Darstellung, Kristallstruktur, Schwingungsspektren und Normalkoordinatenanalyse von $[Os(acac)_3]$

Synthesis, Crystal Structure, Vibrational Spectra, and Normal Coordinate Analysis of $[Os(acac)_3]$

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Tris(acetylacetonato)osmium(III), Crystal Structure, IR Data, Raman Data, Normal Coordinate Analysis

In the reaction of $K_2[OsCl_6]$ with boiling water/acetylacetone (1:1) a mixture of different chloro-acetylacetonato complexes is formed, from which $[Os(acac)_3]$ can be isolated by column chromatography with dichloromethane on silica gel. The crystal structure of $[Os(acac)_3]$ (monoclinic, space group $P2_1/c$, $a = 13.968(5)$, $b = 7.517(5)$, $c = 16.455(5)$ Å, $\beta = 98.939(5)^\circ$, $Z = 4$) has been determined by single crystal X-ray diffraction analysis. High resolution IR and Raman spectra were measured at low temperature (10 K). Based on the molecular parameters of the X-ray structure determination a normal coordinate analysis has been performed and the normal modes of vibration have been assigned. With a set of 32 force constants, taking into account the intraligand vibrations, a good agreement between observed and calculated frequencies has been achieved. The valence force constants are $f_d(OsO) = 3.19$ and $f_d(OC) = 6.74$ mdyn/Å.

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