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crystract: A Crystallography Package in R for .cif Data Processing

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Summary

The Crystallographic Information File (CIF) is the standard format for disseminating crystal structure data, yet parsing and analyzing these files for large-scale computational and statistical analysis is a significant bottleneck for research in the chemical and material sciences(Hall et al., 1991). `crystract` is an R package designed to provide an efficient, open-source solution for the batch processing and statistical analysis of CIF files. The package streamlines the extraction of metadata, unit cell parameters, atomic coordinates, and symmetry operations for a single CIF file or hundreds at the same time. From the information stored in the CIF file, our package can determine the first-neighbor bonding environment around each symmetrically independent atom in a unit cell, with all interatomic distances and bond angles, while propagating experimental uncertainties (i.e., the estimated standard deviations of the unit cell parameters and fractional atomic coordinates). Furthermore, a comprehensive workflow for efficient extraction and processing of these data is provided, centered around the calculation of average interatomic distances, identified as a key parameter for a streamlined comparison of structural features of different compounds. One of the most important features within this workflow is the package's ability to process positional or occupational disorder. To handle positional disorder, a filtering function to eliminate non-physical distances is provided. Occupational disorder is taken into account via the possibility of calculating an occupancy-weighted average interatomic distance. Additionally, filtering functions to calculate average distances, only including user-specified elements or atomic positions, are available. This paper outlines the architecture and core functionalities of `crystract`, demonstrating its utility with a practical example.

Statement of need

Despite the standardization provided by the CIF format, significant practical barriers remain for researchers aiming to perform high-throughput computational analysis, particularly in batch. The first barrier is technical: CIF files, while standardized, often exhibit syntactic variations or errors depending on their originating software or laboratory, which can cause simplistic parsers to fail. The second barrier is conceptual: a CIF file does not typically contain an explicit list of all atoms in the unit cell. Instead, it reports the unique atoms in the asymmetric unit and a set of symmetry operations. A complete structural analysis, therefore, requires the correct application of these symmetry operations to generate the full unit cell and its atomic contents—a non-trivial, error-prone computational task that must be handled by specialized software. This complexity often forces researchers into a fragmented and inefficient workflow, piecing together disparate tools for data validation, structure generation, geometric analysis, and final statistical modeling.

A number of excellent software tools have been developed to address some of these challenges, yet a comprehensive review reveals a specific and critical gap. The most mature ecosystem for computational materials science currently resides in Python, where `pymatgen` stands as a powerful and widely adopted standard(Ong et al., 2013). This extensive library offers robust CIF parsing and a host of advanced analysis functions, including the calculation of interatomic distances and the prediction of bonding environments using sophisticated, data-mining approaches like the CrystalNN algorithm(Pan et al., 2021). While `pymatgen` offers robust CIF parsing and advanced analysis, it has limitations for a complete, statistically rigorous workflow: it does not programmatically propagate the experimental uncertainties reported in CIFs (i.e., the estimated standard deviations of the unit cell parameters and fractional atomic coordinates) for its derived geometric quantities. Furthermore, batch processing requires the user to write custom scripts to loop over files. Filtering presents another challenge: although `pymatgen` includes a function to filter for minimum and maximum distances, they have to be specified one element at a time, one file at a time, by the user. This makes it cumbersome to use `pymatgen` for large-scale datasets and studies.

Other specialized Python tools like `cifkit`—a Python-based command-line tool(Lee & Oliynyk, 2024)—and its companion software, `cif-bond-analyzer` (CBA)—designed for the singular task of exporting bond lists(Tyvanchuk et al., 2024)—provide fast, lightweight, and native batch processing for geometric analysis. However, their scope is intentionally limited to interatomic distances and bond analysis; they also do not provide native functions for calculating bond angles or propagating experimental uncertainties.

Other specialized tools, such as the CCDC's Mercury(Macrae et al., 2006) or the IUCr's enCIFer(Allen et al., 2004), are indispensable for interactive 3D visualization and formal CIF syntax validation, respectively. However, their primary design as graphical user interface (GUI) applications makes them ill-suited for the automated, scriptable, and reproducible workflows required for modern data science without the capability for high-throughput handling.

Within the R ecosystem, the landscape is sparse. The `cry` package provides basic statistics for crystallography computation and falls short of large-scale research and ML-based applications(Foadi et al., 2025). Its design, centered on a custom S3 object system, is not optimized for the high-throughput, data-frame-centric workflows required for large-scale statistical analysis. `cry` is limited to the analysis of crystallographic parameters and diffraction data from individual files. It is not equipped for the geometric analysis of atomic structures, as it is unable to apply symmetry operations to generate a full unit cell from asymmetric coordinates, and is therefore unable to calculate the resulting interatomic distances and angles, or handle the structural disorder commonly found in real materials.

To our knowledge, no package or software—whether in Python, as GUIs, or within R—provides a single, integrated solution capable of combining the automated batch processing of large collections of CIF files and the systematic propagation of experimental uncertainties, while providing additional features indispensable for the structural analysis of large datasets. Such a research software landscape forces researchers into creating fragmented and inefficient workflows, piecing together disparate tools for structure generation, geometric analysis, and finally statistical modeling.

Overview of functionalities provided by existing packages in Python and R.

Task	CIFkit	CBA (CIF Bond analyzer)	pymatgen	cry	crystract
Read/parse singular CIF file	Yes	No, uses cifcit for this	Partially, via importers like CifParser	Yes	Yes

Task	CIFkit	CBA (CIF Bond analyzer)	pymatgen	cry	crystract
Batch / high-throughput processing of many CIFs	Yes	Yes	Yes, but certain tasks require manual scripting	No	Yes
Supercell / unit cell generation / lattice operations	Yes, can generate unit cell and supercell via +/- 1 shifts	Yes, when computing minimum bond lengths for site	Yes, structure operations, transformation, supercell, etc.	No	Yes, can generate unit cell and supercell via +/- 1 shifts
Coordination number determination	Yes	Yes	Yes	No	Yes
Calculation of interatomic distances	Yes	Yes	Yes	No	Yes
Calculation of bond angles	No	No	No	No	Yes
Error propagation	No	No	No	No	Yes
Handling of occupational disorder	Yes	No, uses cifkit	Partial, can read occupancies, but does not use them	No	Yes
Handling of structural disorder	No	No	No	No	Yes, via filtering function
Filtering for specific atoms or crystallographic sites	Yes	Yes	No	No	Yes
Calculation of weighted average accounting for disorder.	No	No	No	No	Yes
Output to multiple formats	No outputs of extracted data, only figures such as histograms or visualizations	No outputs of extracted data, only figures such as histograms or visualizations	No	No	Yes

Crystract

To address these needs, we have developed "`crystract`", an open-source R package designed to provide a seamless, robust, and statistically-minded workflow for crystallographic analysis. `crystract` provides an end-to-end toolkit that operates entirely within the R environment. Its primary contributions are fourfold.

First, it provides a robust and efficient engine for parsing and processing large batches of CIF files. It is designed from the ground up around R's data-centric paradigm, directly presenting all extracted and calculated data in tidy data frames(Wickham, 2014) ready for immediate manipulation and analysis with the wider R ecosystem. `crystract` has been tested to be working on the ICSD(Zagorac et al., 2019), AMCSD(Downs & Hall-Wallace, 2003), and COD(Gražulis et al., 2009); however other databases and formats may also be accepted.

Second, it offers comprehensive geometric analysis. This output includes the CIF file's core metadata and a rich set of derived attributes essential for crystallographic research. These attributes include: a complete list of atomic coordinates after symmetry operations, all interatomic distances based on predicted bonded pairs (using CrystalNN(Pan et al., 2021), MinimumDistanceNN(Zemann, 1966; Zimmermann et al., 2017), BrunnerNN_reciprocal(Brunner, 1977), VoronoiNN(O'Keeffe, 1979), and EconNN(Hoppe, 1979) algorithms), and bond angles—a feature not natively available in other command-line batch-processing tools.

Third, and most uniquely, `crystract` introduces a capability largely absent in other programmatic tools: the rigorous propagation of experimental uncertainties from the CIF through all derived geometric quantities. By reading the estimated standard deviations (e.s.d.s) of the fractional atomic coordinates and unit cell parameters provided in the CIF, the package utilizes standard error propagation theory(Ku, 1966) to compute rigorous standard uncertainties for all calculated interatomic distances and bond angles. This feature facilitates a more sophisticated and honest statistical treatment of structural data, allowing researchers to quantify the confidence in their calculated results.

Fourth, as the most valuable feature for the user community, it provides a suite of integrated filtering functions that are essential for high-throughput analysis and handling complex structures, thus exceeding the capabilities offered by currently existing software tools. Our workflow is centered around the calculation of average interatomic distances, as a key parameter in the structural comparison of different compounds. The average atomic distance can be calculated for all symmetrically independent atoms or a subset of these by prior application of the filtering function based on the user-specified element or atomic site. Furthermore, occupational or positional disorder can be handled via a filtering function to exclude non-physical distances in the process of calculating the average distance. This filtering is based on the automatic recognition of the elements in a structure and the calculation of an expected interatomic distance from their covalent radii(Emsley, 1998; Pyykkö & Atsumi, 2009) or a user-specified list of atomic radii. Partial site occupation occurs in many real compounds and is indispensable for deriving structure-property trends or predicting new functional materials(Jakob et al., 2026). If one simply calculates interatomic distances from the coordinates given in the CIF file without accounting for partial occupation, one obtains non-physical distances between atoms that cannot coexist in the same local configuration. Such artifacts would distort any statistical measure by including interactions that never occur in reality. While taking these features native to real crystal structures into account, a weighted average distance can be calculated, either for all individual atoms or a user-defined subset by the application of the available filtering functions for user-specified atoms or crystallographic sites.

Implications

The availability of packages like "crystract", "pymatgen", "cifkit", and others brings the field of crystallography, mineralogy, and materials science a step closer to realizing the transformative potential of data-driven science. crystract is one part of a larger effort made to develop AI methods to perform comparative studies across hundreds or even thousands of structures, thus providing researchers with the foundations to derive overarching structure-property relationships of minerals and materials to ultimately employ known compounds for new applications or predict new materials.

crystract creates a launchpad for integrating crystallographic data into machine learning pipelines for a variety of application areas. Our package's capability to handle positional or occupational disorder, propagate uncertainties, and generate comprehensive data outputs provides an excellent feature set for predictive modeling efforts.

Finally, as an open source package, "crystract" will be a community-driven, transparent resource that invites extensions and improvements from other researchers who want to use crystallographic data in their own scientific explorations. crystract can be easily installed from CRAN using `install.packages("crystract")`, and the source code is available on GitHub at github.com/PrabhuLab/ml-crystals/tree/main/packages/crystract.

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Author Contributions using the CRediT (Contribution Roles Taxonomy)

Conceptualization – AP, JMH

Data Curation – DN, JMH, AP

Formal Analysis – DN, JMH, AP

Funding Acquisition – AP

Investigation – DN, JMH, AP

Methodology – DN, JMH, AP

Project Administration – AP, JMH

Resources – JMH, SMM, AP, MS

Software – DN, JMH, AP

Supervision – AP, JMH

Validation – DN, JMH, SMM, AP, MS

Writing (Original Draft Preparation) – DN, JMH, AP

Writing (Review & Editing) – DN, JMH, AP, SMM, MS

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