FAKULTÄT FÜR CHEMIE

universität wien

Einladung zum Vortrag im Rahmen des Fakultätskolloquiums von

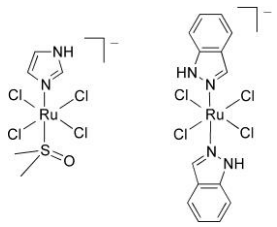
Ass.-Prof. Dr. Dirk Deubel

Institut für Theoretische Chemie der Fakultät für Chemie der Universität Wien

„Quantum Chemical Studies of Metals in Medicine“

The breakthrough of metals in medicine was the discovery and clinical use of cisplatin as an anticancer drug, which increased the cure rate of testicular cancer from nearly 0 to over 90 percent. The therapeutic spectrum of cisplatin is limited, however, as frequent types of cancer are resistant to the drug or become resistant during therapy. Many patients undergo cycles of partial disease remission, resistance, relapse, and treatment with another drug, until further therapy is considered ineffective. Therefore, the search for metal anticancer complexes has continued and extended to complexes of non-platinum metals, most notably ruthenium. Computational studies based on quantum chemical calculations can explore the chemical space and the reactions of metal complexes, because transition structures and activation energies of elementary reaction steps are accessible. We wish to report quantum chemical studies of KP1019 and NAMI-A, two ruthenium(III) complexes being tested in clinical trials. This lecture focuses on the factors controlling the reduction of the Ru(III) anticancer complexes to their Ru(II) analogs, the factors controlling the reactivity of the complexes in both oxidation states to biomolecules, the hypothesis of the intracellular reoxidation of the Ru(II) complexes, and the evaluation of these data to improve our understanding of the mode of action of ruthenium anticancer agents.

Figure 1. NAMI-A (left) and KP1019 (right). Counterions are omitted



Montag, 20. Juni 2016, 16:30 Uhr
Carl Auer von Welsbach Hörsaal
Boltzmanngasse 1, 1090 Wien

Bernhard Keppler Dekan	Lothar Brecker Vizedekan	Veronika Somoza Vizedekanin