Abstract

The formerly reported hydroxyamide $Ph_2PfcC(O)NHCH_2CH_2OH$ **1** and its respective novel congeneric analogues $Ph_2PfcC(O)NHCH_{3-n}(CH_2OH)_n$ (**3**: n = 2; **4**: n = 3) were used to prepare a series of arene-ruthenium(II) complexes $[(\eta^6\text{-arene})RuCl_2(\text{L-}\kappa P)]$ **6-8** (arene = C_6H_6, *p*-cymene, C_6Me_6; L = **1**, **3** or **4**). These complexes were studied as pre-catalysts in redox isomerization of allylic alcohols to carbonyl compounds. Among the compounds prepared, complex **6b** $[(\eta^6\text{-}p\text{-cymene})RuCl_2(\mathbf{1}\text{-}\kappa P)]$ showed best results.

The solid state structure of the product of photolytic decomposition of complex $[(\eta^6\text{-}C_6Me_6)RuCl_2(\mathbf{2}\text{-}\kappa P)]$ (**2** = $Ph_2PfcC(O)N(CH_2CH_2OH)_2$), *viz*, $[(\mu\text{-}Cl)_3\{Ru(\eta^6\text{-}C_6Me_6)\}_2][FeCl_4]$ **9**, was determined by single-crystal X-ray diffraction analysis.

The bis-phosphane complexes $[M^{II}Cl_2(\mathbf{1}\text{-}\kappa P)_2]$ (M = *trans*-Pd (**10**), *cis*-Pt (**11**) and *trans*-Pt (**12**)) together with chalcogenide derivatives $Ph_2P(O)fcC(O)NH(CH_2)_2OH$ (**13**) and $Ph_2P(S)fcC(O)NH(CH_2)_2OH$ (**14**) derived from hydroxyamide **1** were tested *in vitro* for their cytotoxicity against human ovarian A2780 cancer cell line. Complexes tested showed moderate cytotoxicity.

Triol-amide $FcC(O)NHC(CH_2OH)_3$ **15** (Fc = ferrocenyl) reacted with decavanadate $(Bu_4N)_2[H_3V_{10}O_{28}]$ at elevated temperature and prolonged reaction time yielding the hybrid hexavanadate $(Bu_4N)_2[\{FcC(O)NHC(CH_2O)_3\}_2V_6O_{13}]$ **16** capped with the redox-active ferrocenyl pendants. The novel compound was thoroughly studied by standard spectral methods, X-ray diffraction analysis, cyclic voltammetry and theoretical calculations. Single-point DFT calculations performed for the isolated hexavanadate anion gave an insight into the bonding scheme within hexavanadate cage and offered an explanation for electrochemical behavior of the compound.

Conjugation of 1′-(diphenylphosphanyl)ferrocene-1-carboxylic acid (Hdpf) with ω-aminosulfonic acids $H_2N(CH_2)_nSO_3H$ (n = 1-3) afforded amidosulfonates $(Et_3NH)[Ph_2PfcCONH(CH_2)_nSO_3]$ (**17**: n = 1, **18**: n = 2, **19**: n = 3; fc = ferrocene-1,1′-diyl), isolated as the respective triethylammonium salts. These ligands were employed in the synthesis of palladium(II) complexes *trans*-$[PdCl_2(\text{L-}\kappa P)_2]$ (**23**: L = **17**; **24**: L = **18**; **25**: L = **19**) which, in turn, were probed as defined pre-catalysts for aqueous cyanation of aryl bromides with potassium hexacyanoferrate(II).

Keywords: Ferrocene; Phosphane ligands; Aqueous catalysis; Theoretical calculations; Anticancer properties; Polyoxovanadates ; Structure elucidation.