Kristallstrukturen, ^{195}Pt-NMR-Verschiebungen, Schwingungsspektren und Normalkoordinatenanalysen von *trans*-Dihalogeno-bis(oxalato)platinaten(IV), *trans*-$[PtX_2(ox)_2]^{2-}$, X = Cl, Br, I

Crystal Structure, ^{195}Pt NMR Chemical Shifts, Vibrational Spectra, and Normal Coordinate Analyses of *trans*-Dihalogeno-bis(oxalato)platinates(IV), *trans*-$[PtX_2(ox)_2]^{2-}$, X = Cl, Br, I

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trans-Dichloro-bis(oxalato)platinate(IV), *trans*-Dibromo-bis(oxalato)platinate(IV), *trans*-Diiodo-bis(oxalato)platinate(IV), Crystal Structure, Vibrational Spectra

By reaction of $(n\text{-}Bu_4N)_2[Pt(ox)_2]$ with elemental halogens in dichloromethane the complexes *trans*-$[PtX_2(ox)_2]^{2-}$ (X = Cl, Br, I) are formed. The crystal structures of *trans*-$(py_2CH_2)[PtCl_2(ox)_2]\cdot C_4H_6O_3$ (**1**) (monoclinic, space group $P2_1/n$, a = 12.119(3), b = 14.926(2), c = 12.666(4) Å, β = 91.26(3)°, Z = 4), *trans*-$(py_2CH_2)[PtBr_2(ox)_2]$ (**2**) (monoclinic, space group $P2_1/n$, a = 7.402(8), b = 16.997(3), c = 14.898(3) Å, β = 98.15(3)°, Z = 4) and *trans*-$(py_2CH_2)[PtI_2(ox)_2]\cdot C_3H_7NO$ (**3**) (orthorhombic, space group Pnma, a = 10.380(9), b = 13.973(2), c = 17.440(4) Å, Z = 4) have been determined by single crystal X-ray diffraction analysis. Highly resolution IR and Raman spectra were measured at low temperature (10 K). Using the molecular parameters of the X-ray determinations normal coordinate analyses based on a modified valence force field have been performed and the normal modes of vibration are assigned. The valence force constants are f_d(PtCl) = 2.19, f_d(PtBr) = 1.68, f_d(PtI) = 1.28 mdyn/Å and f_d(PtO) ranges from 2.71 to 2.82 mdyn/Å. The observed ^{195}Pt NMR shifts are $\delta(^{195}Pt)$ = 6472.4 (X = Cl), 6027.1 (Br) and 5142.7 ppm (I).

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