

CODデータからCTRDataBaseデータ作成

2025年09月19日

HelperTex Office

概要

CTRのD a t a B a s eはテキストデータを入力として作成される。
本資料では、CODデータを入力とする方法を説明します。
CODで検索すると以下の表示がされます。

☐ Burbankite



Belovitskaya Yu V, Pekov I V, Kabalov Yu K

Crystallography Reports 45 (2000) 26-29

Refinement of the crystal structures of low-rare-earth

and "typical" burbankites by the Rietveld method

Locality: Khibiny Massif, Kola Peninsula, Russia

Sample: B-108

Note: x02 adjusted to satisfy symmetry constraints

_database_code_amcsd 0012365

10.5313 10.5313 6.4829 90 90 120 P6_3mc

atom	x	y	z	occ	Biso	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)
NaA	.5237	.4763	.319	.728	1.7	.006	.006	.011	0	.003	-.003
CaA	.5237	.4763	.319	.231	1.7	.006	.006	.011	0	.003	-.003
YA	.5237	.4763	.319	.01	1.7	.006	.006	.011	0	.003	-.003
SrB	.8410	.1590	0	.633	.88	.0021	.0021	.0091	.0010	.001	-.001
BaB	.8410	.1590	0	.106	.88	.0021	.0021	.0091	.0010	.001	-.001
CeB	.8410	.1590	0	.074	.88	.0021	.0021	.0091	.0010	.001	-.001
LaB	.8410	.1590	0	.038	.88	.0021	.0021	.0091	.0010	.001	-.001
NdB	.8410	.1590	0	.016	.88	.0021	.0021	.0091	.0010	.001	-.001
PrB	.8410	.1590	0	.006	.88	.0021	.0021	.0091	.0010	.001	-.001
CaB	.8410	.1590	0	.047	.88	.0021	.0021	.0091	.0010	.001	-.001
C1	.799	.201	.53		2.7						
C2	0	0	.85		2.0						
C3	1/3	2/3	.49		2.0						
O1	.376	.088	.628		1.6						
O2	.930	.070	.352		2.9						
O3	.406	.594	.49		1.7						
O4	.770	.230	.358		3.1						

[Download AMC data \(View Text File\)](#)

[Download CIF data \(View Text File\)](#)

[Download diffraction data \(View Text File\)](#)

[View Jmol 3-D Structure \(permalink\)](#)

CIF と diffraction データを download し D a t a B a s e の M a k e M y I C D D により作成します。

CODから cif と diffraction を得る。



https://www.crystallography.net/cod/index.php

Crystallography Open Database

COD Crystallography Open Database

COD Home

- Home
- What's new?

Accessing COD Data

- Browse
- Search
- Search by structural formula

Add Your Data

- Deposit your data
- Manage depositions
- Manage/release prepublications

Documentation

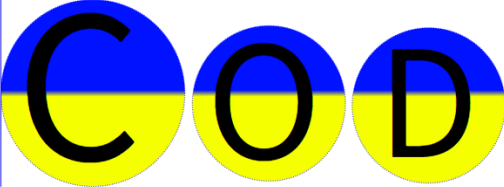
- COD Wiki
- Obtaining COD
- License
- Privacy and GDPR
- Querying COD
- Citing COD
- COD Mirrors
- Advice to donors
- Useful links

Open-access collection of crystal structures of organic, inorganic, metal-organic compounds and minerals, excluding biopolymers.


Including data and *software* from *CrystalEye*, developed by Nick Day at the *department of Chemistry*, the University of Cambridge under supervision of *Peter Murray-Rust*.

All data on this site have been placed in the *public domain* by the contributors.

Currently there are **528013** entries in the COD.
Latest deposited structure: [7250866](#) on 2025-09-18 at 01:25:53 UTC




CIFs Donators




Crystallography Open Database

Main CIF donators :





International Union of Crystallography permits systematic downloads of coordinates files published in *the IUCr journals*; COD is updating its coordinate archive and the database from the IUCr web site on a regular basis. More than 20000 CIF files are downloaded at the moment.



The American Mineralogist Crystal Structure Database

The main source of COD mineral data.

 and 

March 2003 and later, ~7000 CIFs

American Mineralogist Crystal Structure Database

Important Update News

The RRUFF Project is being updated to improve its interface and content. The beta version of the update is accessible to the public at RRUFF.net. New data is only being added to the beta site. Please note that it is in development, and some components are not functional. Existing RRUFF.info links will resolve to the new site after RRUFF.net is officially released.

We are grateful to NASA for the funding of this effort.

American Mineralogist Crystal Structure Database

This site is an interface to a crystal structure database that includes every structure published in the American Mineralogist, The Canadian Mineralogist, European Journal of Mineralogy and Physics and Chemistry of Minerals, as well as selected datasets from other journals. The database is maintained under the care of the Mineralogical Society of America and the Mineralogical Association of Canada, and financed by the National Science Foundation.

Search interface with fields for Mineral, Author, Chemistry Search, Cell Parameters and Symmetry (highlighted), Diffraction Search, and General Search. Search and Reset buttons are present.

Logic interface: ☒ AND ☐ OR

Viewing (About File Formats): ☒ amc long form ☐ amc short form ☐ cif

Download: ☒ amc ☐ cif ☐ diffraction data

People NSF Mineralogical Society of America Mineralogical Association of Canada Extra

Number of Files downloaded since Apr 1, 2003: 1248463276
 Data Last Updated: January 08, 2024
 Web Page Last Updated: July 31, 2018
 This page has been accessed 4958297 times.

格子定数の限定

Cell Parameters and Symmetry

	Lower Range	Upper Range	
a	10.5	11	<input checked="" type="radio"/> Range
b	10.5	11	<input type="radio"/> Tolerance
c	6.4	6.5	
alpha	90	90	
beta	90	90	
gamma	120	120	
space group			
crystal system	hexagonal		

Logic interface:
☒ AND ☐ OR

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Search interface:






- Mineral
- Author
- Chemistry Search
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- General Search
- Search Tips

Search [] Reset []

Logic interface: ☒ AND ☐ OR


Viewing (About File Formats): ☒ amc long form ☐ amc short form ☐ cif

Download: ☒ amc ☐ cif ☐ diffraction data

People      Extra

Number of Files downloaded since Apr 1, 2003: 1248467569
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☐ **Burbankite**

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O4	.770	.230	.358		3.1						

[Download AMC data \(View Text File\)](#)

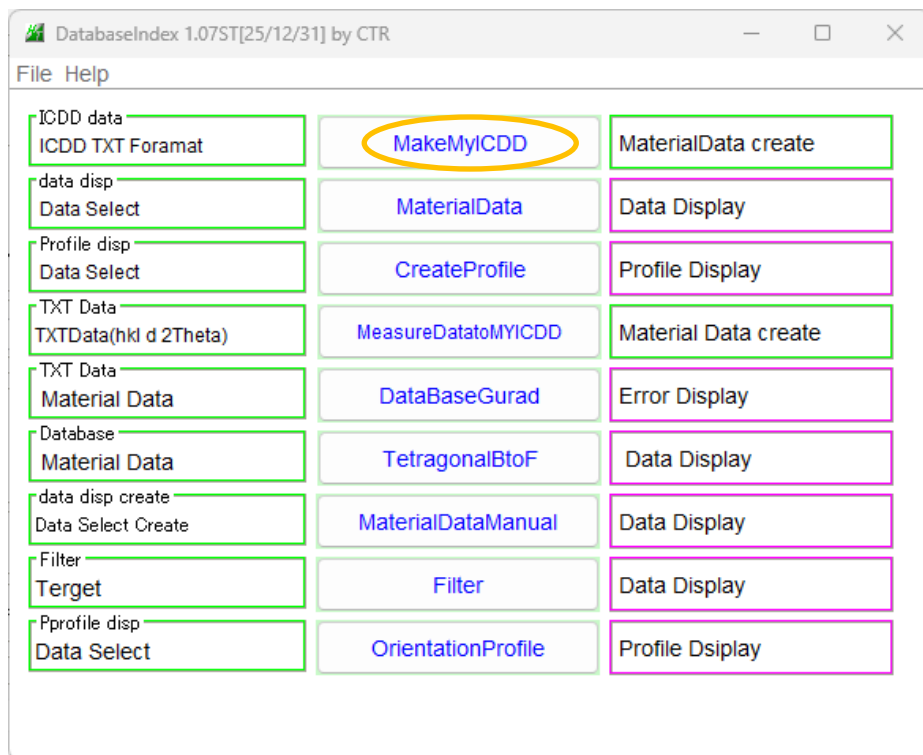
[Download CIF data \(View Text File\)](#)

[Download diffraction data \(View Text File\)](#)

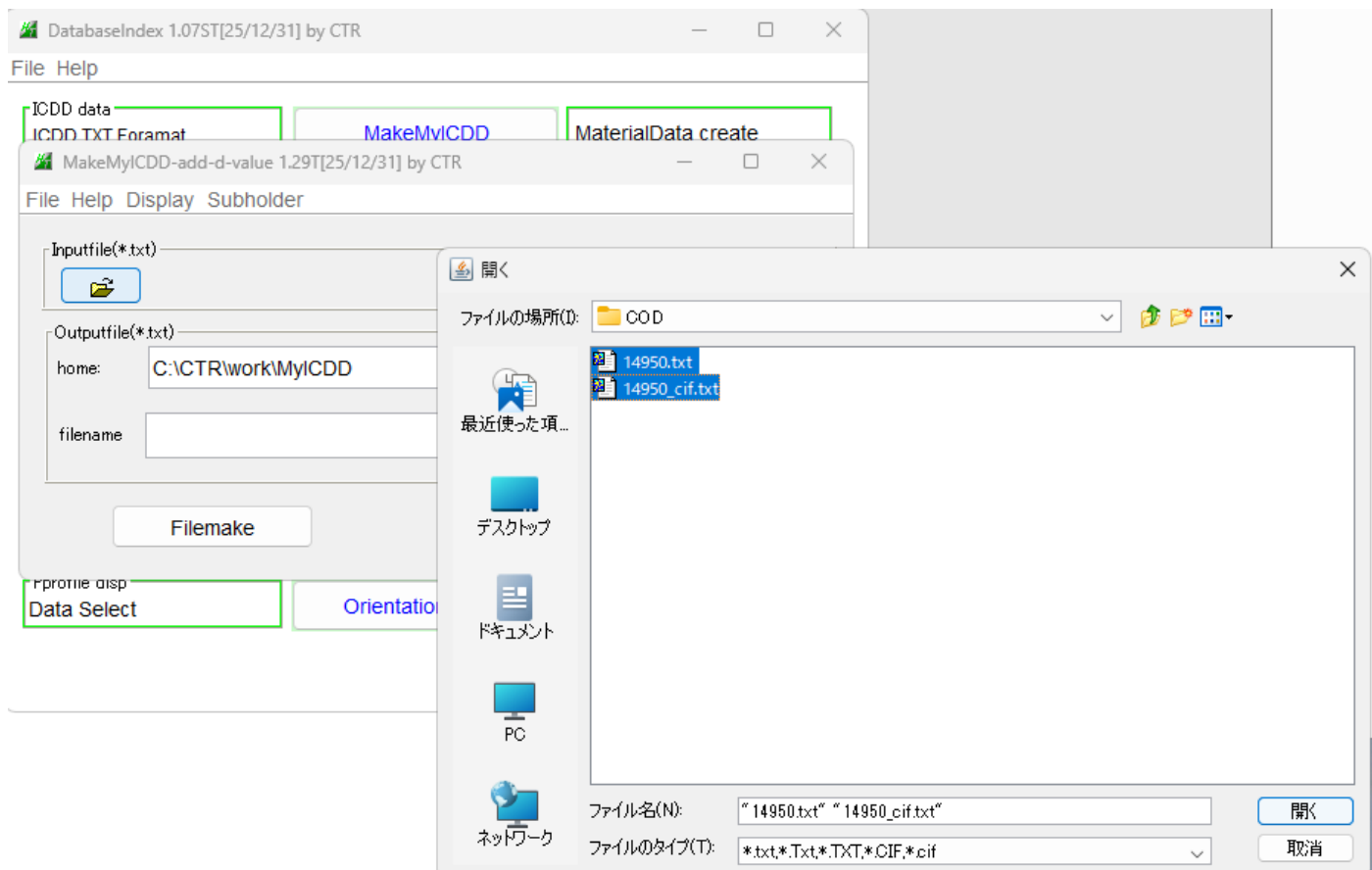
[View Jmol 3-D Structure \(permalink\)](#)

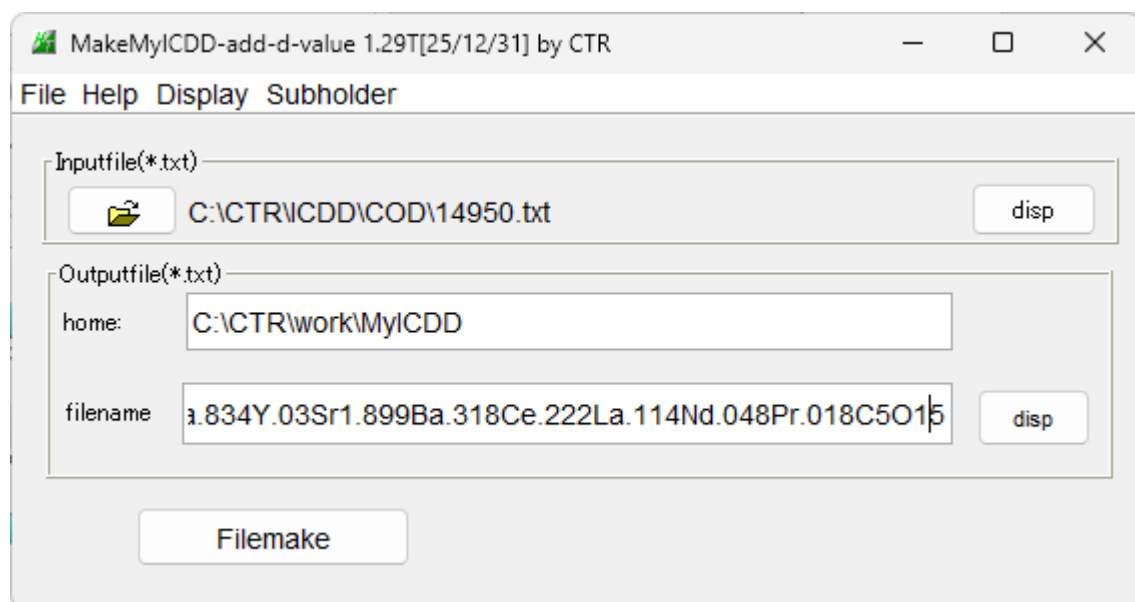
CIF と diffraction データを save する。

s a v e したデータから C T R D a t a B a s e の作成

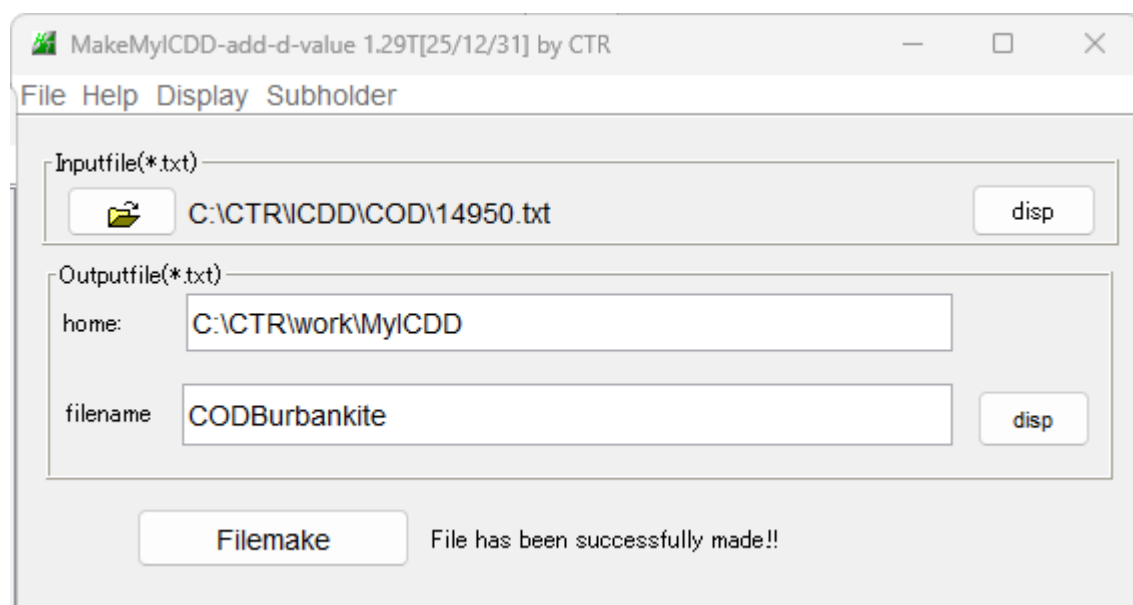
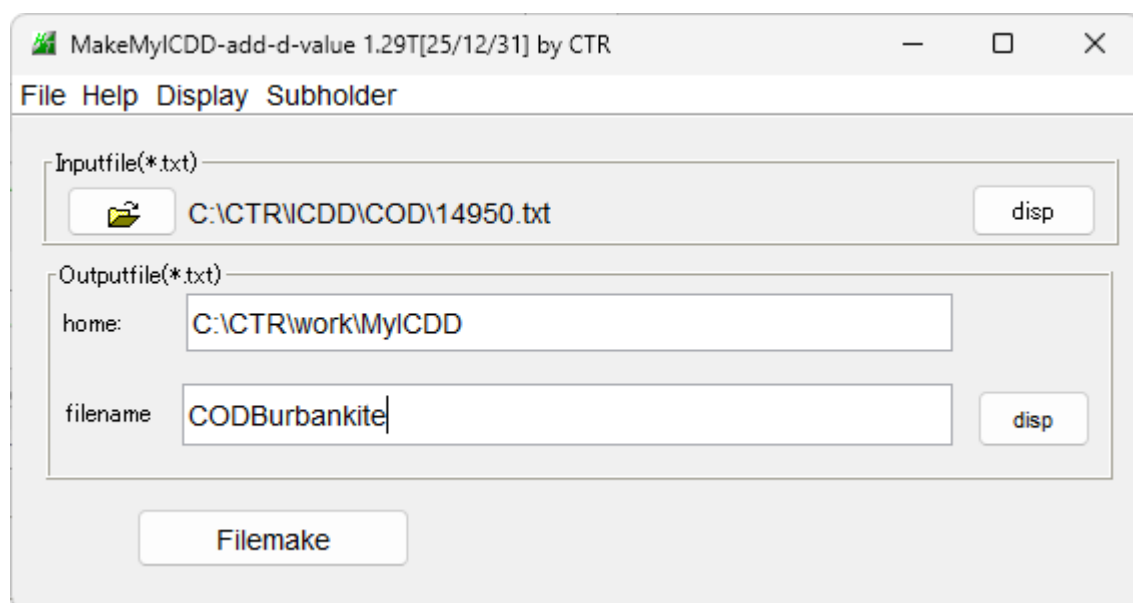


s a v e したデータから M Y I C D D データの作成





filename を変更し作成する。



作成されるファイル

TextDisplay 1.14S C:\CTR\work\MylCDD\CODBurbankite.TXT

File Help

BurbankiteNa2.184Ca.834Y.03Sr1.899Ba.318Ce.222La.114Nd.048Pr.018C5O15

4

10.5313

10.5313

6.4829

90.0

90.0

120.0

1.541838

86

1	0	0	30.17	9.1204	9.70
1	0	1	36.38	5.2840	16.78
1	1	0	37.25	5.2656	16.84
2	0	0	26.24	4.5602	19.47
2	0	1	82.14	3.7299	23.86
2	1	0	13.10	3.4472	25.85
0	0	2	48.04	3.2415	27.52
1	0	2	5.01	3.0543	29.24
2	1	1	81.96	3.0436	29.34
3	0	0	19.24	3.0401	29.38
1	1	2	16.89	2.7604	32.43
3	0	1	28.13	2.7525	32.53
2	0	2	98.65	2.6420	33.93
2	2	0	100.00	2.6328	34.05
3	1	0	3.49	2.5295	35.49
2	1	2	1.85	2.3614	38.11
3	1	1	21.31	2.3565	38.19
4	0	0	8.00	2.2801	39.52

MaterialData 1.38T[25/12/31] by CTR

File Help Disp

Search

Hexagonal

☐ LaboTex($a \leq b \leq c$ $\alpha \leq 90$ $\beta \leq 90$ $\gamma \leq 90$) ☐ Trigonal(to Rhombohedral)

Wave length

1.54056

Select

CODBurbankite.TXT

AluminumOxide.TXT

Beryllium.TXT

CODBurbankite.TXT

Gd2TiO5.TXT

Graphite.TXT

Hematite.TXT

Magnesium.TXT

Nickel-Hexa.TXT

Disp Cancel Return Structure

Chemical formula

Input(e. g. C2 H4) Change