

# Kristallstrukturen, Schwingungsspektren und Normalkoordinatenanalyse von *cis*-(*n*-Bu<sub>4</sub>N)<sub>2</sub>[ReBr<sub>4</sub>(NCS)<sub>2</sub>], *cis*-(*n*-Bu<sub>4</sub>N)<sub>2</sub>[ReBr<sub>4</sub>(NCSe)<sub>2</sub>] und *cis*-(*n*-Bu<sub>4</sub>N)<sub>2</sub>[ReBr<sub>4</sub>(NCS)(NCSe)]

Crystal Structures, Vibrational Spectra and Normal Coordinate Analyses of *cis*-(*n*-Bu<sub>4</sub>N)<sub>2</sub>[ReBr<sub>4</sub>(NCS)<sub>2</sub>], *cis*-(*n*-Bu<sub>4</sub>N)<sub>2</sub>[ReBr<sub>4</sub>(NCSe)<sub>2</sub>] and *cis*-(*n*-Bu<sub>4</sub>N)<sub>2</sub>[ReBr<sub>4</sub>(NCS)(NCSe)]

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*cis*-Tetrabromodithiocyanato(N)-rhenat(IV), *cis*-Tetrabromodiselenocyanato(N)-rhenat(IV), *cis*-Tetrabromo-thiocyanato(N)-selenocyanato(N)-rhenat(IV), Crystal Structure, Vibrational Spectra

The crystal structures of *cis*-(*n*-Bu<sub>4</sub>N)<sub>2</sub>[ReBr<sub>4</sub>(NCS)<sub>2</sub>] (**1**) (triclinic, space group  $\bar{P}1$ ,  $a = 11.475(6)$ ,  $b = 20.096(16)$ ,  $c = 22.144(11)$  Å,  $\alpha = 110.56(6)$ ,  $\beta = 92.97(5)$ ,  $\gamma = 99.77(7)^\circ$ ,  $Z = 4$ ), *cis*-(*n*-Bu<sub>4</sub>N)<sub>2</sub>[ReBr<sub>4</sub>(NCSe)<sub>2</sub>] (**2**) (triclinic, space group  $\bar{P}1$ ,  $a = 11.527(3)$ ,  $b = 20.237(7)$ ,  $c = 22.07(2)$  Å,  $\alpha = 110.05(4)$ ,  $\beta = 93.86(6)$ ,  $\gamma = 99.49(4)^\circ$ ,  $Z = 4$ ) and *cis*-(*n*-Bu<sub>4</sub>N)<sub>2</sub>[ReBr<sub>4</sub>(NCS)(NCSe)] (**3**) (triclinic, space group  $\bar{P}1$ ,  $a = 11.488(2)$ ,  $b = 20.164(6)$ ,  $c = 22.158(5)$  Å,  $\alpha = 110.44(2)$ ,  $\beta = 93.34(2)$ ,  $\gamma = 99.626(18)^\circ$ ,  $Z = 4$ ) 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*-Bu<sub>4</sub>N) salts have been assigned by normal coordinate analysis. The valence force constants are  $f_d(\text{ReN}) = 1.70$  (**1**), 1.70 (**2**) and 1.72 (**3**),  $f_d(\text{ReBr}) = 1.36$  (**1**), 1.30 (**2**) and 1.36 mdyn/Å (**3**).