

Manual for AutoFree v. 1.0

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AutoFree is a Python 2.7/3.5 program for calculating free energies and other properties from DMACRYS output files [1]. The separate program AutoLD can be used to generate input files for DMACRYS.

The program takes the following arguments:

- i Input file. The input file should be a zip archive containing DMACRYS input and output files from lattice dynamics calculations. If no file is given, any dmain and dmaout files in the current directory are used.
- t Temperature in Kelvin. Calculate properties at this temperature.
- b Kernel bandwidth in units of cm^{-1} . This is the bandwidth used for the Epanechnikov KDE. Half of this bandwidth is used for the Gaussian KDE. Default is 6.0/3.0 wavenumbers.

The program reads lattice vectors, phonon eigenvectors and eigenvalues, elastic tensors and Z-values from one or several dmain and dmaout files. The program will automatically determine supercell sizes etc. One dmain file of the original unit cell must be included.

Make sure the Z-value in the dmaout files is correct, especially for $Z' > 1$ and multi-component structures. The thermodynamic properties are calculated with respect to Z formula units per primitive cell.

The speed of sound and the Debye frequency is calculated from the elastic tensor. The Debye contributions should be added to the Neat and KDE-values to improve the convergence of the thermodynamic properties. Note that if the Debye contributions are used, the Neat or kernel contributions should be scaled by $(n - 3)/n$, where n is the number of phonons.

Kernel density estimates are used to improve the convergence of the phonon density of states. Epanechnikov and Gaussian kernel densities are used. The kernel bandwidth should be chosen with some care. It is recommended that convergence tests are carried out to determine suitable supercell sizes and kernel bandwidths.

The program has been tested with DMACRYS versions 2.0.4 and 2.2.2.1. Several example files are included that illustrate the capabilities of the program.

An output text-file with file extension '.dos' is written, containing the phonon frequencies and the phonon densities of states. These can be used to plot the frequency spectrum.

Please see articles by Price, Leslie, Nyman & Day [1, 2, 3, 4] for more details. These articles should be cited appropriately if AutoFree is used in research.

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References

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