Poster Presentation

MS83.P19

Two new platinum complexes containing a chelating safrole-derivative and amine

P. Kimpende[1,3], N. Dinh[2], T. Huan[2], D. Toan[2], L. Van Meervelt[3]

[1]*University of Kinshasa, Chemistry Department, Kinshasa, D. R. Congo,,* [2]*Hanoi National University of Education, Department of Chemistry, Hanoi, Vietnam,* [3]*KU Leuven, Chemistry Department, Heverlee, Belgium*

A series of new platinum(II) complexes containing chelating safrole (or its derivatives) and various amines have been synthesized to evaluate their anticancer activity. Here we report the structure determination of [Pt((MeO)2Ph)(o-toluidine)Cl] (1) and [Pt((MeO)2Ph)(piperidine)Cl] (2), with (MeO)2Ph 3,4-dimethoxyphenyl-2-propene. Plate-like crystals of (1), suitable for x-ray diffraction measurement were obtained by slow evaporation from an ethanol solution. Rod-like crystals of (2) were harvested from ethanol after slow evaporation of acetone from an ethanol-acetone solution. Diffraction data were collected on a diffractometer equipped with a Bruker-AXS SMART 6000 CCD detector and integrated by the program SAINT. A multi-scan absorption correction was performed by the program SADABS. Both structures were solved by direct methods using the SHELXS program and refined according to the least-squares method to R-values of for 0.0204 (1) and 0.0280 for (2). The crystal of (1) to the orthorhombic space group P212121 and that of (2) belongs to the triclinic space group P-1. The asymmetric unit of (1) comprises one molecule of [Pt((MeO)2Ph)(o-toluidine)Cl]. The asymmetric unit of (2) consists of one ethanol molecule and one [Pt((MeO)2Ph)(piperidine)Cl] molecule. Both structures are similar with respect to the configuration and geometry of the Pt complex. Considering the centroid Cg of the allyl C=C bond as one ligand, the coordination geometry of Pt is square planar (other ligands are Cl, N (amine) and C (phenyl ring)). The angle between the best planes through the (MeO)2Ph and amine ligands is 84.3(1)° in (1) and 25.2(5)° in (2). The best plane through the allyl group makes an angle of 55.6(2)° and 56.4(4)° with the best plane through the (MeO)2Ph group, respectively in (1) and (2). The allyl double bond C=C is nearly perpendicular to Pt—Cg line, 89.8(2)° in (1) and 87.4(8)° in (2). For (1) the packing is essentially the result of van der Waals' interactions and two weak hydrogen bonds of type C-H...Cl and C-H...O. In (2) the packing is determined by the O-H...O hydrogen bond (O...O distance 2.870(4) Å) between ethanol and one of the methoxy substituents.

[1] *T.T. Da, Young-Mi Kim, N. T. Thanh, et al., Organometallics, 2008, 27(14), 3611-3613,* ***[2]*** *T.T. Da, L.X. Chien, N.T. Thanh Chi, et al., Journal of Coordination Chemistry, 2012, 65(1), 131-142.,* ***[3]*** *M.J. Hickey, The Journal of Organic Chemistry, 1948,13(3), 443-446*

Keywords: Platinum(II) complex, Safrole derivative, Anticancer activity