

18202 Network for Equilibria and Chemical Thermodynamics Advanced Research

Assoc.Prof. Aleksandar Cvetkovski, PhD (DSc. Chemistry)
Professor of Physical Chemistry & Pharmaceutical Technology
University "Goce Delcev" Stip
Faculty of medical science
Krste Misirkov b.b.
P. fax. 201, 2000 Stip
Republic of Macedonia
e-mail : aleksandar.cvetkovski@ugd.edu.mk

Abstract of lecture:

Development Thermodynamical data sets

The purpose of the STSM is to perform structure-thermodynamics correlation analysis based on the crystallographic data deposited in Cambridge Crystallography Database (CCDC) that relate to structures of particular families of compounds that exerts different properties. In addition, partially to utilize the published crystallographic data (e.g. non-covalent bond energies/ bond distances, mainly different types of H-bonds) as a models for developing case studies with encompass the appropriate data sets that might be used for developing the algorithmams for particular applications in calculation the possible non-covalent interactions in molecular crystals.