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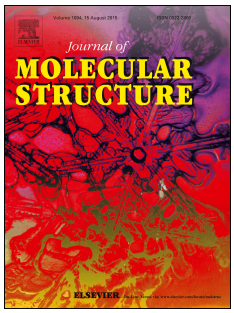

Pd (II) complexes of bidentate chalcone ligands: Synthesis, spectral, thermal, antitumor, antioxidant, antimicrobial, DFT and SAR studies

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Pd (II) Complexes of Bidentate Chalcone Ligands: Synthesis, Spectral, thermal, Antitumor, Antioxidant, Antimicrobial, DFT and SAR Studies

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Abstract

The ligation behavior of two chalcone ligands namely, (E)-3-(4-chlorophenyl)-1-(pyridin-2-yl)prop-2-en-1-one (L^1) and (E)-3-(4-methoxyphenyl)-1-(pyridin-2-yl)prop-2-en-1-one (L^2), towards the Pd(II) ion is determined. The structures of the complexes are elucidated by elemental analysis, spectral methods (IR, electronic and NMR spectra) as well as the conductance measurements and thermal analysis. The metal complexes exhibit a square planar geometrical arrangement. The kinetic and thermodynamic parameters for some selected decomposition steps have been calculated. The antimicrobial, antioxidant and anticancer activities of the chalcones and their Pd(II) complexes have been evaluated. Molecular orbital computations are performed using DFT at B3LYP level with 6-31+G(d) and LANL2DZ basis sets to access reliable results to the experimental values. The calculations are performed to obtain the optimized molecular geometry, charge density distribution, extent of distortion from regular geometry. Thermodynamic parameters for the investigated compounds are also studied. The calculations confirm that the investigated complexes have square planner geometry, which is in a good agreement with the experimental observation.

Keywords: Chalcone, Pd(II) complexes, Antimicrobial, antioxidant, anticancer activity, Molecular modeling

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