

# **EMFDTW: an automated crystallographic identification tool supporting multiple comparison criteria**

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## Supplementary Data

The grouped data of the constructed ionic compound skeleton prototype and crystal structure prototype databases can be found in Supporting Information-2 and Supporting Information-3. Each group of similar structures is given a prototype name in the table. All original crystal structure data are from COD<sup>1</sup> and ICSD<sup>2</sup>. The naming information of the prototype includes the international space group number, international space group symbol, Hall number, and structure ID for this structure, which allows for a clear and unique identification of a particular prototype. The description and data type of the properties in the result tables are shown in Table S1.

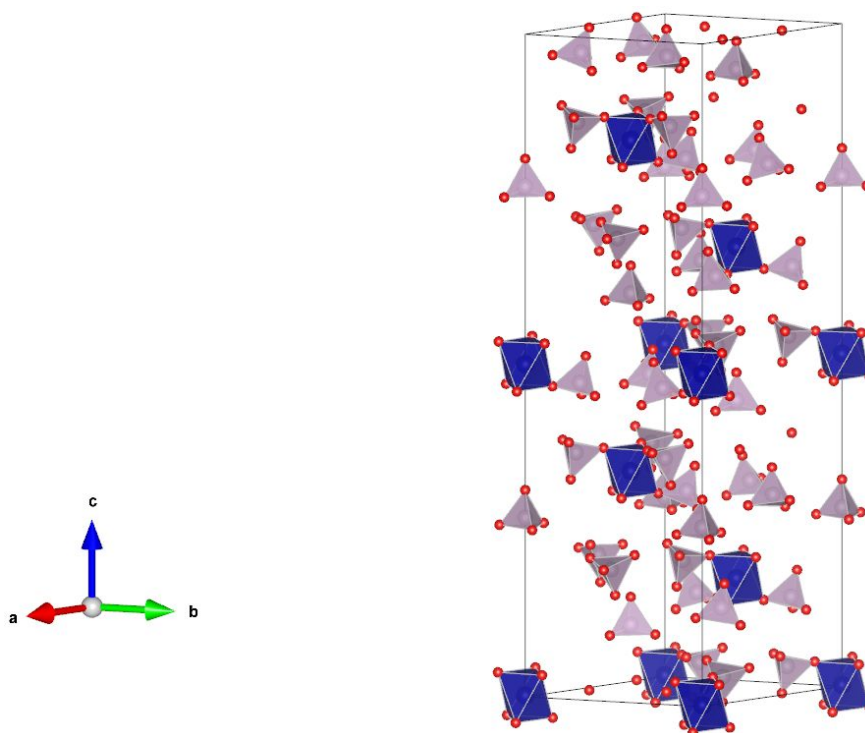
**Table S1. The description and data type of the properties in the result table.**

Property	Description	Data Type
filename	Source and ID of structure data and whether to remove migration ions	String
prototypename	The prototype name to which the current structure belongs	String
similarity_percent	The similarity value between the current structure and its corresponding prototype structure	Number
site_type_composition	Prototype composition information calculated through site type composition analysis algorithm	String
international_space_group_number	The space group number of the prototype	Number
international_space_group_symbol	The space group symbol of the prototype	String
hall_number	The hall number of the prototype	Number
similar_group_id	The similar group id to which the current structure belongs	Number
same_group_id	The same group id to which the current structure belongs	Number
material_type	Ionic compound material type	String

## Ionic compound skeleton prototypes in the skeleton prototype database

The following are some typical skeleton prototypes of electrochemical energy storage materials identified and classified using the EMFDTW algorithm, as well as their organized information stored in the database.

## S1.1 Skeleton Prototype: AB7C28\_161\_R3c\_452\_cod\_2215686\_Ca



**Figure S1.** The skeleton prototype after removing  $\text{Ca}^{2+}$  ions from cod\_2215686.

Material Structure Type: Whitlockite

Site Type Composition: AB7C28

International Space Group Number: 161

International Space Group Symbol: R3c

Hall Number: 452

Origin: COD

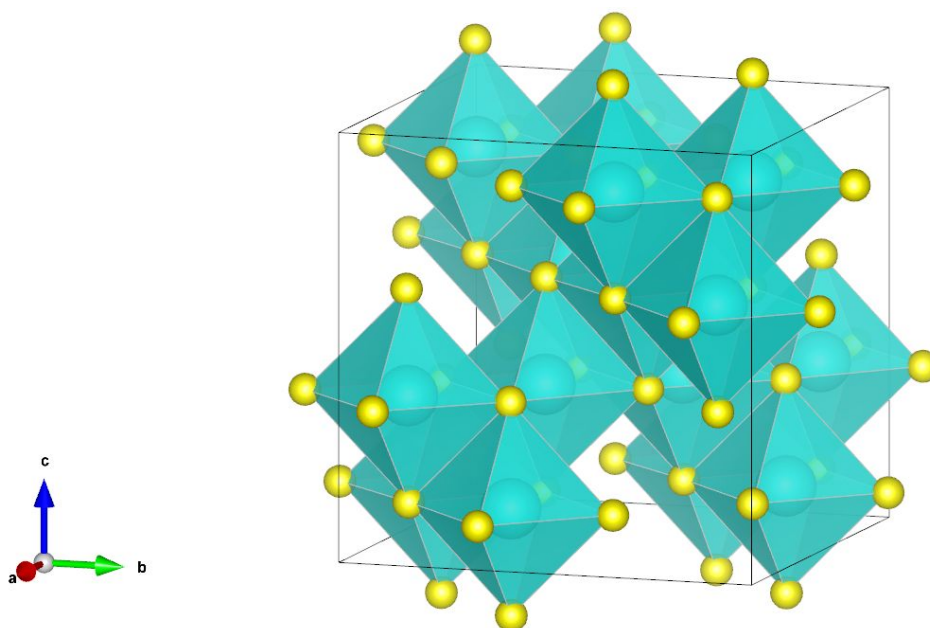
Structure ID: 2215686

Removed Ions:  $\text{Ca}^{2+}$

Similar Group ID:4439

Same Group ID:24841

## S1.2 Skeleton Prototype: AB2\_227\_Fd-3m\_525\_cod\_1536470\_Mg



**Figure S2.** The skeleton prototype after removing  $\text{Mg}^{2+}$  ions from cod\_1536470.

Material Structure Type: Spinel

Site Type Composition: AB2

International Space Group Number: 227

International Space Group Symbol: Fd-3m

Hall Number: 525

Origin: COD

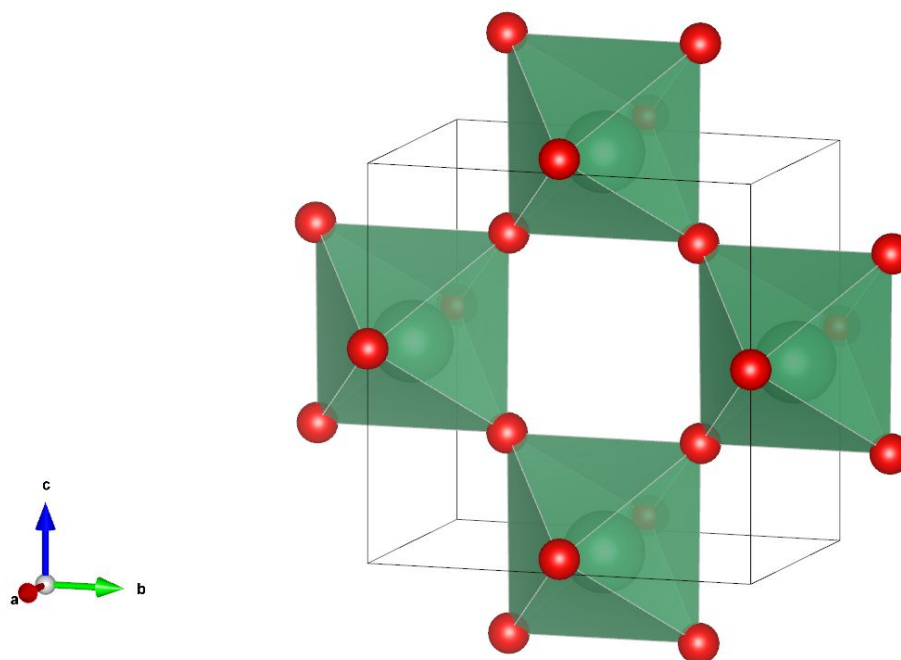
Structure ID: 1536470

Removed Ions:  $\text{Mg}^{2+}$

Similar Group ID:8134

Same Group ID:41605

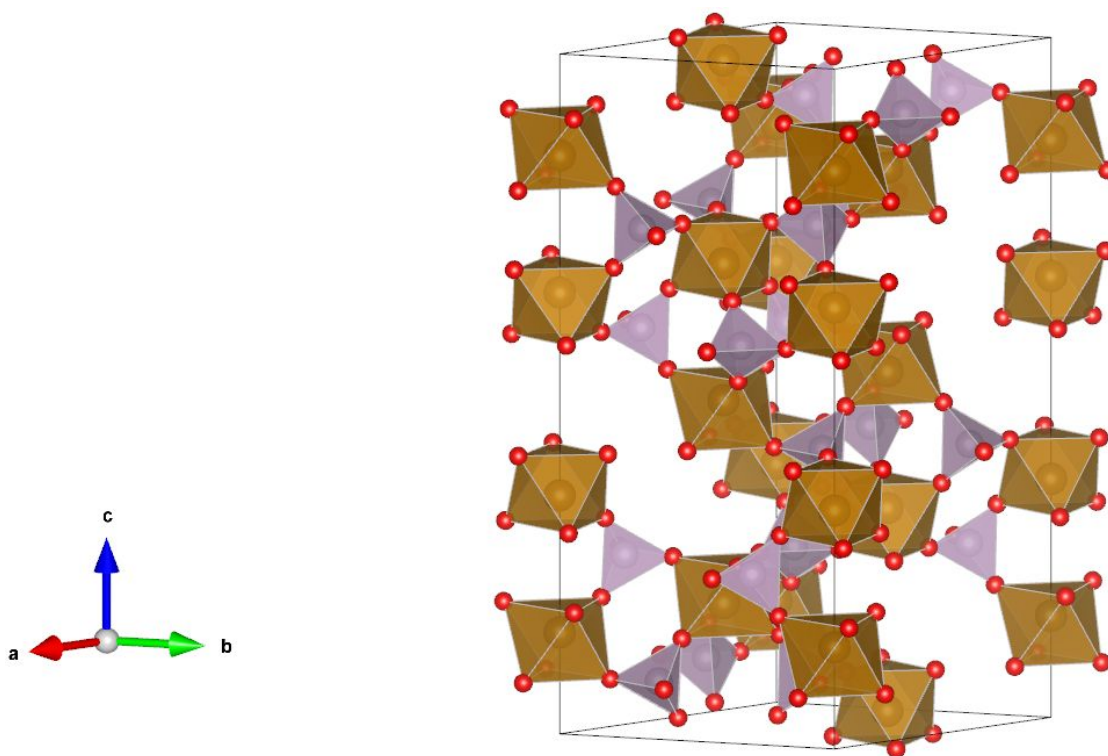
### S1.3 Skeleton Prototype: AB3\_38\_Amm2\_185\_icsd\_009533\_K



**Figure S3.** The skeleton prototype after removing K<sup>+</sup> ions from icsd\_009533.

Material Structure Type: Perovskite  
Site Type Composition: AB3  
International Space Group Number: 38  
International Space Group Symbol: Amm2  
Hall Number: 185  
Origin: ICSD  
Structure ID: 009533  
Removed Ions: K<sup>+</sup>  
Similar Group ID:6499  
Same Group ID:33704

## S1.4 Skeleton Prototype: A2B3C12\_167\_R-3c\_460\_cod\_2221444\_Na



**Figure S4.** The skeleton prototype after removing Na<sup>+</sup> ions from cod\_2221444.

Material Structure Type: NASICON

Site Type Composition: A2B3C12

International Space Group Number: 167

International Space Group Symbol: R-3c

Hall Number: 460

Origin: COD

Structure ID: 1530813

Removed Ions: Na<sup>+</sup>

Similar Group ID:16321

Same Group ID:70825

## S1.5 Skeleton Prototype:

AB2C12\_137\_P4\_2/nmc\_420\_cod\_2107284\_Li

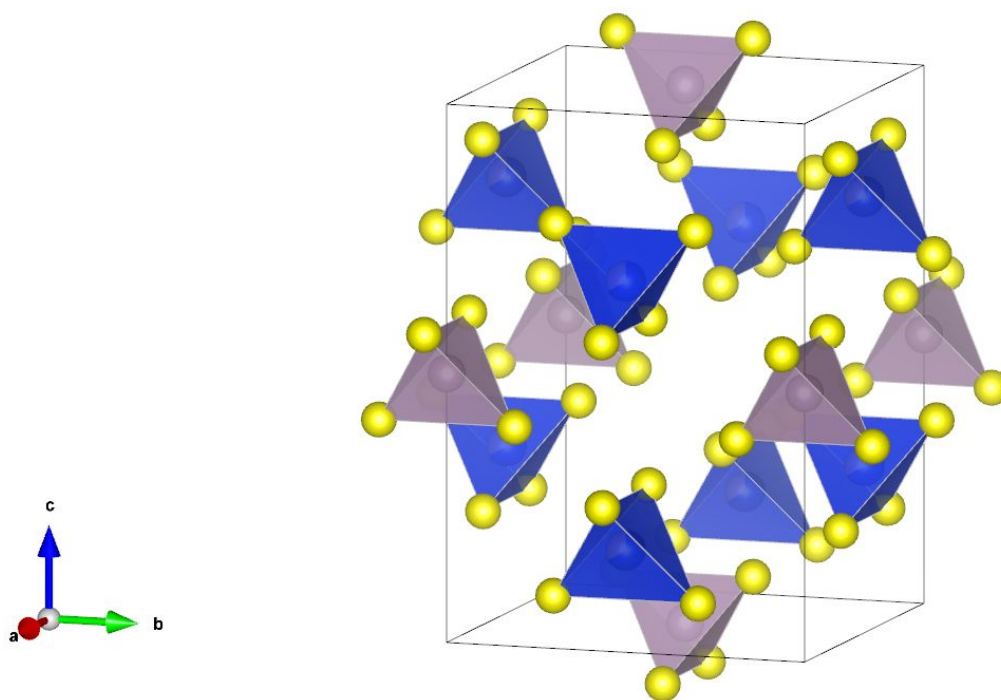


Figure S5. The skeleton prototype after removing  $\text{Li}^+$  ions from cod\_2107284.

Material Structure Type: LGPS

Site Type Composition: AB2C12

International Space Group Number: 137

International Space Group Symbol: P4\_2/nmc

Hall Number: 420

Origin: COD

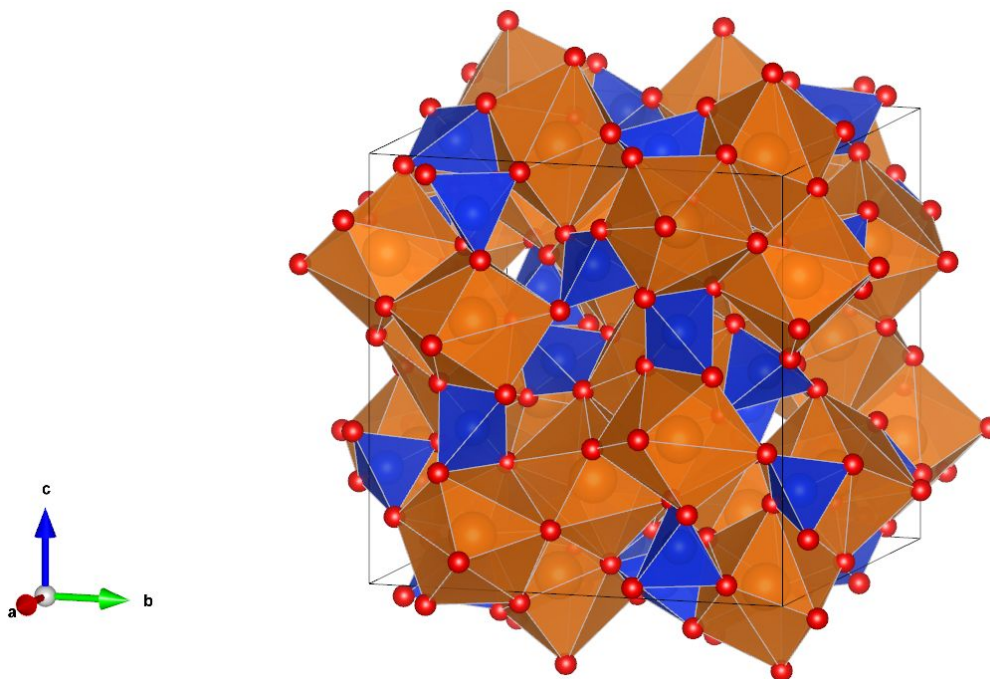
Structure ID: 2107284

Removed Ions:  $\text{Li}^+$

Similar Group ID:11302

Same Group ID:58974

## S1.6 Skeleton Prototype: ABC4\_230\_Ia-3d\_530\_cod\_2108142\_Al



**Figure S6.** The skeleton prototype after removing  $\text{Al}^{3+}$  ions from cod\_2108142.

Material Structure Type: Garnet

Site Type Composition: ABC4

International Space Group Number: 230

International Space Group Symbol: Ia-3d

Hall Number: 530

Origin: COD

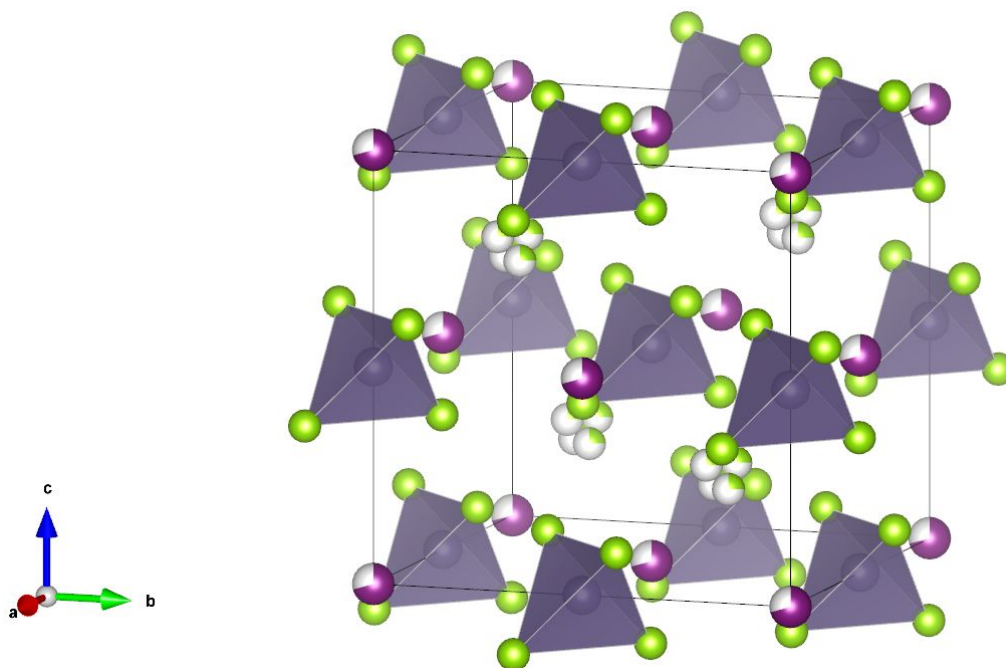
Structure ID: 2108142

Removed Ions:  $\text{Al}^{3+}$

Similar Group ID:2567

Same Group ID:19208

## S1.7 Skeleton Prototype: ABC8\_216\_F-43m\_512\_icsd\_051487\_Ag



**Figure S7.** The skeleton prototype after removing  $\text{Ag}^+$  ions from icsd\_051487.

Material Structure Type: Argyrodite

Site Type Composition: ABC8

International Space Group Number: 216

International Space Group Symbol: F-43m

Hall Number: 512

Origin: ICSD

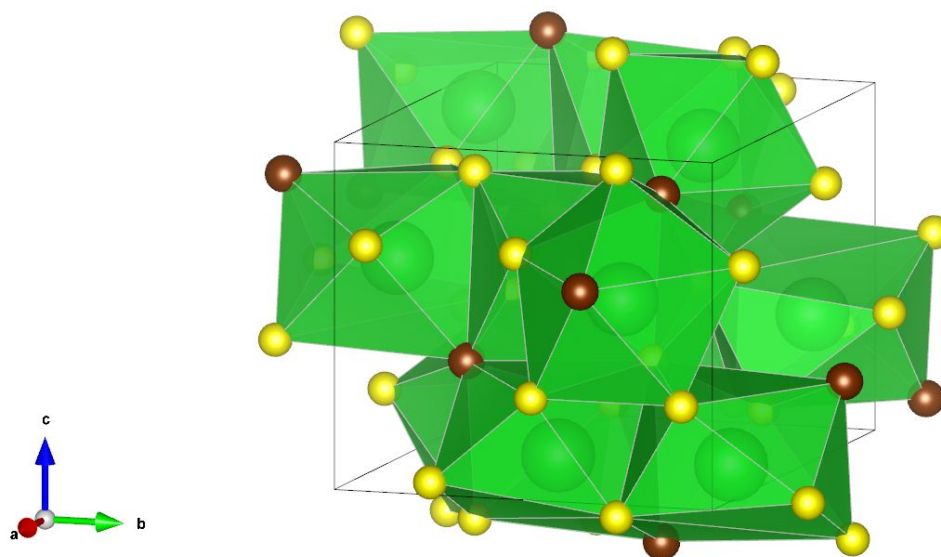
Structure ID: 051487

Removed Ions:  $\text{Ag}^+$

Similar Group ID:1961

Same Group ID:16596

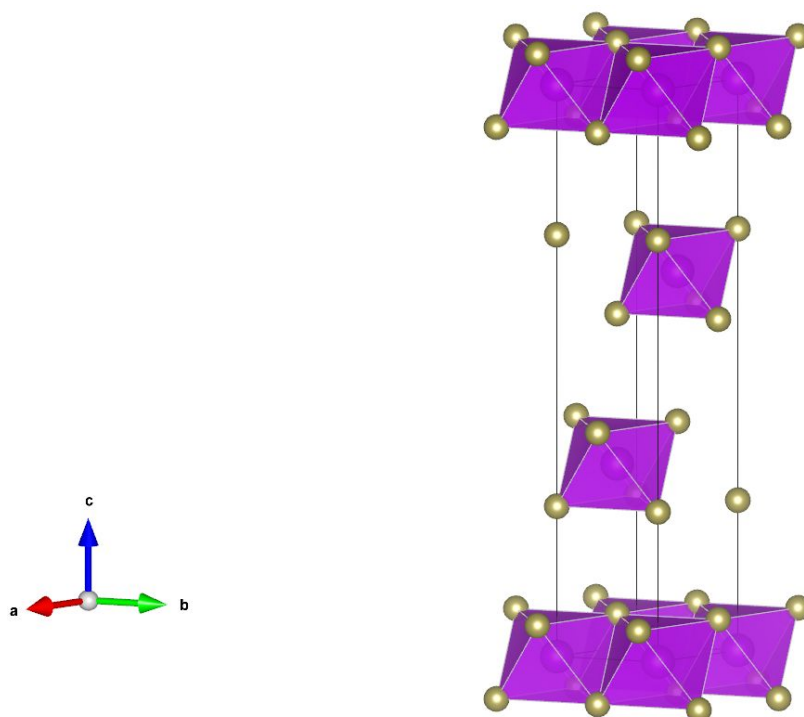
## S1.8 Skeleton Prototype: AB3C4\_62\_Pnma\_292\_cod\_7700681\_Al



**Figure S8.** The skeleton prototype after removing Al<sup>3+</sup> ions from cod\_7700681.

Material Structure Type: Antiperovskite  
Site Type Composition: AB3C4  
International Space Group Number: 62  
International Space Group Symbol: Pnma  
Hall Number: 292  
Origin: COD  
Structure ID: 7700681  
Removed Ions: Al<sup>3+</sup>  
Similar Group ID:7276  
Same Group ID:37834

## S1.9 Skeleton Prototype: AB2\_166\_R-3m\_458\_cod\_1533759\_K



**Figure S9.** The skeleton prototype after removing  $K^+$  ions from cod\_1533759.

Material Structure Type: Chromium Sodium Sulfide

Site Type Composition: AB2

International Space Group Number: 166

International Space Group Symbol: R-3m

Hall Number: 458

Origin: COD

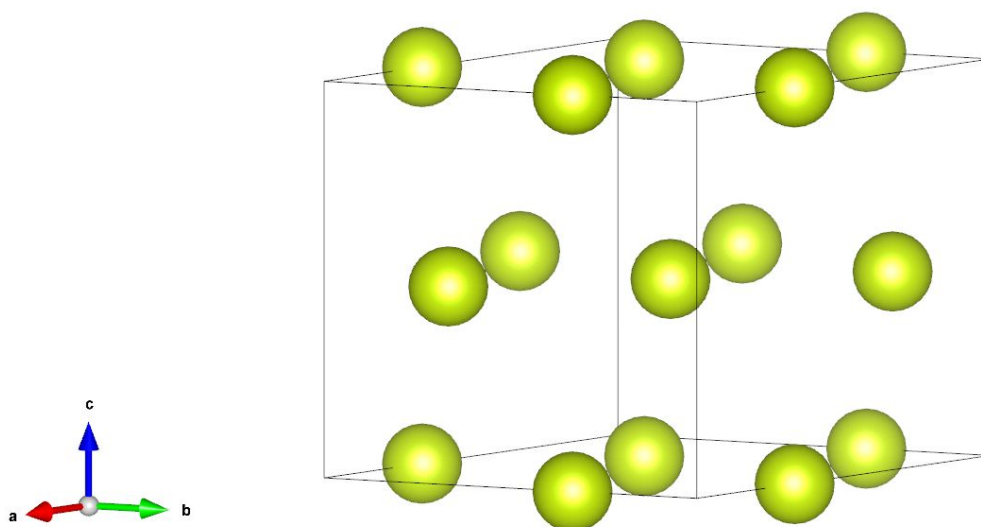
Structure ID: 1533759

Removed Ions:  $K^+$

Similar Group ID:8312

Same Group ID:44603

## S1.10 Skeleton Prototype: A\_194\_P6\_3/mmc\_488\_icsd\_016965\_F



**Figure S10.** The skeleton prototype after removing F<sup>-</sup> ions from icSD\_016965.

Material Structure Type: Corundum

Site Type Composition: A

International Space Group Number: 194

International Space Group Symbol: P6<sub>3</sub>/mmc

Hall Number: 488

Origin: ICSD

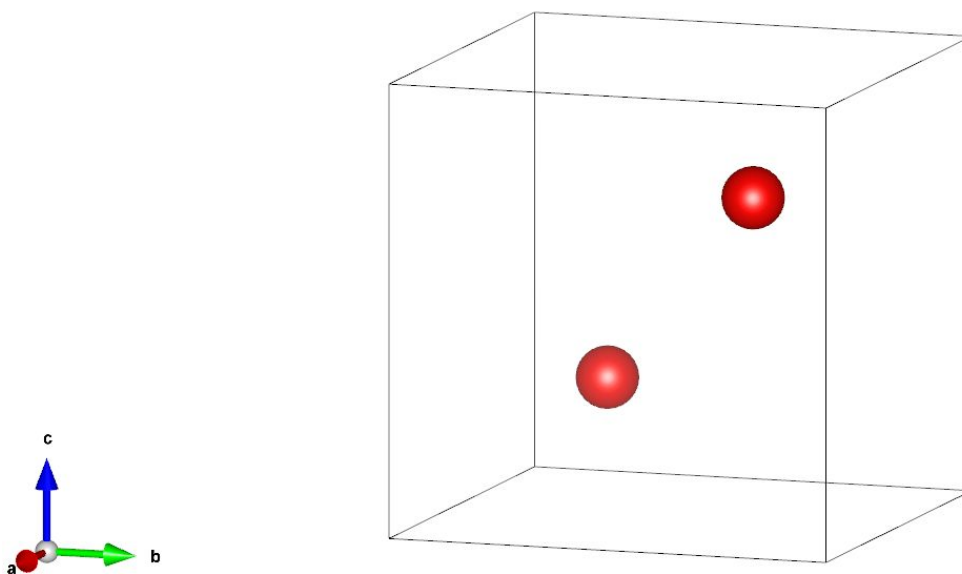
Structure ID: 016965

Removed Ions: F<sup>-</sup>

Similar Group ID:431

Same Group ID:6154

## S1.11 Skeleton Prototype: A\_229\_Im-3m\_529\_icsd\_063281\_Cu



**Figure S11.** The skeleton prototype after removing  $\text{Cu}^{2+}$  ions from icsd\_063281.

Material Structure Type: Cuprite

Site Type Composition: A

International Space Group Number: 229

International Space Group Symbol: Im-3m

Hall Number: 529

Origin: ICSD

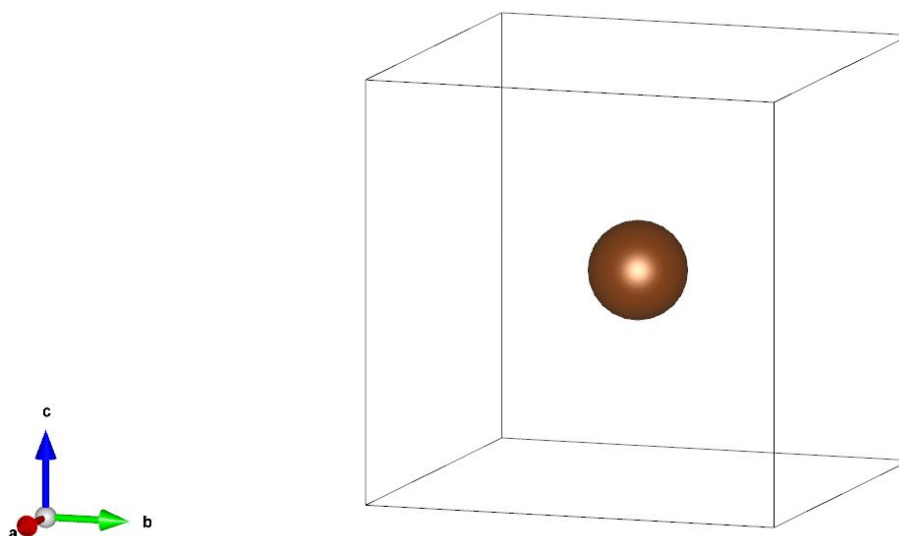
Structure ID: 063281

Removed Ions:  $\text{Cu}^{2+}$

Similar Group ID:262

Same Group ID:1302

## S1.12 Skeleton Prototype: A\_221\_Pm-3m\_517\_icsd\_290580\_K



**Figure S12.** The skeleton prototype after removing  $K^+$  ions from icsd\_290580.

Material Structure Type: Fluorite

Site Type Composition: A

International Space Group Number: 221

International Space Group Symbol: Pm-3m

Hall Number: 517

Origin: ICSD

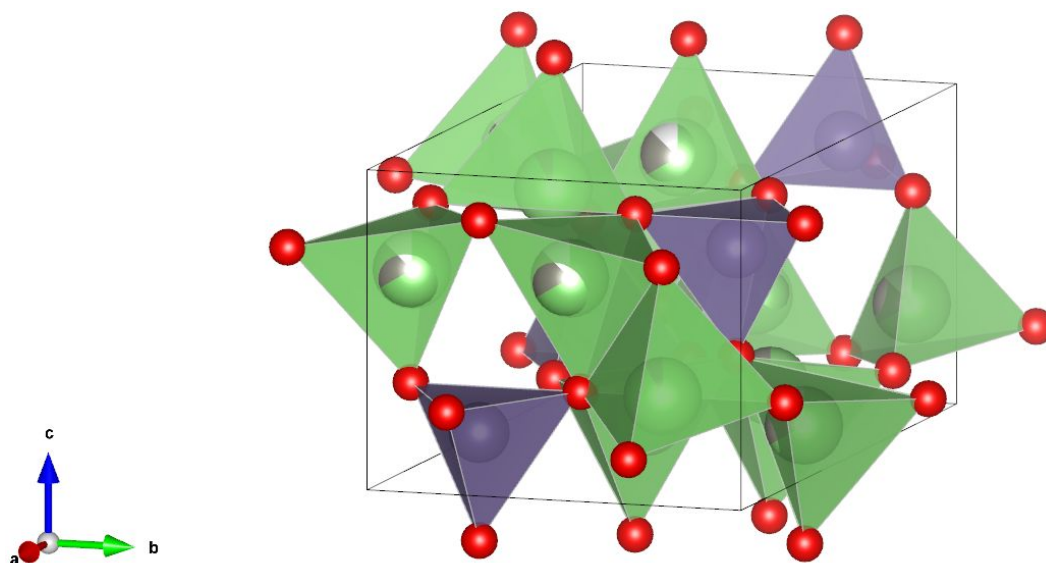
Structure ID: 290580

Removed Ions:  $K^+$

Similar Group ID:305

Same Group ID:3910

### S1.13 Skeleton Prototype: AB3C4\_62\_Pnma\_292\_icsd\_065643\_Li



**Figure S13.** The skeleton prototype after removing Li<sup>+</sup> ions from icsd\_065643.

Material Structure Type: LISICON

Site Type Composition: AB3C4

International Space Group Number: 62

International Space Group Symbol: Pnma

Hall Number: 292

Origin: ICSD

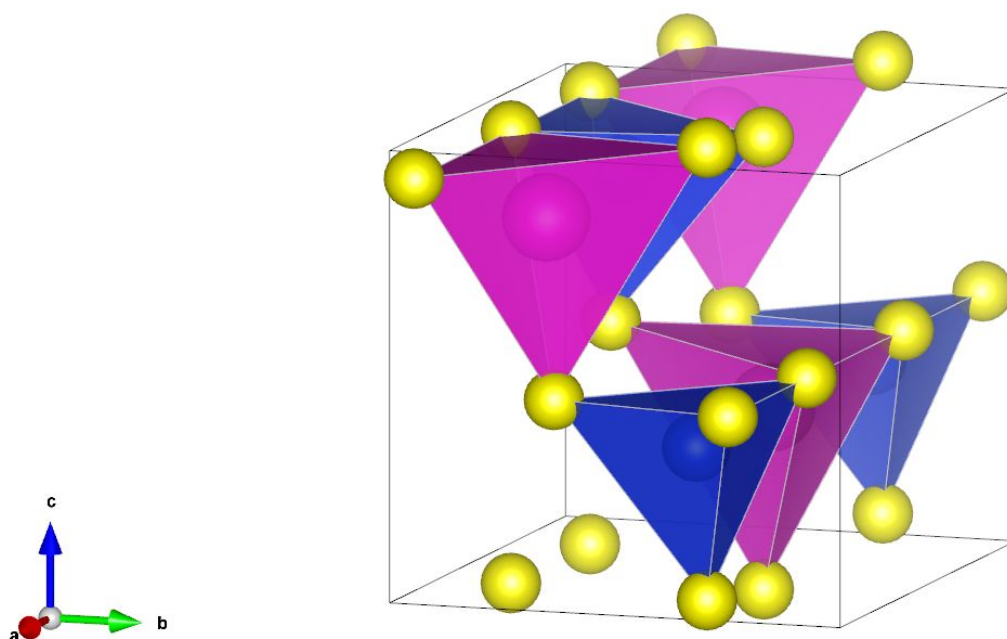
Structure ID: 065643

Removed Ions: Li<sup>+</sup>

Similar Group ID:7275

Same Group ID:37827

## S1.14 Skeleton Prototype: ABC4\_31\_Pmn2\_1\_155\_icsd\_002780\_Cu



**Figure S14.** The skeleton prototype after removing  $\text{Cu}^{2+}$  ions from icsd\_002780.

Material Structure Type: Lithium Iron Silicate

Site Type Composition: ABC4

International Space Group Number: 31

International Space Group Symbol: Pmn2\_1

Hall Number: 155

Origin: ICSD

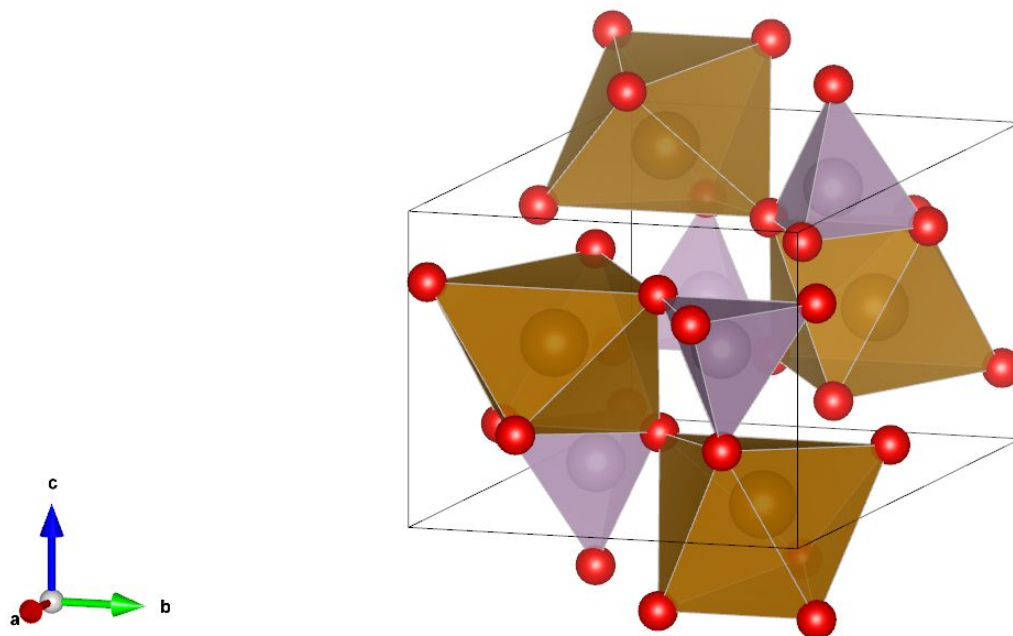
Structure ID: 002780

Removed Ions:  $\text{Cu}^{2+}$

Similar Group ID:2537

Same Group ID:19040

## S1.15 Skeleton Prototype: ABC4\_62\_Pnma\_292\_icsd\_193796\_Li



**Figure S15.** The skeleton prototype after removing  $\text{Li}^+$  ions from icsd\_193796.

Material Structure Type: Olivine

Site Type Composition: ABC4

International Space Group Number: 62

International Space Group Symbol: Pnma

Hall Number: 292

Origin: ICSD

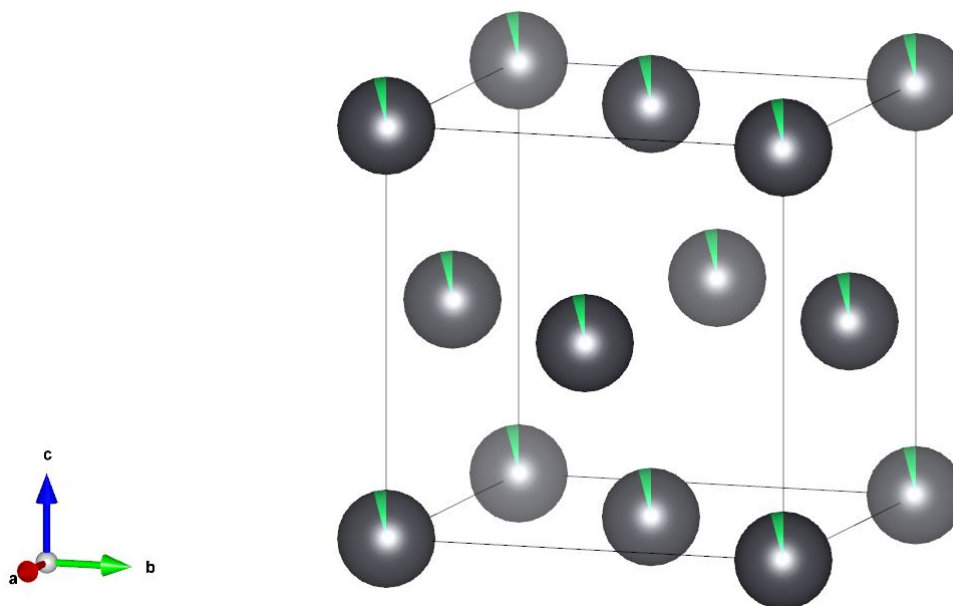
Structure ID: 193796

Removed Ions:  $\text{Li}^+$

Similar Group ID:2451

Same Group ID:18493

## S1.16 Skeleton Prototype: A\_225\_Fm-3m\_523\_cod\_1008610\_F



**Figure S16.** The skeleton prototype after removing F<sup>-</sup> ions from cod\_1008610.

Material Structure Type: Sphalerite

Site Type Composition: A

International Space Group Number: 225

International Space Group Symbol: Fm-3m

Hall Number: 523

Origin: COD

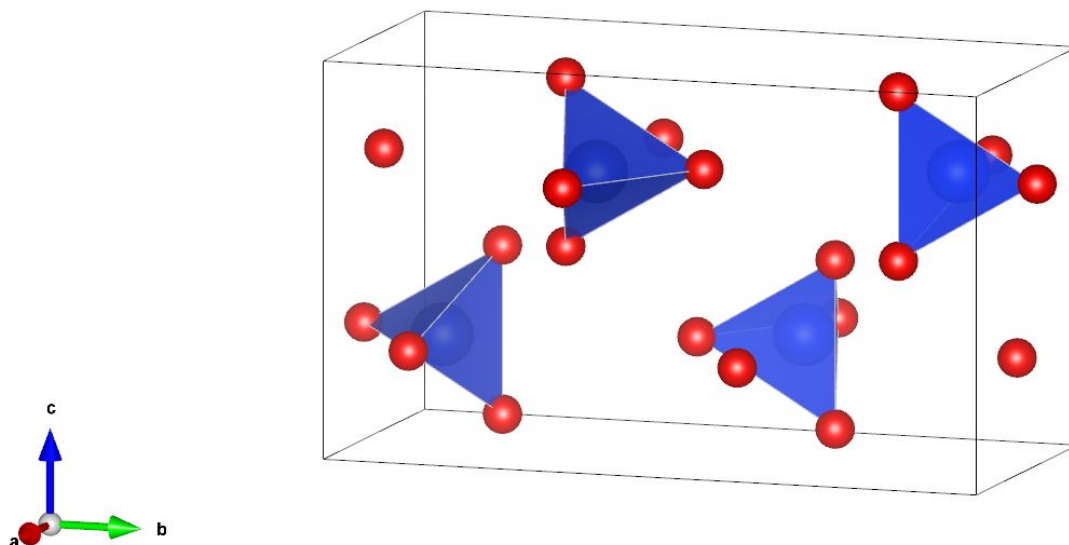
Structure ID: 1008610

Removed Ions: F<sup>-</sup>

Similar Group ID:297

Same Group ID:2394

## S1.17 Skeleton Prototype: AB4\_62\_Pnma\_292\_icsd\_050080\_Mg



**Figure S17.** The skeleton prototype after removing  $\text{Mg}^{2+}$  ions from icsd\_050080.

Material Structure Type: thio-LISICON

Site Type Composition: AB4

International Space Group Number: 62

International Space Group Symbol: Pnma

Hall Number: 292

Origin: ICSD

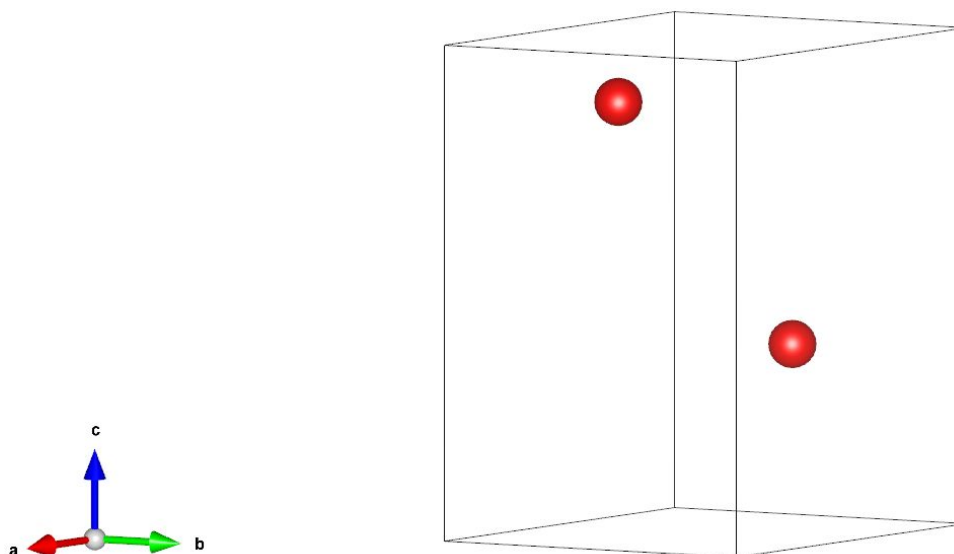
Structure ID: 050080

Removed Ions:  $\text{Mg}^{2+}$

Similar Group ID:5319

Same Group ID:27849

## S1.18 Skeleton Prototype: A\_194\_P6\_3/mmc\_488\_icsd\_157133\_Zn



**Figure S18.** The skeleton prototype after removing  $\text{Zn}^{2+}$  ions from icSD\_157133.

Material Structure Type: Wurtzite

Site Type Composition: A

International Space Group Number: 194

International Space Group Symbol: P6\_3/mmc

Hall Number: 488

Origin: ICSD

Structure ID: 157133

Removed Ions:  $\text{Zn}^{2+}$

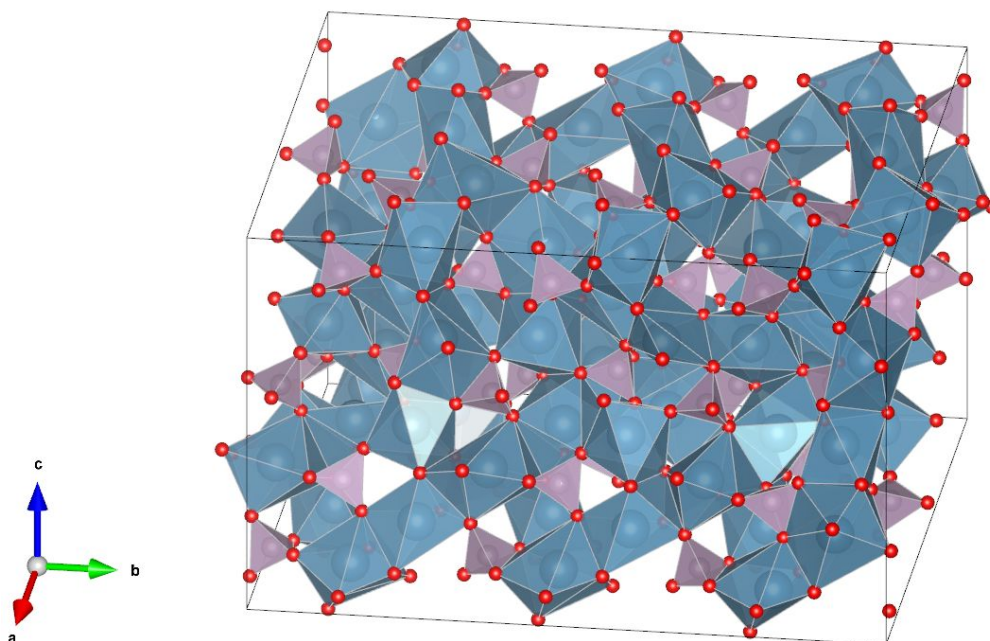
Similar Group ID:418

Same Group ID:5671

## Ionic compound prototypes in the prototype database

The subsequent content presents prototype structure data identified and categorized through the EMFDTW algorithm. Additionally, we also conducted a search for typical prototype structures within the domain of electrochemical energy storage materials.

### S2.1 Prototype: A2B3C8\_14\_P2\_1/c\_81\_cod\_2106194



**Figure S19.** The prototype of cod\_2106194.

Material Structure Type: Whitlockite

Site Type Composition: A2B3C8

International Space Group Number: 14

International Space Group Symbol: P2\_1/c

Hall Number: 81

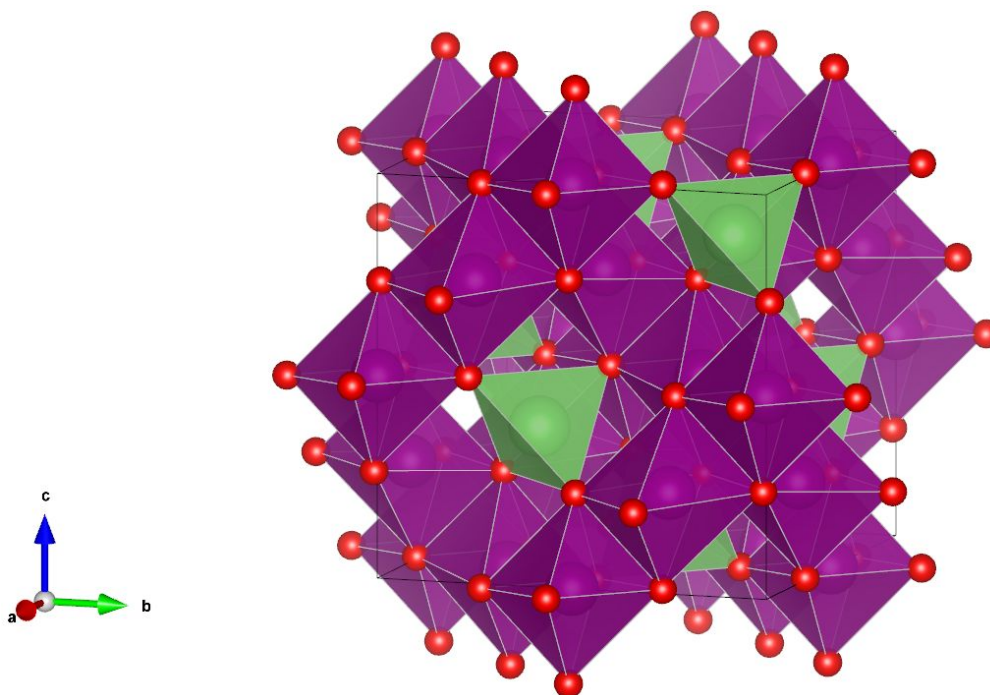
Origin: COD

Structure ID: 2106194

Similar Group ID:21810

Same Group ID:84279

## S2.2 Prototype: AB<sub>2</sub>C<sub>4</sub>\_227\_Fd-3m\_525\_cod\_1513964



**Figure S20.** The prototype of cod\_1513964.

Material Structure Type: Spinel

Site Type Composition: AB<sub>2</sub>C<sub>4</sub>

International Space Group Number: 227

International Space Group Symbol: Fd-3m

Hall Number: 525

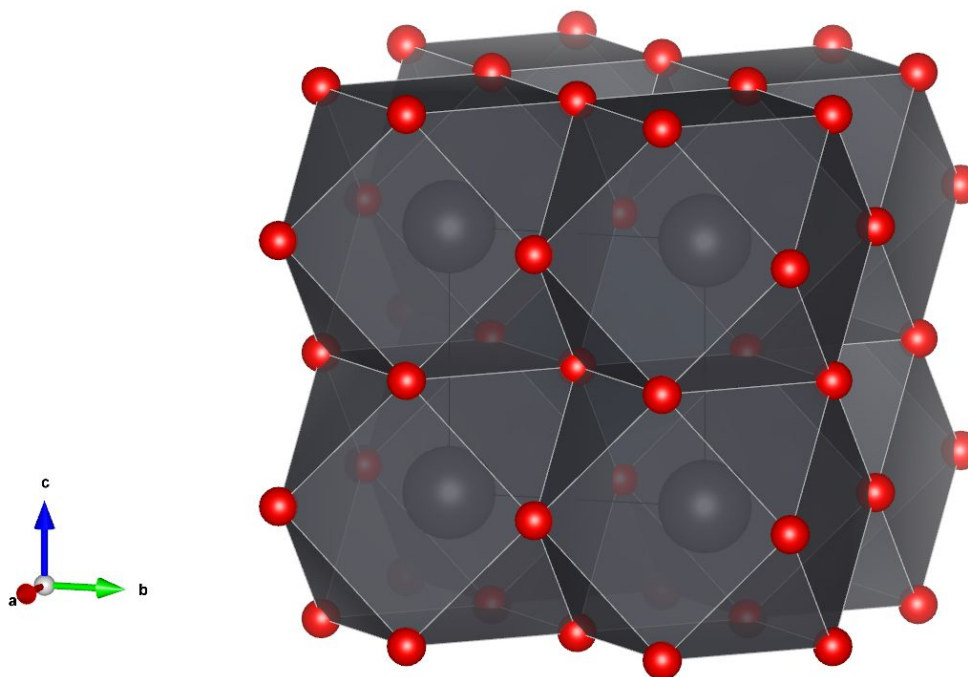
Origin: COD

Structure ID: 1513964

Similar Group ID:12252

Same Group ID:55763

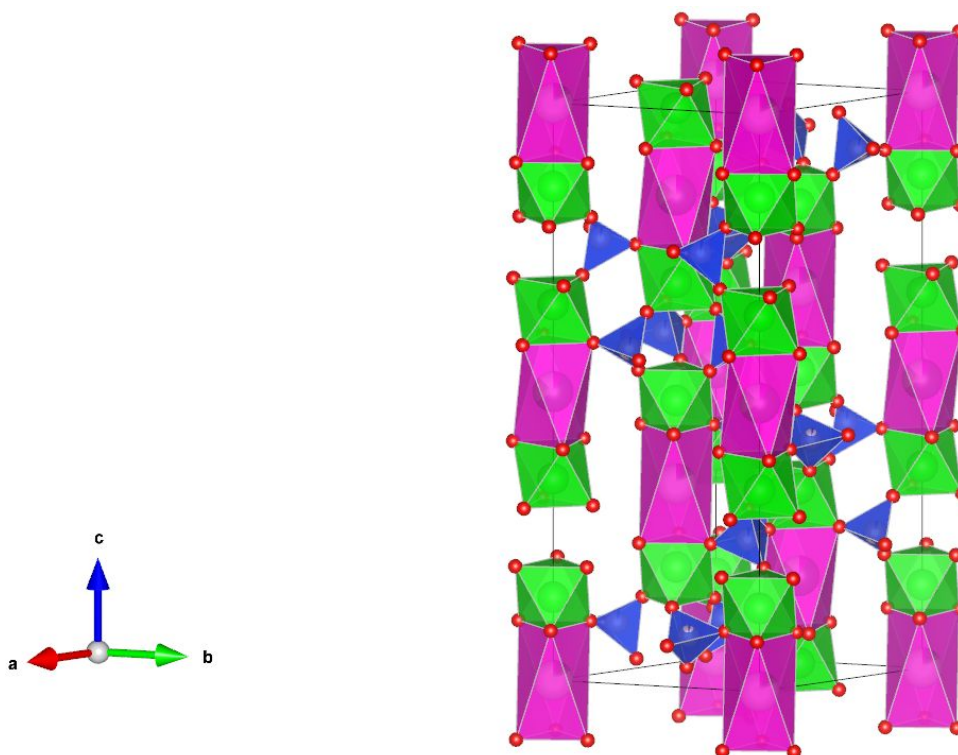
## S2.3 Prototype: ABC3\_221\_Pm-3m\_517\_cod\_1501498



**Figure S21.** The prototype of cod\_1501498.

Material Structure Type: Perovskite  
Site Type Composition: ABC3  
International Space Group Number: 221  
International Space Group Symbol: Pm-3m  
Hall Number: 517  
Origin: COD  
Structure ID: 1501498  
Similar Group ID:3378  
Same Group ID:19036

## S2.4 Prototype: AB<sub>2</sub>C<sub>3</sub>D<sub>12</sub>\_148\_R-3\_436\_cod\_1520808



**Figure S22.** The prototype of cod\_1520808.

Material Structure Type: NASICON

Site Type Composition: AB<sub>2</sub>C<sub>3</sub>D<sub>12</sub>

International Space Group Number: 148

International Space Group Symbol: R-3

Hall Number: 436

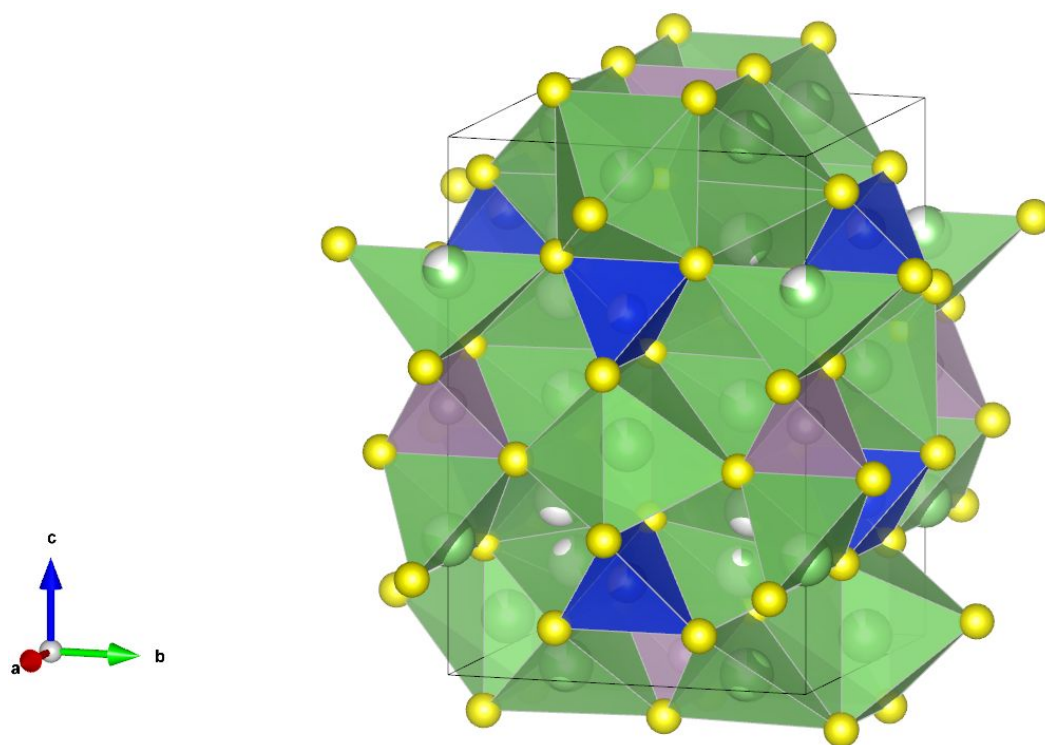
Origin: COD

Structure ID: 1520808

Similar Group ID:13958

Same Group ID:64244

## S2.5 Prototype: AB<sub>2</sub>C<sub>12</sub>D<sub>16</sub>\_137\_P4\_2/nmc\_420\_cod\_2107284



**Figure S23.** The prototype of cod\_2107284.

Material Structure Type: LGPS

Site Type Composition: AB<sub>2</sub>C<sub>12</sub>D<sub>16</sub>

International Space Group Number: 137

International Space Group Symbol: P4<sub>2</sub>/nmc

Hall Number: 420

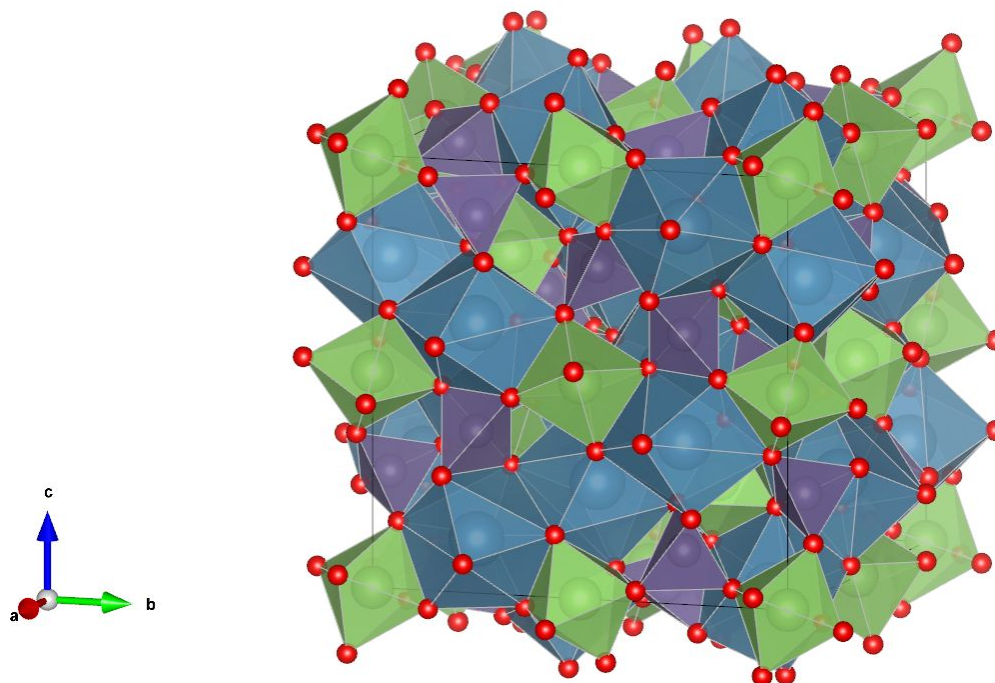
Origin: COD

Structure ID: 2107284

Similar Group ID:15722

Same Group ID:70205

## S2.6 Prototype: A2B3C3D12\_230\_Ia-3d\_530\_cod\_1529480



**Figure S24.** The prototype of cod\_1529480.

Material Structure Type: Garnet

Site Type Composition: A2B3C3D12

International Space Group Number: 230

International Space Group Symbol: Ia-3d

Hall Number: 530

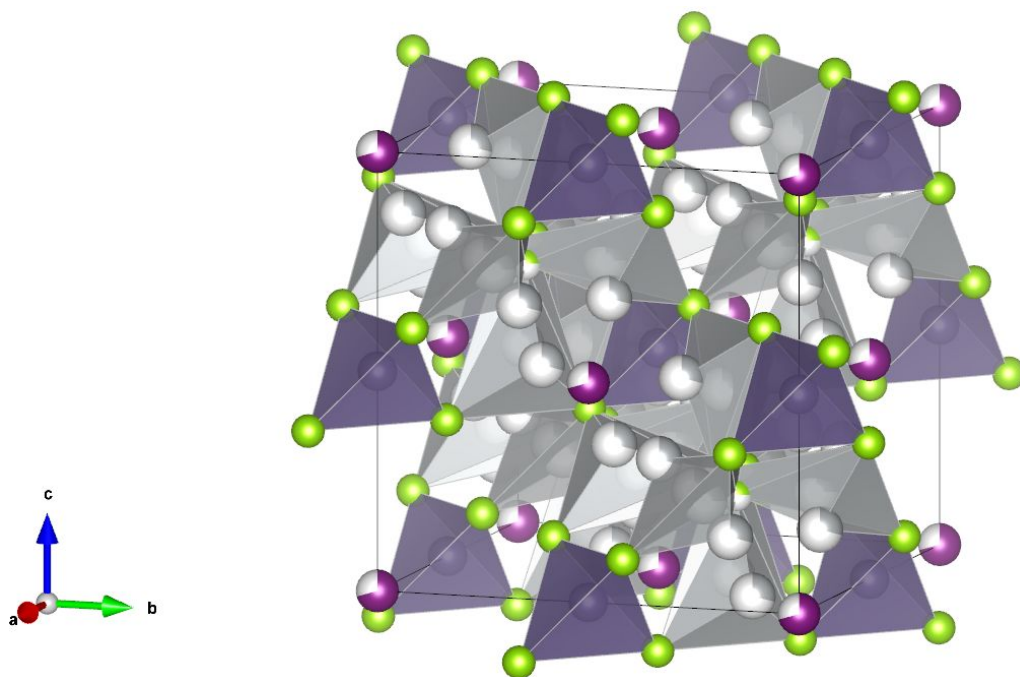
Origin: COD

Structure ID: 1529480

Similar Group ID:22763

Same Group ID:86683

## S2.7 Prototype: ABC8D24\_216\_F-43m\_512\_cod\_1509953



**Figure S25.** The prototype of cod\_1509953.

Material Structure Type: Argyrodite

Site Type Composition: ABC8D24

International Space Group Number: 216

International Space Group Symbol: F-43m

Hall Number: 512

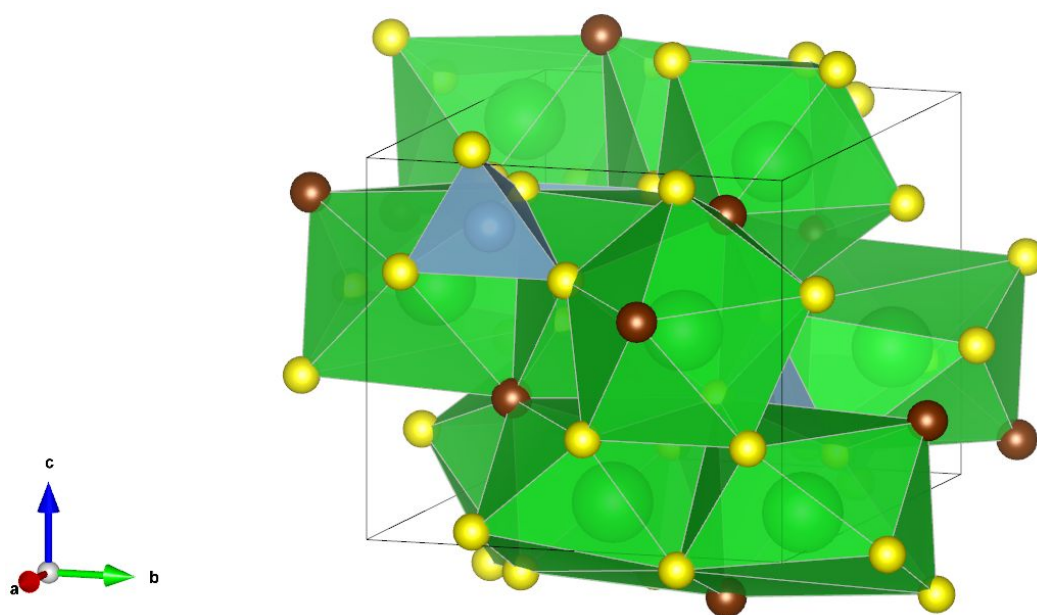
Origin: COD

Structure ID: 1509953

Similar Group ID:2079

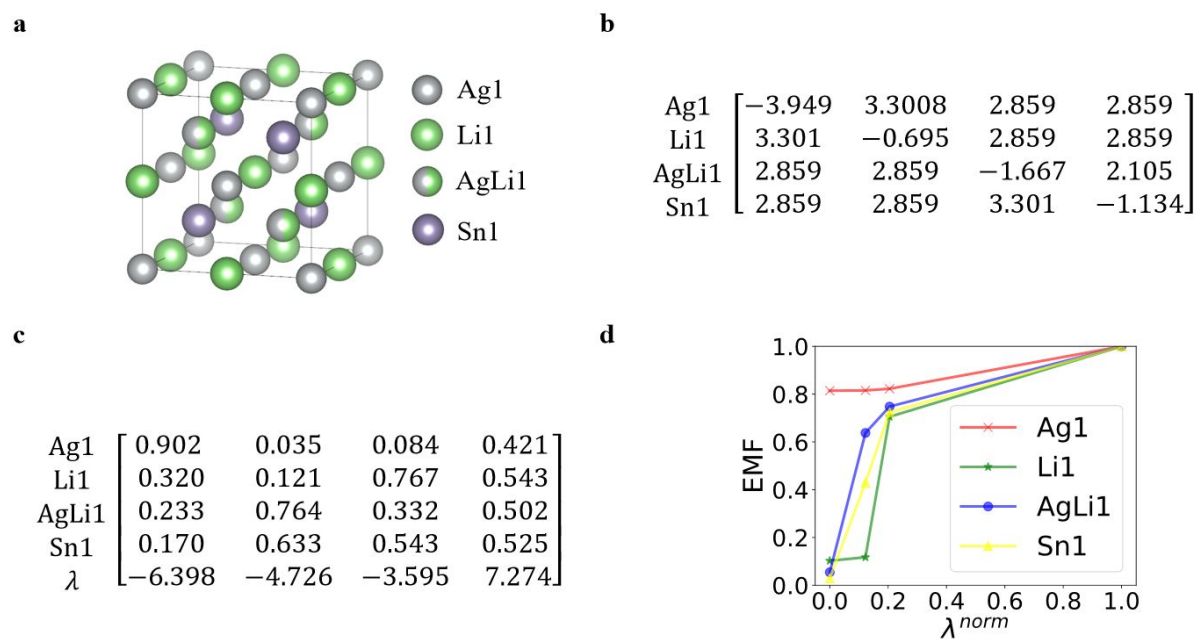
Same Group ID:12596

## S2.8 Prototype: ABC3D4\_62\_Pnma\_292\_cod\_7700681



**Figure S26.** The prototype of cod\_7700681.

Material Structure Type: Antiperovskite  
Site Type Composition: ABC<sub>3</sub>D<sub>4</sub>  
International Space Group Number: 62  
International Space Group Symbol: Pnma  
Hall Number: 292  
Origin: COD  
Structure ID: 7700681  
Similar Group ID:3908  
Same Group ID:23028



**Figure S27.** The process of converting compound  $\text{Ag}_{1.5}\text{Li}_{1.5}\text{Sn}$  into EMFs diagram. a. The structure of compound  $\text{Ag}_{1.5}\text{Li}_{1.5}\text{Sn}$ (icsd\_154087). b. The distance matrix corresponding to  $\text{Ag}_{1.5}\text{Li}_{1.5}\text{Sn}$ . c. The eigen-subspace modular sequence corresponding to each site obtained from the distance matrix. d. The EMFs diagram corresponding to the crystal structure.

**Table S2. Comparison results between DTW and FASTDTW (dataset: 2990 structures).**

	DTW	FASTDTW
Group	454 (threshold = 0.9)	447 (threshold = 0.9)
Time cost	936.5mins	27mins

## References

1. Gražulis, S. *et al.* Crystallography Open Database (COD): an open-access collection of crystal structures and platform for world-wide collaboration. *Nucleic Acids Research* **40**, D420–D427 (2012).
2. Belsky, A., Hellenbrandt, M., Karen, V. L. & Luksch, P. New developments in the Inorganic Crystal Structure Database (ICSD): accessibility in support of materials research and design. *Acta Crystallogr B Struct Sci* **58**, 364–369 (2002).