Kristallstrukturen und Normalkoordinatenanalyse von *trans*-$(n\text{-}Bu_4N)_2[ReCl_4IX]$, X = NCS, NCSe

Crystal Structures and Normal Coordinate Analyses of *trans*-$(n\text{-}Bu_4N)_2[ReCl_4IX]$, X = NCS, NCSe

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trans-Tetrachloromonoiodothiocyanato(N)-rhenate(IV), *trans*-Tetrachloro-monoiodoselenocyanato(N)-rhenate(IV),
Crystal Structure, Normal Coordinate Analysis

The crystal structures of *trans*-$(n\text{-}Bu_4N)_2[ReCl_4I(NCS)]$ (triclinic, space group $P\bar{1}$, a = 11.268(3), b = 11.696(2), c = 18.109(3) Å, α = 98.68(2) β = 106.40(2), γ = 97.58(2)°, Z = 2) and *trans*-$(n\text{-}Bu_4N)_2[ReCl_4I(NCSe)]$ (orthorhombic, space group $P\,2_12_12_1$, a = 11.839(2), b = 12.2679(10), c = 31.136(5) Å, Z = 4) have been determined by single crystal X-ray diffraction analysis. Based on the molecular parameters of the X-ray determinations the low temperature (10 K) IR and Raman spectra of the $(n\text{-}Bu_4N)$ salts have been assigned by normal coordinate analysis. The valence force constants are f_d(ReN) = 1.69(NCS) and 1.65(NCSe) mdyn/Å.