**How to use CIF2PDF:**

1. Download the Crystallographic Information File (CIF) you want to know the atomic distance distribution of, e.g. from [ICSD](https://icsd.fiz-karlsruhe.de/search/basic.xhtml) or [Springer Materials](https://materials.springer.com/), and save it in the “CIF2PDF\CIFs”.
2. Open it in [VESTA](https://jp-minerals.org/vesta/en/download.html).
3. In VESTA navigate to ***File*** *🡪* ***Export Data…*** and save the file as data type .XYZ in the same folder (“CIF2PDF\CIFs”). Make sure the CIF and the XYZ-file name is identical.
4. Open “CIF2PDF\ CIF2PDF.m” in MATLAB.
5. In line 30 set the filename of the XYZ-file.
6. Run the code.

**During the computation several figures and a TXT-file are created. In the list of outputs below a short explanation is given. In *italics* the save path is given for these files.**

Figure 1: Unit cell as saved in the CIF/XYZ-file. You should inspect whether the atomic positions are correct. “*CIF2PDF\Reduced\_Unit\_Cells\*”

Figure 2: Reduced unit cell. “*CIF2PDF\Reduced\_Unit\_Cells\*”

Figure 3: Crystal lattice constructed from the reduced unit cell. The size of the lattice is such that a sphere with radius RMax=20 Å (also depicted in the coordinate system) fits into the lattice. This is also the distance up to which the atomic distances are calculated. It can be changed in line 300. Increasing RMax also increases the computation time. “*CIF2PDF\Integrated\_Lattices\*”

Figure 4: Shows the relative occurrence of atomic distances broken down by the different atomic species. This distribution is representative of a pair distribution function of the input crystal system. “*CIF2PDF\PDFs\*”

TXT-File: Table representation of the relative occurrence of atomic distances broken down by the different atomic species. “*CIF2PDF\PDFs\*”

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