Kristallstrukturen, Schwingungsspektren und Normalkoordinatenanalyse von *cis*- und *trans*-$[ReCl_4(NCSe)(SeCN)]^{2-}$

Crystal Structures, Vibrational Spectra, and Normal Coordinate Analysis of *cis*- and *trans*-$[ReCl_4(NCSe)(SeCN)]^{2-}$

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cis-Tetrachloroselenocyanato(N)-selenocyanato(Se)-rhenate(IV),
trans-Tetrachloroselenocyanato(N)-selenocyanato(Se)-rhenate(IV),
Crystal Structure, Vibrational Spectra, Normal Coordinate Analysis

The crystal structures of *cis*-$(n\text{-}Bu_4N)_2[ReCl_4(NCSe)(SeCN)]$ (monoclinic, space group P $2_1/n$ a = 10.794(3), b = 11.687(3), c = 35.716(4) Å, β = 96.97(1)°, Z = 4) and *trans*-$(CH_2Py_2)[ReCl_4(NCSe)(SeCN)]$ (monoclinic, space group P $2_1/c$, a = 8.348(2), b = 7.518(1), c = 31.295(7) Å, β = 97.12(2)°, 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 $f_d(ReN)$ = 1.68 and $f_d(ReSe)$ = 1.15 mdyn/Å.

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