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Crystallographic report

p-Bis(*N*-methylimidazolyl)xylylene tetra (selenocyanate)cadmium(II), $[XylIm_2][Cd(SeCN)_4]$

Daojie Liu* and Dacheng Li

Department of Chemistry, Liaocheng University, Liaocheng, Shandong 252059, People's Republic of China

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The title compound $[XylIm_2][Cd(SeCN)_4]$ [$XylIm_2$ = *p*-bis(*N*-methylimidazolyl)xylylene] comprises discrete *p*-bis(*N*-methylimidazolyl)xylylene cations and $[Cd(SeCN)_4]^{2-}$ anions in which the cadmium atoms are tetrahedrally coordinated by four selenium atoms. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: cadmium; selenocyanate; imidazolium; crystal structure

COMMENT

The structure of the title compound comprises discrete *p*-bis(*N*-methylimidazolyl)xylylene cations and $[Cd(SeCN)_4]^{2-}$ anions, as shown in Fig. 1. The cadmium atom is situated on a two fold axis and is tetrahedrally coordinated by four *Se*-coordinated $SeCN^-$ ions, and the nitrogen atoms remain uncoordinated. The average Se–Cd–Se angle is 109.5°, which is close to the ideal value of a tetrahedron. Remarkably, the Cd–Se bond distances [2.6510(5) Å and 2.6693(5) Å] are relatively short. The average Cd–Se distance is 0.18 Å shorter than those of $[Et_4N[Cd(SeCN)_3]$ (average 2.82 Å).[1] The anions stack into a one-dimensional linear chain with the Cd···Cd···Cd angle being 180°. The Cd···Cd distance is 4.53 Å, which is the shortest Cd···Cd distance found in cadmium–XCN^- (X = S, Se) complexes.[1]

*Correspondence to: Daojie Liu, Department of Chemistry, Liaocheng University, Liaocheng, Shandong 252059, People's Republic of China.
E-mail: liudjchem@yahoo.com

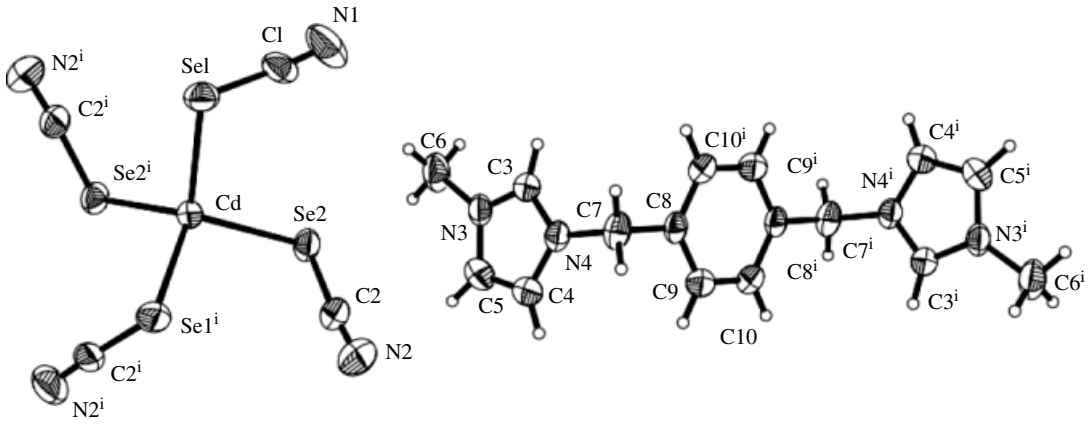

Figure 1. View of $[XylIm_2][Cd(SeCN)_4]$ with atomic numbering scheme showing 50% probability ellipsoids. Important geometric parameters: Cd–Se1 2.6508(7), Cd–Se2 2.6696(7), C2–Se2 1.830(7), C1–Se1 1.827(8), C1–N1 1.143(11), C2–N2 1.169(10), N1–C1–Se1 175.9(8), N2–C2–Se2 174.9(7), $Se1^i$–Cd–Se1 111.84(4), $Se1^i$–Cd–$Se2^i$ 106.53(2), Se1–Cd–$Se2^i$ 108.46(3), $Se1^i$–Cd–Se2 108.46(3), Se1–Cd–Se2 106.53(2), $Se2^i$–Cd–Se2 115.11(3), C1–Se1–Cd 99.7(2), C2–Se2–Cd 101.5(2). Symmetry codes: i, $-x+3/2, y, -z+1/2$.

EXPERIMENTAL

p-Bis(*N*-methylimidazolyl)xylylene dichloride was added to the premixed solution of 1 ml of $Cd(NO_3)_2{\cdot}4H_2O$ (1 mol L^{-1}) and 3 ml of KSeCN (1 mol l^{-1}). Colorless crystals were obtained by slow evaporation of the filtrate at room temperature. Yield: 92%. Anal. Found: C, 29.87; H, 2.59; N, 13.68. Calc. for $C_{20}H_{20}CdN_8Se_4$: C, 30.00; H, 2.52; N, 13.99%.

X-ray diffraction data were collected on a Siemens SMART CCD diffractometer using graphite monochromated Mo Kα radiation ($\lambda = 0.710\,73$ Å) at room temperature. Crystallographic data: $C_{20}H_{20}CdN_8Se_4$, $M = 800.68$, monoclinic, $P2/n$, $a = 12.134(3)$, $b = 4.5246(10)$, $c = 23.799(5)$ Å, $\beta = 90.898(4)°$, $V = 1306.4(5)$ Å^3, $Z = 2$, 2953 unique reflections, R_1, wR_2 (all data): 0.074, 0.192. Programs used: SAINT, SHELXL97, ORTEP. CCDC deposition number: 183573.

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