ＣＯＤデータからＣＴＲＤａｔａＢａｓｅデータ作成

２０２５年０９月１９日

ＨｅｌｐｅｒＴｅｘ　Ｏｆｆｉｃｅ

概要

ＣＴＲのＤａｔａＢａｓｅ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**

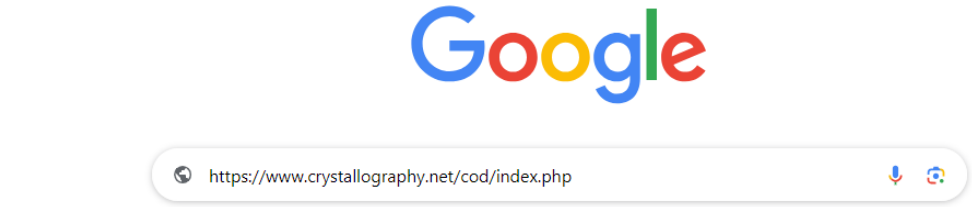
Belovitskaya Yu V, Pekov I V, Kabalov Yu K
Crystallography Reports 45 (2000) 26-29
Refinement of the crystal structures of low-rare-earth
and "typical" burbankites by the Rietveld method
Locality: Khibiny Massif, Kola Peninsula, Russia
Sample: B-108
Note: x02 adjusted to satisfy symmetry constraints
_database_code_amcsd 0012365
10.5313 10.5313 6.4829 90 90 120 P6_3mc

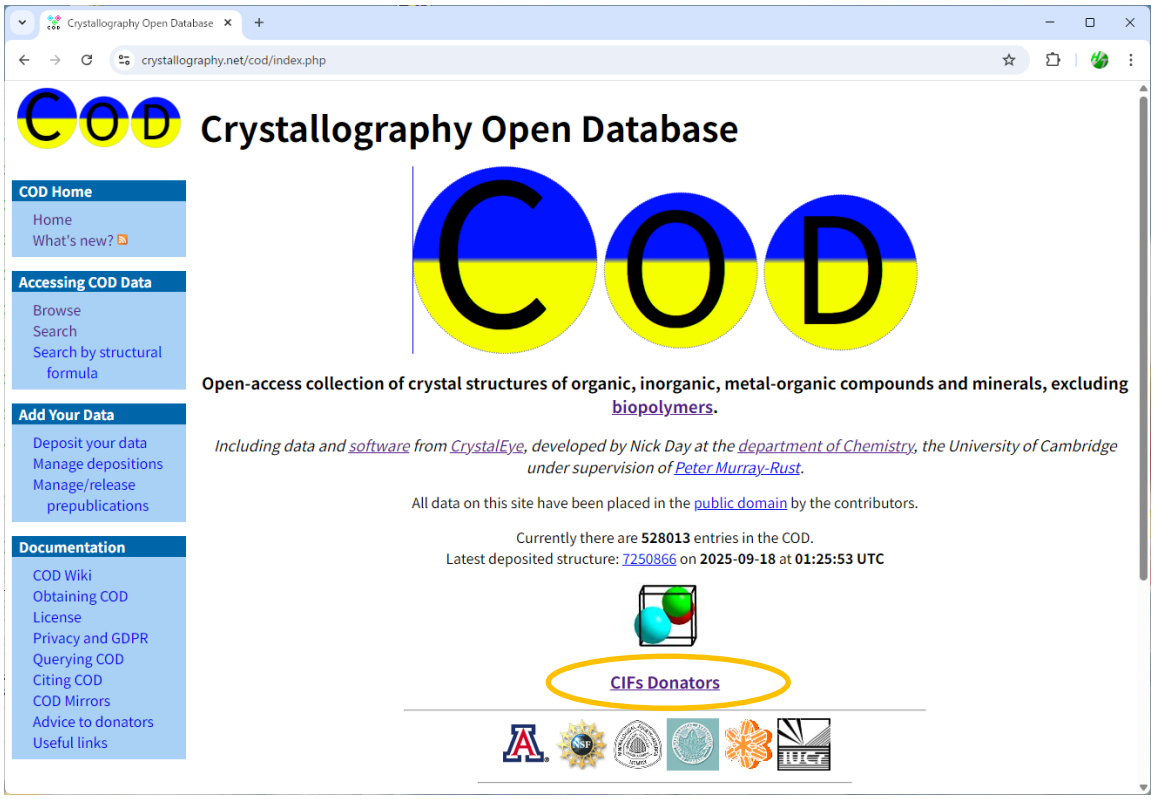
atom	x	y	z	occ	Biso	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)
NaA	.5237	.4763	.319	.728	1.7	.006	.006	.011	0	.003	-.003
CaA	.5237	.4763	.319	.231	1.7	.006	.006	.011	0	.003	-.003
YA	.5237	.4763	.319	.01	1.7	.006	.006	.011	0	.003	-.003
SrB	.8410	.1590	0	.633	.88	.0021	.0021	.0091	.0010	.001	-.001
BaB	.8410	.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						

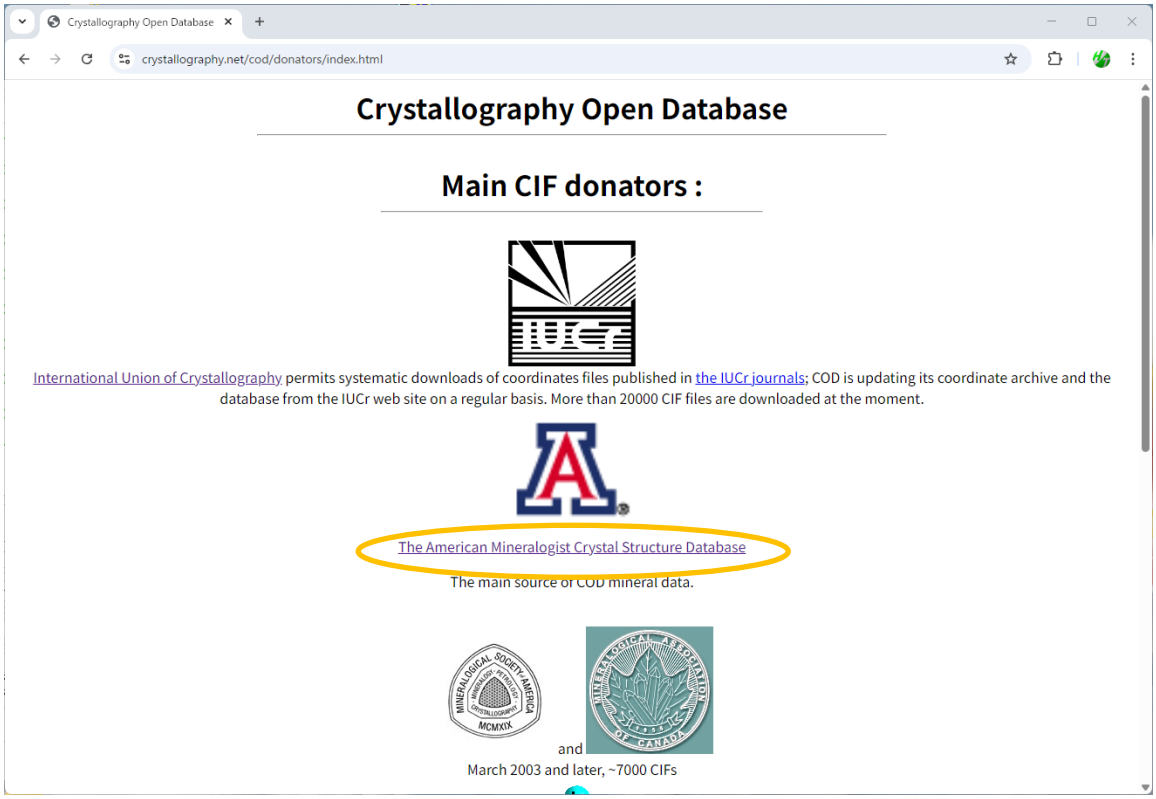
Download AMC data (View Text File)
Download CIF data (View Text File)
Download diffraction data (View Text File)
View JMOL 3-D Structure (permalink)

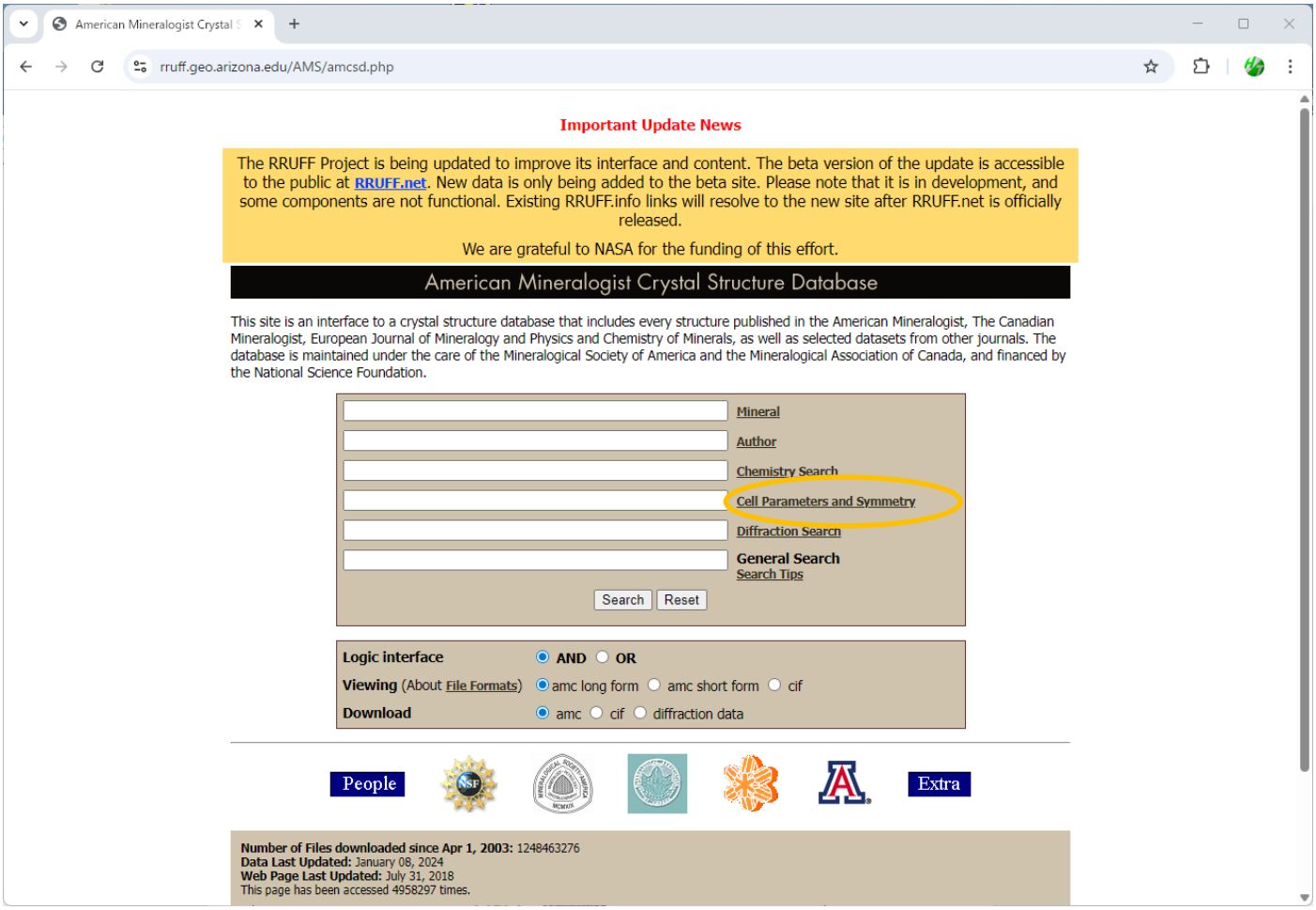
CIF と diffraction データを download しＤａｔａＢａｓｅのＭａｋｅＭｙＩＣＤＤにより作成します。

ＣＯＤから cif と diffraction を得る。








American Mineralogist Crystal S
rruff.geo.arizona.edu/AMS/amcsd.php
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.
Mineral
Author
Chemistry Search
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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
People
Extra
Number of Files downloaded since Apr 1, 2003: 1248463276
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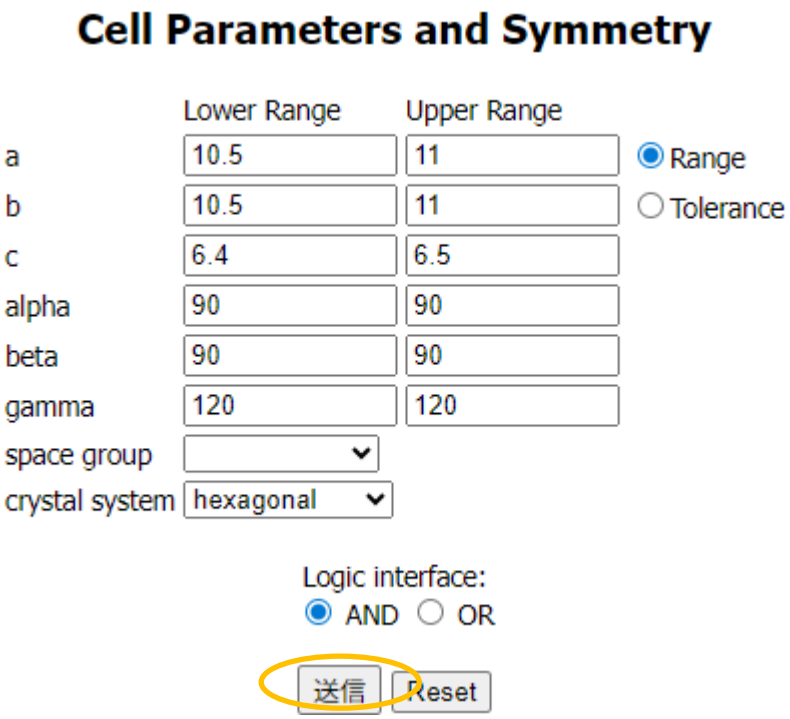
Web Page Last Updated: July 31, 2018
This page has been accessed 4958297 times.

格子定数の限定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Lower Range
Upper Range
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10.5
11
Range
b
10.5
11
Tolerance
c
6.4
6.5
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gamma
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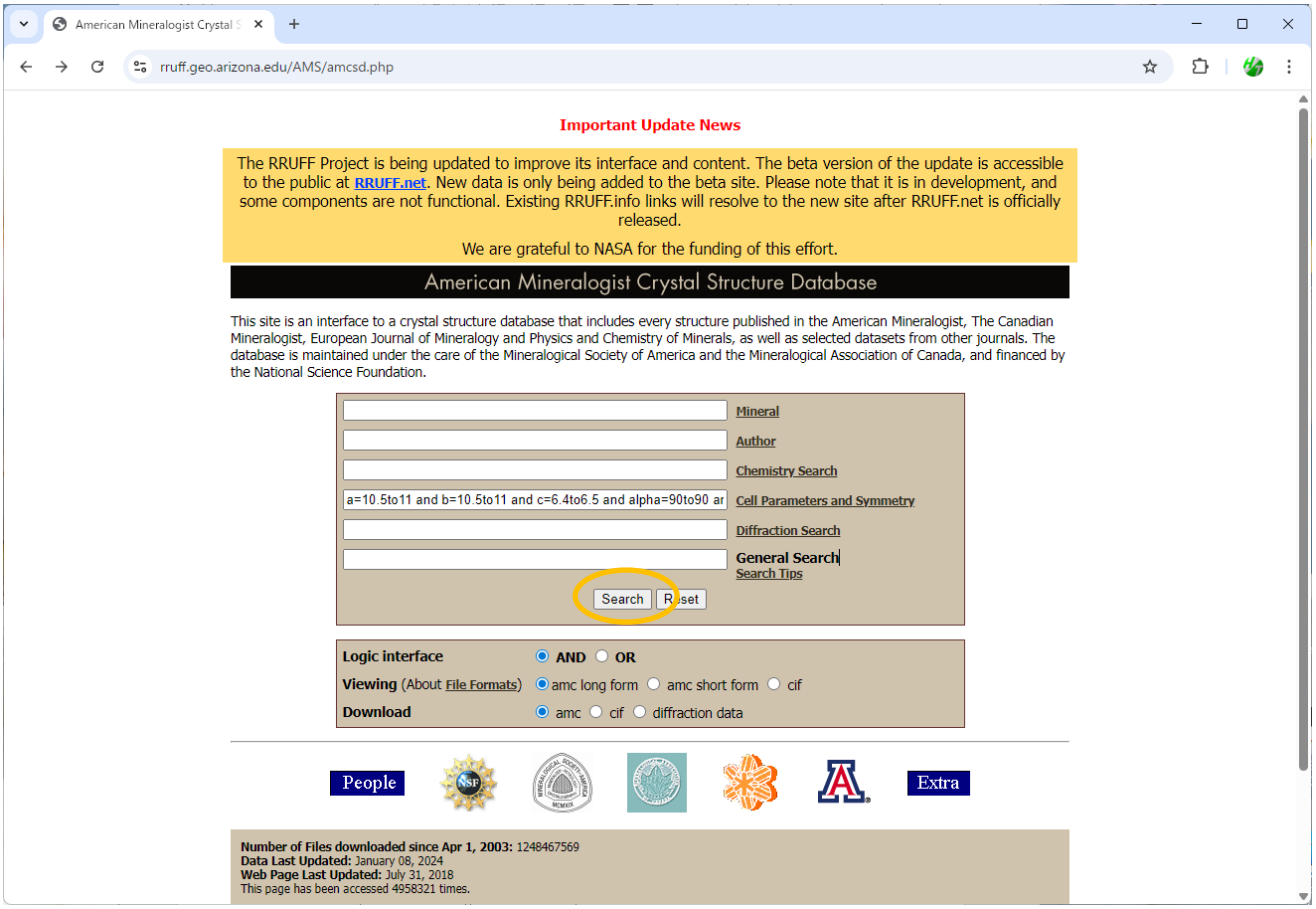
space group
crystal system
hexagonal
Logic interface:
AND
OR
送信
Reset



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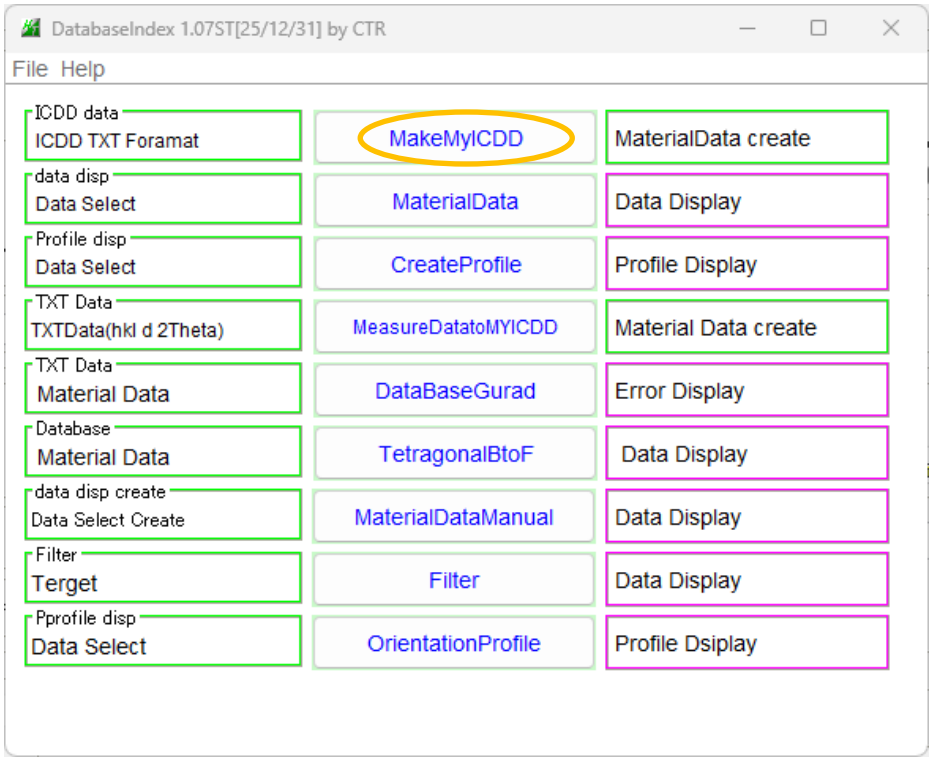
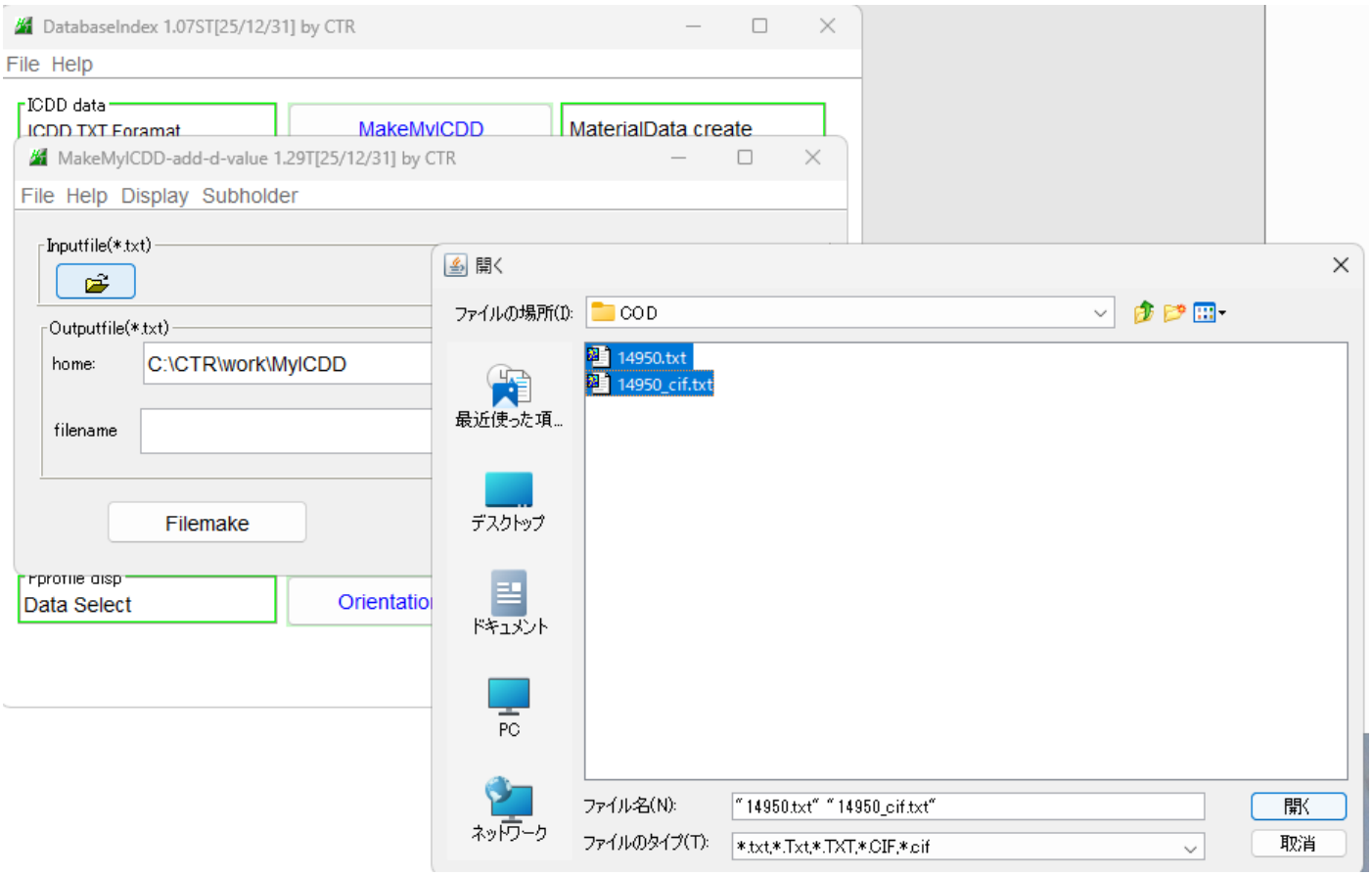
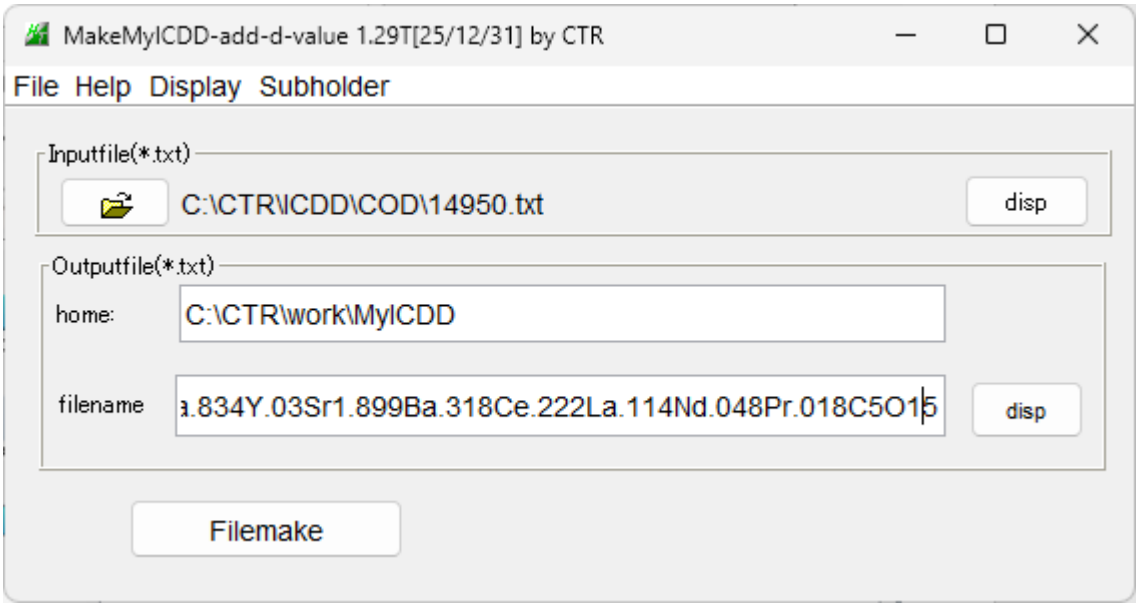
CIF と diffraction データを ｓ ａ ｖ ｅする。

ｓａｖｅしたデータからＣＴＲＤａｔａＢａｓｅの作成



ｓａｖｅしたデータからＭＹＩＣＤＤデータの作成





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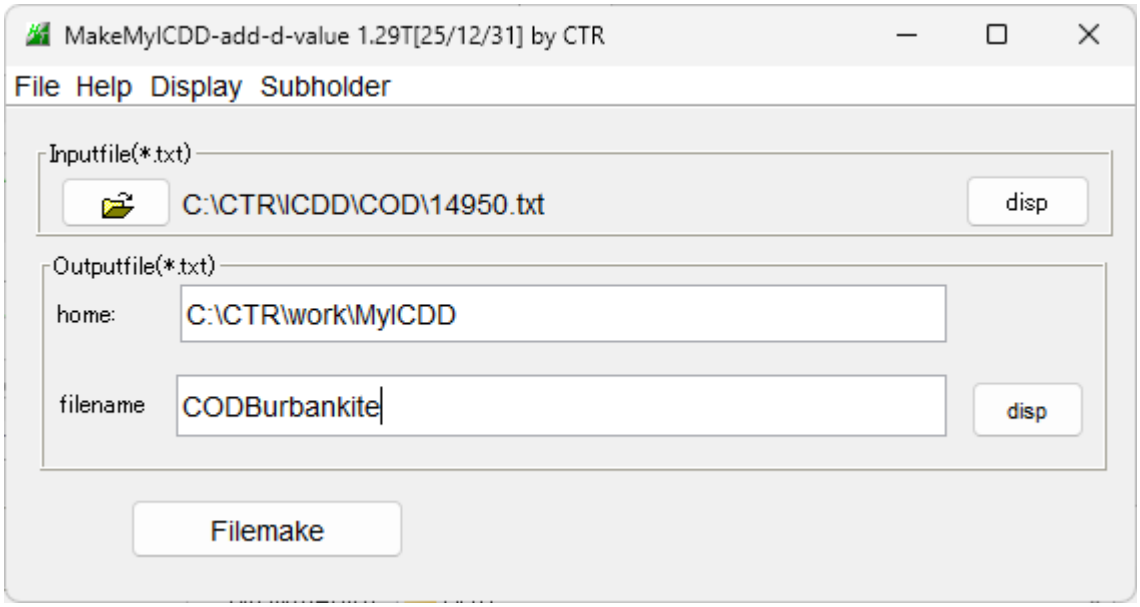

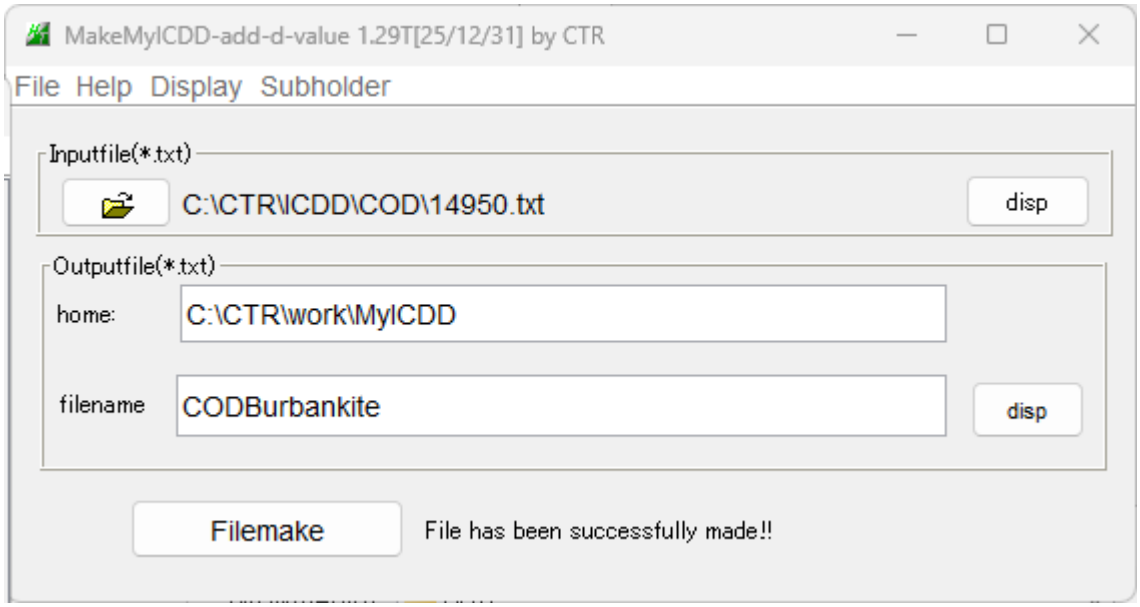

作成されるファイル

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File Help

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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

Ｄａｔａ Ｂａｓｅ登録の確認