

match – online

Joachim Braun, Adalbert Kerber, Reinhard Laue
Lehrstuhl II für Mathematik
University of Bayreuth
D-95440 Bayreuth, Germany

match is now going online, which means that under the address

<http://www.mathe2.uni-bayreuth.de/match/online/links.html>

links can be found, where basic calculations can be done online. The idea is to extend these in the future, and to ask the audience of **match** to contribute.

To begin with, we offer:

- A check if a given molecular formula (of an organic molecule) is admissible, which means that there exist corresponding structural formulae, subject to default values of the valences of the atoms involved. Later on we shall also allow to input valences that differ from the usual default values.
- An online evaluation of the number of connectivity isomers corresponding to a given admissible molecular formula. (The server will run for 1 minute and tell the user how many connectivity isomers were evaluated and if this number is the complete number or not.)
- An online inspection of the first 1000 connectivity isomers that were constructed.

It is important to note, that these checks are *mathematical* checks, i.e. no chemical stability arguments are used, no substructures excluded, and all the mathematically possible structural formulae are evaluated.