MS30-P24 Molecular and crystal structures of hydroxyl and ester functionalized N-heterocyclic carbene complexes of iridium(I)

Merve İzmirli[1], Aytaç G. Gökçe[1], Derya Gülcemal[2], Süleyman Gülcemal[2], Muhittin Aygün[1]

1. Department of Physics, Dokuz Eylul University, 35160 Buca, İzmir, Turkey.
2. Department of Chemistry, Ege University, 35100 Bornova, İzmir, Turkey

email: muhittin.aygun@deu.edu.tr

Because of their extraordinary properties, N-heterocyclic carbenes (NHCs) have found access to a great variety of catalytic processes which include C-C coupling reactions, formation of furans, cyclopropanation, olefin metathesis, hydroformylation, polimerization and hydrosilylation reactions.[1-5] The crystal and molecular structures of Ir(I) NHC complexes have been determined by single crystal x-ray diffraction technique. In both complexes, the coordination geometries around the iridium centers, formed by the coordination to the metal of the two olefinic bonds of the cyclooctadiene ligand, the carbon atom of the NHC ligand and the chlorine atom, are slightly distorted square-planar (Figure 1). The Ir–C(NHC) distances are within the expected range and consistent with other NHC-supported [Ir(COD)Cl] complexes.

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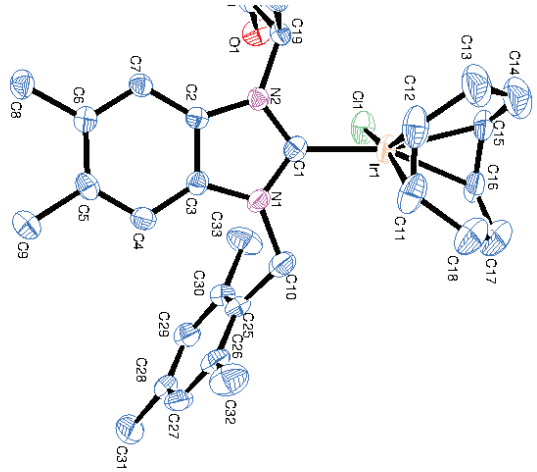

Figure 1. The molecular structure of the complex with displacement ellipsoids drawn at the 30% probability level and hydrogen atoms have been omitted for clarity.

Keywords: N-heterocyclic carbene, Ir(I) complex, hydroxyl and ester functionalization, crystal structure