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NOTE

DiRef, A Database of References Associated with the Spectra of Diatomic Molecules

For some years now we have been compiling references related to the spectra of diatomic molecules. The ultimate (but still distant) goal is to update Huber and Herzberg's classic book on the constants of diatomic molecules (*1*). Our work is based largely on the Berkeley Newsletters (*2*), which contain references to papers on the spectra of diatomic and small polyatomic molecules. DiRef (short for Diatomic Reference Database) currently consists of about 30,000 references covering the period 1974–2000. DiRef contains all of the diatomic references from the Berkeley Newsletters from these years, corrected if necessary, and with some additional citations. The starting year was chosen to ensure adequate overlap with the references found in Huber and Herzberg (*1*). We endeavor to keep DiRef current through updates several times per year.

An on-going project (about half completed) is the addition of Huber and Herzberg's references to DiRef. The National Institute of Standards and Technology (NIST) has placed Huber and Herzberg's book on line (http://webbook.nist.gov/chemistry), although we have found that this "WebBook" is not a completely faithful reproduction. The NIST WebBook, however, does contain a nearly complete set of titles for the articles cited as well as author initials. To save space, Huber and Herzberg did not include titles of references or author initials in their book.

DiRef is a free, Web-based database that can be accessed at the internet address http://diref.uwaterloo.ca. Each entry in the database includes a title for each reference and the molecular formula in the form AB, AA, $AB+n$, $AB-n$, $AA+n$, or $AA-n$, where A and B are the usual symbols for elements and n is an integer for charged species. Searches are carried out primarily by chemical formula. The search can be restricted by year(s) or by author name(s). Unfortunately, "*et al.*" is used extensively in the database for long lists of authors, so using the author option can result in missed references. We have considered the possibility of trying to restore the missing authors but the amount of work involved is considerable.

The database engine used for DiRef is PostgreSQL (http://www.postgresql.org), an open source SQL (Structured Query Language) software package available for numerous platforms. The user interface is written in PHP (an embedded scripting language; see http://www.php.net) and we are currently running the program on a Sun Ultra 5 workstation. A useful feature of the interface is that if the user mouse clicks on the journal name or article title, the program attempts to connect to the journal home page. Depending on the particular electronic journals that your institution subscribes to, and the year of the reference, the user can rapidly retrieve the article. In any case, a list of journal Web sites for all cited journals is also available.

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2. J. G. Phillips, S. P. Davis, and D. M. Eakin, "Berkeley Newsletter, Analysis of Molecular Spectra," University of California, Berkeley, Berkeley, CA 94720. For more information contact S. Davis at the Department of Physics.

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