10^{-7} \text{ mol dm}^{-3}$ ,  $c_{\text{Lig}} = 1.7 \times 10^{-5} \text{ mol dm}^{-3}$ ) at different pH values.



**Figure S4**

Correlation of rate constant  $k_H$  for dissociation of the yttrium(III) complexes with the first protonation constant of the ligands. The solid line was fitted for all the studied ligands and the dotted line was fitted only through three the most similar ligands ( $H_4dota$ ,  $H_5do3ap^{PrA}$  and  $H_4do3ap^{ABn}$ ).

