between the host and guest molecules by the computational method (electrostatic surface charge distribution, heat of formation and so on) and we found the important contribution of CH–π interactions which probably act to stabilize the guest molecule inside the cavity of host molecule.

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MS11.01.06 INCLUSION COMPOUNDS: RELATING STRUCTURE TO THERMAL STABILITY.

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Research on inclusion compounds has largely concentrated on the synthesis of novel host compounds, aimed at selective enclathration of targeted guest molecules. We have directed our program to the understanding of the intermolecular forces which are responsible for the process of molecular recognition between host and guest, in order to explain the physical properties of inclusion compounds.

We have synthesised a variety of host-guest complexes comprising bulky hosts containing the hydroxyl moiety, have elucidated their crystal structures and measured their thermodynamic stabilities with a variety of analytical techniques. The kinetics of enclathration of a gaseous guest by a solid host has been studied using a novel magnetic suspension balance, while the kinetics of thermal decomposition of labile clathrates has allowed us to elucidate the mechanism of the desolvation reactions. Competition experiments between close isomers of a guest have been carried out both in solution and with the host in suspension, and we have extended this principle to solid-solid systems.

The results of both the dynamic and equilibrium experiments are rationalised in terms of the molecular structures and the crystal packings of the host-guest compounds concerned.

MS11.01.07 MOLECULAR RECOGNITION OF ANIONS: HYDROGEN-BONDING PROPERTIES OF SULFATE, THIOCYANATE AND PICRATE ANIONS.

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Ions play an important role in biological systems, as substrates (ATP, peptidic side-chains..) or as structural elements at interfaces (membranes, micelles). Whereas the environment of cations is well studied, our goal is to analyse the structural characteristics of anion binding, very little[1] being written on this topic (aside of halogens).

The anions we started to study are geometrically very different: spherical, (sulfate dianion), linear (SCN) and flat (picrate). Sulfate plays a role in protein architecture, SCN has 2 acceptor centers and is very small, and picrate has a flat aromatic (hydrophobic) core. The method used was the search through Cambridge Crystallographic Data Bank, and we analysed the H-bonding possibilities of each anion observed in the retrieved crystal structures.

Discrete sulfate dianion principal characteristic is to form as many H-bonds as possible, short and direct, up to 12 per dianion. This quality gives sulfate a character of strong linker in forming molecular associations. The O-bonded sulfate (monoanion) is much less attractor and more directional. The H-binding property of SO_4^{2-} will depend on its complexing environment. SCN$^-$ has a very unusual behaviour. To our knowledge, this systematic analysis of its binding properties is the first one based on experimental results: isolated, this linear anion binds by both ends to H-donors; when coordinated to a metal by one end, it can binds to H-donors by the other end. Metal cations fall into different classes whether they

bind to S or to N. Correlations between the charge (or size) of the cation and its position with respect to the anionic cylinder were found. Picrate forms strong hydrogen bonds which might involve the ortho nitro groups. The most evident result is the formation of intimate ion pairs. Other observed aggregation modes are infinite chains and macrorings.

The structural data assembled in these analyses can be useful to predict molecular associations, and in certain cases (sulfate[1]), agree quite well with similar analyses in biological systems. Moreover, our results provide the first picture of the coordination behaviour of SCN$^-$.

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PS11.01.09 MODEL STUDY OF THE RECOGNITION CENTER INVOLVING PYRIMIDINE BASES AND AMIDE GROUP OF AMINO ACIDS.

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In the frames of the problem of molecular recognition this work is aimed at the investigation of hydrogen bond formation of the amide group with nucleic acid bases in the crystal structure of a specific repressor-operator complex of bacteriofage 434. The interactions between the monomers of nucleic acids and proteins, which lead to hydrogen bonds formation, were studied on the systems (consisting of nitrogen bases 1,3-dimetUra and 1-metThy and acrylamide) which are good models of interactions, involving specific aminoacid side chains of Gln and Asn and free atomic groups of nucleic base Thy in single or double stranded DNA. Thermodynamic parameters of interactions were obtained using a method of temperature dependent field ionization mass spectrometry and theoretically by the atom-atom potential functions calculations. Under the mass spectrometric conditions the associates of molecules were formed in the gas phase; variation of the temperature allowed to obtain relative association constants and to calculate the enthalpies of associates formation (DH, kcal/mole) using Vant-Hoff plots. A good agreement between experimental and theoretical data for acrylamide complexes with 1,3-dimetUra (9.7 vs 10.1) and 1-metThy (6.8 vs 6.6) was observed. Proposed schemes of the energetically favourable hydrogen bonding are as follows: a) for the complex of acrylamide with 1,3- dimetUra: N1-H...O2 ; b) for the complex of acryl- amide with 1-metThy: O1...H-N2 or N1-H...O2. The data obtained enabled us to determine hydrogen bond for formation and mutual positions of molecules in the crystals and can be used for quantitative estimates of the probability of recognition.

PS11.01.10 MOLECULAR RECOGNITION OF THE PHYTOHORMONE AUXIN AND RELATED COMPOUNDS.

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A molecular recognition approach was applied to the auxin family (indol-3-yl acetic acid, IAA), the most intensively studied plant hormone. The final goal of the research is to offer a mechanism of hormone binding to receptor(s) and to provide data for QSAR of indole and non-indole auxins. The study includes natural and synthetic alkylated and halogenated analogues of IAA. Both, active and inactive analogues have been included in the analyses. The problem has been tackled in three directions: analysis of the molecular geometry, study of electron redistribution by substitution effects, and correlation of the physico-chemical parameters with substitution effects and bioactivity. The analysis has been based on the results of X-ray structure analysis, computational chemistry, FT-IR, UV & NMR spectroscopies, physico-chemical parameters such as lipophilicity and acid-base properties of the