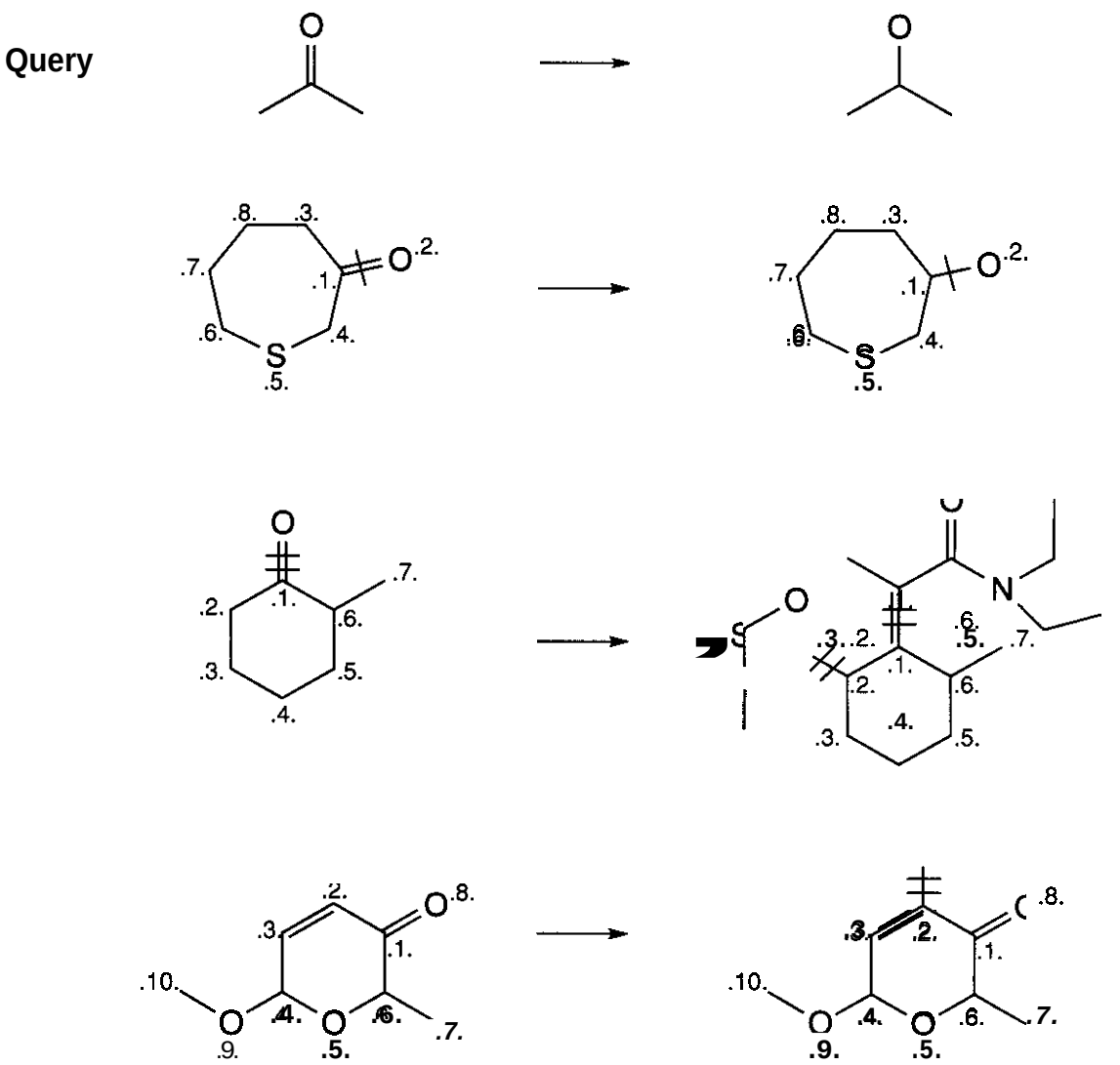

Figure 9.15. Reaction substructure search query and some example hits. If no reacting center or mapping information is used, all three hits are found. If reading bond information is used, hit c is excluded. If both reacting atom and reacting bond information is included, then false hits b and c are excluded.

(89), material safety data sheets (90), and chemical suppliers (91). Some useful tools include the Accord ChemExplorer program, which allows searching word processor documents and files for particular chemical structures, and the CambridgeSoft ChemFinder for Word (92).

3.4 Chemical Information Management Systems and Databases

A number of software and database vendors provide programs and database systems to implement representation, registration, and searching of chemical information in a corporate environment. Some of these vendors have smaller personal chemical database systems that support registration and searching on a personal computer. A handful of academic and public domain systems are also available. Finally, an increasing number of chemical information systems are being made available on the Internet. Some representative systems that are being sold or have been discussed recently in the literature are discussed below.

3.5 Commercial Database Systems for Drug-Sized Molecules

Accelrys. A subsidiary of Pharmacopeia, Inc, Accelrys was originally a provider of molecular modeling software. They recently acquired several companies that provide offerings in the chemical information and bioinformatics areas. The company provides unique databases including several for reactions.

- BioCatalysis—biomolecules as catalysts
- BioSter—pairs of biologically similar structures for bioisosterism applications
- Biotransformations—developed in conjunction with the Royal Society of Chemistry