The molecular and crystal structures of derivatives of the 7-aryl-4,7-dihydro-1,2,3-triazolo[1,5-a]pyrimidine and 4-aryl-1,2,3,4-tetrahydro-2-thiopyrimidine which contain flexible six-membered rings have been studied. Results of calculations by AM1 method show that substituents in the phenyl rings do not influence on equilibrium conformation of the di- and tetrahydrodipyrimidine rings (boat and half-chair respectively). However, experimental data, especially for 4,7-dihydrodiazolopyrimidine derivatives, indicate considerable change of endocyclic torsion angles. In the case of the nitro group presence in the dihydropyrimidine ring a chair conformation of aryl-4,7-dihydro-1,2,3-triazolo[1,5-a]pyrimidine and 4-aryl-dihydroazolopyrimidine derivatives, indicate considerable change of endocyclic torsion angles. All these effects can be explained by quantum-chemical calculations. Analysis of the crystal packing showed that strengthening of some non-bonded interactions in the crystal (for example, hydrogen bond) causes a decrease of puckering of the pyrimidine ring. Dependence between energy of intermolecular interactions calculated by atom-atom potential method and magnitudes of torsion angles has been investigated. Analysis of the non-bonded interaction potential gradient agrees well with molecules deformation in the crystals as compared with the gas phase.

A semiempirical quantum chemical method based on a perturbative approach [1] is presented which retains the original meaning of the contributions (dispersion, electrostatic, induction, and repulsion energy) to the lattice energy. These components are obtained using the results of the semiempirical MINDO/3 method [2]. Thus the dispersion energy is calculated by means of the London formula employing MINDO/3-FP [3] atom-in-molecule polarizabilities and vertical (Koopmans) ionization potentials. Only the Coulomb part of the electrostatic energy is considered employing MINDO/3 atomic charges which are also used together with the polarizabilities to obtain the induction energy. An approximate method is used to calculate the exchange repulsion energy which includes the repulsive part of the lattice energy via MINDO/3 molecular orbitals and overlap integrals.

Results obtained for several organic compounds including some polymorphs are presented. The choice of the molecular model is discussed, emphasizing the importance of a correct positioning of the hydrogen atoms.