ESRF	**Experiment title:** Electronic structure characterization by RIXS spectroscopy of photoactivatable Pt anticancer agents	**Experiment number**: CH-3108
Beamline: 18	**Date of experiment**: from: 21 July 2010 to: 28 July 2010	**Date of report**:
Shifts: ID26 BM26	**Local contact(s)**: Dr. Pieter Glatzel and Kristina Kvashnina	*Received at ESRF:*

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Report: The aim of this proposal was to investigate by X-ray absorption and emission spectroscopy (RIXS/RXES) the electronic structure of a series of Pt(IV) platinum complexes with general formula [Pt(pyridine)2(OH)2(N3)2] **(F)** and [Pt(terpyridine)Cl] **(G)**. These systems have demonstrated high potential as anticancer agents. The experiment was successfully performed thanks to the high quality of the recorded and currently studied data. To summarize, the measurements were performed using the (311) reflections of the Si monochromator for selecting the incident energy and a Si(311) analyzer crystal using the reflection 933 (Bragg angle at 79.16). The combined energy resolution (incident and emitted beam) was 1.2 eV. Because of the dilution of most of the samples we take advantage of a Ketek detector (SDD detector), available at ID26, instead of the avalanche photo diode (APD) adopted in the last beamtimes (see proposal/report CH2988-CH3107). We started measuring at the L$_3$ edge, Pt-based reference materials as PtCl$_4$ and PtCl$_6$, collecting XANES spectra, normal XES spectra (REALLY?) and valence to core (VTC) RXES map. The obtained VTC RXES maps are shown in **Figure 1**. Following the indications obtained from these samples we have measured for **F** and **G** (after careful radiation damage studies) in pellet (diluted and concentrated) the XANES, non-resonant XES spectra and full VTC RXES maps. The radiation damage was avoided (see report CH-3107) and the time per point was keep under the RDT (radiation damage time). The collected VTC map for **F** is shown in **Figure 2**. We studied of the same compound the modification induced on the electronic structure by means of the interaction with different solvents. We measured in distillate water (5mM, 10 mM, 20mM), ethanol (5mM, 10 mM, 20mM), methanol (5mM, 10 mM, 20mM), and isopropyl alcohol (5mM, 10 mM, 20mM). In the case of **G,** in order to improve our knowledge on the interaction with water, we measured our system in different concentrations (5 mM, 10 mM, 20 mM, 40 mM) in order to investigate the modifications of the electronic structure and to compare with the solid (note that in ethanol, methanol and isopropyl the solubility is very low, less than 0.5mM).

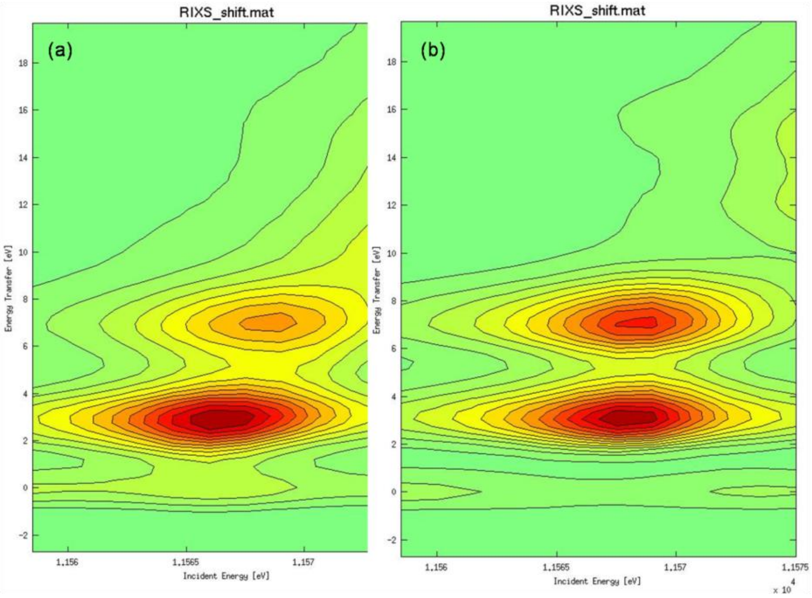

Figure 1. VTC RXES maps for (a) PtCl4 and (b) PtCl6. The measurements were performed on pellets at room temperature

At this point of our analysis we can state that the collected VTC RXES maps evidence interesting differences in the peak positions and structures that have to be understood (**Figure 3)**.

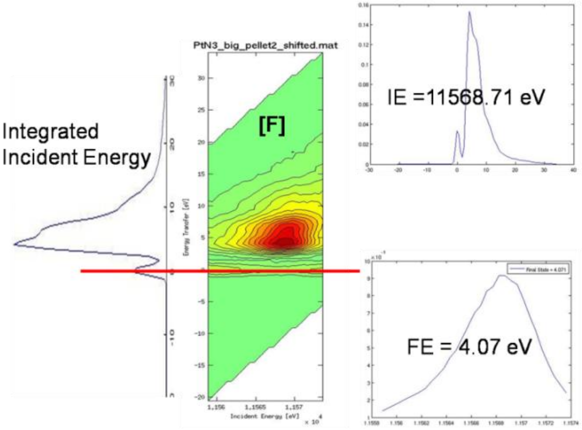

*Figure 2. VTC RXES map for **F** (center), Integrated incident energy (left), fixed incident energy IE (right, top) and final state energy FE (right, bottom)*

At the same edge we also collected XANES, non-resonant XES spectra and full VTC RXES maps for two types of Pt-metallorganic framework (MOF) and a Pt linker. In order to investigate also the edge L_1 edge we changed the crystal using Ge(211) with the reflection (844) and we collected XANES spectra reference compounds and for **F** (pellet concentrated and diluted, different solvent) and **G** (pellet con concentrated and diluted, water) as done previously. Also in this case we collected spectra of the MOF systems. The same procedure was applied for the Lα where Ge(220) crystals were mounted using the reflection (660). The collected data will be interpreted using TDDFT codes and compared with our UV-Vis and measurements.

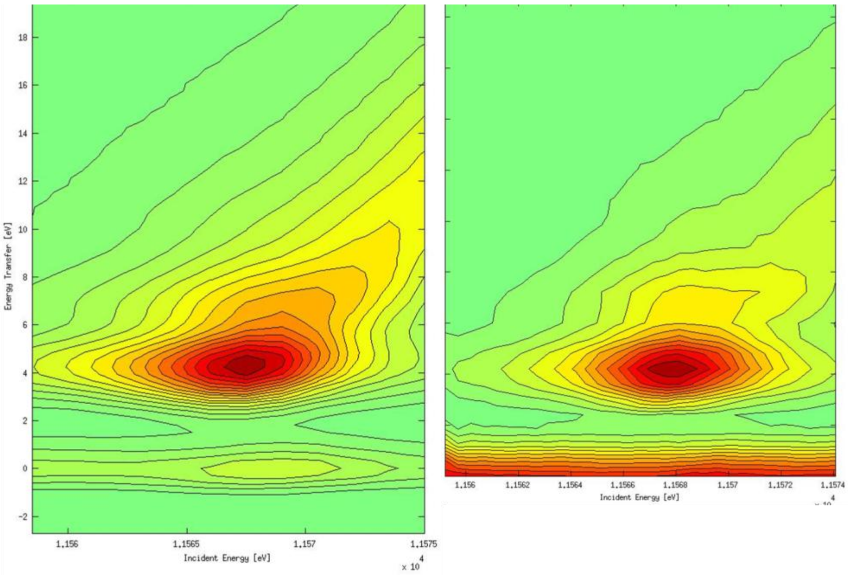

Figure 1.Comparison between G-pellet (left) and G 20mM in distillated water(right)

Acknowledgements: We thank all the staff of ID26 and BM26 for their help.