Solution and solid state NMR studies of some selenium analogues of auranofin (an anti-arthritic gold drug). Wazeer, Mohammed I. M.; Isab, Anvarhusein A.; Ahmad, Saeed. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. Journal of Coordination Chemistry (2005), 58(5), 391-398. Publisher: Taylor & Francis Ltd.

Abstract

Three mixed ligand complexes of Au(I) with phosphines and selenones, [Et3PAu(Se:C<)]Br [Se:C< = imidazolidine-2-selenone (ImSe), N-methylimidazolidine-2-selenone (MeIMSe), 1,3-diazinane-2-selenone (DiazSe)] as analogs of auranofin (Et3PAuSR) were prepd. and characterized by elemental anal., IR and NMR methods. A decrease in the IR frequency of the C:Se mode of selenones upon complexation is indicative of selenone binding to Au(I) via a selenone group. An upfield shift in 13C NMR for the C:Se resonance of the selenones and downfield shifts in 31P NMR for the R3P moiety are consistent with the Se coordination to Au(I). 13C solid state NMR shows the chem. shift difference between free and bound selenone to Au(I) for ImSe and DiazSe to be .apprx.10 and 17 ppm resp. Large 77Se NMR chem. shifts (55 ppm) upon complexation in the solid state for [Et3PAuDiazSe]Br compared to [Et3PAuImSe]Br (10 ppm) indicates the former to be more stable and the Au-Se bond to be stronger than in the latter complex.