# Manual for AutoLD v. 1.0

Jonas Nyman

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AutoLD v. 1.0 is a Python 2.7/3.5 script for automatically making input files to DMACRYS [1] for lattice dynamics calculations on supercells. The script creates dmain files containing supercells, the size of which can be selected automatically, according to methods described in ref. [2] and [3]. The lattice dynamics algorithm implemented in DMACRYS is described in ref. [4] and [5].

The AutoLD program takes the following arguments, all of which are optional.

**-i** A string specifying the name of the input file. A DMACRYS (dmain) input file. This should be generated by other means, such as with NEIGHCRYS. If no name is specified and there is exactly one dmain file in the working directory, that file will be used.

**-k** A float, the target **k**-point distance in units of $Å^{-1}$. The default is 0.12.

**-l** A string: 'yes' or 'no', to generate linear supercells or not. This is 'yes' by default

**-s** A string: 'yes' or 'no', to split linear supercells into shorter cells with mutually co-prime expansion coefficients. This defaults to 'yes'. This has no effect if rectangular cells are made.

**-c** A string specifying one or several supercell dimensions to be generated, for example [1,1,2][1,2,1][2,1,1]. This allows the user to input a set of supercell dimensions determined by other methods.

The default method for choosing expansion coefficients is to specify a target distance between **k**-points in reciprocal space, typically around 0.2 ($Å^{-1}$). Three supercells, expanded along lattice vectors **a**, **b** or **c** respectively are then generated. A lattice vector **a** is expanded until $\mathbf{a}^*$ is strictly shorter than the target distance.

Lattice dynamics calculations work best with unit cells that do not have very acute or obtuse angles. Suitable 'reduced cells' can be obtained with the Krivý-Gruber algorithm [6], or the ADDSYMM routine in PLATON. Experimental crystal structures rarely require any modification.

If the three linear supercells are very long, it can be cost-effective to split them into several smaller supercells, each sampling different **k**-points. A co-prime splitting

method [3] is implemented and is used by default. This allows a larger number of **k**-points to be sampled with distances down to about 0.05 $Å^{-1}$. Up to 26 **k**-points can be sampled in each direction.

It is also possible to generate a single rectangular supercell, which samples **k**-points in a regular grid in reciprocal space. Again, the optimal expansion coefficients are selected in order to make the supercell as close to a cube as possible. A target **k**-point distance of about 0.45 is recommended for rectangular supercells.

The user can also just pass in a list of dimensions to be generated. This is particularly useful for quasi-harmonic calculations and facilitate sampling the same **k**-points in unit cells with different lattice parameters.

The dmain files may contain Williams, FIT or custom atom types, *i.e.* of the format C_W1__, C_F1__, C_01__ or C_C1__. Such atom types should work for H, C, N, O, F, S, Cl, Xe and 'virtual' atoms with atom type V_01, see below.

A few example dmain files are provided for testing purposes. AutoLD has been tested together with DMACRYS versions 2.0.4 and 2.2.2.

- ACETAC_FIT is an acetic acid structure. The dmain file uses the FIT potential (with H foreshortening).
- AKOVOL01 contains sulfur so the S_01 atom type is used together with the Williams potential.
- CUKCIU contains 1,4-dioxane with the Williams potential.
- CO2_V demonstrates the use of virtual, non-interacting, dummy atoms.
- Fluorophenol_Xe demonstrates how lone atoms are treated. These must be placed last in the BASI block and given the molecule number 0. Atom type Xe01 is used for xenon. The fluorine has atom type F_01 and anisotropic repulsion.
- FORMII has custom atom types and uses the DBUC potential. Only for DMACRYS 2.2.x.

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# References

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[3] J Nyman, O Sheehan Pundyke, and G M Day. Accurate force fields and methods for modelling organic molecular crystals at finite temperatures. *Physical Chemistry Chemical Physics*, 18:15828–15837, 2016.

[4] G M Day, S L Price, and M Leslie. Atomistic calculations of phonon frequencies and thermodynamic quantities for crystals of rigid organic molecules. *The Journal of Physical Chemistry B*, 107(39):10919–10933, 2003.

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