QCLDB II: Quantum Chemistry Literature Data Base II.

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Quantum Chemistry Literature Data Base (QCLDB) is a database of those papers published after 1978 which treat only ab initio calculations of atomic and molecular electronic structure. From about thirty core journals they are collected, surveyed, and given proper tags revealing the content and essence of the paper by the group of young Japanese quantum chemists. Those theoretical works even without reporting any computational results are also collected which are judged to have significant relevance to ab initio calculations, while no semi-empirical calculations are included. QCLDB is finally edited and copyrighted by Quantum Chemistry Data Base Group (QCDBG).

QCLDB provides quite useful information not only to chemists but also to both theoretical and experimental scientists, who want to know the state of the art theoretical aspects of chemical substances and materials.

QCLDB was first published in a book form in 1982 by Elsevier, and has been supplemented annually as a special issue of THEOCHEM (Journal of Molecular Structure). The supplement was carried into a special issue of the Journal of Computer Chemistry Japan from 2005. Besides the printed version the users could use its electronic version with a retrieval program, either by making direct access to the computer at the Institute for Molecular Science (IMS), Okazaki, or by subscribing for the on-line version to the Japan Association for International Chemical Information (JAICI). From its very beginning we have been occasionally modifying the policy of data collection and the format of the database in order to keep up with the rapid progress and popularization of ab initio calculations. In 2001 we began to test the internet web-version for a limited group of users.

We announce the opening of our new web-version of QCLDB II [1] from April 1, 2004, which is offered the registered users free usage of the updated database including all the previous data. The login window is shown in figure 1. The new QCLDB II will help your research activities more efficiently than before. In this presentation, we will demonstrate QCLDB II through internet if it is possible.

Figure 1 Login window of QCLDBII

This work was partially supported by the Ministry of Education, Culture, Sports, Science and Technology, Grant-in-Aid for Scientific Research (B), 16350009, and for Publication Scientific Research in 2004.

[1] N. Koga et al. QCLDBII, \texttt{http://qcldb2.ims.ac.jp/}