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Crystallographic report

Bis(isonicotinonitrile)cadmium diselencyanate, $[Cd(SeCN)_2(pyCN)_2]$ (pyCN = isonicotinonitrile)

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The title compound, $[Cd(SeCN)_2(pyCN)_2]_\infty$, adopts an extended one-dimensional chain structure in which the neighboring cadmium atoms are bridged by two selenocyanate ions. The central cadmium atom has a distorted octahedral geometry defined by two isonicotinonitrile and four selenocyanate ions in a 4*N*2*Se* fashion. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: cadmium; selenocyanate; isonicotinitrile; crystal structure; coordination polymer

COMMENT

The asymmetric unit comprises half a formula unit of $[Cd(SeCN)_2(pyCN)_2]$ with the cadmium atom located at a center of symmetry. The cadmium(II) atoms are bridged by two $SeCN^-$ ions, one of them is *Se*-coordinated and the other one is *N*-coordinated to the same side of the metal atom, thereby forming an infinite linear chain structure, as shown in Fig. 1. The Cd...Cd separation within the polymer is 5.970(9) Å, which matches the reported value in $[Cd(SCN)_2(pyCN)_2]_\infty$.[1] Each cadmium atom is coordinated by two $SeCN^-$ selenium atoms, two $SeCN^-$ nitrogen atoms, and two pyridyl nitrogen atoms, and each pair of the same donating atoms is in a *trans*-configuration, leading to an octahedral geometry. The cyano nitrogen atoms of isonicotinonitrile remain uncoordinated.

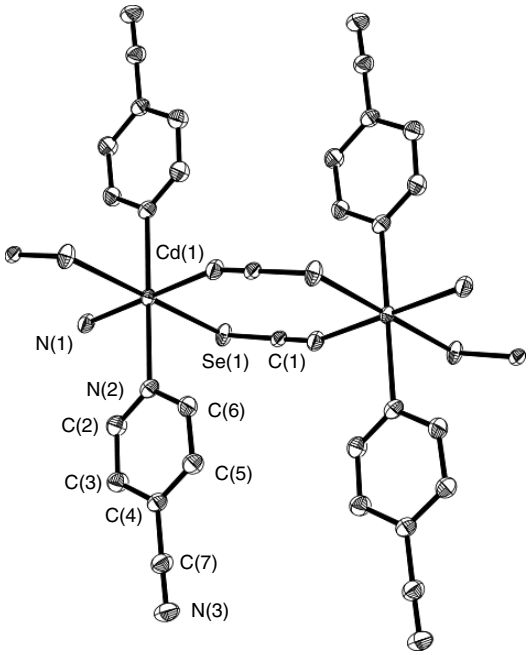

Figure 1. View of $[Cd(SeCN)_2(pyCN)_2]_\infty$ with atomic numbering scheme showing 50% probability ellipsoids (hydrogen atoms are omitted for clarity). Important geometric parameters: Cd(1)–Se(1) 2.8306(4), Cd(1)–N(1) 2.322(3), Cd(1)–N(2) 2.394(3), C(1)–Se(1) 1.811(3), C(1)–N(1)^{i} 1.154(4) Å, N(1)–Cd–Se(1) 85.93(7), N(1)–Cd–N(2) 90.56(9), N(2)–Cd–Se(1) 86.06(6), N(1)–Cd–N(2)^{ii} 89.44(9), N(1)^{i}–C(1)–Se(1) 179.0(3), N(1)^{ii}–Cd–Se(1) 94.07(7), N(2)^{ii}–Cd–Se(1) 93.94(6), Cd–N(1)–C(1)^{iii} 161.2(2), Cd–Se(1)–C(1) 94.37(9), Cd–N(2)–C(2) 119.0(2), Cd–N(2)–-C(6) 122.7(2)°. Symmetry codes: *i*, $x-1$, y, z; *ii*, $-x+2$, $-y$, $-z$; *iii*, $x+1$, y, z.

EXPERIMENTAL

To a solution of $Cd(NO_3)_2$ (1 mmol) in H_2O (10 ml) was added KSeCN (2 mmol). The resulting colorless solution was treated with an ethanolic solution of isonicotinonitrile (2 mmol). Upon standing and slow evaporation, colorless crystals were obtained. Yield: 87%. Anal. Calc. for $C_{14}H_8CdN_6Se_2$: C, 31.69; H, 1.52; N, 15.84. Found: C, 31.24; H, 1.68; N, 15.51%.

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X-ray diffraction data were collected at −150 °C on a Siemens Smart-CCD diffractometer using graphite-monochromated Mo Kα radiation ($\lambda = 0.71073$ Å) on a crystal $0.19 \times 0.21 \times 0.44$ mm^3. Crystallographic data: $C_{14}H_8CdN_6Se_2$, $M = 530.58$, monoclinic, $P2_1/n$, $a = 5.9702(10)$, $b = 17.740(3)$, $c = 8.7425(15)$ Å, $\beta = 109.351(3)°$, $V = 873.6(3)$ Å^3, $Z = 2$, $D = 2.017$ Mg m^{-3}, 5163 reflections collected, 1938 unique ($R_{int} = 0.079$), Goodness-of-fit on $F^2 = 1.07$, final R indices [$I > 2\sigma(I)$], 0.034, 0.087. Programs used: SAINT, SHELXL97, ORTEP. CCDC deposition number: 169248.

REFERENCE

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