

Bretherick's Reactive Chemical Hazards Database. Version 1.00

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Bretherick's Reactive Chemical Hazards Database—version 1.00 is available from Butterworth-Heinemann Ltd. and is essentially a computer-readable version of the *Handbook of Chemical Reactive Hazards*. The program, like the book, addresses historical reports of accidents associated with procedures, reactions, and analytical methods. I found the software as thorough as the printed book and somewhat more convenient. The database is organized in the same way as the 4th edition of the *Handbook of Chemical Reactive Hazards*, providing two sections and several appendices. The first section provides information on chemicals listed alphabetically by formula. The second section gives information by subject class. The appendices cover journal abbreviations used, fire-related data (simple table format), glossary, hazards overview, and organization of the database.

The hardware required is an IBM-compatible, MS-DOS 2.1 or higher, 640K memory, floppy drive (3.5-in. 1.44MB or 5.25-in. 1.2MB), hard disk with at least 6M available, and EGA or Hercules display. The software can provide hard-copy (screen dumps) to Epson or Laserjet printers. I tested the software on a SUN 386i in an MSDOS window and made printouts on a postscript printer using an Epson-2-postscript filter (not provided with the software). I encountered a problem with the diskette copy protection that is reportedly

an artifact of using the 386i rather than the usual IBM-compatible machine. The original diskettes were replaced by the publisher, and installation proceeded without further incident. The installation instructions are provided in the user's manual and are not complicated. Once the software was installed I encountered no difficulties in using it, and I experienced no software crashes. I found the program sufficiently easy to use so that the manual was consulted only for making screendumps and only then because of my need to print on an unsupported (postscript) printer.

The user moves through the database by means of a window system and function keys. The database provides for searching by name or formula, and there is very good cross-referencing of related items. Searches may be conducted for hazards by class or topic and also partial name searches are allowed. There is online help available along with the ability to back-out after following a chain of cross-referenced items. Figure 1 shows a typical screen display. This display also reveals the only error that I encountered—the use of the symbol Zn instead of Zr for zirconium.

A few entries have simple line-drawings which can be selected (displayed) as shown in Figure 2. It is not possible

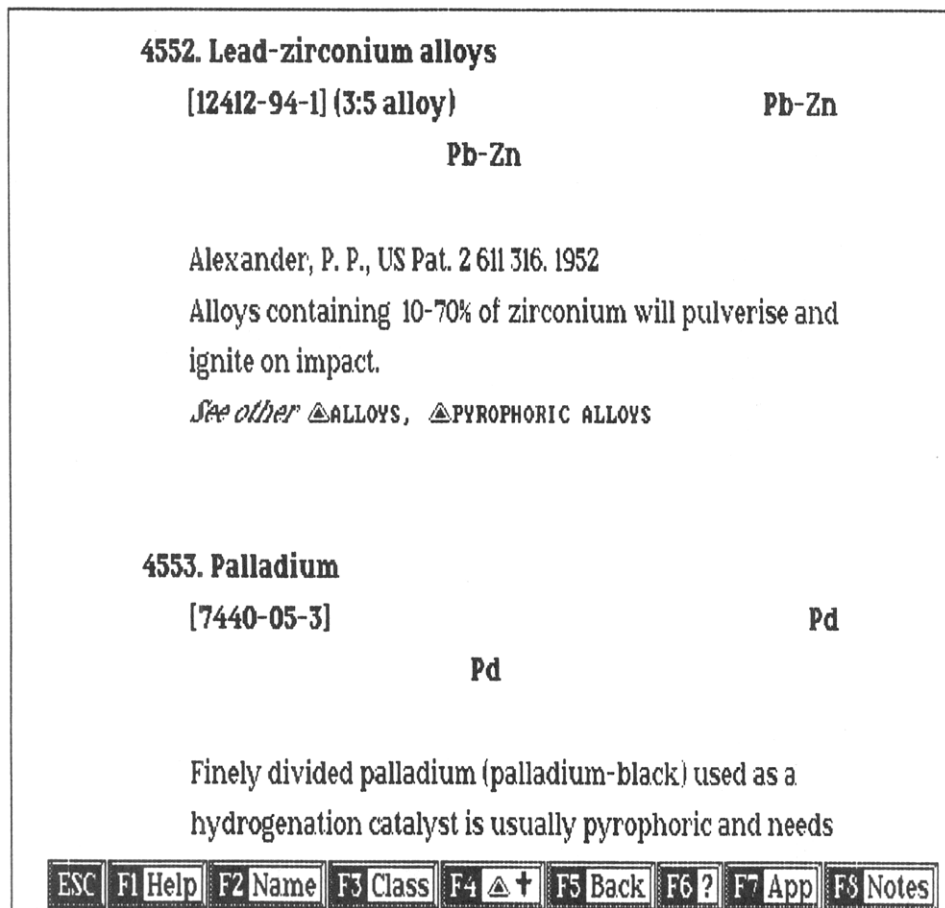


Figure 1. Typical screen display.

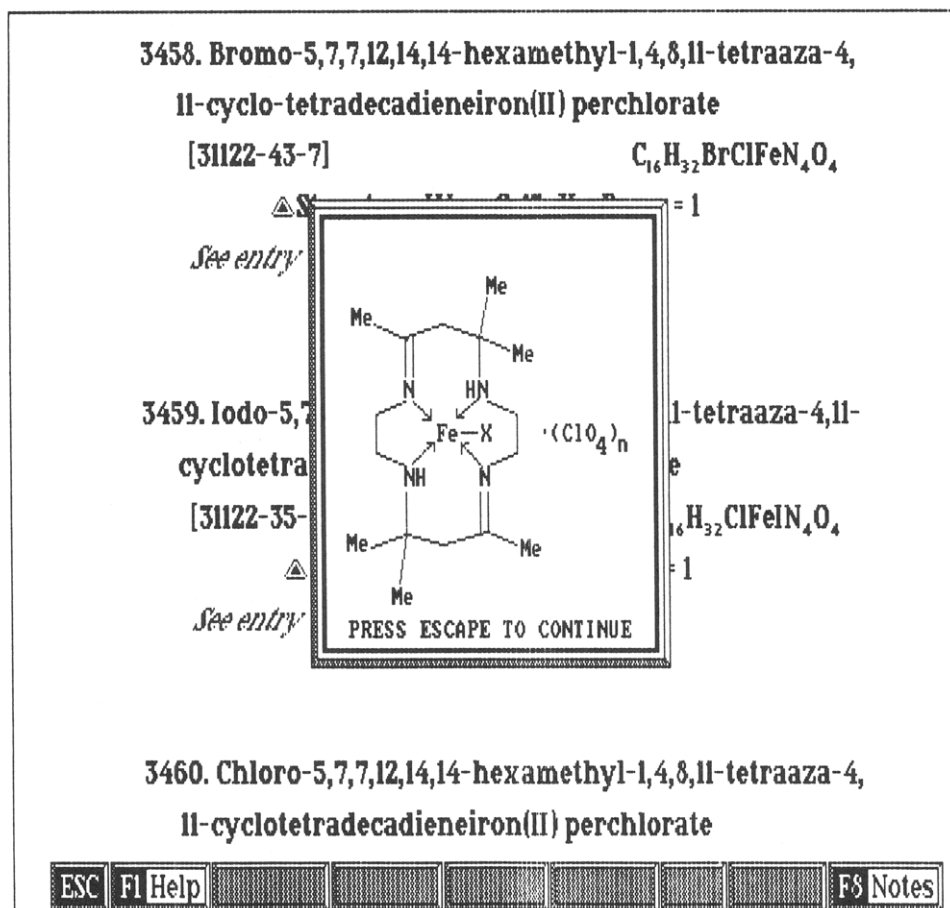


Figure 2. Ring compound with structure displayed over main window.

APPENDIX 2 Fire-Related Data				
	Formula	B.P., °C	E.L., °C	A.I.T., °C
Acetone	C_3H_6O	-17	2,6-12,8	-
Methyl vinyl ether	C_3H_6O	-5,5	-56(o)	2,6-39,0
Oxetane	C_3H_6O	50	-28	-
2-Propen-1-ol	C_3H_6O	-21	3,0-18,0	-
Propionaldehyde	C_3H_6O	49	-9	2,9-17
Propylene oxide	C_3H_6O	34	-37	3,1-27,5
1,3-Dioxolane	$C_3H_6O_2$	-2	-	-
Ethyl formate	$C_3H_6O_2$	-34	2,7-13,5	-
Methyl acetate	$C_3H_6O_2$	-9	3,1-16	-
Dimethyl carbonate	$C_3H_6O_3$	18	-	-
2-Propene-1-thiol	C_3H_6S	-10	-	-
1-Bromopropane	C_3H_7Br	-1	4,6-?	-
2-Bromopropane	C_3H_7Br	1	-	-
1-Chloropropane	C_3H_7Cl	47	<-18	2,6-11,1
2-Chloropropane	C_3H_7Cl	36	-32	2,8-10,7
Chloromethyl ethyl ether	C_3H_7ClO	15	-	-
2-Iodopropane	C_3H_7I	20	-	-
3-Aminopropane	C_3H_7N	-29	2,2-22	-
Azetidine	C_3H_7N	61	-20	-
Cyclopropylamine	C_3H_7N	1	-	-
2-Methylaziridine	C_3H_7N	-10	-	-
Isopropyl nitrite	$C_3H_7NO_2$	40	<10	-
Propyl nitrite	$C_3H_7NO_2$	47	<20	-
Isopropyl nitrate	$C_3H_7NO_3$	11	?-100	175
Propyl nitrate	$C_3H_7NO_3$	20	2-100	-
Propane	C_3H_8	-45	-104	2,2-9,5
Ethyl methyl ether	C_3H_8O	11	-37	2-10,1
Propanol	C_3H_8O	15	2,5-13,5	-
2-Propanol	C_3H_8O	12	2,3-12,7	-

ESC FI Help FS Notes

Figure 3. Fire-related data displayed.

to search by structure, but for most that should not be a problem. An example of an appendix with fire-related data is shown in Figure 3. Note that there are gaps in the data.

Using nearly 2 years of back issues and current issues of *Chemical Engineering News*, I compared letters to the editor regarding safety issues with a search using this database. In general the database did quite well in providing information that should have been helpful in preventing the accidents that were described in C&EN.

On the negative side, there is no provision for pasting information from the database to a text file (there is a simple editor for making notes), the screen dump for output is rather inefficient, and postscript printers, in common use, are not supported. A simple text interface would have allowed access over a network which would be desirable with the increasing

presence of networks and workstations. The original software that was received was copy protected and that proved inconvenient. The database is a faithful representation of the printed text but is faster and easier to use but as such some of the referenced material is dated. As the name suggests it addresses only *reactive hazards*. A database as thorough and easy to use as this but that also included health-exposure data would be of even greater value.

The Reactive Chemical Hazards Database is no substitute for careful thought and literature review when dealing with hazardous materials and processes; there are omissions and errors, but it is a good first step. It is also not without some humor; the entry before 'carbaboranes' is 'can of beans'—a screen dump of this display (not shown) now resides on the side of the laboratory's oven door.