CRYSTAL STRUCTURE OF (ACETYLACETONATO) (DICARBONYL)IRIDIUM(I)

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The structure of $Ir(CO)_2(acac)$ is determined by XRD at room temperature. Crystallographic data for $C_7H_7IrO_4$ are: $a = 6.4798(5)$ Å, $b = 7.7288(5)$ Å, $c = 9.1629(10)$ Å, $\alpha = 105.738(2)°$, $\beta = 90.467(3)°$, $\gamma = 100.658(2)°$, space group $P\bar{1}$, $V = 433.24(6)$ Å^3, $Z = 2$, $d_{calc} = 2.662$ g/cm^3, $R = 0.0167$. The structure is built of isolated mononuclear molecules. The central iridium atom has a square coordination environment formed by two oxygen atoms that belong to the acetylacetonate ligand and two carbon atoms of carbonyl groups. The average Ir–O and Ir–C bond lengths are 2.045(3) Å and 1.832(6) Å respectively. Molecules are stacked in such a way that the planes of coordination squares turn out to be parallel to the Ir…Ir distances between the nearest neighbors in the stack of 3.242 Å and 3.260 Å.

Keywords: iridium(I), acetylacetone, carbonyl, XRD.