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Optimization and centralization of working processes in computational chemistry

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During the last years it became usual to do computations at molecules on high performance servers. This procedure required a relatively large amount of work, since first a molecule had to be modelled and an input file was produced. This, in the next step had to be handed over to the computing server, which returned the results of the computations as output files, which still had to be evaluated by the user.

Administration and storage of the output was task of the user and often required some IT-related knowledge to handle the data. This decentralization of the tasks can be reduced with WebMO [1] in connection with a Wiki-based system. Molecules will become furthermore only drawn in a Java based 3D-editor made available by WebMO itself, a method is selected and the results are presented in a formatted form. WebMO supports a number of different common computation programs, so methods can be compared among themselves.

For the implementation of such a system first a Linux – based web server must be set up, in our case an openSuSE 10.3 system with an Apache 2 web server had been chosen. WebMO and the mediaWiki [2] system we chose were installed.

With this system now 20 organic compounds were computed with different methods and compared amongst each other. The results now can be transferred into the Wiki and be seen by all other users and changed or supplemented if necessary. In particular the extension by topic-related additional information represents a revaluation of the results.

Since it concerns a web-based solution, all results and information are world-wide available. This connection of WebMO and mediaWiki can contribute to the Teamwork, as a substantial component of the research work.

References

1. **WebMO – Computational Chemistry on the Web** [http://www.webmo.net/]
2. **mediaWiki** [http://www.mediawiki.org/wiki/MediaWiki]