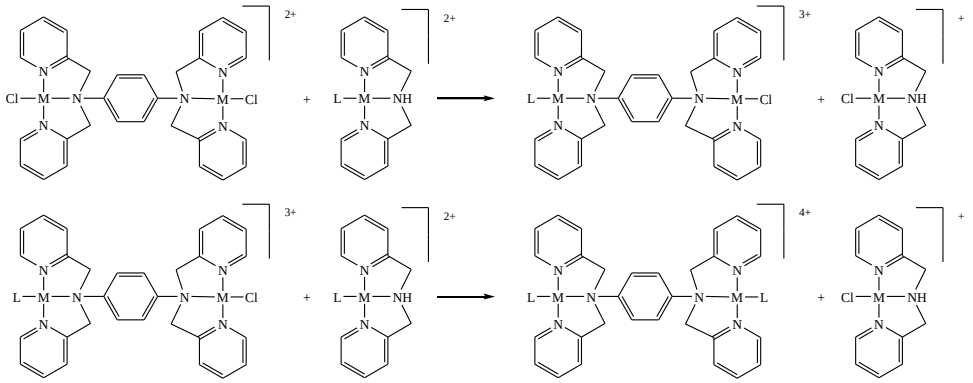
Relative stability of homo- and hetero-bimetallic Pd(II) and Pt(II) complexes compared to their mononuclear analogues

Dušan Ćoćić,[a] Snežana Jovanović,[a] Ralph Puchta,[b] Biljana Petrović[a]

[a] Faculty of Science, University of Kragujevac, Radoja Domanovića 12, P. O. Box 60, 34000 Kragujevac, Serbia; [b] Department of Chemistry and Pharmacy, Faculty of Science, Friedrich-Alexander University Erlangen-Nuremberg, Egerlandstr. 1, 91058 Erlangen, Germany

Notwithstanding the success story of cisplatin, there are number of problems that need to be considered during the treatment of cancer with cisplatin. As a result of these negative properties, research in recent years has focused more on non-classical multinuclear platinum and palladium complexes. [1]

In order to get insight in relative stability of bimetallic palladium(II) and platinum(II) complexes against their mononuclear analogues, we calculated the following model equation:



where M represent Pd(II) and Pt(II), and L stands for Tu, Gua, $S(CH_3)_2$, $HSCH_3$.

The B3LYP functional was used to optimize the geometries and to perform the frequency calculations of the examined systems. In all calculations, def2-SVP basis set was employed. The influence of solvent (water) was evaluated using CPCM formalism [2]. These calculations were performed using the Gaussian 09 program package [3].

Comparing the CPCM-energies of our model equation and considering the reliability of applied DFT method, we tend to consider our bimetallic Pd(II) and Pt(II) complexes and mononuclear analogues as equally stable.

[1] C. Manzotti, G. Pratesi, E. Menta, R.Di Domenico, E. Cavalletti, H.H. Fiebig, L.R. Kelland, N. Farrell, D. Polizzi, R. Supino, G. Pezzoni, F. Zunino, *Clin. Cancer Res.* **2000**, *6*, 2626-2634.

[2] a) V. Barone, M. Cossi, *J. Phys. Chem. A*, **1998**, *102*, 1995–2001.
b) M. Cossi, N. Rega, G. Scalmani, V. Barone, *J. Comput. Chem.*, **2003**, *24*, 669-681.

[3] M. J. Frisch, *et al.*, *Gaussian 09, Revision B.01,* **2009**, Gaussian Inc., Wallingford CT.