

Resource Summary Report

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Cambridge Structural Data Base

RRID:SCR_007310

Type: Tool

Proper Citation

Cambridge Structural Data Base (RRID:SCR_007310)

Resource Information

URL: <http://www.ccdc.cam.ac.uk/Solutions/CSDSystem>

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Description: It records bibliographic, chemical and crystallographic information for organic molecules and metal-organic compounds whose 3D structures have been determined using X-ray diffraction and neutron diffraction.

The CSD records results of single crystal studies and powder diffraction studies which yield 3D atomic coordinate data for at least all non-H atoms. In some cases the CCDC is unable to obtain coordinates, and incomplete entries are archived to the CSD.

The CSD includes crystal structure data arising from:

- * publications in the open literature
- * Private Communications to the CSD (via direct data deposition)

The Cambridge Structural Database System (CSDS) is a single product that comprises the following components: The Cambridge Structural Database (CSD); CSDS Software: search and information retrieval (ConQuest), structure visualization (Mercury), statistical analysis of retrieved data (VISTA), and software for database creation (PreQuest); Knowledge bases derived from the CSD: Mogul (intramolecular geometry) and IsoStar (intermolecular interactions, including data from the PDB).

Cambridge Structural Database (CSD) is the world repository of small-molecule crystal structures. For example, the crystal structures supported by the National Institute on Drug Abuse are deposited here.

Abbreviations: CSD

Synonyms: Cambridge Structural Database

Resource Type: database, software resource, data or information resource

Keywords: 3d structure, crystal, crystal studies, csd, metal-organic compounds, neutron diffraction, organic molecules, powder diffraction, x-ray diffraction

Funding:

Resource Name: Cambridge Structural Data Base

Resource ID: SCR_007310

Alternate IDs: DOI:10.25504/FAIRsharing.vs7865, nif-0000-00174, DOI:10.5517, DOI:10.25505, DOI:10.17616/R36011

Alternate URLs: <http://www.ccdc.cam.ac.uk/products/csd/>, <https://doi.org/10.17616/R30P93>, <https://doi.org/10.17616/r36011>, <https://doi.org/10.5517/>, &&<https://doi.org/10.25505/>, , <https://dx.doi.org/10.5517/>, <https://dx.doi.org/10.25505/>, <https://fairsharing.org/10.25504/FAIRsharing.vs7865>

Record Creation Time: 20220129T080241+0000

Record Last Update: 20250416T063503+0000

Ratings and Alerts

No rating or validation information has been found for Cambridge Structural Data Base.

No alerts have been found for Cambridge Structural Data Base.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 132 mentions in open access literature.

Listed below are recent publications. The full list is available at [FDI Lab - SciCrunch.org](#).

Inagaki Y, et al. (2014) A Diels-Alder super diene breaking benzene into C₂H₂ and C₄H₄ units. Nature communications, 5, 3018.

Buro C, et al. (2014) Imatinib treatment causes substantial transcriptional changes in adult *Schistosoma mansoni* in vitro exhibiting pleiotropic effects. PLoS neglected tropical diseases, 8(6), e2923.

Mabied AF, et al. (2014) Crystal structure and stereochemistry study of 2-substituted benzoxazole derivatives. *ISRN organic chemistry*, 2014, 728343.

Li D, et al. (2014) Synthesis, crystal structure, and thermal decomposition of the cobalt(II) complex with 2-picolinic acid. *TheScientificWorldJournal*, 2014, 641608.

Acosta-Reyes FJ, et al. (2014) In and out of the minor groove: interaction of an AT-rich DNA with the drug CD27. *Acta crystallographica. Section D, Biological crystallography*, 70(Pt 6), 1614.

Chygorin EN, et al. (2014) Tetra-kis(2-[[1,1-bis-(hydroxy-methyl)-2-oxidoethyl]imino-methyl]-6-nitro-pheno-lato)tetra-copper(II). *Acta crystallographica. Section E, Structure reports online*, 70(Pt 2), m54.

Zhao H, et al. (2014) Complex self-assembly of pyrimido[4,5-d]pyrimidine nucleoside supramolecular structures. *Nature communications*, 5, 3108.

Hu Y, et al. (2014) A carbonate-forming Baeyer-Villiger monooxygenase. *Nature chemical biology*, 10(7), 552.

Zang HY, et al. (2014) Discovery of gigantic molecular nanostructures using a flow reaction array as a search engine. *Nature communications*, 5, 3715.

Li D, et al. (2014) Synthesis and Crystal Structure of the Bioinorganic Complex [Sb(Hedta)]·2H₂O. *Bioinorganic chemistry and applications*, 2014, 461605.

Ahmed Hassan LE, et al. (2014) Crystal structure elucidation and anticancer studies of (-)-pseudosemiglabrin: a flavanone isolated from the aerial parts of *Tephrosia apollinea*. *PloS one*, 9(6), e90806.

Jennifer SJ, et al. (2014) Design of co-crystals/salts of some Nitrogenous bases and some derivatives of thiophene carboxylic acids through a combination of hydrogen and halogen bonds. *Chemistry Central journal*, 8, 20.

Rahaman A, et al. (2014) Bioinspired Hydrogenase Models: The Mixed-Valence Triiron Complex [Fe₃(CO)₇(η⁵-edt)₂] and Phosphine Derivatives [Fe₃(CO)_{7-x}(PPh₃)_x(η⁵-edt)₂] (x = 1, 2) and [Fe₃(CO)₅(η²-diphosphine)(η⁵-edt)₂] as Proton Reduction Catalysts. *Organometallics*, 33(6), 1356.

Chavda JK, et al. (2014) Synthetic Studies Towards the Core Structure of Nakadomarin A by a Thioamide-Based Strategy. *European journal of organic chemistry*, 2014(1), 129.

Tanaka H, et al. (2014) Unique behaviour of dinitrogen-bridged dimolybdenum complexes bearing pincer ligand towards catalytic formation of ammonia. *Nature communications*, 5, 3737.

Li HJ, et al. (2014) Induced marine fungus *Chondrostereum* sp. as a means of producing new sesquiterpenoids chondrosterins I and J by using glycerol as the carbon source. *Marine*

drugs, 12(1), 167.

Barakat A, et al. (2014) Tandem Aldol-Michael reactions in aqueous diethylamine medium: a greener and efficient approach to dimedone-barbituric acid derivatives. Chemistry Central journal, 8(1), 9.

Hemamalini M, et al. (2014) Investigation of supramolecular synthons and structural characterisation of aminopyridine-carboxylic acid derivatives. Chemistry Central journal, 8, 31.

Sun CY, et al. (2013) Efficient and tunable white-light emission of metal-organic frameworks by iridium-complex encapsulation. Nature communications, 4, 2717.

Diring S, et al. (2013) Localized cell stimulation by nitric oxide using a photoactive porous coordination polymer platform. Nature communications, 4, 2684.