

s9.m2.o1 **Structure and Reactivity of Supramolecular Compounds: Mise en Scene.** L.R. Nassimbeni¹ and E. Weber², ¹*Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa.* ²*Institut für Organische Chemie, T U Bergakademie Freiberg, Leipziger Strasse 29 D-09596 Freiberg/Sachsen, Germany.*
Keywords: host design, molecular recognition, reactivity.

Molecular recognition lies at the heart of host-guest chemistry and the formation of an inclusion compound depends on the strengths and directions of the various intermolecular forces acting on the multi-component system.

Since the 1970's considerable effort has been put into the synthesis of host molecules with specific properties. These hosts are generally of two types: first, those that form molecular complexes by accepting convex guests into a cavity, e.g. cyclodextrins, cavitands and carcerands. The second type are those hosts which form lattice inclusion compounds by packing in a manner that leaves channels or cavities in the crystal structure.

The presentation will give a brief historical review of host-guest chemistry. This will be followed by a discussion of the synthetic strategies adopted for the synthesis of specific host molecules. The physical properties of the ensuing inclusion compounds will be considered. In particular, we will highlight the methods used in measuring their thermal stabilities, the kinetics of formation and desolvation, and the evaluation of enthalpies and entropies of enclathration. The question of selective enclathration of a given guest from a mixture of guests will be examined, and the results correlated with lattice energy calculations.

s9.m2.o2 **Effect of pressure on the intramolecular reactions. in solid coordination compounds.** E.V. Boldyreva. *Institute of Solid State Chemistry and Mechanochemistry, Siberian Division Russian Academy of Sciences and Novosibirsk State University, Kutateladze, 18, Novosibirsk, 630128 Russia, FAX: +7-3832-322847, email: elena@solid.nsc.ru*

Keywords: molecular interactions, supramolecular compounds.

Studies of the effects of the environment on the intramolecular reactions in crystals are important for a better understanding of the interplay between intra- and intermolecular interactions. Applying high hydrostatic pressure to the samples, one can distort the structure in a continuous way, preserving the same polymorph, and this makes this method of distorting the environment of a reacting fragment advantageous in many respects, as compared with studying the same reaction in different polymorphs of the same compound, or, even more problematic, in different (more or less related) compounds.

In the present contribution we summarize the published data on the effects of pressure on the kinetics of intramolecular reactions in solid coordination compounds. Effects of pressure on the thermal nitrito \rightarrow nitro and on the photochemical nitro \rightarrow nitrito isomerization in Co(III)-pentammine complexes will be considered in more details. Pressure accelerates thermal nitrito-nitro isomerization, although the molar volume during this reaction increases (at 0.84 %). The unusual effect is due to the anisotropy of structural distortion of the nitrito-complexes under pressure and in the course of nitrito-nitro isomerization: particular crystallographic directions contract strongly (up to 3.4 %) in the course of nitrito-nitro isomerization despite the overall volume increase, and the same directions are compressed under pressure. Similarly, a comparison of the anisotropy of structural distortion during nitro-nitrito photoisomerization with that induced by elastic loading of crystals made it possible to explain the decrease in the quantum yield in the elastically compressed parts of the crystal, although the molar volume decreases in the course of the reaction.