

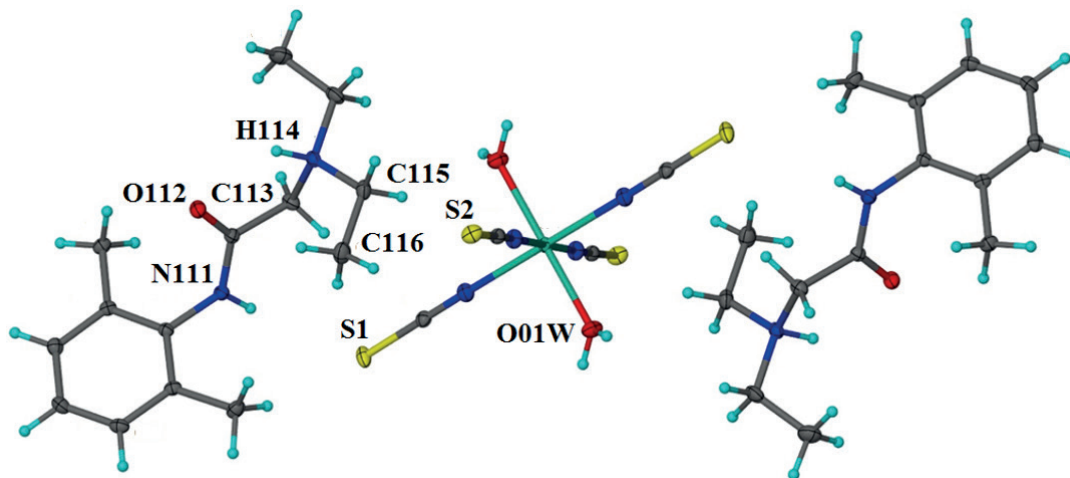
## STRUCTURE OF BIS(LIDOCAINE) TETRATHIOCYANONICKELATE(II) DIHYDRATE

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Lidocaine is a drug used as an anesthetic and for the treatment of chronic pain. Nickel(II) complex of lidocaine was prepared in water-methanol solution (pH=7) with 1:2:4 molar ratio of the nickel chloride, lidocaine, and potassium thiocyanate. Resulting bis(lidocaine) tetrathiocyanatonickelate(II) dihydrate,  $(\text{LidH})_2[\text{Ni}(\text{NCS})_4] \cdot 2\text{H}_2\text{O}$ , crystallizes in the monoclinic space group  $P2_1/c$  with  $a = 18.3509(5)$ ,  $b = 7.6532(2)$ ,  $c = 14.9585(4)$  Å,  $\beta = 109.964(2)^\circ$ ,  $V = 1974.57(9)$  Å<sup>3</sup>, and  $Z = 2$  (CCDC 1859310). Coordination of the  $\text{Ni}^{2+}$  ion with ligands generates octahedral anion  $[\text{Ni}(\text{NCS}_4)2\text{H}_2\text{O}]^{2-}$  with N-bonded thiocyanates, while two protonated cations  $\text{LidH}^+$  remain in an outer coordination field.



The anion and cation are also associated by H-bonds: the sulfur atom S1 interacts with hydrogen atoms covalently bonded to the nitrogen N111 and carbon C113 atoms, and the atom S2 forms a H-bond with the atom C116. The atom H114 of protonated diethylamino-N-group forms a bifurcated H-bond with the carbonyl atom O112 and the sulfur atom S1<sup>iv</sup> of neighboring unit cell, the carbon atom C115 forms a weak H-bond with O01W<sup>i</sup> of the water molecule in neighboring unit cell, and hydrogen atoms of water molecule are included in hydrogen bonding between the oxygen atom O01W and the sulfur atoms S2<sup>ii</sup> and S2<sup>iii</sup> of the neighboring unit cells.