$Ru_3(CO)_{12}$. Why D_{3h}?

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$M_3(CO)_{12}$ (M= Fe, Ru, Os) may, in theory, adopt D_3, D_{3h}, C_{2v} symmetries. Iron carbonyl has a C_{2v} structure, ruthenium and osmium carbonyls have D_{3h} structures and only their derivatives show the least hindered D_3 configuration. The D_{3h} structure of $Ru_3(CO)_{12}$ has been justified theoretically using steric or electronic parameters. Only a marginal attention was paid to the deformation of axial CO groups, and it has been attributed to steric repulsion among oxygen atoms or to a more efficient orbital superposition between Ru atoms and C atoms. X-ray intensities of a $Ru_3(CO)_{12}$ crystal have been collected at low temperature and to them a multipole analysis has been applied; the electron density distribution obtained has been studied with the QTAIM and the topological and energetic parameters of intra- and inter-molecular interactions have been determined. Significant $C_{ax}\cdots C_{ax}$ interactions have been detected. The unexpected features of experimental electron density maps will be discussed.

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