

DMACRYS 2.3

Category

Software/Material Modelling

DMACRYS models crystals of rigid molecules, allowing lattice energy minimization and the calculation of second derivative properties.

Energy minimization package to simulate rigid molecules with multipoles

Product Specification

DMACRYS models crystals of rigid molecules, allowing lattice energy minimization and the calculation of second derivative properties.

Product Description

DMACRYS is a software programme to model perfect crystals of rigid polyatomic molecules, allowing lattice energy minimization and calculation of second derivative properties including the elastic tensor and lattice modes. DMACRYS is designed to use anisotropic atom-atom model intermolecular potentials, particularly distributed multipole electrostatic models. It can also handle a range of other potentials that are being developed for organic molecules, including the foreshortening of bonds to hydrogen of the Williams01 potential. The latest version 2.3 models larger molecules and unit cells more efficiently.

The distribution includes the input file processing package NEIGHCRY, a test-suite with harness and notes, and some utility scripts. Further information, including links to the manuals are on <http://www.chem.ucl.ac.uk/cposs/dmacrys/index.html>

Training may be required, and this can be organised with the program author through our partner organisation UCL Consultants Ltd. For information on rates and availability, please contact them on 020 7679 9794 or info@uclconsultants.com, quoting "XIP product DMACRYS"

Product Requirements

DMACRYS has been tested on the following hardware and software and this represents our approved list.

AMD 64 processor running Linux operating system version 3.16.0-5-amd64 using ifort FORTRAN compiler version 15.0.1.

Other hardware/software combinations have been used successfully and there is no reason why the codes should not run on other systems.

References

1. Day, Karamertzanis, Price, Habgood, Welch, Leslie, Price(2010) , <http://pubs.rsc.org/en/Content/ArticleLanding/2010/CP/c004164e>, <http://pubs.rsc.org/en/journals/journalissues/cp>, 12, 8478-8490