Platinum complexes with thiourea derivatives as ligands: looking for their bonding scheme

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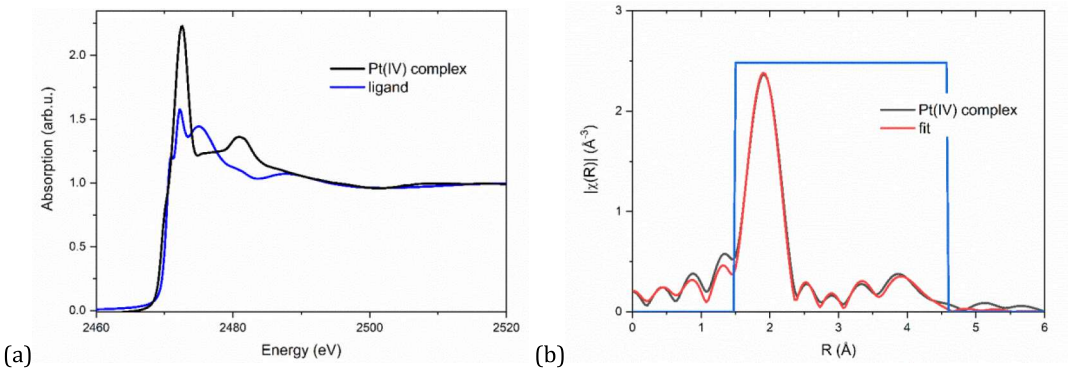
A. Drzewiecka-Antonik[1]*, A. Wolska[1], P. Rejmak[1], D. Szulczyk[2],
A. Maximenko[3] and M. Klepka[1]

[1]*Institute of Physics, Polish Academy of Sciences, 02-668 Warsaw, Poland*
[2]*Medical University of Warsaw, 02-097 Warsaw, Poland*
[3]*SOLARIS National Synchrotron Radiation Centre, 30-392 Krakow, Poland*

*e-mail: adrzew@ifpan.edu.pl

Over the last three decades, there has been increasing interest in platinum complexes with *N,S*- donor ligands as thiourea derivatives. Such complexes may exhibit either higher anticancer activity or reduced toxicity compared to known metal containing drugs, such as cisplatin[1]. Therefore, a series of platinum complexes containing thiourea moieties in their structure was synthesized and their cytotoxicity was assessed. The novel complexes show high activity (IC_{50} ≤10 μM) against human primary colon cancer (SW620) and human breast cancer (MDA-MB-231), while showing no toxicity towards the normal cell line.

The synthesized compounds have been structurally characterized. The metal cation to ligand ratio is 1:1 and the presence of chloride anions (derived from the salt used for synthesis) in their structure has been observed. The Pt L3-edge and Cl K-edge XANES spectra indicated the presence of Pt(IV) and Pt(II) complexes in the analyzed group of compounds. A comparison of S K-edge XANES spectra (Fig. 1a) indicated the coordination of the S atom to the metal cation. The shift of the bands, in the ATR-IR spectra, corresponding to the vibrations of the C=S group within the ligand-complex pair confirmed that ligand coordinate to matal cation via S atom of thiourea moiety. The analysis of Pt L3-edge EXAFS spectra for representative Pt(IV) complex (Fig. 1b) revealed four Cl anions (from inorganic salt) and two S atoms (from organic ligand) around metal cation. Based on experimental data and DFT calculations, the molecular structure of the studied complexes has been proposed.



(a) (b)

Figure 1 (a) Comparison of S K-edge XANES spectra for representative thiourea ligand–Pt(IV) complex pair; (b) EXAFS fitting of the experimental oscillations (black line) and the fitting result (red line).

Acknowledgements: The authors acknowledge SOLARIS Centre for the access to the ASTRA beamline, under the provision of the Polish Ministry of Science and Higher Education project "Support for research and development with the use of research infra-structure of the National Synchrotron Radiation Centre SOLARIS" under contract no. 1/SOL/2021/2.

References

1. Q. Pena et al., Chem. Soc. Rev. 51 (2022) 2544.