

Finding Optical Rotation Data for Organic Compounds

Handbook of Data on Organic Compounds

Crerar, 1st Floor Reference Collection QD257.7.H360 1989

Find compound by name or CAS no. in Index (volume 7). Using the 5-digit HODOC number, find the entry for the compound in volumes 1-6. A key to abbreviations used in entries and a description of specific rotation appears in the introductory pages of each volume.

Specific rotation (or optical rotation) entries examples as they appear in HODOC appear below:

α : $[\alpha]^{25/D} 28.1 \text{ 95\% al}$

Temperature 25 degrees Celsius, 589.3 nm wavelength, 95% concentrated solution in ethyl alcohol, +28.1 degrees rotation

α : $[\alpha]^{20/D} -65.5 \text{ (w)}$

Temperature 20 degrees Celsius, 589.3 nm wavelength, water as solvent but no concentration given, -65.5 degrees rotation

Merck Index

Crerar, 1st Floor Reference Collection RS356.M552 (latest edition) OR

Crerar, 2nd Floor Bookstacks RS356.M552 (older edition)

Find compound by name/synonym or CAS No. Look for the symbol for specific or optical rotation – $[\alpha]^{20}$. You may also see information about other controlled variables, light wavelength of light used, solvent, concentration of solution, temperature (indicated by the superscript 20), etc. This information is often highly abbreviated, so consult the key or explanatory information found at the front of the volume.

Dictionary of Organic Compounds

Crerar, 1st Floor Reference Collection QD291.H464

Also available online as **Combined Chemical Dictionaries**: <http://www.lib.uchicago.edu/h/ccd>

Look up compound in index volume by name/synonym or CAS no. and find entry in the appropriate volume. In the online resource, optical rotation is very clearly labeled as such:

Optical Rotation $[\alpha]^{20}_D +126.8$

In the print volumes, you will need to look for the $[\alpha]$ symbol with the accompany abbreviated information:

C21H28O2 M 312

Anabolic steroid. Mp 166-9° . $[\alpha]^{20}_D +105^\circ \text{ (c, 0.539 in CH}_2\text{Cl}_2\text{/Et}_2\text{O)}$

where c refers to concentration (usually as a weight/volume percentage) and the solvent is a dichloromethane/diethyl ether mixture, the sodium-D line (589.3 nm wavelength) of light was used at 20 degrees Celsius. If path length is not one of the specified variables, you can assume it is standard 10 decimeters

If you can't find your compound in any of these resources, ask a librarian at the Crerar Library for help.