Crystal Structures of Zn(II) and Cd(II) Thiocyanate Complexes with N,N-diethylethylenediamine

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The crystal structures of Zn(II) and Cd(II) thiocyanate complexes with N,N-diethylethylenediamine(L), $Zn(NCS)_2L$ (**1**) and $[Cd(SCN)_2L]_n$ (**2**), have been determined by single-crystal X-ray diffraction methods. The discrete Zn(II) complex (**1**) crystallizes in the monoclinic system, $P2_1/c$ space group with a = 9.462(1) Å, b = 10.589(2) Å, c = 13.729(4) Å, β = 100.79(1)°, V = 1351.2(5) Å^3, Z = 4, D_c = 1.464 g/cm^3, D_o = 1.457 g/cm^3, R = 0.0599, and ωR = 0.139. The zinc(II) atom is tetra-coordinated being ligated with two isothiocyanato N atoms and two N atoms of N,N-diethylethylenediamine chelating ligand. The coordination geometry of central zinc(II) atom is close to tetrahedron with the average of distance of Zn-N(L), 2.050 Å and the average of distance of $Zn\text{-}N_{(NCS)}$, 1.928 Å. The one-dimensional Cd(II) complex (**2**) crystallizes in the monoclinic system, $P2_1/c$ space group with a = 13.277(1) Å, b = 9.400(1) Å, c = 10.800(4) Å, β = 92.98(1)°, V = 1346.1(5) Å^3, Z = 4, D_c = 1.701 g/cm^3, D_o = 1.656 g/cm^3, R = 0.0313, and ωR = 0.0745. The cadmium(II) atom is hexa-coordinated being ligated with two thiocyanato S atoms, two isothiocyanato N atoms, and two N atoms of N,N-diethylethylenediamine chelating ligand. The coordination geometry of central cadmium(II) atom is close to octahedron with the averages of distance of $Cd\text{-}N_{(L)}$, of $Cd\text{-}N_{(NCS)}$, of $Cd\text{-}S_{(SCN)}$, which are 2.377 Å, 2.367 Å, and 2.705 Å. Each cadmium(II) atom is doubly bridged by SCN ligands, thus it is forming one-dimensional polymeric linear chain structures.