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UNIMOLIS – A Computer-aided Course on Molecular Symmetry and Isomerism

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We here announce a computer-assisted course on molecular symmetry and isomerism, for undergraduate and graduate students in the first place, though it will be useful as a refreshment and update of knowledge in stereochemistry for researchers and practitioners of organic chemistry, biochemistry, pharmaceutics, etc.. The course is made freely accessible on the Web. In UNIMOLIS we tried to produce a visual and interactive course, introducing as few technical terms as possible and illustrating every new concept by means of objects from everyday life.

The contents of the course are as follows. After an introduction a short first chapter on the elemental composition familiarizes the beginner with isomeric compounds. The second chapter deals with constitution, constitutional isomerism and topological symmetry. Here the user is given access to the molecular generator MOLGEN. The ensuing chapters treat 3D geometry and stereoisomerism in some depth: Chapter 3 is on the basics of 3D structure of molecules, chapter 4 introduces geometrical symmetry in 3-space. After these foundations are laid, the concepts of chirality (chapter 5) and topicity (chapter 6) are treated. Both are discussed mainly in terms of the absence or presence of

symmetry in molecules, not in terms of so-called elements of chirality. Finally, in chapter 7 on diastereomorphic interactions the importance of chirality and topicity for the molecular scientist is demonstrated, discussing examples from ^{1}H NMR spectroscopy and stereoselective synthesis as well as from everyday life.

Each chapter except the first is accompanied by problems with solutions, which are an integral part of the course. While the main text is reserved for principles, in the problems the student is encouraged to deal with some ramifications.

Throughout, we strive for clean definitions, without ever intimidating the student with mathematical formalism. Rather, many pictures and 3D molecular models (mostly in the Chime format, some in VRML) are given that can be manipulated by a user in various ways.

The URL of UNIMOLIS is http://btm2d7.mat.uni-bayreuth.de/unimolis.