

Prediction of properties and structure of molecular solids (crystals comprising molecules bonded by non-covalent interactions) from ab-initio calculation is a challenging problem. Binding energies of such structures require usage of precise ab-initio methods, which are computationally extremely demanding. Potentials which can be fitted on ab-initio data, or whose parameters can be obtained from a precalculated density matrix, can be used to reduce the number of computations by describing interactions of distant molecules. One method aiming to describe electrostatic contributions is distributed multipole expansion, which expands a density matrix into spherical tensors around several points on a molecule. We have developed a program that can obtain coefficients of multipole expansion from two different codes integrating the density matrix, calculate electrostatic contributions to intermolecular energy, and rotate multipole expansion. This can be done up to an arbitrary order of expansion. We study properties of calculated coefficients depending on ab-initio method, basis of the density matrix, and the code that was used for the integration of the density matrix. We test the prediction of electrostatic energy on dimer datasets of molecular solids with different physical/chemical properties – methanol, methane, ammonia, and carbon dioxide. Furthermore, we also tried to fit the coefficients of single multipole expansion on dimer dataset. To test the possibility of description of distributed properties, we tried fitting a simple model of correlation energy by using classical fitting procedures as well as techniques from machine learning.