A new structural motif for cadmium dithiocarbamates: crystal structures and Hirshfeld surface analyses of homoleptic zinc and cadmium morpholine dithiocarbamates

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Abstract
The crystal and molecular structures of two homoleptic morpholine-derived dithiocarbamates of zinc, bisnuclear [Zn(S2CNR1H2)(2)(O)(2)](2)(2) (1), and cadmium, - one-dimensional coordination polymer [Cd(S2CNR1H2)(2)(O)(2)](2)(2) (2), are described. In 1, a centrosymmetric binuclear molecule is found as there are equal numbers of chelating and bidentate bridging dithiocarbamate ligands; weak transannular Zn center dot center dot center dot S interactions are found within the resultant eight-membered (center dot center dot center dot center dot center dot center dot O) ring which has the form of a chair. The resultant 4+1 S-5 donor set is highly distorted with the geometry tending towards a square-pyramid. By contrast, a square-planar geometry is found in centrosymmetric 2 defined by symmetrically chelating dithiocarbamate ligands. The presence of Cd center dot center dot center dot center dot center dot center dot O secondary bonding in the crystal of 2 leads to a distorted +2 S-6 octahedron and a linear coordination polymer, which is unprecedented in the structural chemistry of cadmium dithiocarbamates. The analyses of the Hirshfeld surfaces for 1 and 2 show the dominance of H center dot center dot center dot H interactions and X-ray diffraction; zinc.

Keywords:
Author Keywords: cadmium; coordination polymer; crystal structure analysis; dithiocarbamate; Hirshfeld surface; X-ray diffraction; zinc

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