



Univerzita Karlova v Praze, Přírodovědecká fakulta

Sekce chemie PŘF UK v Praze
zve všechny zájemce na přednášku z cyklu

Quo Vadis Chemie

Combined NMR and DFT approaches to investigate the solution structure of metal complexes

kterou přednese

Dr. Carlos Platas-Iglesias



pracoviště

**Universidade da Coruña, A Coruña,
Španělsko**

dne **1. prosince** v **15:00 hod.**

**v posluchárně CH2, v budově chemických kateder PŘF UK
Hlavova 8, Praha 2**

Abstrakt: Determining the structure in solution of coordination compounds is important for the rational design of complexes with pre-determined properties. Many metal ions are paramagnetic and, therefore, they induce important paramagnetic shifts in their ^1H and ^{13}C NMR spectra. These paramagnetic shifts encode useful structural information that can be analyzed with the aid of density functional theory (DFT) calculations. Several examples of this combined NMR/DFT approach, applied to complexes of the lanthanide(III) ions and transition metal ions of the *d*-block, will be presented.

