IR - Sadtler Steroids 2 - Wiley

Spectra - 245

Description

The steroids database of 245 FT-IR spectra represents important classes of compounds for steroid research.

Additional Information

All compounds are of at least 98% purity and each spectrum is labeled with the following information (when available): CAS name, structural formula, molecular formula, molecular weight, physical data, source of sample, and method of sample preparation.

Classifications

Carboxylic Acids - 14
Carboxylic Acids Esters - 94
Aldehydes - 1
Ketones - 104
Primary Alcohols - 17
Secondary Alcohols - 20

Technique

All data were measured at an optical retardation of 0.25 which corresponds to 4 cm^{-1} nominal spectral resolution. Standard techniques have been developed in our laboratories to ensure that the spectra published are of the best possible quality and reproducible for comparison and identification purposes. The preferred sample preparation methods are capillary cells for liquids, cast films from a suitable solvent for samples with melting points below 72°C, and KBr wafers for solids with melting points above 72°C. When the KBr method cannot be used for solids due to a reaction between KBr and the compound, the split mull sample preparation technique is used. The sample is mulled in mineral oil, spread between AgCl plates and the entire spectrum is measured. The sample is then mulled in a perfluorinated hydrocarbon, spread between AgCl plates and the spectrum is measured again. Finally, the two spectra are merged where the perfluorinated hydrocarbon data are used from 4000 cm^{-1} to 1330 cm^{-1} and the mineral oil data are used from 1330 cm^{-1} to 450 cm^{-1}. This method provides a complete spectrum of the compound without interference from the mineral oil or the perfluorinated hydrocarbon mulling compounds.

This collection has been subject to the Sadtler Data Review Protocol™ to provide you with the highest standard in spectral data today. These rigorous qualifying procedures start at data acquisition and continue throughout the database development process.