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A new structural motif for cadmium dithiocarbamates : Crystal structures and Hirshfeld surface analyses of homoleptic zinc and cadmium morpholine dithiocarbamates (Article)

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Abstract

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The crystal and molecular structures of two homoleptic morpholine -derived dithiocarbamates of zinc , binuclear {Zn[S 2 CN(CH 2 CH 2) 2 O) 2] 2 } 2 (1), and cadmium , one-dimensional coordination polymer {Cd[S 2 CN(CH 2 CH 2) 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···S interactions are found within the resultant eight-membered {···SCSZn} 2 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···S secondary bonding in the crystal of 2 leads to a distorted 4+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···H, S···H/H···S and O···H/H···O contacts to the surface , i.e. contributing around 90 and 80%, respectively. © 2019 Walter de Gruyter GmbH, Berlin/Boston.

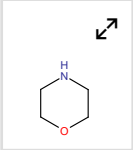
SciVal Topic Prominence

Topic: Ligands | Crystal structure | Dithiocarbamate ligands

Prominence percentile: 84.652

Chemistry database information

Substances



Author keywords

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