

MS30-O2 Structure and function of coordination compounds for radiopharmaceutical application

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Many dynamic processes occur at the molecular level; thus fundamental understanding of structural behavior, and the associated influence on (kinetic) properties is still of prime importance. Herein we emphasize the continued relevance of small molecule crystallography in coordination chemistry in conjunction with an *integrated* mechanistic approach utilising spectroscopic techniques and specifically reaction kinetics, to counteract trivialized conclusions based on thermodynamic observations alone [1].

We highlight dynamics in small coordination compounds utilised as model radiopharmaceuticals and the importance of structure of the compounds on some functions thereof. The 4th and 5th row elements of the manganese triad, and in particular the ^{99m}Tc, ¹⁸⁸Re, ¹⁸⁶Re isotopes, find widespread application in nuclear medicine [2,3]. Thus, the *fac*-[M(CO)₃]⁺ core (M = ^{99m}Tc, ⁹⁹Tc, ¹⁸⁸Re, ¹⁸⁶Re) is of continued interest due to its potential in biomedical applications since it is a low-valent, low-spin, kinetically inert organometallic core with high *in vivo* stability. It coordinates many types of ligands which determine the hydro- and lipophilic properties.

Many overarching aspects of radiopharmaceuticals are imperative for its successful application; in particular, those associated with and directly influencing the kinetic stability and/or reactivity, and can be quite diverse. It is therefore important to consider these aspects in an overarching approach to enable better understanding and consequent potential more accurate prediction of *in vivo* behavior thereof [1, 3-6].

This presentation will underline some of the above mentioned aspects on small coordination compounds, and illustrate the importance of structure and concurrent different processes/ factors which significantly influence the *kinetics* in metal complexes and the structures thereof, including radiopharmaceutical models.

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MS30-O3 Guest-responsive metal-organic frameworks based on asymmetric bridging ligands

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Polymeric coordination compounds, and their subset metal-organic frameworks (MOFs) have provided a rich source of interest to researchers in solid state functional materials [1]. The inherent porosity achievable for 2D and 3D network structures generated from bridging ligands coordinated to metal ions allows for applications as diverse as catalysis, gas storage, separation and extraction [2]. While interpenetration can sometimes appear as a hindrance to engineering highly porous materials, it may hold some advantages in terms of thermal stability and increased functionality. Examples from our recent work will be presented, including MOFs incorporating Co(II) and Zn(II) with flexible pyridylcarboxylate ligands. These MOFs are robust to solvent loss. New crystalline phases result from the exposure of the empty frameworks to various solvents (Figure 1). The resulting solvatochromism has been correlated to solvent properties [3, 4].

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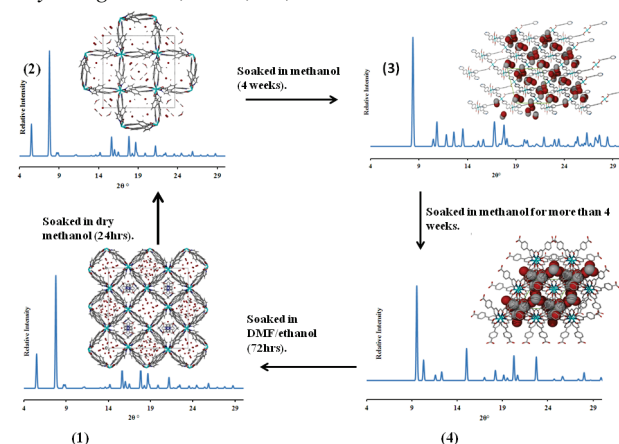


Figure 1. Phase transformations in a Co(II) MOF.

Keywords: MOF, solvatochromism, thermochromism, coordination compound