PS07.00.50 STRUCTURE OF A NEW HYDRIODO-(METHOXO)-IRIDIUM(III) COMPLEX RELATED TO CATALYTIC REDUCTION OF ALKynes. Tsunetake Yamagata, Kazumide Tani, Department of Chemistry, Faculty of Engineering Science, Osaka University

Hydrido(alkoxy) complexes of transition metals play important roles of catalytic processes involving hydride transfer and alcohol homologation. Here we will report the preparation and structural characterization of a new dinuclear hydrido(methoxy-iridium(III) complex.

The hydrido(methoxy) complex, [Ir2(η6-bis-methoxy)(η6-O2CMe2)(η6-O2CN(Me))]2+, was prepared by treating [Ir2(η6-bis-methoxy)(η6-O2CNMe)]Cl with NaOMe. The complex co-crystallized with MeOH and was obtained as yellow needles.

The structure was determined by X-ray diffraction. The complex is sevenfold coordinated to the iridium(I) atoms, with two methoxy groups, two carbonyl groups, and three methanol molecules.

In contrast to the anionic coordination compounds, a series of compounds exist from β-diketones in which the iridium atom forms cation or neutral complexes. We have determined two crystal structures which contain the central Bq4-tetrahedron.


In complex I the boron atom is coordinated to one dioxy ligand and one Bβ-diketone ligand. The boron-oxygen tetrahedron is due to the unequal B-O bond lengths, symmetrical distorted. Bond lengths are B-O(alkoxy) 1.46(3) Å, B-O(keto) 1.49(3) Å, C-O(keto) 1.50(3) Å, C-O(alkoxy) 1.296(5) Å. Bond angles are O on B from 107.4(6)° to 110.7(3)°.

In the structure II the four O atoms adopt an almost perfect tetrahedral arrangement about the boron with bond lengths B-O mean 1.46(1) Å, bond angles O-B-O are between 107.6(2)° and 112.5(2)°. Bond lengths O-C are 1.31 (2) Å. All heterocycles in both compounds are non-planar.


Our thanks are due to O.Krookfich from the University of Vladivostok for the supply of complexes I and II for re-crystallization.