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LaTeX, the word-processing system for mathematically oriented articles

LaTeXis *the* word processing system for mathematically oriented articles, and therefore also for publication in MATCH. In connection with Ramek's CHEMSTRUCT (see the Computer Corner of MATCH **30**) it provides most of the tools necessary for publication in mathematical chemistry, and *it provides book printing quality.* (Cf., for example, the article on MOLGEN in MATCH **27**.)

There is also a software tool that allows to transform LaTeX-files (after some easy changes) into hypertext: LATEX2HTML.

LaTeXis availabe from most of the servers via anonymous ftp. In Germany, for example, from the well known server at the university of Stuttgart:

ftp.uni – stuttgart.de

Moreover, LaTeX, together with many other useful programs in contained in LINUX, which is very cheap or even free, and there is also a DOS-version called emtex.

Therefore, LaTeXis strongly recommended for people who intend to submit publications for MATCH.

A. Kerber

News from MOLGEN

Chr. Benecke, R. Grund, A. Kerber, R. Laue, Th. Wieland

Since we reported about MOLGEN last time [1], a lot of features have been modified and added. In this short overview we want to describe those extended possibilities. The differences comprise a new generating method, capabilities for handling spatial information and an improved user interface.

1 The generation method

As described in [1], the former generator constructed all the isomers starting from pre-calculated and catalogued cyclic subgraphs. This method, however, turned out to be hardly extensible, since more powerful catalogs grew to 100 MB and more. For this and several further reasons, a completely new algorithm was developed, see [2]. It is now based on *orderly generation*, an idea introduced in [3]. A catalog is no longer needed, so that range and speed could be increased remarkably.
Moreover, two other features have been added. First the expander, which brings macroatoms used in the generation process to their actual size, no longer must be run separately, but can be switched on as part of the generator. On the other hand, substructures in the goodlist (and badlist) may now be "open", which means that two free valences — attached to different atoms — may after generation form a single bond and need not necessarily join these two atomes with to different other ones.

2 Processing threedimensional information

A new module, called **MolView**, has been developed capable of visualizing the results of the optimizer which calculates a spatial placement of a given isomer by minimizing an energy function similar to MM2 [4].
Moreover, there is the option to compute all configurational isomers corresponding to a given structural isomer (see article [5] in this issue). A lot of effects are taken into account, like asymmetric tetravalent atoms, spirans, double bonds, allens, etc. If possible, spatial realizations of these isomers are constructed geometrically. The display of R/S and cis/trans descriptors is available, too.

3 User environment

The current version of MOLGEN is distributed on a DOS user interface requiring VGA graphics. A free demo version can be obtained from the authors or from

`ftp://btm2x7.mat.uni-bayreuth.de/dist/molgen_e.exe`

via Internet. This is a self-expanding DOS-file which should be placed in an appropriated directory before calling.
Having access to the WWW you may take a look at our MOLGEN-pages starting from

`http://btm2xd.mat.uni-bayreuth.de/molgen/mghome.html`.

The next generation of MOLGEN user interfaces is currently under development and will be released at the beginning of 1995. These are cross-platform programmed versions that are available for MS-Windows, IBM OS/2, SUN Solaris and IBM RS6000 (further systems on request). They'll enhance the work with MOLGEN by making use of the features of the window environments like drag & drop, multi-windowing, clipboard-copying, system printer support, and many more. Additionally, import and export of data in **MDL/MOLFILE**-format has now become available.

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SYMMETRICA, a computer algebra package for representations of the symmetric group

SYMMETRICA is a computer algebra package devoted to the representation theory, the combinatorics, the invariant theory and the applications of symmetric groups and of related classes of groups, for example, alternating groups and general linear groups. It should run on any computer with a C-compiler, but, honestly, it is much better if you run it on a workstation. Here are some of the topics:

- Characters of symmetric and alternating groups, also of wreath products of symmetric groups,
- irreducible matrix representations of symmetric and of alternating groups, polynomial representations of general linear groups $GL_m(\mathbf{C})$,
- irreducible projective representations of symmetric groups,
- multivariate polynomials and in particular Schubert polynomials, also zonal polynomials,
- algebra of symmetric functions, including plethysm,
- Schur polynomials as well as several other series of symmetric polynomials together with base change matrices,
- zonal polynomials and Jack symmetric functions,
- cycle indicator polynomials for combinatorial enumeration,
- the group algebra of the symmetric groups, including manipulation of tableaux.

Using these structures and appropriate procedures, you can evaluate irreducible characters, and decompose reducible ones. You can do combinatorial enumeration to some extent, and you can also apply symmetry adapted bases by an application of irreducible matrix representations, which can be evaluated explicitly.
SYMMETRICA is still in progress, at present the main emphasize lies on projective matrix representations of symmetric groups, on finite group actions, and on the constructions of discrete structures. It is public domain, it can be fetched, via anonymous ftp, from
btm2x7.mat.uni-bayreuth.de:dist/SYM.tar.Z
After uncompressing and unpacking you find in the subdirectory USER (USER.tex) a LaTeX-file of the manual and many example files. If you have questions, please contact

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