

Darstellung und Schwingungsspektren von *cis*- und *trans*-[OsXY(acac)₂], X ≠ Y = Cl, Br, I sowie Normalkoordinatenanalyse von *trans*-[OsClBr(acac)₂]

Synthesis and Vibrational Spectra of *cis*- and *trans*-[OsXY(acac)₂], X ≠ Y = Cl, Br, I, and Normal Coordinate Analysis of *trans*-[OsClBr(acac)₂]

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Dihalogeno-bis(acetylacetonato)osmium(IV), IR Data, Raman Data,
Normal Coordinate Analysis, *trans* Influence

In the reaction of K₂ [OsX₃ Y₃] with boiling water/acetylacetonone (1:1) the six mixed complexes *cis*- and *trans*-[OsX₂(acac)₂] (X ≠ Y = Cl, Br, I) are formed, which have been purified by column chromatography with toluene on silica gel. The IR and Raman spectra (10 K) show the intraligand vibrations of the acac groups with nearly constant frequencies and the stretching vibrations of OsO in the range 460-696, of OsCl at 315-345, of OsBr at 210-225, and of OsI at 160-175 cm⁻¹. A normal coordinate analysis based on a modified valence force field was performed for *trans*-[OsClBr(acac)₂] and the vibrational modes 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_l (OsCl[•]) = 1.75, f_d(OsBr') = 1.63 and f_d (OsO) = 3.27 mdyne/Å.

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