

[Look Up Full Text](#)[Full Text from Publisher](#)[Find PDF](#)[Export...](#)[Add to Marked List](#)

◀ 1 of 1 ▶

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

By: [Ahmad, J](#) (Ahmad, Jimmy)^[2]; [How, FNF](#) (How, Fiona N-F)^[2]; [Halim, SNA](#) (Halim, Siti Nadiyah Abdul)^[3]; [Jotani, MM](#) (Jotani, Mukesh M.)^[4]; [Lee, SM](#) (Lee, See Mun)^[1]; [Tiekink, ERT](#) (Tiekink, Edward R. T.)^[1]

ZEITSCHRIFT FUR KRISTALLOGRAPHIE-CRYSTALLINE MATERIALS

Volume: 234 Issue: 5 Pages: 341-349

DOI: 10.1515/zkri-2018-2141

Published: MAY 2019

Document Type: Article

[View Journal Impact](#)

Abstract

The crystal and molecular structures of two homoleptic morpholine-derived dithiocarbamates of zinc, binuclear $[Zn(S_2CN(CH_2CH_2)_2O)_2]_2$ (1), and cadmium, - one-dimensional coordination polymer $[Cd(S_2CN(CH_2CH_2)_2O)_2]_2$ (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 $\{center dot center dot center dot SCSZn\}_2$ 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 center dot center dot center dot S 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, S center dot center dot center dot H/H center dot center dot center dot S and O center dot center dot center dot center dot H/H center dot center dot center dot O contacts to the surface, i.e. contributing around 90 and 80%, respectively.

Keywords

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

KeyWords Plus: INTERMOLECULAR INTERACTIONS

Author Information

Reprint Address: Tiekink, ERT (reprint author)

Sunway Univ, Res Ctr Crystalline Mat, Sch Sci & Technol, Bandar Sunway 47500, Selangor Darul, Malaysia.

Addresses:

[1] Sunway Univ, Res Ctr Crystalline Mat, Sch Sci & Technol, Bandar Sunway 47500, Selangor Darul, Malaysia

+ [2] Int Islamic Univ Malaysia, Dept Chem, Kulliyyah Sci, Jalan Sultan Ahmad Shah, Kuantan 25200, Pahang, Malaysia

+ [3] Univ Malaya, Dept Chem, Kuala Lumpur 50603, Malaysia

[4] Bhavans Sheth RA Coll Sci, Dept Phys, Ahmadabad 380001, Gujarat, India

E-mail Addresses: edwardt@sunway.edu.my

Funding

Funding Agency	Grant Number
Sunway University	

[View funding text](#)

Publisher

WALTER DE GRUYTER GMBH, GENTHINER STRASSE 13, D-10785 BERLIN, GERMANY

Citation Network

In Web of Science Core Collection

0

Times Cited

[Create Citation Alert](#)

35

Cited References

[View Related Records](#)

Use in Web of Science

Web of Science Usage Count

1

Last 180 Days

1

Since 2013

[Learn more](#)

This record is from:

Web of Science Core Collection
- Science Citation Index Expanded

[Suggest a correction](#)

If you would like to improve the quality of the data in this record, please [suggest a correction](#).

Journal Information

Impact Factor: [Journal Citation Reports](#)

Categories / Classification

Research Areas: Crystallography

Web of Science Categories: Crystallography

[See more data fields](#)

◀ 1 of 1 ▶

Cited References: 35

Showing 30 of 35 [View All in Cited References page](#)

(from Web of Science Core Collection)

- 1. INVESTIGATION OF A NEW XANTHATE LIGAND - THE CRYSTAL AND MOLECULAR-STRUCTURES OF NICKEL AND CADMIUM (METHOXYETHYL)XANTHATES** Times Cited: 26
By: ABRAHAMS, BF; HOSKINS, BF; TIEKINK, ERT; et al.
AUSTRALIAN JOURNAL OF CHEMISTRY Volume: 41 Issue: 7 Pages: 1117-1122 Published: 1988
- 2. SYNTHESIS, STRUCTURE, AND SPECTROSCOPIC PROPERTIES OF COPPER(II) COMPOUNDS CONTAINING NITROGEN SULFUR DONOR LIGANDS - THE CRYSTAL AND MOLECULAR-STRUCTURE OF AQUA[1,7-BIS(N-METHYLBENZIMIDAZOL-2'-YL)-2,6-DITHIAHEPTANE]COPPER(II) PERCHLORATE** Times Cited: 7,187
By: ADDISON, AW; RAO, TN; REEDIJK, J; et al.
JOURNAL OF THE CHEMICAL SOCIETY-DALTON TRANSACTIONS Issue: 7 Pages: 1349-1356 Published: 1984
- 3. Title: [not available]** Times Cited: 679
By: Alcock, N.W.
Adv. Inorg. Chem. Radiochem. Volume: 15 Pages: 1 Published: 1972
- 4. catena-Poly[cadmium-bis(mu-N,N-dimethyldithiocarbamato-kappa S-3,S'-S)]** Times Cited: 7
By: Bing, Yue; Li, Xing; Zha, Meiqin; et al.
ACTA CRYSTALLOGRAPHICA SECTION E-STRUCTURE REPORTS ONLINE Volume: 66 Pages: M1500-U1551 Part: 11 Published: NOV 2010
- 5. VAN DER WAALS VOLUMES + RADII** Times Cited: 16,920
By: BONDI, A
JOURNAL OF PHYSICAL CHEMISTRY Volume: 68 Issue: 3 Pages: 441-+ Published: 1964
- 6. Title: [not available]** Times Cited: 54
By: Brandenburg, K.
DIAMOND Published: 2006
Publisher: Crystal Impact GbR, Bonn, Germany
- 7. Crystal structures of 2,2'-bipyridine adducts of two cadmium O-alkyl dithiocarbonates: rationalisation of disparate coordination geometries based on different crystal packing environments** Times Cited: 18
By: Chen, DL; Lai, CS; Tiekink, ERT
ZEITSCHRIFT FUR KRISTALLOGRAPHIE Volume: 218 Issue: 11 Pages: 747-752 Published: 2003
- 8. Title: [not available]** Times Cited: 4
By: Clegg, W.
CSD Communication (Private Communication) Published: 2016
- 9. Structural features of zinc(II) bis(O-alkyldithiocarbonate) and zinc(II) bis(N,N-dialkyldithiocarbamate) compounds** Times Cited: 41
By: Cox, MJ; Tiekink, ERT
ZEITSCHRIFT FUR KRISTALLOGRAPHIE Volume: 214 Issue: 3 Pages: 184-190 Published: 1999
- 10. Rigaku Oxford Diffraction** Times Cited: 9
Group Author(s): CrysAlis PRO
CRYALIS PRO Published: 2014

11. **WinGX and ORTEP for Windows: an update** Times Cited: 5,659
By: Farrugia, Louis J.
JOURNAL OF APPLIED CRYSTALLOGRAPHY Volume: 45 Pages: 849-854 Part: 4 Published: AUG 2012
12. **Secondary Bonding** Times Cited: 32
By: Haiduc, I.
Encyclopedia of Supramolecular Chemistry Pages: 1215 Published: 2004
Publisher: Marcel Dekker Inc., New York
13. Title: [not available] Times Cited: 1
By: Halim, S. N. A.
Personal communication to the Cambridge Structural Database Published: 2015
Refcode: QUQTED
14. **TONTO-A System for Computational Chemistry** Times Cited: 1
By: Jayatilaka, D.; Grimwood, D. J.; Lee, A.; et al.
TONTO A SYSTEM FOR C Published: 2005
Available at
URL: <http://hirshfeldsurface.net/>
[Show additional data]
15. **Supramolecular association in the triclinic (Z'=1) and monoclinic (Z'=4) polymorphs of 4-(4-acetylphenyl)piperazin-1-ium 2-amino-4-nitrobenzoate** Times Cited: 6
By: Jotani, Mukesh M.; Wardell, James L.; Tiekink, Edward R. T.
ZEITSCHRIFT FUR KRISTALLOGRAPHIE-CRYSTALLINE MATERIALS Volume: 234 Issue: 1 Pages: 43-57 Published: JAN 2019
16. **Supramolecular association in (mu(2)-pyrazine)-tetrakis(N,N-bis(2-hydroxyethyl)dithiocarbamato)dizinc(II) and its di-dioxane solvate** Times Cited: 10
By: Jotani, Mukesh M.; Poplaukhin, Pavel; Arman, Hadi D.; et al.
ZEITSCHRIFT FUR KRISTALLOGRAPHIE-CRYSTALLINE MATERIALS Volume: 232 Issue: 4 Pages: 287-298 Published: APR 2017
17. **Bis[bis(N-2-hydroxyethyl,N-isopropyl-dithiocarbamato)mercury(II)](2): crystal structure and Hirshfeld surface analysis** Times Cited: 17
By: Jotani, Mukesh M.; Tan, Yee Seng; Tiekink, Edward R. T.
ZEITSCHRIFT FUR KRISTALLOGRAPHIE-CRYSTALLINE MATERIALS Volume: 231 Issue: 7 Pages: 403-413 Published: JUL 2016
18. **Potassium morpholine-4-carbodithioate monohydrate** Times Cited: 4
By: Mafud, Ana C.
ACTA CRYSTALLOGRAPHICA SECTION E-CRYSTALLOGRAPHIC COMMUNICATIONS Volume: 68 Pages: M1025+ Part: 8 Published: AUG 2012
19. **Noncovalent bonding: Stacking interactions of chelate rings of transition metal complexes** Times Cited: 28
By: Malenov, Dusan P.; Janjic, Goran V.; Medakovic, Vesna B.; et al.
COORDINATION CHEMISTRY REVIEWS Volume: 345 Pages: 318-341 Published: AUG 15 2017
20. **Novel tools for visualizing and exploring intermolecular interactions in molecular crystals** Times Cited: 1,026
By: McKinnon, JJ; Spackman, MA; Mitchell, AS
ACTA CRYSTALLOGRAPHICA SECTION B-STRUCTURAL SCIENCE Volume: 60 Pages: 627-668 Part: 6 Published: DEC 2004
21. **Towards quantitative analysis of intermolecular interactions with Hirshfeld surfaces** Times Cited: 995
By: McKinnon, Joshua J.; Jayatilaka, Dylan; Spackman, Mark A.
CHEMICAL COMMUNICATIONS Issue: 37 Pages: 3814-3816 Published: 2007
22. **Electron delocalization mediates the metal-dependent capacity for CH/pi interactions of acetylacetonato chelates** Times Cited: 66
By: Milcic, Milos K.; Medakovic, Vesna B.; Sredojevic, Dusan N.; et al.
INORGANIC CHEMISTRY Volume: 45 Issue: 12 Pages: 4755-4763 Published: JUN 12 2006
23. **Hirshfeld Surfaces Identify Inadequacies in Computations of Intermolecular Interactions in Crystals: Pentamorphic 1,8-Dihydroxyanthraquinone** Times Cited: 222
By: Rohl, Andrew L.; Moret, Massimo; Kaminsky, Werner; et al.
CRYSTAL GROWTH & DESIGN Volume: 8 Issue: 12 Pages: 4517-4525 Published: DEC 2008

24. **A short history of SHELX** Times Cited: 70,402
By: Sheldrick, George M.
ACTA CRYSTALLOGRAPHICA A-FOUNDATION AND ADVANCES Volume: 64 Pages: 112-122 Part: 1 Published: JAN 2008
25. **Crystal structure refinement with SHELXL** Times Cited: 11,640
By: Sheldrick, George M.
ACTA CRYSTALLOGRAPHICA SECTION C-STRUCTURAL CHEMISTRY Volume: 71 Pages: 3-8 Part: 1 Published: JAN 2015
26. **Electrostatic potentials mapped on Hirshfeld surfaces provide direct insight into intermolecular interactions in crystals** Times Cited: 339
By: Spackman, Mark A.; McKinnon, Joshua J.; Jayatilaka, Dylan
CRYSTENGCOMM Volume: 10 Issue: 4 Pages: 377-388 Published: 2008
27. **Single-crystal structure validation with the program PLATON** Times Cited: 13,921
By: Spek, AL
JOURNAL OF APPLIED CRYSTALLOGRAPHY Volume: 36 Pages: 7-13 Part: 1 Published: FEB 2003
28. **Supramolecular Isomerism in a Cadmium Bis(N-Hydroxyethyl, N-isopropylthiocarbamate) Compound: Physicochemical Characterization of Ball (n=2) and Chain (n = infinity) Forms of {Cd[S2CN(iPr)CH2CH2OH](2)center dot solvent}(n)** Times Cited: 56
By: Tan, Yee Seng; Sudlow, Anna L.; Molloy, Kieran C.; et al.
CRYSTAL GROWTH & DESIGN Volume: 13 Issue: 7 Pages: 3046-3056 Published: JUL 2013
29. **Persistence of C-H center dot center dot center dot pi(chelate ring) interactions in the crystal structures of Pd(S2COR)(2). The utility of Pd(S2COR)(2) as precursors for palladium sulphide materials** Times Cited: 17
By: Tan, Yee Seng; Halim, Siti Nadiyah Abdul; Molloy, Kieran C.; et al.
CRYSTENGCOMM Volume: 18 Issue: 7 Pages: 1105-1117 Published: 2016
30. **Exploring the crystallization landscape of cadmium bis(N-hydroxyethyl, N-isopropylthiocarbamate), Cd[S2CN(iPr)CH2CH2OH] (2)** Times Cited: 17
By: Tan, Yee Seng; Halim, Siti Nadiyah Abdul; Tiekink, Edward R. T.
ZEITSCHRIFT FUR KRISTALLOGRAPHIE-CRYSTALLINE MATERIALS Volume: 231 Issue: 2 Pages: 113-126 Published: FEB 2016

Showing 30 of 35 [View All in Cited References page](#)

Clarivate

Accelerating innovation

© 2019 Clarivate [Copyright notice](#) [Terms of use](#) [Privacy statement](#) [Cookie policy](#)

Sign up for the Web of Science newsletter [Follow us](#)

