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Crystallographic report

N,N′-Dimethylimidazolium tris(selenocyanate) cadmium(II), $[Me_2Im][Cd(SeCN)_3]$ (Me_2Im = *N,N′*-dimethylimidazolium)

Daojie Liu* and Dacheng Li

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

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The title structure, $[Me_2Im][Cd(SeCN)_3]$ (Me_2Im = *N,N′*-dimethylimidazolium), comprises triply bridged one-dimensional cadmium-selenocyanate chains in which the cadmium atoms are octahedrally coordinated within 3*Se*3*N* geometries. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: cadmium; selenocyanate; imidazolium; coordination polymer

COMMENT

The cadmium atom is 3*N*3*Se*-hexacoordinated and exists within a distorted octahedral geometry in which the three nitrogen atoms are in a *fac* configuration, implying that each selenium atom is in a *trans* position to a nitrogen atom (Fig. 1). The average Cd–N, Cd–Se bond distances and the Cd–Se–C and Cd–N–C angles are normal and match the values found in $[Et_4N][Cd(SeCN)_3]$.[1] Adjacent cadmium atoms are linked by three virtually linear $SeCN^-$ ions, thus forming one-dimensional zigzag chains. The Cd···Cd separation is 5.60 Å and the Cd···Cd···Cd angle is 146°. The infinite zigzag chains are parallel to each other and are separated by *N,N′*-dimethylimidazolium cations.

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

EXPERIMENTAL

$[Me_2Im]I$ (224 mg, 1.0 mmol) was added to the pre-mixed 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}).

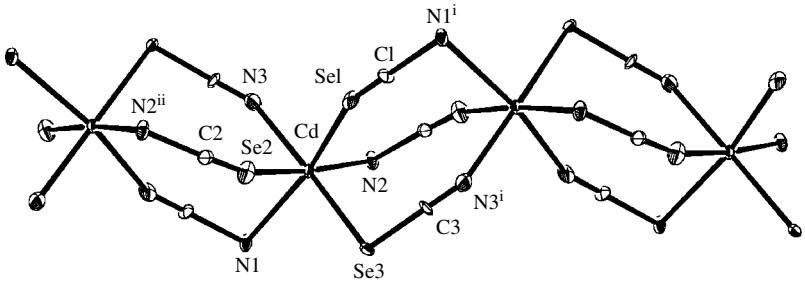

Figure 1. View of $[Me_2Im][Cd(SeCN)_3]$. Important geometric parameters: Cd–Se1 2.7840(10), Cd–Se2 2.7881(10), Cd–Se3 2.7691(10), Cd–N1 2.3748, Cd–N2 2.3497, Cd–N3 2.376(8), C1–Se1 1.809(8), C2–Se2 1.814(7), C3–Se3 1.816(8), C1–$N1^i$ 1.156(11), C2–$N2^{ii}$ 1.149(11), C3–$N3^i$ 1.145(11) Å; $N1^i$–C1–Se1 177.5(7), $N2^{ii}$–C2–Se2 178.8(8), $N3^i$–C3–Se3 179.1(8), N1–Cd1–N2 86.7(3), N2–Cd–N3 81.8(3), N1–Cd–N3 81.1(3), N2–Cd–Se3 93.64(19), N1–Cd–Se3 88.64(19), N3–Cd–Se3 169.0(2), N2–Cd–Se1 92.41(18), N1–Cd–Se1 173.88(19), N3–Cd–Se1 92.78(19), Se3–Cd–Se1 97.46(3), N2–Cd–Se2 170.94(17), N1–Cd–Se2 87.98(19), N3–Cd–Se2 90.10(19), Se3–Cd–Se2 93.58(3), Se1–Cd–Se2 92.07(3)°. Symmetry codes: i, $-x+2$, $y+1/2$, $-z+3/2$; ii, $-x+2$, $y-1/2$, $-z+3/2$.

Colorless crystals were obtained by slow evaporation of the solution at room temperature. Yield: 89%. Anal. Found: C, 18.21; H, 1.95; N, 13.10. Calc. for $C_8H_9CdN_5Se_3$: C, 18.32; H, 1.73; N, 13.35%.

X-ray diffraction data were collected on a Siemens SMART CCD diffractometer using graphite monochromated Mo Kα radiation ($\lambda = 0.710\,73$ Å) at $-150\,^{\circ}$C. Crystallographic data: $C_8H_9CdN_5Se_3$, $M = 524.48$, orthorhombic, $P2_12_12_1$, $a = 9.6586(17)$, $b = 10.6975(19)$, $c = 13.627(3)$ Å, $V = 1408.0(4)$ Å^3, $Z = 4$, $D = 2.474$ Mg m^{-3}, 3075 reflections unique, R_1, wR_2 (all data): 0.049, 0.121. Programs used: SAINT, SHELXL97, ORTEP. CCDC deposition number: 183 572.

REFERENCE

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