

Kristallstrukturen, Schwingungsspektren und Normalkoordinatenanalyse von *cis*-(*n*-Bu₄N)₂[ReBr₄(NCS)(SCN)], *trans*-(*n*-Bu₄N)₂[ReBr₄(NCS)(SCN)] und *trans*-(*n*-Bu₄N)₂[ReBr₄(NCSe)(SeCN)]

Crystal Structures, Vibrational Spectra and Normal Coordinate Analyses of *cis*-(*n*-Bu₄N)₂[ReBr₄(NCS)(SCN)], *trans*-(*n*-Bu₄N)₂[ReBr₄(NCS)(SCN)] and *trans*-(*n*-Bu₄N)₂[ReBr₄(NCSe)(SeCN)]

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cis/trans-Tetrabromothiocyano(N)-thiocyanato(S)-rhenat(IV), *trans*-Tetrabromoseleno-
cyanato(N)-selenocyanato(Se)-rhenat(IV), Crystal Structure, Vibrational Spectra, Normal
Coordinate Analysis

The crystal structures of *cis*-(*n*-Bu₄N)₂[ReBr₄(NCS)(SCN)] (**1**) (monoclinic, space group P2₁/n, *a* = 11.203(3), *b* = 11.738(5), *c* = 35.218(7) Å, β = 93.434(4)°, Z = 4), *trans*-(*n*-Bu₄N)₂[ReBr₄(NCS)(SCN)] (**2**) (monoclinic, space group P2₁/n, *a* = 11.644(7), *b* = 13.695(3), *c* = 29.028(8) Å, β = 95.96(4)° Z = 4) and *trans*-(*n*-Bu₄N)₂[ReBr₄(NCSe)(SeCN)] (**3**) (monoclinic, space group P2₁/n, *a* = 11.894(2), *b* = 13.737(2), *c* = 28.869(7) Å, β = 96.98(10)° Z = 4) have been determined by single crystal X-ray diffraction analysis. Based on these molecular parameters 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_d(ReN) = 1.70 (**1**), 1.75 (**2**) and 1.75 (**3**), f_d(ReS) = 1.32 (**1**) and 1.37 (**2**) and f_d(ReSe) = 1.20 mdyn/Å (**3**).