Thermogravimetric and IR spectroscopic hints of structure validated by X-ray crystallography, János Madarász,[a*] Petra Bombicz[b] and György Pokol[a], [a]*Institute of General and Analytical Chemistry, Budapest University of Technology and Economics, H-1521 Budapest, Hungary, and* [b]*Institute of Chemistry, Chemical Research Centre, Hungarian Academy of Sciences, P.O. Box 17, H-1525 Budapest, Hungary*. E-mail: madarasz@tki.aak.bme.hu

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The molecular moieties, their arrangement and intermolecular interactions within a crystal strongly affect its thermal stability and FTIR absorption. Usually we try to explore the building blocks in a set of related substances applying combustion analysis, thermal analysis (thermogravimetry and coupled techniques) FTIR-spectroscopy, in combination before single crystal X-ray diffraction. The former methods may provide initial information on stoichiometry, ionic states and binding strengths of the constituents. Sometimes the results give also a hint of the structure. *Vice versa* the knowledge of the structure and especially of the H bonds from single crystal X-ray diffraction helps to explain decomposition behavior and FTIR absorption spectra of the materials. This complex application of the methods helps us to reveal structure-property relationships and based on the gained implications we can conclude on related polycrystalline samples, even on a clearing up of reaction pathway.

One of our investigated systems is a set of amine complexes of Cu(II) containing theophyllinate anions, for modeling chelating of DNA-bound guanine [1-3]. The other is a set of lattice compounds of theophylline with compounds related to ethylenediamine for collecting information on the possible structure of anti-asthmatic drug aminophylline [4-6]. The third system [7-9] contains various thiourea-metal precursors of semiconductive sulfide thin films. They are Cu(I), Sn(II), Zn(II) complexes containing thiourea ligands in various stoichiometric composition

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