

三方晶系の菱面体格子の扱い

2025年09月27日

概要

三方晶系の空間群は143から167の25の空間群が含まれる。

六方晶ブラベ格子 (P 18空間群)、菱面体ブラベ格子 (R 7空間群)

菱面体ブラベ格子は、六方晶と三方晶の表現が可能であるが、六方晶ブラベ格子は六方晶表現のみ
菱面体ブラベ格子は

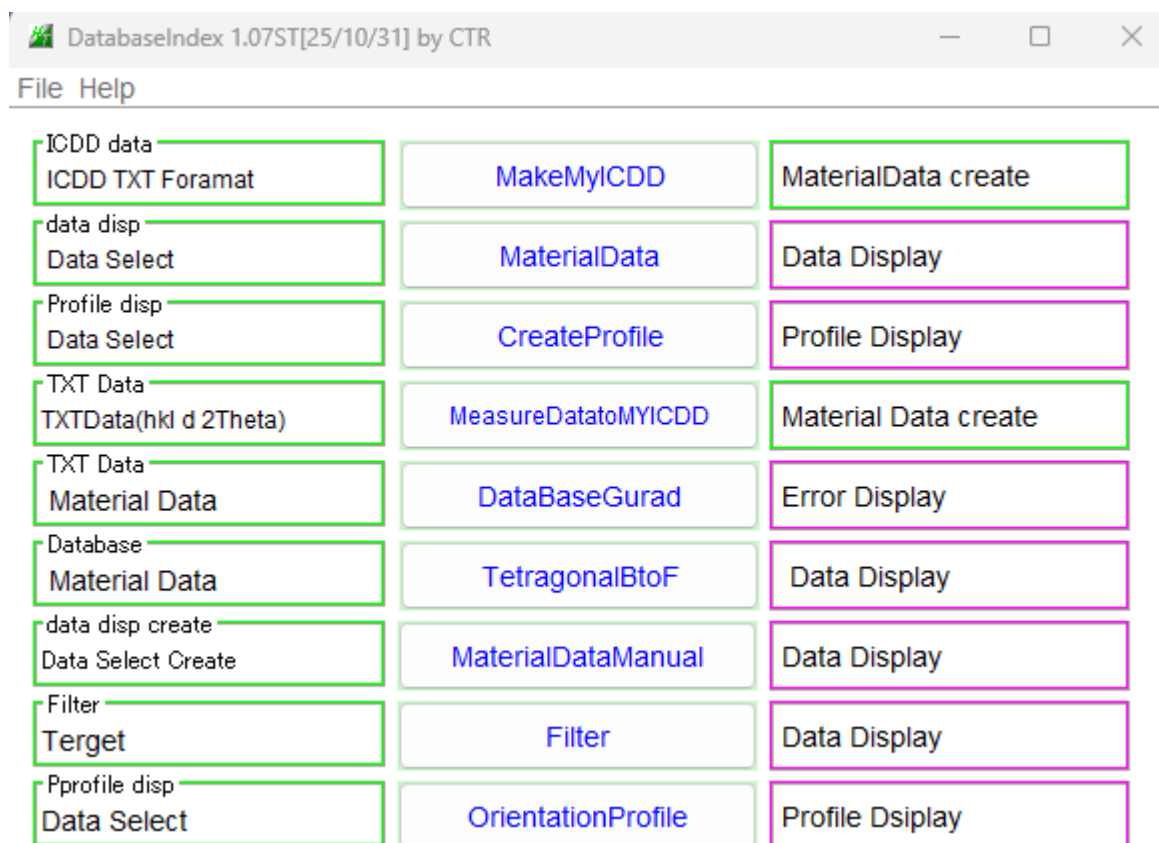
146 R3 148 R-3 155 R32 160 R3m
161 R3c 166 6R-3c1 167 R-3c

で六方晶表現で $-H+K+L=3n$ が成立している。

以下に7空間群の六方晶と三方晶表現を示す。

Hexagonal (六方晶系 P) とは区別される。

Hexagonalの空間群は、168から194である。



CODデータをMakeMyICDDで変換しMaterialDataで表示しています。

MakeMyICDDによる登録はHexagonalに登録 (4)

MaterialData表示はHexagonalで選択、表示はTrigonal
六方晶ブラベ格子はTrigonalに登録 (3)

MaterialData表示はTrigonalで選択

0000022
Cronstedtite
Formula: Si₅Fe_{1.4}O_{4.001}H_{1.667}
_symmetry_space_group_name_H-M 'R3'
_symmetry_Int_Tables_number 146
_Symmetry 3

登録は Hexa に分類

146HRDISP

Trigonal

3.16 (1.0)
3.16 (1.0)
21.25 (6.7247)

90.0
90.0
120.0
1.54056

29					
0	0	3	18.05	7.0833	12.486
0	0	6	100.0	3.5417	25.123
1	0	1	39.31	2.7142	32.974
0	1	2	5.26	2.6501	33.794
1	0	4	68.95	2.4328	36.917
0	0	9	4.18	2.3611	38.081
0	1	5	33.68	2.3009	39.118
1	0	7	5.62	2.0326	44.538
0	1	8	7.26	1.906	47.673
0	0	12	1.79	1.7708	51.568
1	0	10	28.22	1.6784	54.637
1	1	0	19.59	1.58	58.355
0	1	11	10.84	1.5782	58.428
2	-1	3	2.83	1.5421	59.934
1	1	3	2.83	1.5421	59.934
2	-1	6	6.75	1.4429	64.53
1	1	6	6.75	1.4429	64.53

146HRDISP

Rhombohedral or Trigonal

7.3145 (1.0)
7.3145 (1.0)
7.3145 (1.0)

24.9494
24.9494
24.9494
1.54056

29					
1	1	1	18.05	7.0833	12.486
2	2	2	100.0	3.5417	25.123
1	0	0	39.31	2.7142	32.974
1	1	0	5.26	2.6501	33.795
2	1	1	68.95	2.4328	36.917
3	3	3	4.18	2.3611	38.081
2	2	1	33.68	2.3009	39.118
3	2	2	5.62	2.0326	44.538
3	3	2	7.26	1.906	47.673
4	4	4	1.79	1.7708	51.568
4	3	3	28.22	1.6784	54.637
1	0	-1	19.59	1.58	58.356
4	4	3	10.84	1.5782	58.428
2	0	1	2.83	1.5421	59.934
2	1	0	2.83	1.5421	59.934
3	1	2	6.75	1.4429	64.53
3	2	1	6.75	1.4429	64.53

148 R-3 Dolomite

0000086

Dolomite

Formula: CaMgC2O6

_symmetry_space_group_name_H-M 'R-3'

_symmetry_Int_Tables_number 148

_Symmetry 3

148HRDISP

Trigonal

4.815 (1.0)

4.815 (1.0)

16.119 (3.3477)

90.0

90.0

120.0

1.54056

33

1	0	1	2.05	4.037	21.999
0	1	2	2.21	3.7036	24.008
1	0	4	100.0	2.8977	30.831
0	0	6	4.6	2.6865	33.324
0	1	5	5.19	2.5505	35.157
1	1	0	11.44	2.4075	37.32
1	1	3	17.99	2.197	41.048
2	-1	3	5.68	2.197	41.048
0	2	1	4.13	2.0677	43.743
2	0	2	13.87	2.0185	44.867
0	2	4	4.36	1.8518	49.16
0	1	8	18.07	1.8142	50.249
1	1	6	6.78	1.7929	50.888
2	-1	6	12.85	1.7929	50.888
0	0	9	1.24	1.791	50.946
3	-1	1	2.51	1.5686	58.821
2	1	1	1.93	1.5686	58.821
1	2	2	3.0	1.5468	59.734

148HRDISP

Rhombohedral or Trigonal

6.0496 (1.0)

6.0496 (1.0)

6.0496 (1.0)

46.9018

46.9018

46.9018

1.54056

33

1	0	0	2.05	4.037	21.999
1	1	0	2.21	3.7036	24.008
2	1	1	100.0	2.8978	30.831
2	2	2	4.6	2.6865	33.323
2	2	1	5.19	2.5505	35.157
1	0	-1	11.44	2.4075	37.32
2	1	0	17.99	2.197	41.048
2	0	1	5.68	2.197	41.048
1	1	-1	4.13	2.0677	43.742
2	0	0	13.87	2.0185	44.866
2	2	0	4.36	1.8518	49.16
3	3	2	18.07	1.8142	50.249
3	2	1	6.78	1.7929	50.887
3	1	2	12.85	1.7929	50.887
3	3	3	1.24	1.791	50.945
2	-1	0	2.51	1.5686	58.82
2	0	-1	1.93	1.5686	58.82
2	1	-1	3.0	1.5468	59.734

155 R32 Tincalconite

0000321

Tincalconite

Formula: NaB2O6H5

_symmetry_space_group_name_H-M 'R32'

_symmetry_Int_Tables_number 155

_Symmetry 32

155DISP

Trigonal

11.09 (1.0)

11.09 (1.0)

21.07 (1.8999)

90.0

90.0

120.0

1.54056

100

1	0	1	10.9	8.7391	10.113
0	1	2	1.31	7.0975	12.461
0	0	3	19.26	7.0233	12.593
1	1	0	12.73	5.545	15.97
0	2	1	41.18	4.682	18.938
1	0	4	2.95	4.6185	19.202
2	0	2	58.72	4.3696	20.307
1	1	3	36.77	4.3521	20.389
0	1	5	6.48	3.8589	23.029
2	1	1	9.08	3.5774	24.869
0	2	4	6.41	3.5488	25.072
1	2	2	64.6	3.432	25.94
2	0	5	6.04	3.1674	28.15
2	1	4	29.8	2.989	29.868
1	1	6	14.55	2.9668	30.097
0	3	3	7.25	2.913	30.665
3	0	3	92.75	2.913	30.665
1	0	7	9.68	2.8722	31.112

155DISP

Rhombohedral or Trigonal

9.5039 (1.0)

9.5039 (1.0)

9.5039 (1.0)

71.3868

71.3868

71.3868

1.54056

100

1	0	0	10.9	8.7392	10.113
1	1	0	1.31	7.0975	12.461
1	1	1	19.26	7.0234	12.593
1	0	-1	12.73	5.545	15.97
1	1	-1	41.18	4.6821	18.938
2	1	1	2.95	4.6185	19.201
2	0	0	58.72	4.3696	20.307
2	1	0	36.77	4.3521	20.389
2	2	1	6.48	3.8589	23.028
2	0	-1	9.08	3.5774	24.869
2	2	0	6.41	3.5488	25.072
2	1	-1	64.6	3.432	25.94
3	1	1	6.04	3.1674	28.15
3	1	0	29.8	2.989	29.867
3	2	1	14.55	2.9668	30.097
2	2	-1	7.25	2.9131	30.665
3	0	0	92.75	2.9131	30.665
3	2	2	9.68	2.8723	31.112

1 6 0 R 3 m S i C

0000031

SiC-IV

Formula: Si7C7

_symmetry_space_group_name_H-M 'R3m'

_symmetry_Int_Tables_number 160

_Symmetry 32

160HRDISP

Trigonal

3.073 (1.0)
3.073 (1.0)
52.78 (17.1754)

90.0

90.0

120.0

1.54056

41

1	0	1	3.35	2.6579	33.693
0	1	2	12.23	2.6479	33.824
1	0	4	38.45	2.6088	34.347
0	1	5	48.28	2.5805	34.734
0	0	21	100.0	2.5133	35.694
1	0	7	99.95	2.5096	35.75
0	1	8	55.49	2.4681	36.372
1	0	10	37.61	2.3763	37.828
0	1	11	30.29	2.3273	38.656
1	0	13	15.99	2.2257	40.495
0	1	14	23.58	2.1742	41.5
1	0	16	9.06	2.0713	43.664
0	1	17	5.8	2.0206	44.818
1	0	19	2.22	1.9217	47.26
0	1	23	1.75	1.7379	52.619
1	0	25	8.88	1.654	55.513
0	1	26	10.49	1.614	57.01
1	0	28	28.91	1.5382	60.1

160HRDISP

Rhombohedral or Trigonal

17.6826 (1.0)
17.6826 (1.0)
17.6826 (1.0)

9.9698

9.9698

9.9698

1.54056

41

1	0	0	3.35	2.6579	33.693
1	1	0	12.23	2.6479	33.824
2	1	1	38.45	2.6088	34.347
2	2	1	48.28	2.5805	34.734
7	7	7	100.0	2.5133	35.694
3	2	2	99.95	2.5096	35.75
3	3	2	55.49	2.4681	36.372
4	3	3	37.61	2.3763	37.828
4	4	3	30.29	2.3273	38.656
5	4	4	15.99	2.2257	40.495
5	5	4	23.58	2.1742	41.5
6	5	5	9.06	2.0713	43.664
6	6	5	5.8	2.0206	44.818
7	6	6	2.22	1.9217	47.26
8	8	7	1.75	1.7379	52.619
9	8	8	8.88	1.654	55.513
9	9	8	10.49	1.614	57.01
10	9	9	28.91	1.5382	60.1

161 R3c Whitlockite
 0000445
 Whitlockite
 Formula: (Mg.587Fe.413)Ca9.095P7O28
 _symmetry_space_group_name_H-M 'R3c'
 _symmetry_Int_Tables_number 161
 _Symmetry 32

161HRDISP

Trigonal

10.33 (1.0)

10.33 (1.0)

37.103 (3.5918)

90.0

90.0

120.0

1.54056

120

0	1	2	6.86	8.058	10.971
1	0	4	29.69	6.4392	13.741
0	0	6	1.48	6.1838	14.311
1	1	0	42.72	5.165	17.154
1	1	3	1.2	4.7661	18.602
0	1	8	2.38	4.1174	21.565
0	2	4	14.02	4.029	22.044
1	0	10	36.08	3.4272	25.977
2	1	1	10.28	3.3673	26.447
1	2	2	6.96	3.3265	26.778
1	1	9	3.19	3.222	27.663
2	1	4	63.78	3.1768	28.065
1	2	5	1.94	3.0769	28.995
3	0	0	10.48	2.982	29.939
0	2	10	100.0	2.8557	31.297
1	2	8	30.68	2.7322	32.75
0	3	6	3.02	2.686	33.33

161HRDISP

Rhombohedral or Trigonal

13.7306 (1.0)

13.7306 (1.0)

13.7306 (1.0)

44.193

44.193

44.193

1.54056

120

1	1	0	6.86	8.0581	10.971
2	1	1	29.69	6.4392	13.741
2	2	2	1.48	6.1838	14.311
1	0	-1	42.72	5.165	17.154
2	1	0	1.2	4.7661	18.602
3	3	2	2.38	4.1175	21.564
2	2	0	14.02	4.029	22.044
4	3	3	36.08	3.4272	25.977
2	0	-1	10.28	3.3673	26.447
2	1	-1	6.96	3.3265	26.778
4	3	2	3.19	3.2221	27.663
3	1	0	63.78	3.1768	28.065
3	2	0	1.94	3.0769	28.995
2	-1	-1	10.48	2.982	29.939
4	4	2	100.0	2.8557	31.297
4	3	1	30.68	2.7322	32.75
3	3	0	3.02	2.686	33.33

0000016

Alunite

Formula: $\text{K}_2\text{Al}_3\text{O}_{14}\text{H}_6$

_symmetry_space_group_name_H-M 'R-3m'

_symmetry_Int_Tables_number 166

_Symmetry 32

160HRDISP

Trigonal

6.96 (1.0)
 6.96 (1.0)
 17.35 (2.4928)

90.0

90.0

120.0

1.54056

40

1	0	1	7.2	5.6937	15.55
0	1	2	25.65	4.95	17.905
1	1	0	18.16	3.48	25.576
0	1	5	4.86	3.0073	29.682
1	1	3	100.0	2.9818	29.942
0	2	1	29.21	2.9693	30.071
0	0	6	3.63	2.8917	30.898
0	2	4	9.53	2.475	36.266
1	0	7	30.24	2.2923	39.27
2	0	5	4.75	2.2754	39.574
2	1	1	2.21	2.2588	39.877
1	1	6	1.03	2.2241	40.527
1	2	2	4.66	2.2035	40.923
0	0	9	1.88	1.9278	47.102
0	2	7	3.44	1.9143	47.454
0	3	3	24.66	1.8979	47.89
2	0	8	2.26	1.7603	51.899
2	2	0	31.45	1.74	52.551

160HRDISP

Rhombohedral or Trigonal

7.0423 (1.0)
 7.0423 (1.0)
 7.0423 (1.0)

59.2282

59.2282

59.2282

1.54056

40

1	0	0	7.2	5.6937	15.55
1	1	0	25.65	4.95	17.905
1	0	-1	18.16	3.48	25.576
2	2	1	4.86	3.0073	29.682
2	1	0	100.0	2.9818	29.942
1	1	-1	29.21	2.9693	30.071
2	2	2	3.63	2.8917	30.898
2	2	0	9.53	2.475	36.266
3	2	2	30.24	2.2923	39.27
3	1	1	4.75	2.2754	39.574
2	0	-1	2.21	2.2588	39.877
3	2	1	1.03	2.2241	40.527
2	1	-1	4.66	2.2035	40.923
3	3	3	1.88	1.9278	47.103
3	3	1	3.44	1.9143	47.454
2	2	-1	24.66	1.8979	47.89
4	2	2	2.26	1.7603	51.899
2	0	-2	31.45	1.74	52.551

1 6 7 R - 3 c C a l s i t e

0000098

Calcite

Formula: CaCO3

_symmetry_space_group_name_H-M 'R-3c'

_symmetry_Int_Tables_number 167

_Symmetry 32

167HRDISP

Trigonal

4.99 (1.0)

4.99 (1.0)

17.0615 (3.4191)

90.0

90.0

120.0

1.54056

23

0	1	2	8.1	3.855	23.052
---	---	---	-----	-------	--------

1	0	4	100.0	3.0357	29.398
---	---	---	-------	--------	--------

0	0	6	2.43	2.8436	31.434
---	---	---	------	--------	--------

1	1	0	13.71	2.495	35.965
---	---	---	-------	-------	--------

1	1	3	20.16	2.2848	39.405
---	---	---	-------	--------	--------

2	0	2	14.26	2.0946	43.154
---	---	---	-------	--------	--------

0	2	4	6.16	1.9275	47.109
---	---	---	------	--------	--------

0	1	8	19.67	1.9125	47.502
---	---	---	-------	--------	--------

1	1	6	20.02	1.8754	48.5
---	---	---	-------	--------	------

2	1	1	3.73	1.6259	56.556
---	---	---	------	--------	--------

1	2	2	9.18	1.6042	57.392
---	---	---	------	--------	--------

2	1	4	5.28	1.5253	60.661
---	---	---	------	--------	--------

2	0	8	2.41	1.5179	60.992
---	---	---	------	--------	--------

1	1	9	3.18	1.5094	61.369
---	---	---	------	--------	--------

1	2	5	2.29	1.4733	63.045
---	---	---	------	--------	--------

3	0	0	6.84	1.4405	64.652
---	---	---	------	--------	--------

0	0	12	3.91	1.4218	65.608
---	---	----	------	--------	--------

2	1	7	1.51	1.3569	69.170
---	---	---	------	--------	--------

167HRDISP

Rhombohedral or Trigonal

6.3753 (1.0)

6.3753 (1.0)

6.3753 (1.0)

46.0779

46.0779

46.0779

1.54056

23

1	1	0	8.1	3.8551	23.052
---	---	---	-----	--------	--------

2	1	1	100.0	3.0357	29.398
---	---	---	-------	--------	--------

2	2	2	2.43	2.8436	31.433
---	---	---	------	--------	--------

1	0	-1	13.71	2.495	35.965
---	---	----	-------	-------	--------

2	1	0	20.16	2.2848	39.404
---	---	---	-------	--------	--------

2	0	0	14.26	2.0946	43.153
---	---	---	-------	--------	--------

2	2	0	6.16	1.9275	47.109
---	---	---	------	--------	--------

3	3	2	19.67	1.9125	47.502
---	---	---	-------	--------	--------

3	2	1	20.02	1.8754	48.5
---	---	---	-------	--------	------

2	0	-1	3.73	1.6259	56.555
---	---	----	------	--------	--------

2	1	-1	9.18	1.6042	57.391
---	---	----	------	--------	--------

3	1	0	5.28	1.5254	60.66
---	---	---	------	--------	-------

4	2	2	2.41	1.5179	60.992
---	---	---	------	--------	--------

4	3	2	3.18	1.5095	61.368
---	---	---	------	--------	--------

3	2	0	2.29	1.4733	63.045
---	---	---	------	--------	--------

2	-1	-1	6.84	1.4405	64.651
---	----	----	------	--------	--------

4	4	4	3.91	1.4218	65.608
---	---	---	------	--------	--------

4	2	1	1.51	1.3569	69.178
---	---	---	------	--------	--------

変換が成立しないケース

1 4 3 P 3 c a p p e l e n i t e

MaterialData 1.40T[25/10/31] by CTR

File Help Disp

Search

Rhombohedral or Trigonal

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

Wave length

1.54056

Select

143.TXT

0000935
Cappelenite-(Y)
Formula: BaY6Si3B6O24F2
_symmetry_space_group_name_H-M 'P3'
_symmetry_Int_Tables_number 143
_Symmetry 3

Disp

Disp2

Cancel

Return Structure

Chemical formula

Input(e. g. C2 H4) BaY6Si3B6O24F2

Change

Trigonalに分類

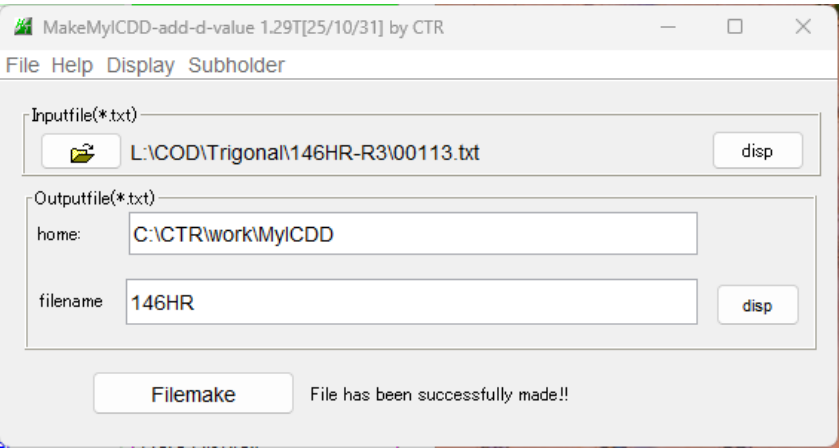
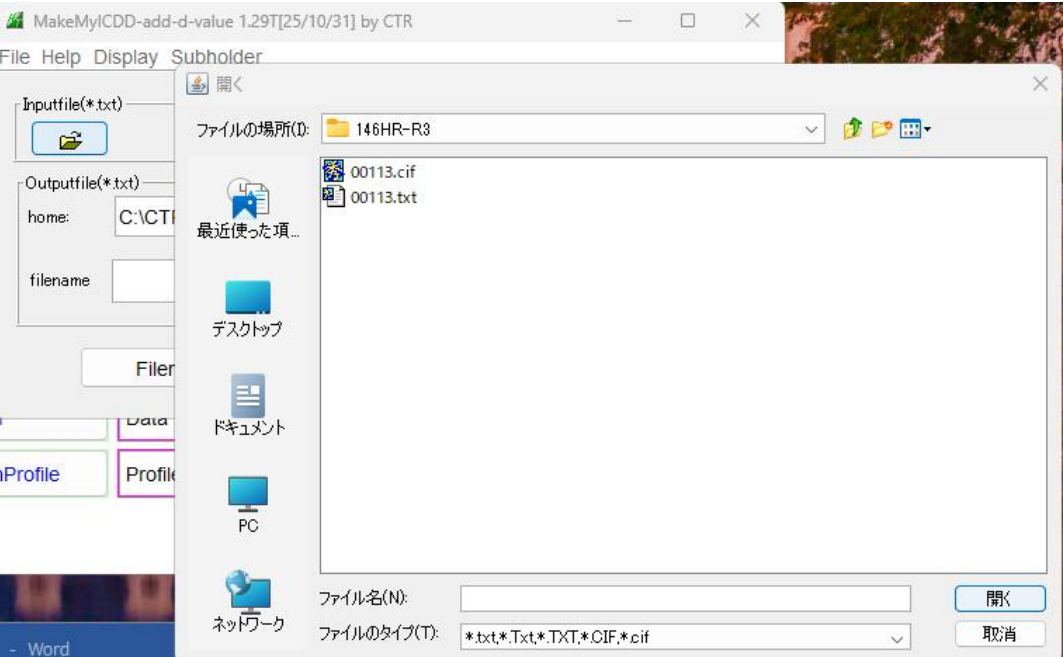
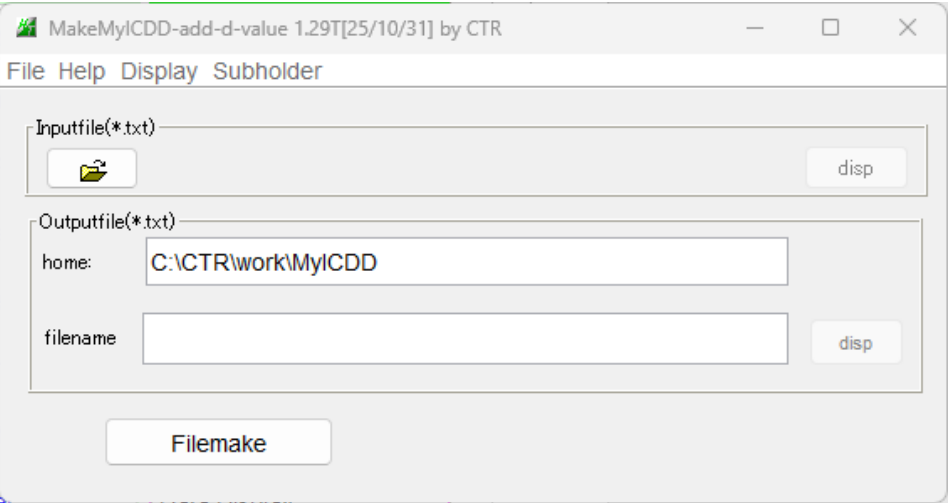
143DISP					
Rhombohedral or Trigonal					
10.67	(1.0)				
10.67	(1.0)				
4.68	(0.4386)				
30.0					
30.0					
120.0					
1.54056					
72					
1	0	0	1.99	9.2405	9.563
3	0	1	23.95	4.68	18.947
1	0	1	1.02	4.1751	21.263
1	1	1	6.03	3.5182	25.294
2	-1	1	6.0	3.5182	25.294
1	2	0	17.37	3.4926	25.482
2	1	0	17.11	3.4926	25.482
3	2	1	6.36	3.2879	27.098
2	0	1	4.24	3.2879	27.098
-1	3	1	25.59	2.7991	31.947
1	2	1	26.03	2.7991	31.947
2	1	1	24.46	2.7991	31.947
3	-1	1	23.93	2.7991	31.947
2	2	0	6.26	2.6675	33.568
3	0	1	2.16	2.5729	34.841
3	0	2	4.96	2.34	38.438
4	-2	1	1.18	2.3175	38.826
2	2	1	1.36	2.3175	38.826

$-H + K + L = 3n$ が成立していない
三方晶表現変換出来ません。

MakeMyICDD

CODからdownloadしたデータ

 00113.cif	2025/9/27 7:08	CIF ファイル	2 KB
 00113.txt	2025/9/27 7:09	テキスト文書	4 KB



MaterialData 1.40T[25/10/31] 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

143.TXT

0000935
Cappelenite-(Y)
Formula: BaY6Si3B6O24F2
_symmetry_space_group_name_H-M 'P3'
_symmetry_Int_Tables_number 143
_Symmetry 3

Disp Disp2 Cancel Return Structure

Chemical formula

Input(e. g. C2 H4) BaY6Si3B6O24F2 Change

Trigonal変換 ($-H+K+L=3n$) 選択すると143.TXT (P3) は表示されません。

MaterialData 1.40T[25/10/31] 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

146HR.TXT

146HR.TXT

148HR.TXT

155.TXT

160HR.TXT

161HR.TXT

166HR.TXT

167HR.TXT

CronstedtiteSi.5Fe1.4O4.001H1.667.TXT

Disp Disp2 Cancel Return Structure

Chemical formula

Input(e. g. C2 H4) Si.5Fe1.4O4.001H1.667 Change