An analysis of spectroscopic signatures, DFT calculations and anti-bacterial activity of newly synthesized Cu(II) and Pd(II) complexes of 2-aminoquinolin-8-ol and 2-(naphthalen-1-ylmethyl)-4,5-dihydro-1*H*-imidazole

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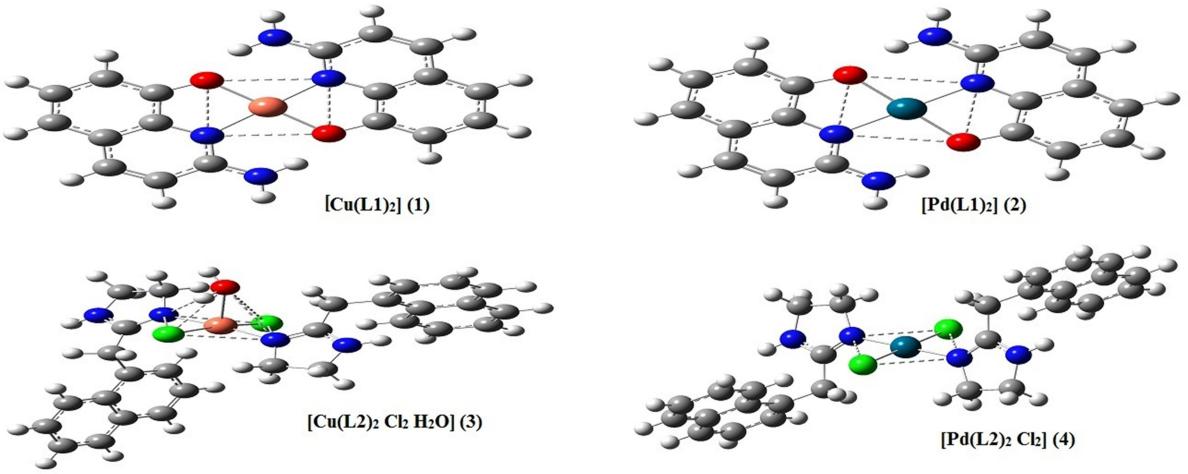

Abstract

Copper(II), Palladium(II) complexes [Cu(L1)2] (1), [Pd(L1)2] (2), [Cu(L2)2Cl2.H2O] (3), [Pd(L2)2Cl2] (4), of 2-aminoquinolin-8-ol (L1) and 2-(naphthalen-1-ylmethyl)-4,5-dihydro-1*H*-imidazole (L2) were synthesized and physico-chemically characterized by spectroscopic techniques like IR, UV-Visible and elemental analysis. The structures of the ligands and their complexes were optimized by density functional theory (DFT) method using B3LYP/6-311++G(d,p) basic set for L1 and L2 and B3LYP/LanL2DZ basic set for 1, 2, 3 and 4, respectively. The bond lengths and bond angles of complexes were compared with the literature values which were in good agreement. The results revealed that 1, 2 and 4 complexes were in square planar geometry and square pyramidal geometry for complex 3. Frontier orbital analysis and global reactivity parameters were also computed at same basic set in the same phase. In

addition, DOS and COOP analysis were also performed using Gauss Sum 3.0 programme for compound 4. All the ligands and complexes were screened for anti-bacterial activity and the metal complexes exhibited highest anti-bacterial activity when compared to ligands.
Keywords: Cu(II), Pd(II) complexes, DFT studies, anti-bacterial activity