Kristallstrukturen, Schwingungsspektren und Normalkoordinatenanalyse von *cis*-$[ReCl_4X_2]^{2-}$, X = NCS, NCSe

Crystal Structures, Vibrational Spectra and Normal Coordinate Analysis of *cis*-$[ReCl_4X_2]^{2-}$, X = NCS, NCSe

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cis-Tetrachlorodi[thiocyanato(N)]-rhenate(IV), *cis*-Tetrachlorodi[selenocyanato(N)]-rhenate(IV), Crystal Structure, Vibrational Spectra, Normal Coordinate Analysis

The crystal structures of *cis*-$(n\text{-}Bu_4N)_2[ReCl_4(NCS)_2]$ (triclinic, space group $P\bar{1}$, a = 11.245(1), b = 20.174(3), c = 21.320(8) Å, α =109.06(2), β = 96.46(2), γ = 98.22(5)°, Z = 4) and *cis*-$(Ph_4P)_2[ReCl_4(NCSe)_2]\cdot 2CH_2Cl_2$ (triclinic, space group P1, a = 10.341(2), b = 13.436(3), c = 19.616(4) Å, α = 92.70(2), β = 92.02(2), γ = 89.99(1)°, Z = 2) have been determined by single crystal X-ray diffraction analysis. Both ambidentate ligands NCS and NCSe are bonded via the N atom. Using the molecular parameters of the X-ray determinations the low temperature (10 K) IR and Raman spectra of the (n-Bu_4N) salts have been assigned by normal coordinate analysis based on a modified valence force field. The valence force constants f_d(ReN) are 1.78(NCS) and 1.79(NCSe) mdyn/ Å.

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