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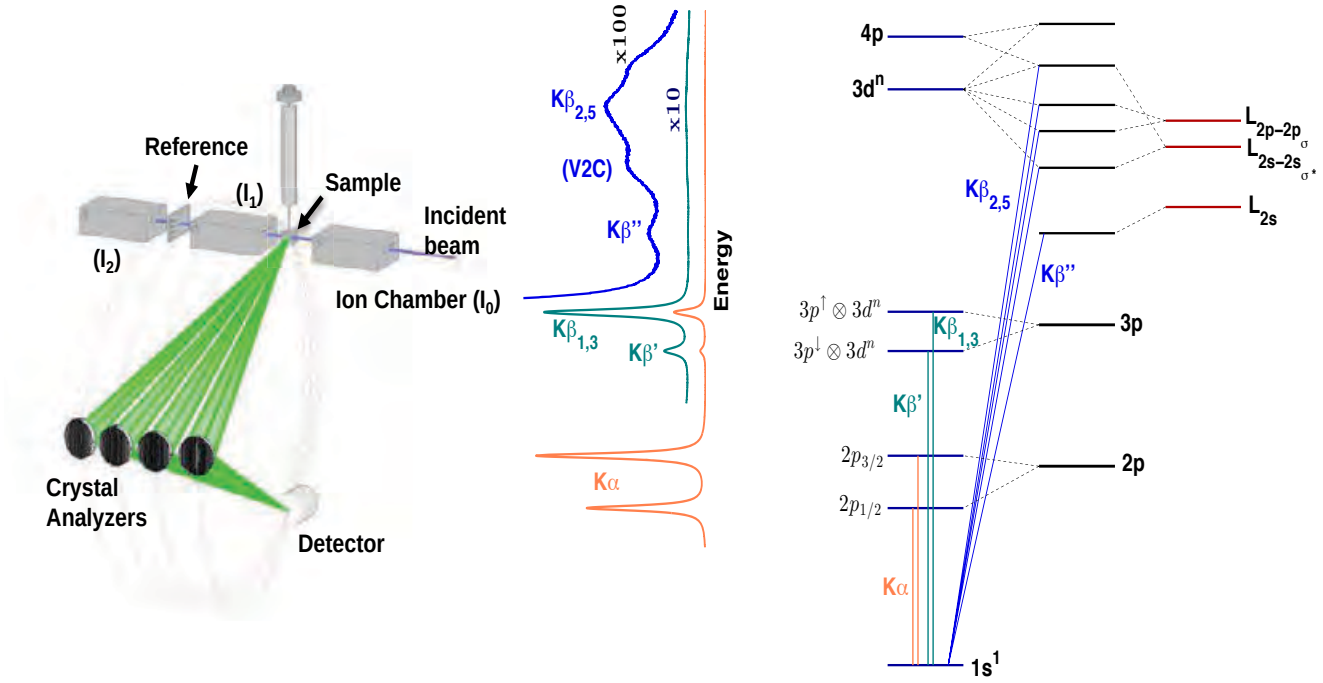
V2C X-Ray Emission Spectroscopy as an Experimental Probe for Ligand Identity

M. Delgado-Jaime[1], S. De Beer[1,2]

[1]*The Max Planck Institute for Chemical Energy Conversion, Muelheim an der Ruhr, Germany,* [2]*Cornell University, Department of Chemistry and Chemical Biology, Ithaca, New York, United States*

The development of valence-to-core (V2C) x-ray emission spectroscopy as an experimental technique for probing the electronic structure of transition metal complexes relevant to catalysis in chemistry and biology has been one of the main focuses of our group. Our level of understanding on this technique has greatly being benefited from DFT calculations based on the single particle model, as implemented in ORCA [1]. The combination of experiment and computations has allowed us to elucidate the underlying fundamental origins of the factors that affect the spectra and has also allowed us to identify specific fingerprints [2] of a diverse number of ligands and protonation states, including the signature of small light atoms in large proteins [3]. A description of the technique will be presented and their applicability will be demonstrated and discussed using different examples.

[1] *F. Neese, Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 73–78,* ***[2]*** *a) M. A. Beckwith, M. Roemelt, M.-N. Collomb, C. DuBoc, T.-C. Weng, U. Bergmann, P. Glatzel, F. Neese and S. DeBeer, Inorganic Chemistry 2011, 50, 8397-8409; b) M. U. Delgado-Jaime, B. R. Dible, K. P. Chiang, W. W. Brennessel, U. Bergmann, P. L. Holland a,* ***[3]*** *K. M. Lancaster, M. Roemelt, P. Ettenhuber, Y. Hu, M. W. Ribbe, F. Neese, U. Bergmann and S. DeBeer, Science 2011, 334, 974-977*



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