Houben-Weyl and *Science of Synthesis*, Web Versions

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Houben-Weyl (*Methoden der organischen Chemie*/*Methods of Organic Chemistry*), published by Georg Thieme, is a well-known treatise covering synthetic methods in organic chemistry and has been published in four editions and a supplementary series under that title. The fifth and most recent edition, which began publication in 2000, has undergone a major editorial change, as reflected in its new title: *Science of Synthesis* (*Methods of Molecular Transformations*), but the content and structure are still more or less the same: a logical arrangement of classes of organic compounds, followed by various synthetic strategies. Reviews of individual volumes of the new series have been published in numerous places. These reviews have generally been positive; any concerns voiced focused on occasional omissions or brevity of treatment of some classes of compounds.[1]

Thieme has recently made available electronic versions of both *Houben-Weyl* and *Science of Synthesis*. While the interfaces for these two sources are superficially similar, there are some sizable and significant differences in several areas, including procedures for text and structure searching and the display of search results. Because of the familiarity of the chemistry community with *Houben-Weyl* and *Science of Synthesis*, this review will not examine their content but will focus primarily on their respective user interfaces and the general ease of use of the electronic versions.

The *Houben-Weyl* portion of the database currently includes the entirety of the 2nd, 3rd, and 4th editions as well as nearly all of the E-series. The E22 volumes, which cover peptides, are missing; however, it is the intention of the publisher to establish a separate peptide database corresponding to these volumes. The search screen is divided into two sections. On the left is a table of contents index with headings corresponding to the editions, volumes, chapters, and section headings of the original work. All headings are in English, regardless of the language of the original document. On the right is the *Houben-Weyl* section currently being viewed, displayed as a pdf document.

Two search modes are available to the user: a simple search on key words within the chapter headings and subheadings using the search box at the top of the left-hand screen, or an enhanced search, which allows users to include volume number, page number, or publication date in their search strategy. Additionally, the "Index" button on the enhanced search screen enables the user to browse chapter or subheading key words. When the user selects the enhanced search, a search screen replaces the document display screen on the right. At this writing, only the 4th edition and the E-series are searchable, and the older editions can be searched only by browsing using the table of contents screen; however, a new release is planned that will include the indexes of the earlier editions.

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One additional mode of access is available: by clicking on the "Structure Templates" button, the user can bring up a display of structure fragments (including simple ring systems) and special topics. Clicking on a particular fragment provides the user with a set of more specific choices, until the specific class of compounds desired has been located. Alternatively, one can select one of the "special volumes" to view sections dealing with particular classes of compounds. In the absence of structure/substructure searching capabilities, this mode of access provides a means of locating relevant documents based on chemistry rather than purely verbal descriptors. Again, as with the other search modes, only the 4th edition and the E-series are searchable at this writing.

Neither of these two search modes produces a list of results. Instead, on the left side of the screen, a red number is displayed next to the edition in which the hits can be found, indicating the total number of hits per edition. The user has to click through to the various volumes, following the red numbers until a red dot appears, identifying a specific document. On displaying the pdf document, the user can use the "Go to" button either to add the next group of pages to what is currently on the screen or to skip ahead to the next group of pages.

Thus, the current structure of the *Houben-Weyl* database closely parallels that of the print volumes, for which no comprehensive index exists. In the older editions, each volume had its own index, while the 4th edition and the E-series have a comprehensive index covering only those volumes. The full text can only be displayed, not searched: only the chapter headings and subheadings can be searched. Since the pdf documents are image only files, users cannot even perform simple text searches using the Acrobat Reader search engine.

As stated above, *Science of Synthesis* is a major, comprehensive revision of *Houben-Weyl*. It is intended to incorporate all the data contained in previous editions as well as the most current information. Nevertheless, *Science of Synthesis* is not intended to replace *Houben-Weyl* in either the print or electronic form. The new edition does not repeat the information contained in the old, in fact, *Science of Synthesis* contains references back to *Houben-Weyl* where appropriate. *Science of Synthesis* does not include the general laboratory methods sections found in *Houben-Weyl*: all sections of all volumes deal with the preparation or synthesis of specific classes of compounds. It is still in the process of being written and published; at this date, only eight of the 48 expected volumes have been released. The last volumes are expected to appear in 2008. *Science of Synthesis* is published in both electronic and print editions: the content of each new volume is released simultaneously in both formats.

As previously stated, the interface for *Science of Synthesis* is superficially similar to *Houben-Weyl*. The user is presented

with a table of contents listing on the left side of screen, and the text is displayed (as html, not pdf) on the right. As with *Houben-Weyl*, the user can browse the database using the table of contents. The similarity ends there. The *Science of Synthesis* interface, while more sophisticated in terms of its search and display characteristics, is much easier to use. For basic browsing, once a portion of text is displayed, the user can easily move to the previous or following section by clicking on the arrows adjacent to the status box. The status box displays a number that indicates which section user is currently viewing, but the number is difficult to interpret. It is much easier to simply look at the top of the current document, which displays the exact section number currently being viewed as well as indicating the corresponding volume and page number in the print version. The text display includes only the references associated with that section; clicking on the in-text references allows the user to jump to that reference, but it is not possible to jump back to the text. Clicking on the full reference brings up a FIZ-Karlsruhe document request pop-up screen, allowing the user to purchase the original document if desired. Unfortunately, it does not seem to be possible to specify other vendors for purchasing the document, nor are there links to full text.

The *Science of Synthesis* interface offers many more search options than *Houben-Weyl*, from simple full text to chemical structures. When users select "Search" from the menu bar, they are presented with a screen enabling the combination of up to three search terms by means of four different Boolean operators: AND, OR, NOT, and NEAR. Text search fields include Basic Index (in full text); Journal Title, Author, and Publication Year (references); *Science of Synthesis* volume number; Catalyst Name, Solvent Name, Product Yield, and Temperature (reaction conditions). The "..." button allows the user to browse the dictionary for nonnumerical text terms. Three types of structure search are also available: substructure, exact structure, and reaction with substructures. Structure searching requires the ISIS/Draw software from MDL together with the appropriate plug-in to establish communication between ISIS/Draw and the user's Web browser. Thus, a basic knowledge of ISIS/Draw is essential for effective structure searching.

Once a result set has been generated, the user can jump directly to the text by selecting "Go to hits". The text displayed will be the first hit; the user can then browse through the results sequentially by using the status box arrows described above. Alternatively, selecting "View hit list" brings up a separate window that lists all the resultant hits. Clicking on any hit will display the text in the main window. Thus, displaying the full text is much simpler under the *Science of Synthesis* interface than under *Houben-Weyl*. Again, the user may browse forward and backward using the status box arrows. Result sets can be combined by selecting "Hitlists" from the pull-down menu on the search screen; however, the sets must first be saved by clicking on "Save hit list". Such hit lists are saved on the Thieme server only for as long as the search session is open. Closing the session either by logging out or by letting it time out automatically deletes all saved hit lists. The user may designate descriptive names for the hitlists and may also browse them using the "..." button.

In terms of ease of use, the *Science of Synthesis* interface compares favorably with other chemistry databases, such as *SciFinder Scholar* (SFS) and *Beilstein CrossFire Commander* (BCF). Because of differences in the nature of these databases, it is not possible to make direct comparisons: SFS is perhaps less sophisticated, with fewer search options in some key areas, while BCF, because of its great variety of search keys and options, is considerably more sophisticated. Taking all of these factors into account, the interface for *Science of Synthesis* is quite easy to use. While this review was being written, a new release came out that was a considerable improvement over the initial version.

The current release of the *Houben-Weyl* and *Science of Synthesis* databases lacks certain key functions. For example, no context-sensitive or searchable online help system is available. The "Help" button in *Science of Synthesis* only displays the "Getting Started Manual" as a pdf document. There is no help button in the *Houben-Weyl* database. Also problematic are the sizable differences between the *Houben-Weyl* and *Science of Synthesis* databases and their search interfaces, which make it a bit difficult to switch back and forth between the two when searching for similar information. Most critical in this regard is the lack of both full text and structure searching capabilities within *Houben-Weyl*. As stated above, even such text searching as exists is limited to chapter headings and subheadings in only the 4th edition and the E-series. Future releases (another is expected in late 2003) are expected to resolve these issues as well as add other capabilities to both databases. For example, the references to *Houben-Weyl* in *Science of Synthesis* will be linked in the Fall 2003, enabling users to jump directly from *Science of Synthesis* text to the relevant *Houben-Weyl* sections.

Providing electronic access to the material in *Houben-Weyl* and *Science of Synthesis* is a major step in improving the usability of these sources. While they are clearly databases in transition, the ultimate goal of providing comprehensive linked access to and between the various sections of the database seems achievable, as each new release significantly expands and improves functionality and depth of access. Although it does not provide access at the level one might desire, the release current at this writing is a significant improvement over the print editions. Any institution supporting active research in organic synthesis will find these databases useful.

REFERENCES AND NOTES

(1) Schmidbaur, H. Book Review: Science of Synthesis. *Angew. Chem., Int. Ed.* **2003**, *42*, 715−716.

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