ＭａｔｅｒｉａｌＤａｔａソフトウエア用データ作成

ＭａｋｅＭｙ ＩＣＤＤソフトウエア

Ver1.29

２０２４年１２月１７日

HelperTex Office

*Version1.101　2010/09/15 結晶系によっては正しく変換出来なかった修正
* Version 1.104　2011/06/08　trigonal で gamma=120 は Hexagonal 登録
*version 1.21X　2012/06/11 新しい管理に移行
*version 1.22X　2013/03/07 波長を wavelength=から取得
*Version 1.23X　2013/10/02　日本結晶学会データに対応（結晶系が明記されていない）
* Version 1.24X　2013/10/29　変換データＤｉｓｐが機能していない修正
* Version 1.25X　2013/11/02　物質名にカンマが入っている場合、アンダーバーに変換
*Version 1.26　2017/02/12 d-value を追加
*Version 1.27　2021/01/09 空間群に対応
*Version 1.29　2024/12/17 COD 対応,SpaceG の見直し

概要

ＭａｔｅｒｉａｌＤａｔａソフトウエア用データをＩＣＤＤテキストデータから変換するソフトウエア

入力データ

ＩＣＤＤが表示されている画面でＣｏｐｙとして editor に貼り付ける。

```
No: 00-004-0783
Name: Silver-3C, syn
Chemical Formula: Ag
Formula: Ag
Z value: 4
Space Group: Fm-3m(225)
Cell:  4.0862  4.0862  4.0862  90.000  90.000  90.000
Volume:   68.227
Crystal System: Cubic
Quality: I
RIR(I/Ic):    5.20
Subfile: Inorganic, Mineral, Alloy&Metal, Common Phase, Educational Pattern, Forensic, NBS Pattern
---------- Experiment
Radiation: CuKa1  lambda: 1.54056
Reference: Swanson, Tatge. Natl. Bur. Stand. (U.S.), Circ. 539I(1953)23.
CAS: 7440-22-4
---------- Physical
Dmeas: 10.500
Dcalc: 10.501
Melting Point: 1233.600---------- Comment
Additional Patterns: See PDF 01-087-0597. Analysis: Spectrographic analysis indicated faint traces of Ca, Fe and Cu. Color:
Light gray metallic. General Comments: Purity >99.999%. Melting Point: 1233.6 K. Opaque Optical Data: Opaque mineral optical
data on specimen from Great Bear Lake, Canada: RR2Re=94.1, Disp.=16, VHN100=55-63, Color values .314, .321, 94.2, Ref.: IMA
Commission on Ore Microscopy QDF. Sample Source or Locality: Sample obtained from Johnson Matthey Company, Ltd. Temperature of
Data Collection: Pattern taken at 300 K. Unit Cell Data Source: Powder Diffraction.
---------- d-I list (2theta are calculated with wavelength=1.54059)
2theta range:   38.12 -  134.89
   2theta     d        I      (hkl)
  38.12   2.359   100.0  (1,1,1)
  44.28   2.044    40.0  (2,0,0)
  64.43   1.445    25.0  (2,2,0)
  77.47   1.231    26.0  (3,1,1)
  81.54   1.180    12.0  (2,2,2)
  97.89   1.021     4.0  (4,0,0)
 110.50   0.938    15.0  (3,3,1)
 114.93   0.914    12.0  (4,2,0)
 134.89   0.834    13.0  (4,2,2)
```

変換出来なかった場合、入力データを点検して下さい。

区切り文字がおかしくありませんか

例えば、

```
)eleted Or Rejected By: Deleted by 00-04
)iffraction.¥par
---------- d-I list (2theta are ca
'theta range:   30.99 -  180.00¥par
   2theta     d        I      (hkl)¥par
  30.99   3.348   100.0  (0,0,2)¥par
  49.74   2.127     3.0  (1,0,0)¥par
  52.37   2.027    15.0  (1,0,1)¥par
  59.78   1.795     3.0  (1,0,2)¥par
```

或いは、最終行に空白がありませんか？

```
137.39    0.960      1.0   (2,0,3)¥par
 180.00    0.872      1.0   (1,0,7)¥par
180.00    0.837      1.0   (0,0,8)¥par
 180.00    0.833      1.0   (2,0,5)¥par
180.00    0.826      4.0   (1,1,6)¥par
180.00    0.798      2.0   (2,1,1)¥par
}
```

もしこれらの事があるならエディッタで編集して下さい。

```
 129.20    0.990      4.0   (1,1,4)↓
 137.39    0.960      1.0   (2,0,3)↓
 180.00    0.872      1.0   (1,0,7)↓
 180.00    0.837      1.0   (0,0,8)↓
 180.00    0.833      1.0   (2,0,5)↓
 180.00    0.826      4.0   (1,1,6)↓
 180.00    0.798      2.0   (2,1,1)↓
[EOF]
```

が正常な入力データです。

このように編集すれば変換が可能になります。

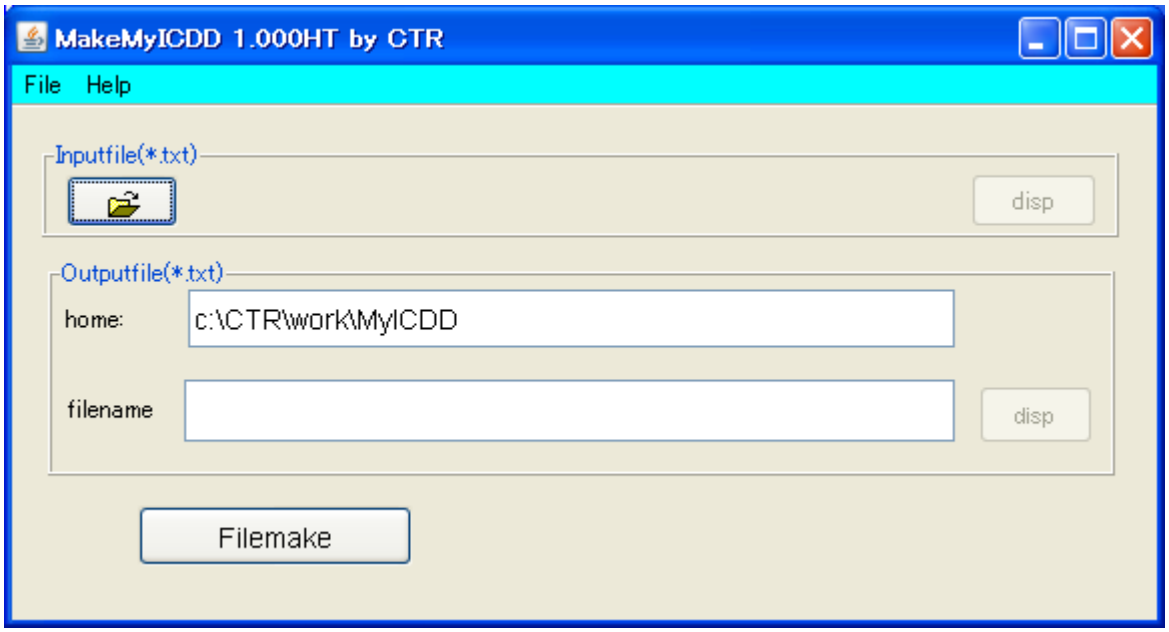
```
Graphite, syn
4
2.456
2.456
6.696
90.0
90.0
120.0
1.54178
19
0       0       2       100.0   30.99
1       0       0       3.0     49.74
1       0       1       15.0    52.37
1       0       2       3.0     59.78
0       0       4       6.0     64.60
1       0       3       4.0     71.03
1       0       4       1.0     85.69
1       1       0       4.0     93.51
1       1       2       6.0     101.77
1       0       5       1.0     104.24
0       0       6       1.0     106.55
2       0       1       1.0     116.79
1       1       4       4.0     129.20
2       0       3       1.0     137.39
1       0       7       1.0     180.00
0       0       8       1.0     180.00
2       0       5       1.0     180.00
1       1       6       4.0     180.00
2       1       1       2.0     180.00
Graphite, syn                                   Formula: C
```

出力データ

```
Silver-3C, syn
0
4.0862
4.0862
4.0862
90.0
90.0
90.0
1.54056
9
1       1       1       100.0   38.12
2       0       0       40.0    44.28
2       2       0       25.0    64.43
3       1       1       26.0    77.47
2       2       2       12.0    81.54
4       0       0       4.0     97.89
3       3       1       15.0    110.50
4       2       0       12.0    114.93
4       2       2       13.0    134.89
00-004-0783                                     Silver-3C, syn
```

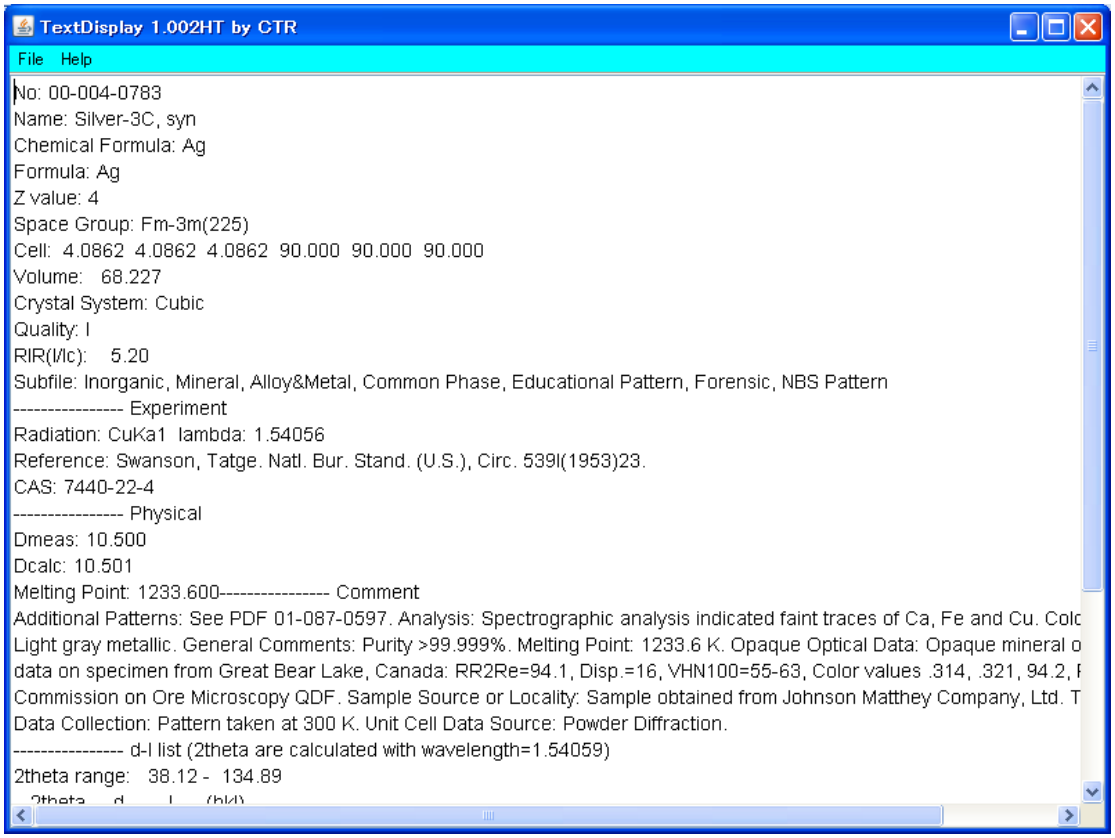
使い方

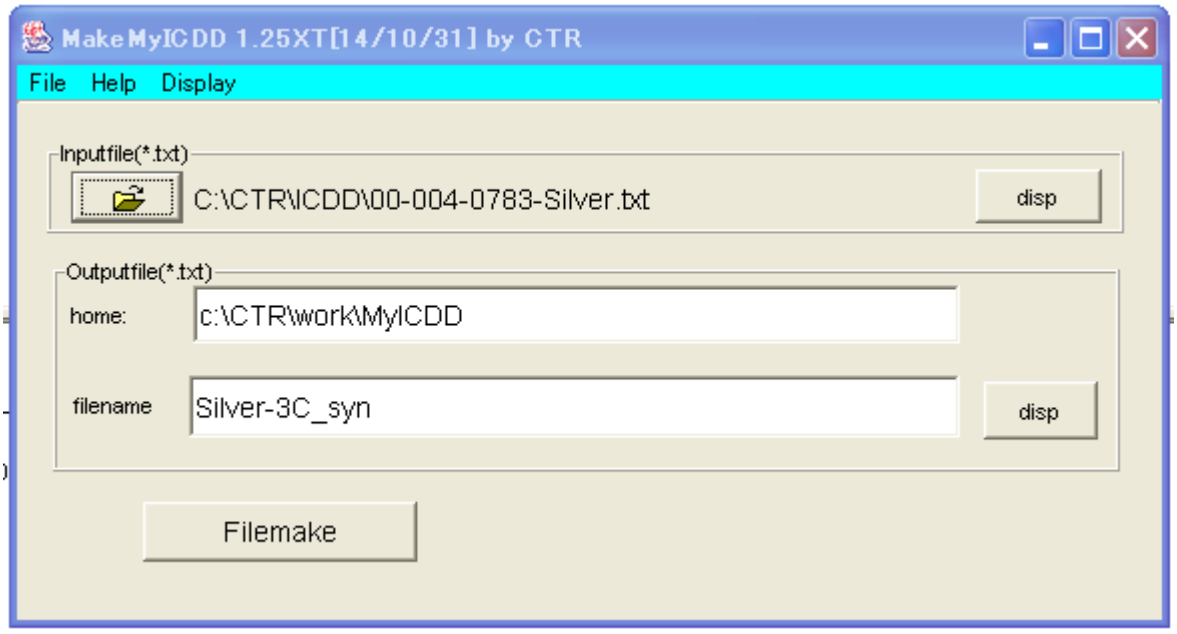
起動　c:¥CTR¥bin¥MakeMyICDD.jar



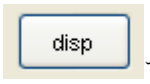
ＩＣＤＤの出力ファイルを指定する

Ｄｉｓｐでファイルを表示

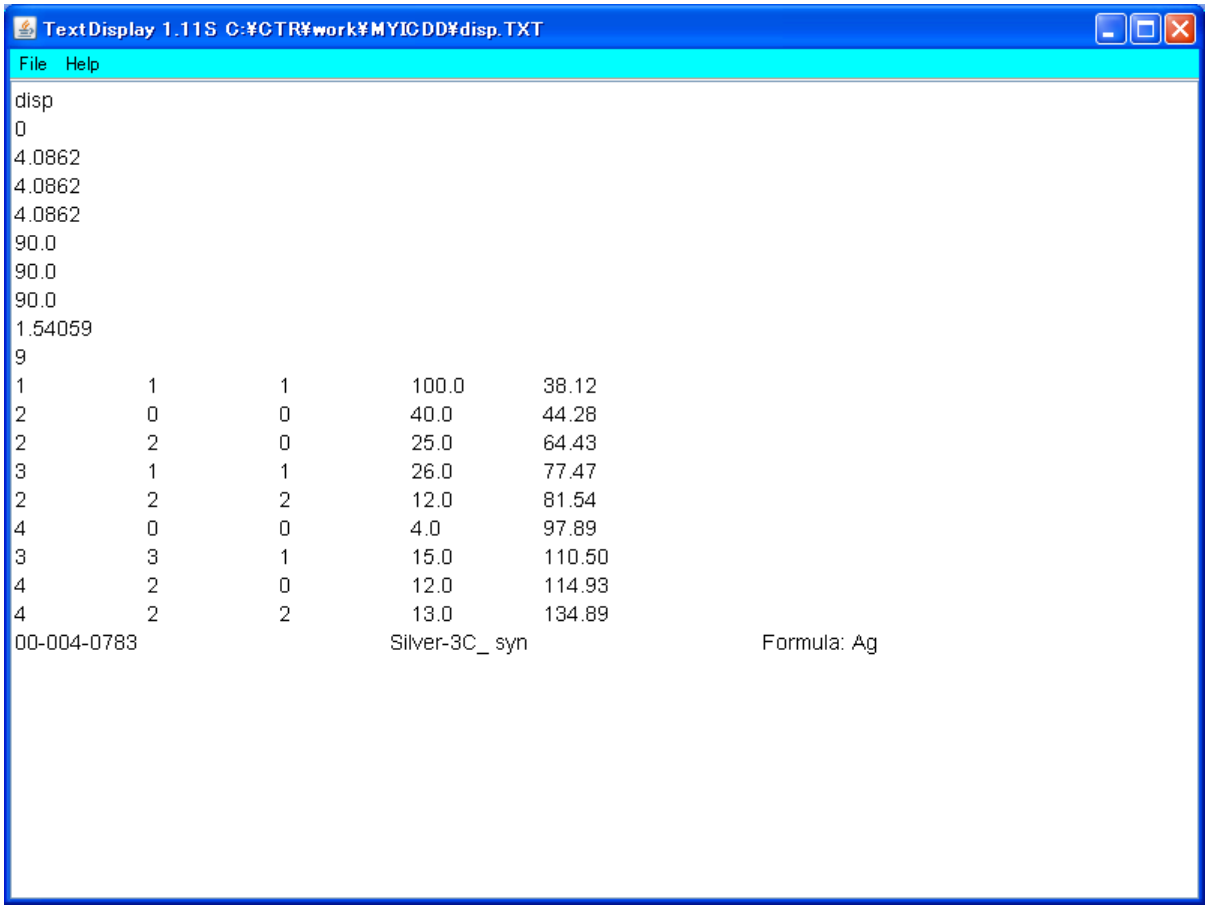




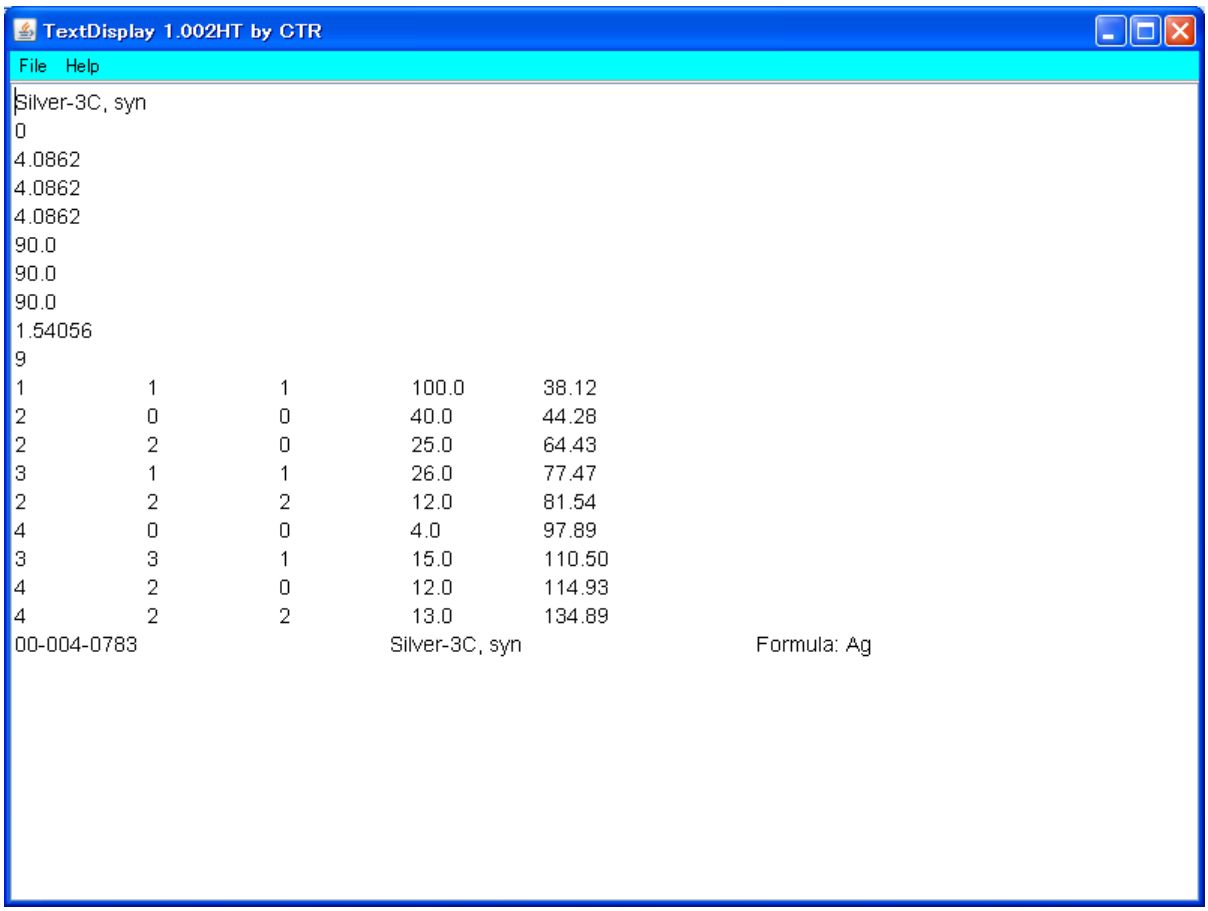
ファイル指定で、自動的にファイル名が作成される。



で作成予定のファイルが出力される。



で所定の場所にファイルが作成される。



ＣＯＤデータに対応

ＣＯＤでは、ｃｉｆとｄｉｆｆｅｒａｃｔｉｏｎデータがｄｏｗｎｌｏａｄ出来る。

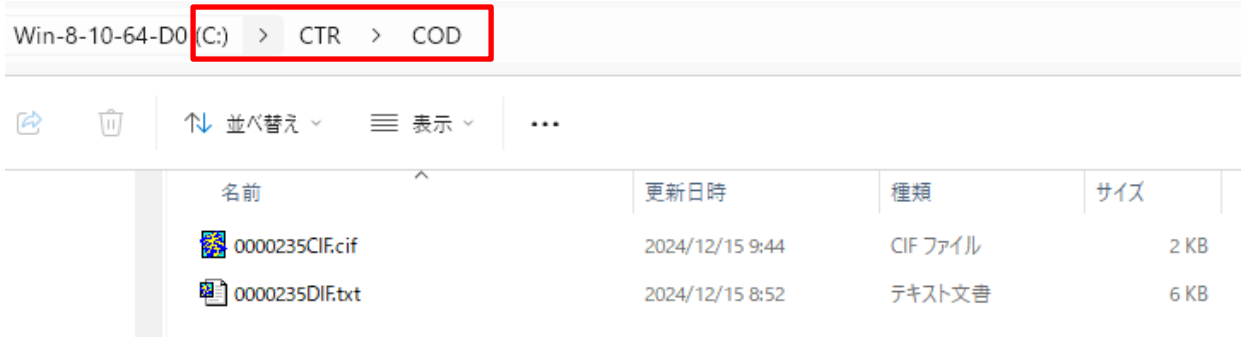
リガクｉｃｄｄデータと異なり、ｄｉｆｆｅｒａｃｔｉｏｎデータでは情報が少なく、

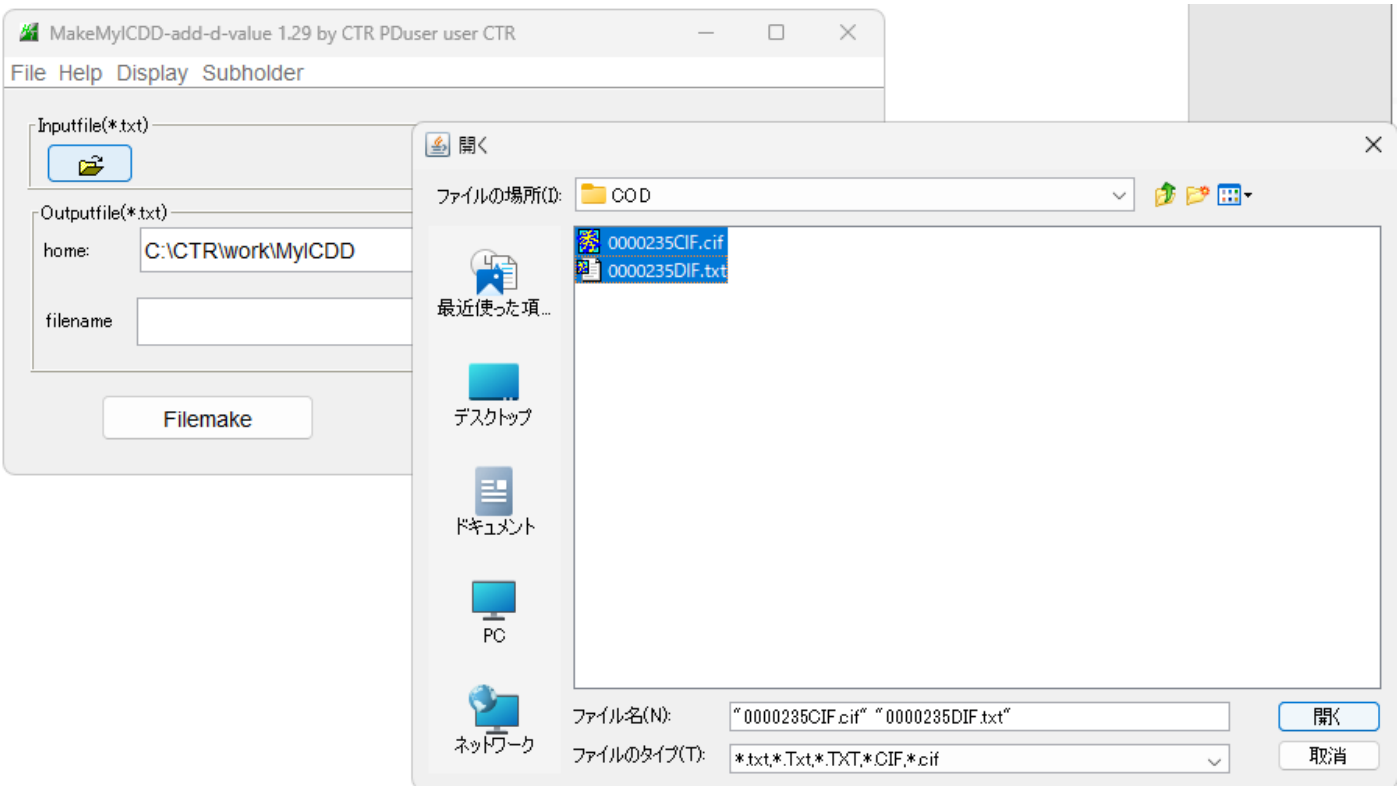
ｃｉｆデータと共に読み込まないとＭＹＩＣＤＤデータは完結しない。

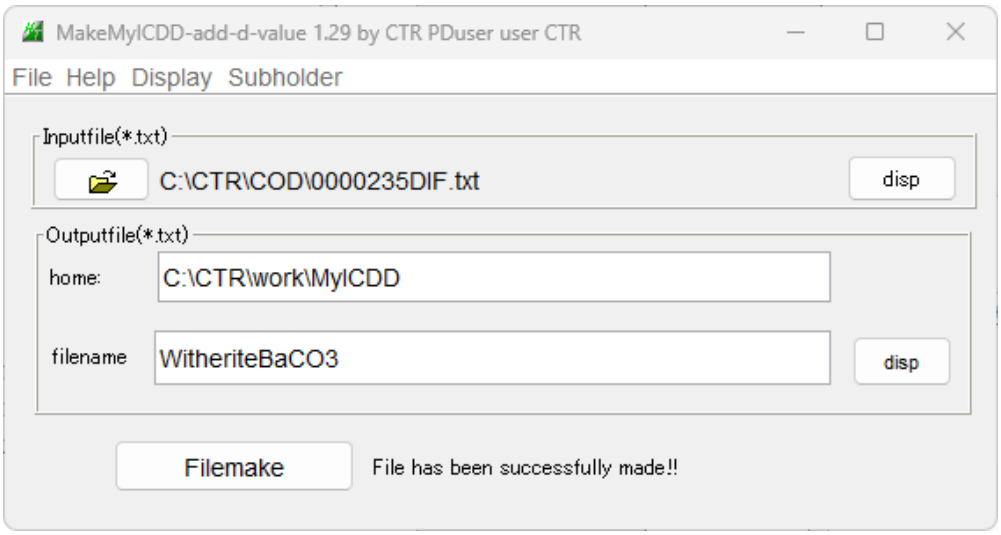
ＭａｋｅＭｙＩＣＤＤソフトウエアにＣＯＤデータ読み込みを追加した。

ＣＯＤデータのｃｉｆとｄｉｆｆｅｒａｔｉｏｎデータ（ｔｘｔ）をｄｏｗｎｌｏａｄし

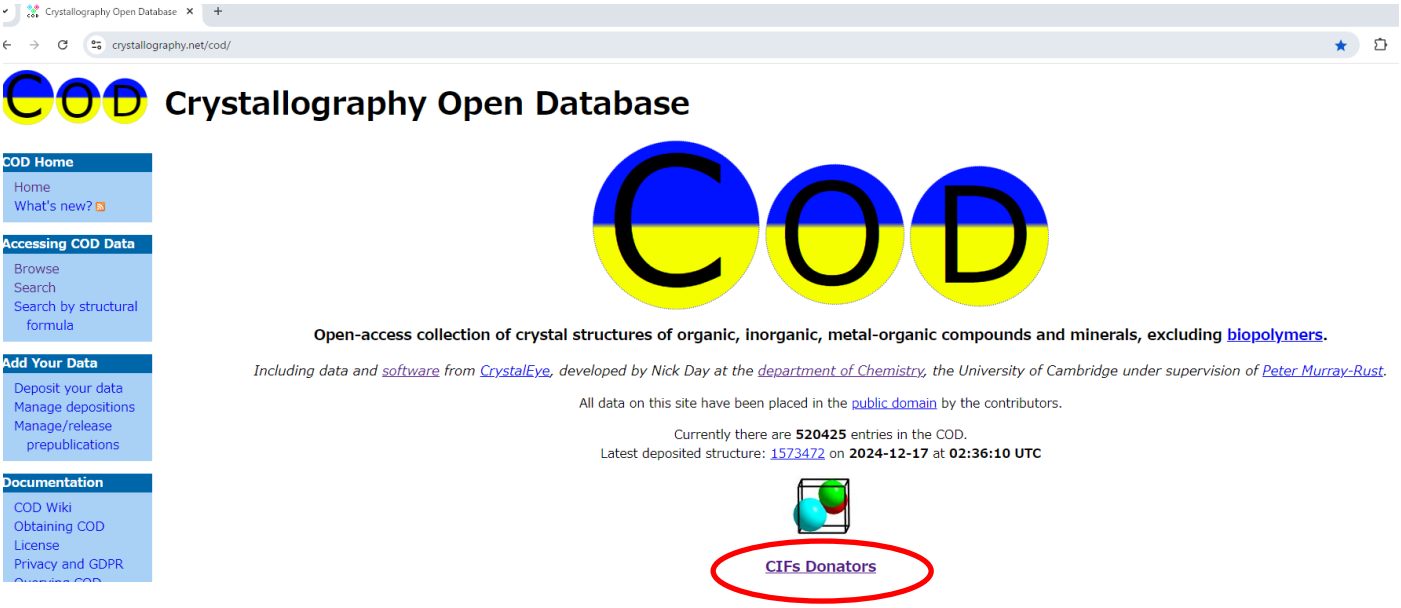
ＣＴＲ￥ＣＯＤホルダにｃｏｐｙを行い読み込む







ＣＯＤでの処理


Crystallography Open Database
crystallography.net/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
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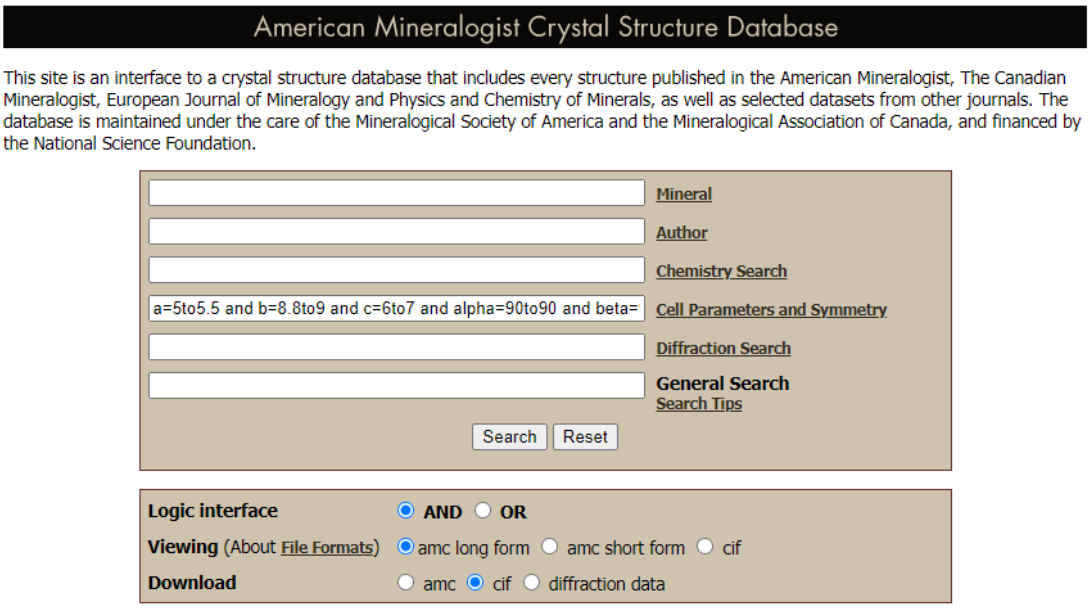
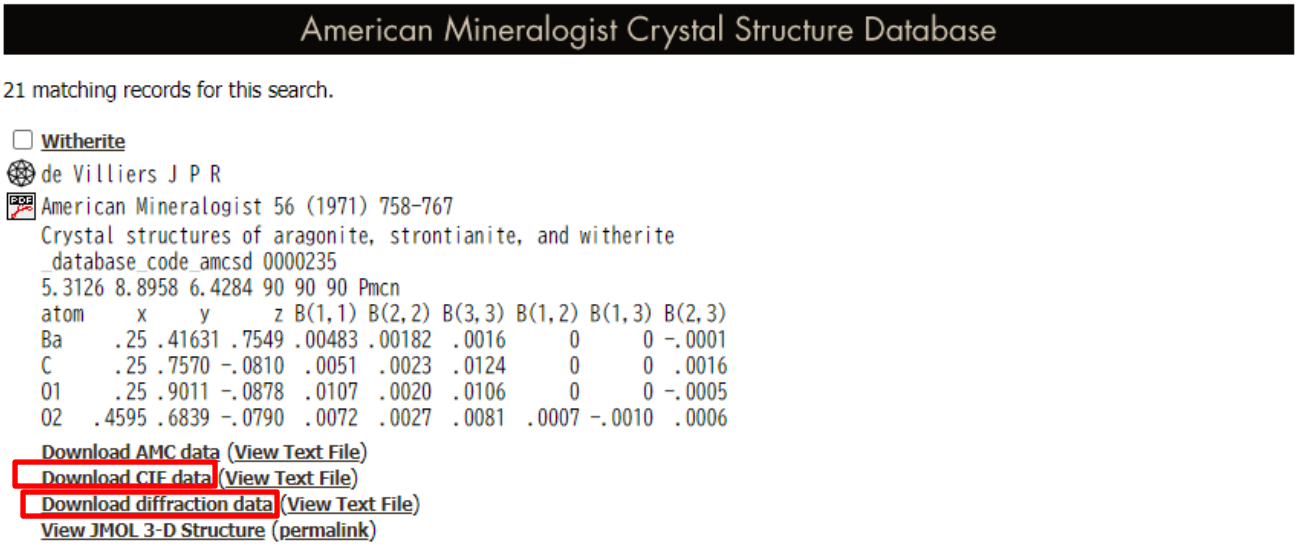
Open-access collection of crystal structures of organic, inorganic, metal-organic compounds and minerals, excluding biopolymers.
Including data and software from CrystalEye, developed by Nick Day at the department of Chemistry, the University of Cambridge under supervision of Peter Murray-Rust.
All data on this site have been placed in the public domain by the contributors.
Currently there are 520425 entries in the COD.
Latest deposited structure: 1573472 on 2024-12-17 at 02:36:10 UTC
CIFs Donators


Crystallography Open Database
crystallography.net/cod/donators/index.html
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.


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.
Mineral
Author
Chemistry Search
a=5to5.5 and b=8.8to9 and c=6to7 and alpha=90to90 and beta=
Cell Parameters and Symmetry
Diffraction Search
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

Ｓｅａｒｃｈを行い


American Mineralogist Crystal Structure Database

21 matching records for this search.

Witherite
de Villiers J P R
American Mineralogist 56 (1971) 758-767
Crystal structures of aragonite, strontianite, and witherite
_database_code_amcsd 0000235
5.3126 8.8958 6.4284 90 90 90 Pmcn

atom	x	y	z	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)
Ba	.25	.41631	.7549	.00483	.00182	.0016	0	0	-.0001
C	.25	.7570	-.0810	.0051	.0023	.0124	0	0	.0016
O1	.25	.9011	-.0878	.0107	.0020	.0106	0	0	-.0005
O2	.4595	.6839	-.0790	.0072	.0027	.0081	.0007	-.0010	.0006

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データとｄｉｆｆｒａｃｔｉｏｎデータを
Ｃ：￥ＣＴＲ￥ＣＯＤにコピーを行う。