

ML. 18-H4 CRYSTAL STRUCTURE AND PROPERTIES OF MOLECULES.
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The study of drugs binding to specific receptor sites is nowadays one of the most promising fields in structure-properties relationships. Two different facts, the unknown nature of receptors and the ascertained stereospecificity of drug-receptor interactions, concur to focus our attention on the molecular structure of drugs as the only way for obtaining valuable information on the geometry of the receptor itself.

Unfortunately this simple idea often fails owing to the extraordinary complexity of the mechanisms of action of biological systems. Future developments will depend on the following factors: 1. The formulation of a wider concept of 'structure', including stereochemical as well as electronic and lipophilic aspects; 2. A better understanding of non-bonded forces responsible for the drug-receptor interaction; 3. A more precise definition of molecular 'properties' in biological systems by complementing the pharmacological profile with 'in vitro' binding studies and 'in vivo' pharmacokinetics data.

Examples will be taken from drugs exerting their action on the GABA/benzodiazepine/barbiturate receptor chloride channel complex which is post-synaptically localized in the inhibitory GABAergic synapses of the central nervous system. In particular the new classes of compounds chemically unrelated to benzodiazepines but binding to their receptor will be discussed. Rather surprisingly they display a spectrum of pharmacological properties ranging from full benzodiazepine-like properties (agonists) to opposite ones (inverse agonists) through pure binding to the receptor without any 'per se' effect (antagonists). These compounds seem to propose a well defined stereochemical problem as agonists, antagonists and inverse agonists must possess a common chemical moiety responsible for the binding to the same receptor site while agonists and inverse agonists should have additional and different stereochemical features able to trigger opposite pharmacological effects.

EL. 13-H6 KRISTALLE IN TECHNIK UND ALLTAG (CRYSTALS IN MODERN LIFE). By Th. Hahn, Institut für Kristallographie der RWTH, 5100 Aachen, FRG.

This public lecture will be in German and is addressed to the general population of the City of Hamburg. It will try to bring out the foundations of modern crystallography as well as some important results and applications of this science.

First, an introduction into the solid state and the world of periodicity and symmetry will be presented, as found in everyday life, art and, of course, crystals. A survey of the most important crystalline materials and their atomic structures follows.

On the basis of the fourth group of the periodic table and the diamond structure the differences between insulators, semi-conductors, and metals will be discussed, followed by organic and biological molecules (starting from carbon) and by silicates and minerals (starting from silicon). Diffraction methods are presented as the key to the wonderland of three-dimensional order of atoms, molecules, tetrahedra, rings, chains, and helices.

The growth of large single crystals with special desired physical properties, e.g. ferroelectric and piezoelectric properties, is the domain of 'materials science' and forms the basis for many important technological applications, as do mass-produced technical materials such as steel, concrete, and sugar.