Crystal Structure of trans-[Co{N(CN)₂}₂(L)₂]_n, (L=1-vinylimidazole)

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The reaction of cobalt nitrate, 1-vinylimidazole (L) and NaN(CN)₂ provided the polymeric complex $[Co\{N(CN)_2\}_2(L)_2]_n$. The crystal structure of the light red complex was determined by X-ray crystallography. Crystal data at 293K are a=9.092(2)Å, b=14.332(2) Å, c=7.291(2) Å, $\beta=113.60(2)^{\circ}$, $P2_{1}/c$, V=870.6(3) Å³, Z=2, $D_{c}=1.447$ g/cm³, λ (Mo K_{α})=0.71073Å, R=0.062, and ωR =0.076 for 1603 observed reflections. The structure consists of octahedrally coordinated cobalt atoms in which the coordination sites are occupied by four N-terminal atoms of dicyanamide ligands and two N atoms of two 1-vinylimidazole ligands in trans arrangement. Two of the dicyanamide ligands act as end-to-end bridging ligands with one neighboring cobalt atom, and the other two also act as end-to-end bridging ligand with the other neighboring cobalt atom, giving a uniform one-dimensional system. The bond distances of Co(1)-N(1) and Co(1)-N(3b) are 2.123(5) Å and 2.129(5) Å, respectively. The angles of Co(1)-N(1)-C(1) and Co(1)-N(3b)-C(2b) are also observed to be 160.3(5)° and 161.0(6)°, respectively. The dicyanamide ligand is angular with 117.6(6)° of the C(1)-N(2)-C(2) and with averaged 175.8° of two adjacent linear N-C-N units. Intrachain Co···Co distance is 7.291 Å (c axis of the cell).