

Darstellung, Schwingungsspektren und Normalkoordinatenanalyse von bindungsisomeren Halogenoselenocyanatorhenaten(IV) sowie Kristallstrukturen von *mer*-(Ph₄P)₂[ReCl₃(NCSe)₂^{cis}(SeCN)] und *mer*-(*n*-Bu₄N)₂[ReCl₃I(NCSe)₂^{cis}]

Synthesis, Vibrational Spectra and Normal Coordinate Analysis of Linkage Isomeric Halogenoselenocyanatorhenates(IV) and Crystal Structures of *mer*-(Ph₄P)₂[ReCl₃(NCSe)₂^{cis}(SeCN)] and *mer*-(*n*-Bu₄N)₂[ReCl₃I(NCSe)₂^{cis}]

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fac-Trichlorotriselenocyanato(N)-rhenate(IV), *mer*-Trichloro-*cis*-diselenocyanato(N)-selenocyanato(Se)-rhenate(IV), *mer*-Trichloromonoiodo-*cis*-diselenocyanato(N)-rhenate(IV), Crystal Structure, Normal Coordinate Analysis

By treatment of *fac*-[ReCl₃I₃]²⁻ with (SeCN)₂ in dichloromethane *fac*-[ReCl₃(NCSe)₃]²⁻ (**1**), *mer*-[ReCl₃(NCSe)₂^{cis}(SeCN)]²⁻ (**2**) and *mer*-[ReCl₃I(NCSe)₂^{cis}]²⁻ (**3**) are formed which have been separated by ion exchange chromatography on diethylaminoethyl cellulose. The crystal structures of *mer*-(Ph₄P)₂[ReCl₃(NCSe)₂^{cis}(SeCN)] (triclinic, space group P $\bar{1}$, *a* = 16.099(1), *b* = 16.729(3), *c* = 21.026(2) Å, α = 70.194(10), β = 73.958(10), γ = 83.929(10)°, *Z* = 4) and *mer*-(*n*-Bu₄N)₂[ReCl₃I(NCSe)₂^{cis}] (monoclinic, space group P2₁/c, *a* = 11.838(1), *b* = 12.796(2), *c* = 30.767(2) Å, β = 97.419(6)°, *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*-Bu₄N) salts have been assigned by normal coordinate analysis. The valence force constants are *f*_q(ReN) = 1.79 (**1**), 1.71 (**2**), 1.71 (**3**) and *f*_q(ReSe) = 1.15 (**2**) mdyn/Å.