High-throughput site analysis for binary and ternary compounds in .cif files

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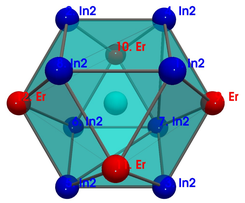
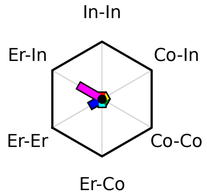
Introduction

Our research colleague identified a new phase of the $PrCo_2Ga$-type in RE-Co-In (RE=Er). To rationalize this observation, we developed an interactive open-source Python tool called CIF Bond Analyzer (CBA) for high-throughput bond pattern analysis from cif files. Additionally, we introduce Python open-source projects designed to preprocess, filter, and analyze cif files.



coordination environment



Formula: $Er_{11}Co_4In_9$
Structure: $Nd_{11}Pd_4In_9$

bond distribution

Motivation from Experimental Synthesis

$PrCo_2Ga$-type phase in the ***RE***–Co–In systems was reported up to Ho:

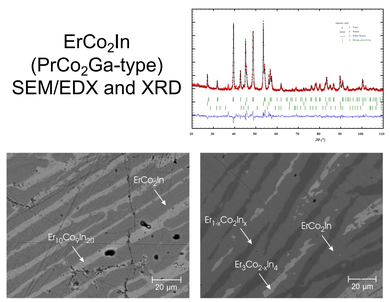
Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
✓	✓	✓	✓	✗	✗	✗	✗

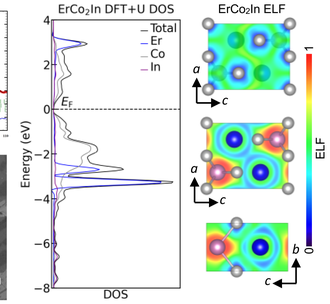
Our experiment[1] indicates $PrCo_2Ga$-type phase was observed in in **Er**Co_2In.

Q. In addition to DFT and diffraction data, can we further rationalize our observation?

[1]*Journal of Alloys and Compounds*, **976**, (173241) (2024)

$ErCo_2In$ ($PrCo_2Ga$-type) SEM/EDX and XRD

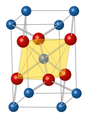




Collaboration with Yuriy Tyvanchuk, Volodymyr Babizhetskyy, Volodymyr Smetana, Mariya Dzevenko

CIF Bond Analyzer (CBA)

We developed an interactive tools to visualize site bonding patterns from .cif files

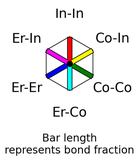


CBA
Crystallographic Information File
Bond
Analyzer

Available here:
github.com/bobleesj/cif-bond-analyzer

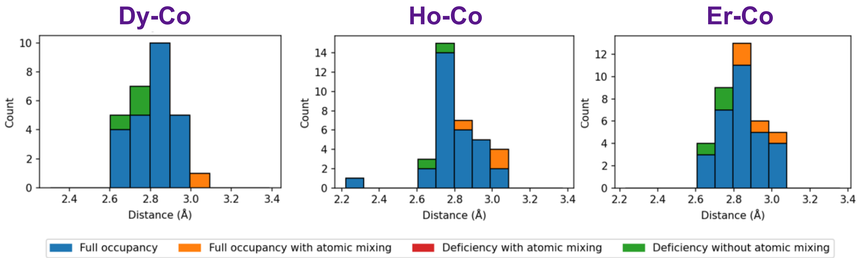
1) System and Coordination Analysis

Visualize bond fractions acquired from site analysis or bond fractions in coordination number geometries.



2) Site/Element analysis

Generate histograms of shortest interatomic distances from each site analyzed in *RE*-Co-In systems.



Q. Are you interested in observing bonding patterns in your system? CBA supports all .cif files and no programming is required!

CIF Cleaner

We developed an interactive Python tool to filter and copy files based on specific attributes

```
Welcome! Please choose an option to proceed:
[1] Move files based on unsupported format after pre-formatting
[2] Move files based on unreasonable distance
[3] Move files based on supercell atom count
[4] Move files based on tags
[5] Move files based on composition type
[6] Move files based on elements
[7] Move files based on coordination number
[8] Copy files based on atomic occupancy and mixing
[9] Get file info in the folder

Enter your choice (1-9): 6
You have chosen: Get file info in the folder

Available folders containing CIF files:
1. elements CIF, 1787 files
2. binary R-X CIF, 3757 files
3. binary R-M CIF, 5510 files
4. binary M-X CIF, 2026 files
5. 20240706_test, 28 files
6. ternary R-M-X CIF, 11418 files

Enter the number corresponding to the folder containing .cif files: 1
```

Available here:
github.com/bobleesj/cif-cleaner

[1] Filter by error

- 250119.cif
- 250120.cif
- 250363.cif
- 250364.cif
- 250365.cif
- 250366.cif
- 250367.cif
- 250368.cif
- 250369.cif
- error_duplicate_labels
- error_wrong_loop_value

cifkit

We developed an easy-to-use Python open-source package for high-throughput analysis of .cif files

CI passing | codecov 97% | python 3.10 | python 3.11 | python 3.12 | pypi v1.0.2 | License MIT

Google Colab Open

Preprocess: standardize site labels and sort ill-formatted files

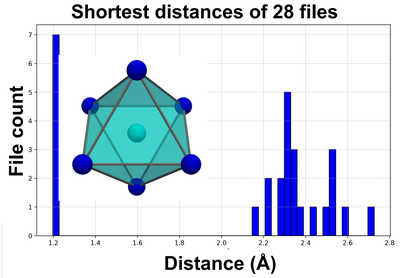
Visualize distribution: count files by supercell size, tags, coordination numbers, elements

Filter: copy, move, and sort .cif files based on attributes

Coordination geometry: extract nearest neighbors from each site

cifkit
Python library for .cif high-throughput analysis

Shortest distances of 28 files



Available here:
github.com/bobleesj/cifkit

GitHub URLs:
CIF Bond Analyzer (CBA): github.com/bobleesj/cif-bond-analyzer
CIF Cleaner: github.com/bobleesj/cif-cleaner
cifkit: github.com/bobleesj/cifkit

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