IRD 3 Application Brief

Aromatic Substitution Isomers

Introduction

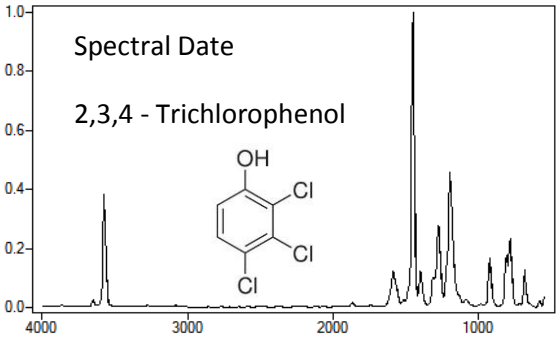
The trichlorophenols are used as fungicides, bactericides and wood preservatives. The 2,4,5-isomer is used in the manufacture of herbicides and insecticides. There is toxilogical and environmental concern since the trichlorophenols can be absorbed through the skin in toxic amounts and they are fairly persistent in the environment. This is one of many examples.

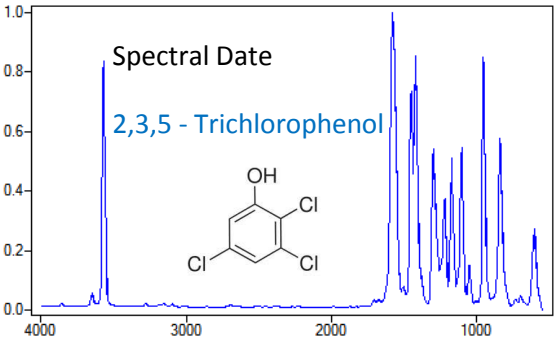
The trichlorophenols are one of many examples of polysubstituted aromatic characterization in general where there is frequent need to know which isomer is present and which are not.

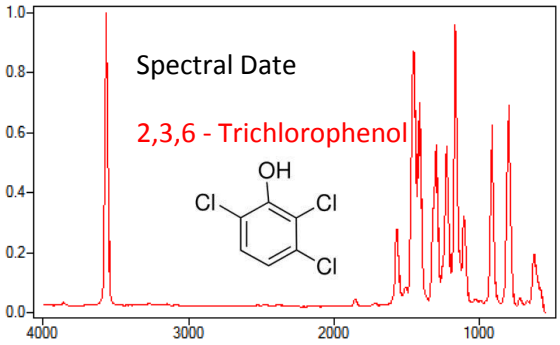
The mass spectra of the trichlorophenol isomers are virtually identical. This is not unexpected since the same fragments will occur with the typical 70eV electron impact process.

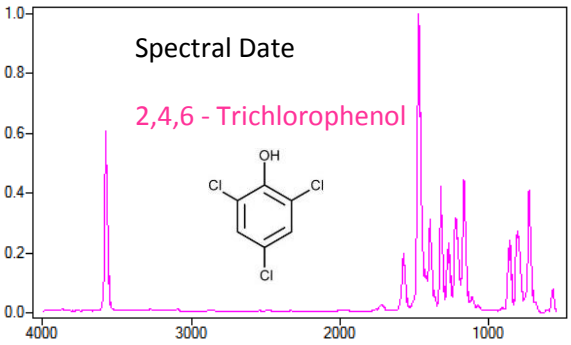
Results

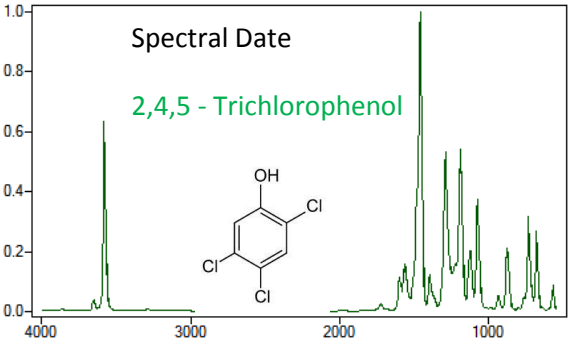
The infrared spectrum of each of the trichlorophenols is unique. However, accurate assignment of all of the bands is complicated. In these tetra substituted compounds the C-H out-of-plane deformations occur in the region from 800 to 870 cm^{-1}. Ring vibrations occur from 1430 to 1625 cm-1. The interactions of the O-H deformation and the C-O stretching produces the bands from 116- to 1200 cm-1 and those around 1300 cm-1. The bands from 3500 to 3700 cm-1 are due to O-H stretching vibrations. Other bands are due to combinations and overtones of the strong low frequency C-Cl.











1511 Neave Street
Covington, KY 41011

p. 859-581-6990
f. 859-581-6821

info@asapanalytical.com
www.asapanalytical.com