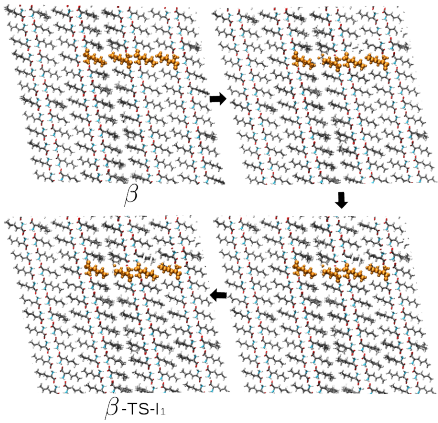

Figure 1. The initial stages of the β to α transition through intermediate state I1 towards the first transition state as obtained by Nudged Elastic Band calculations. A large simulations cell is used to assess the deviations from perfect cooperative motion.

Keywords: phase transitions, molecular dynamics simulations, DL-norleucine, martensitic

MS35-P2 Single Crystal Structures and Spectroscopic Analysis in Metal Complex Dynamics

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Since many dynamic processes (still) occur at the molecular level and at metal cores, fundamental understanding of structural behavior, and the associated influence on (kinetic) properties are of continued and prime importance. In this presentation we emphasize this in conjunction with an *integrated mechanistic approach* to evaluate bonding and reactivity, utilizing small molecule crystal structure data, spectroscopic techniques and reaction kinetics, to counteract trivialized conclusions often based on thermodynamic observations alone [1].

As example, we focus on dynamics in small coordination compounds ustilised as model radiopharmaceuticals, in particular incorporating the ^{99m}Tc, ^{188}Re, ^{186}Re isotopes [2,3]. We discuss some basic characteristics, and the dynamics of the versatile synthon *fac*-$[M^{I}(CO)_3]^+$ and complexes thereof, which include its low-valent, low-spin, kinetically 'inert' organometallic core and the high potential for *in vivo* stability. This starting material and its characteristics must be well understood both in terms of structure and the dynamics therein, before utilization is possible. It coordinates many types of ligands and allows bifunctional chelator ligand design which determines different properties and significantly influences the reactivity in these organometallic molecular materials [1, 3-4].

The above arguments also hold for the dynamics in other processes, in particular homogeneous catalysis [4].

This presentation will underline some of these aspects of small coordination compounds, and illustrate the importance of structure and kinetics and concurrent different processes/ factors which may significantly influence the course of the reaction and the dynamics therein [1, 3-4].

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Keywords: Small Molecules, Reaction Mechanism, Kinetics, Dynamics, Spectroscopy