



# A novel polymeric Cd[SSe<sub>2</sub>N<sub>2</sub>] central core five-coordinate complex: Synthesis, X-ray structure and <sup>113</sup>Cd, <sup>77</sup>Se CP MAS NMR characterization of catena(bis(μ<sub>2</sub>-selenocyanato-N,Se)-(N,N'-dimethylimidazolidine-2-thione-S)-cadmium(II))

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Received 28 October 2007; accepted 8 November 2007

Available online 19 November 2007

## Abstract

Cadmium(II) selenocyanate reacts with *N,N'*-dimethylimidazolidine-2-thione (Me<sub>2</sub>Imt) at a 1:1 ratio forming a polymeric [(Me<sub>2</sub>Imt)Cd(SeCN)<sub>2</sub>]<sub>∞</sub> complex. The metal ion is bonded to one imidazolidine thione through the sulfur atom, two selenocyanate ions through their selenium atoms and two other selenocyanates through their nitrogen atoms. The metal complex coordination sphere Cd[SSe<sub>2</sub>N<sub>2</sub>] adopts a distorted trigonal bipyramidal geometry with the chalcogen atoms occupying the equatorial positions and the nitrogen atoms in the axial positions. The <sup>77</sup>Se CP MAS NMR data are consistent with two different selenium sites and the shielding tensor parameters of <sup>113</sup>Cd point to a near axial symmetry for the cadmium environment.

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**Keywords:** *N,N'*-Dimethylimidazolidine-2-thione; Cadmium selenocyanate; X-ray structure; <sup>113</sup>Cd; <sup>77</sup>Se CP MAS NMR

Metalloproteins with zinc–sulfur centers are known to be targets of selenium redox biochemistry and selenium compounds catalyze the release of zinc from metallothionein in different biochemical reactions [1,2]. Therefore, there is a need of structural elucidation of sulfur and selenium-based coordination chemistry of zinc in particular and group 12 metals in general. The X-ray structures reported so far for zinc and cadmium complexes with [SSe] donor ligands are rare [3–6]. The cadmium complexes present a significant advantage over their zinc counterparts from the structural characterization point of view since <sup>113</sup>Cd NMR spectroscopy stands a sensitive probe of the coordination sphere of the cadmium ion. It has in fact developed into a useful probe of metal environments in metal proteins because Cd<sup>2+</sup> may often be exchanged for other divalent metals such as Zn<sup>2+</sup> in proteins [7]. In this

context, the chemistry of imidazolidine-2-thione and its derivatives has attracted considerable attention because of the potential thione ↔ thiol equilibrium [8] and the various potential donor sites available in these ligands [9]. Several studies have been carried out on their coordinating ability mainly with the aim of determining the coordination mode both in the solid-state and in solution [10]. In this paper, we report on a rare example of a five-coordinate polymeric cadmium complex with Cd[SSe<sub>2</sub>N<sub>2</sub>] coordination sphere. To the best of our knowledge, this is the first X-ray structure ever reported for a cadmium complex having simultaneously sulfur, selenium and nitrogen atoms in its coordination sphere. The structural characterization includes <sup>113</sup>Cd, <sup>77</sup>Se CP MAS NMR studies.

The reaction of Me<sub>2</sub>Imt with Cd(SeCN)<sub>2</sub> in an acetonitrile/methanol mixture leads to the formation of the title compound [11]. The X-ray structure is depicted in Fig. 1 [12]. The complex has a polymeric structure (Fig. 2). The metal ion is bonded to one imidazolidine thione through

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