

Online applications of MOLGEN

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1 The application of MOLGEN

The program system **MOLGEN** is devoted to the computation of all structural formulae (=connectivity isomers) that correspond to a given molecular formula, with (optional) further conditions (e.g. substructures). **MOLGEN** arose from the idea to provide an efficient and portable tool for molecular structure elucidation in both chemical industry, research and education.

Now, as a first step, it is possible to calculate all structural formulae to a given molecular formula *online* via

<http://www.mathe2.uni-bayreuth.de/molgen4/>

Push the button "Molgen Online" to obtain the Molgen input window (see figure 1), where you can enter the molecular formula. Using the "Send" button you can transmit your request to the MOLGEN server which starts the generation of the isomers. MOLGEN constructs several thousand isomers per second, but it is easy to find formulae with an astronomic number of isomers (e.g. C_{60}). Therefore the generator stops automatically after at most three minutes. As a first result you will get the desired number of isomers (see figure 2) according to the given formula (or the number of isomers constructed within the first three minutes). The MOLGEN server saves up to 1000 structures and there is the possibility to view these structures in a 2-dimensional layout (figure 3).

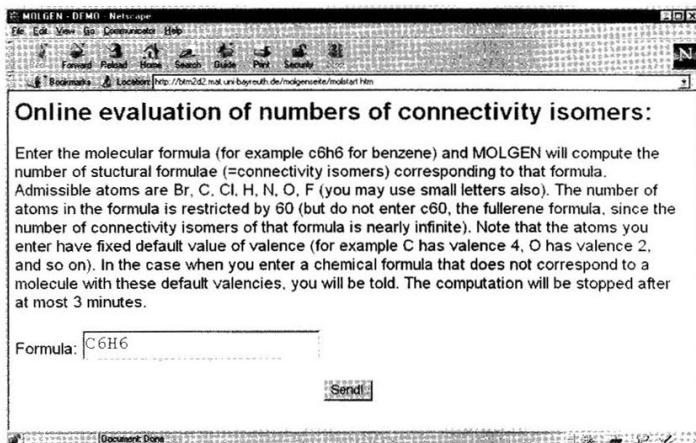


Figure 1: Input of the molecular formula

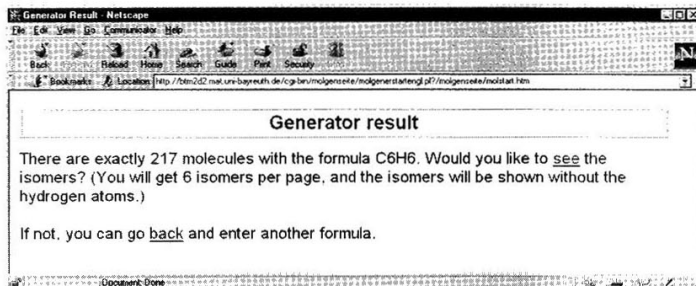


Figure 2: The number of isomers

The MOLGEN-Online tool was first developed for a teaching unit treating several kinds of isomerism in chemistry. The teaching unit is thought for pupils in schools and students at universities. Therein the possibilities of hypertext and scientific software with graphics will be joined resulting in a multimedia tool with much more facilities than either scripts or software can provide. During the development process more of the MOLGEN input restrictions will be implemented so that the MOLGEN-Online

page will be expanded in future.

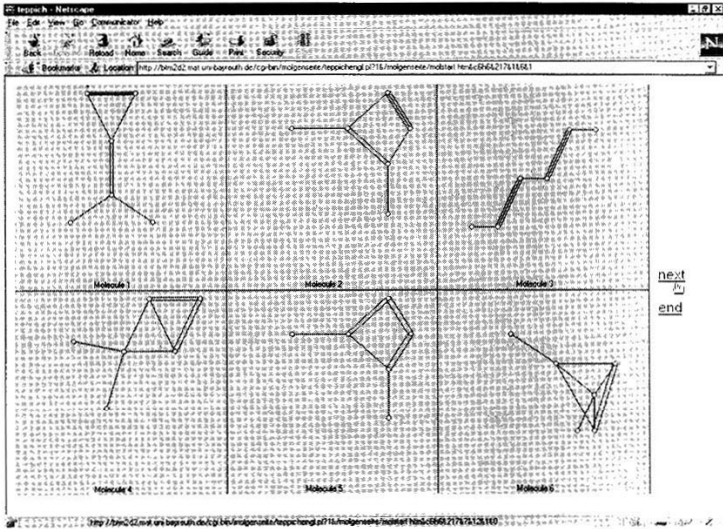


Figure 3: The molecular graphs

References

- [1] G. PÓLYA. Kombinatorische Anzahlbestimmungen für Gruppen, Graphen und chemische Verbindungen. *Acta mathematica*, **68**, pp. 145–253, 1937.
- [2] T. WIELAND. Konstruktionsalgorithmen bei molekularen Graphen und deren Anwendung. *MATCH*, **36**, pp. 5–155, 1997.