Mgr Karolina Dysz

ABSTRACT

In this work sixteen complexes of 7-azaindole and its halo-derivatives (L) - monosubstituted (3-chloro-, 4-chloro-, 3-bromo-, 4-bromo-, 5-bromo-7-azaindole) and disubstituted (3-bromo-4-chloro-7-azaindole and 5-bromo-3-chloro-7-azaindole) with Pt(II) and Pd(II) ions of the formula $[MCl_2(L)_2]$ have been obtained. All investigated complexes of Pd(II) ions with halo-derivatives of 7-azaindole and two complexes of Pt(II) ions with 4-bromo-7-azaindole and 3-bromo-4-chloro-7-azaindole have been synthesized for the first time. The crystal and molecular structures of the 7-azaindole complex with Pd(II) ions and 4-bromo-7-azaindole with Pt(II) ions were confirmed by X-ray analysis. The molecular structures of all *cis*-$[PtCl_2(L)_2]$ and *trans*-$[PdCl_2(L)_2]$ isomers in the solid state were determined using vibrational spectroscopy (FT-IR and FT-Raman) in combination with DFT calculations. On the basis of the calculated potential energy distributions, a full band assignments in the vibrational spectra of these complexes were made.

The crystal and molecular structures, as well as the vibrational spectra of halo-derivatives of 7-azaindole, were also investigated. For the first time, a single crystal X-ray diffraction was performed for four of them: 3-chloro-, 3-bromo- and 4-bromo-7-azaindole as well as 5-bromo-3-chloro-7-azaindole. Theoretical studies of molecular structures and vibrational spectra of monomers and dimers (with N–H···N double hydrogen bonds between pyrrole and pyridine rings) of ligands and their N-deuterated derivatives were carried out using the DFT method. Detailed assignments of bands in the vibrational spectra of isotope isomers were made based on the calculated potential energy distributions.

This work also evaluated the *in vitro* antiproliferative activity of selected ligands and their *cis*-$[PtCl_2(L)_2]$ and *trans*-$[PdCl_2(L)_2]$ complexes on tumour cell lines of various origin and against normal cells. The ligands selected for the research did not show any cytotoxic activity in the tested tumour cell lines, *trans*-$[PdCl_2(L)_2]$ isomers showed low cytotoxicity compared to cisplatin, while *cis*-$[PtCl_2(L)_2]$ isomers were more cytotoxic than cisplatin, although they also showed a strong antiproliferative effect on normal cells compared to cisplatin.

Karolina Dysz

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