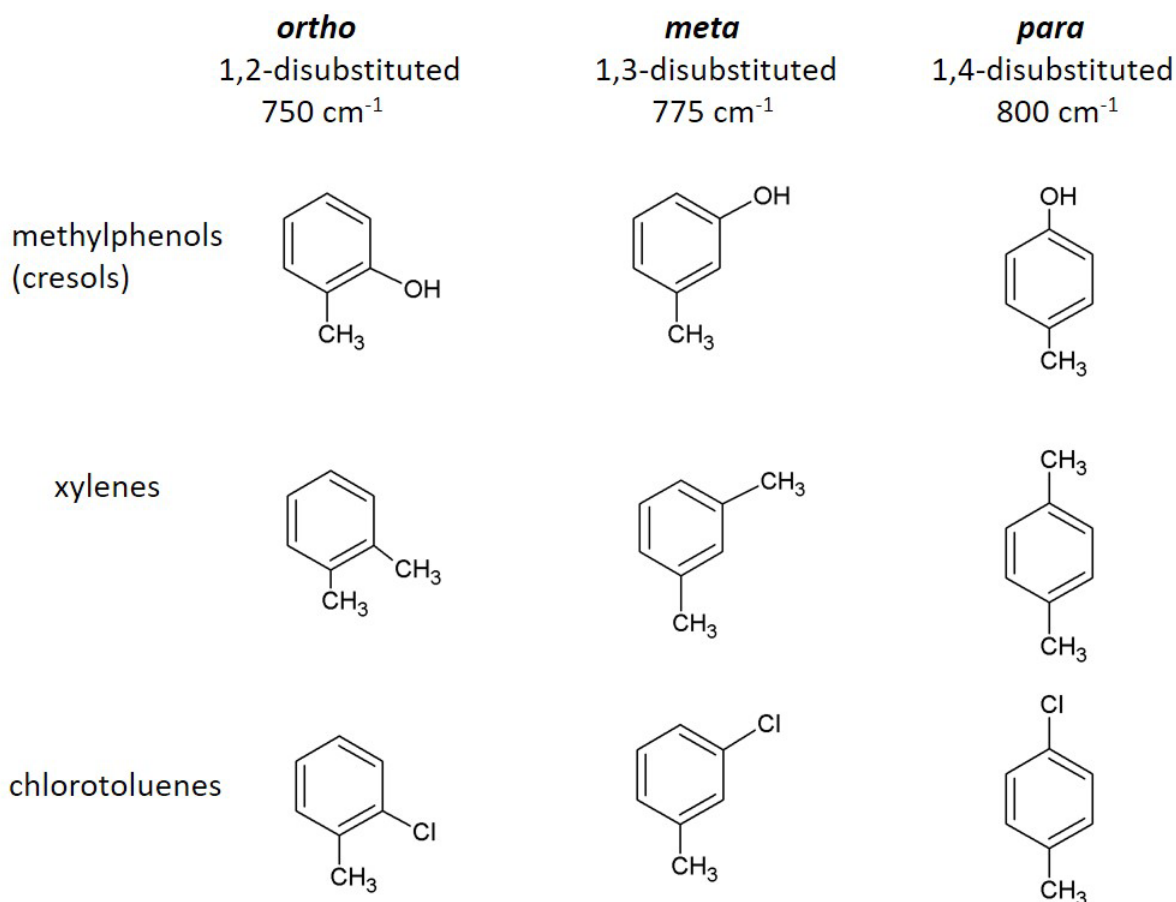
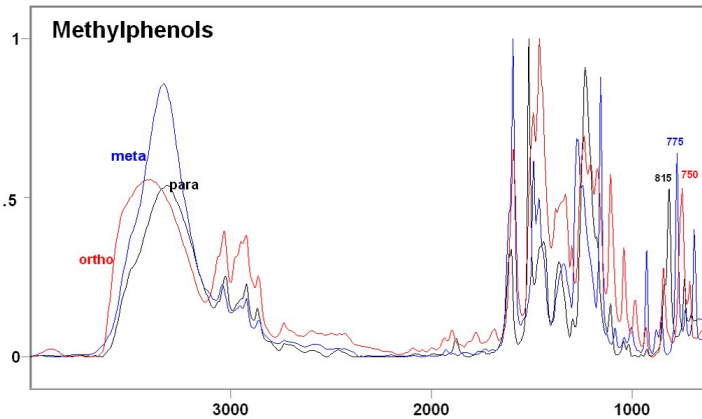
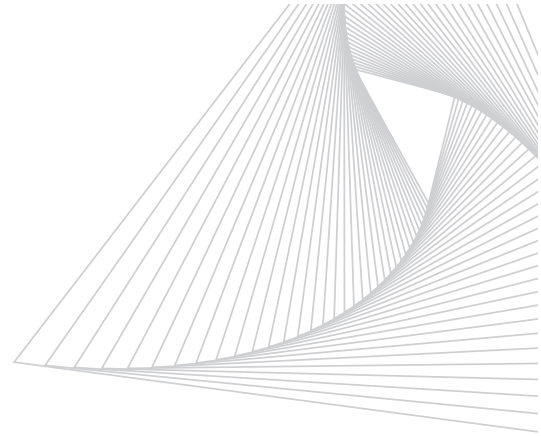
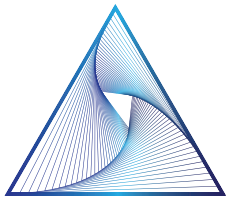


APPLICATION NOTE 024

Determining benzene ring substitution patterns from IR spectra

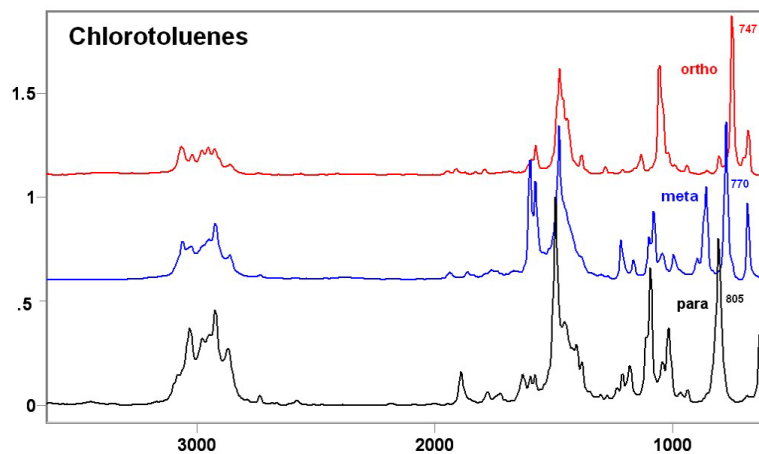
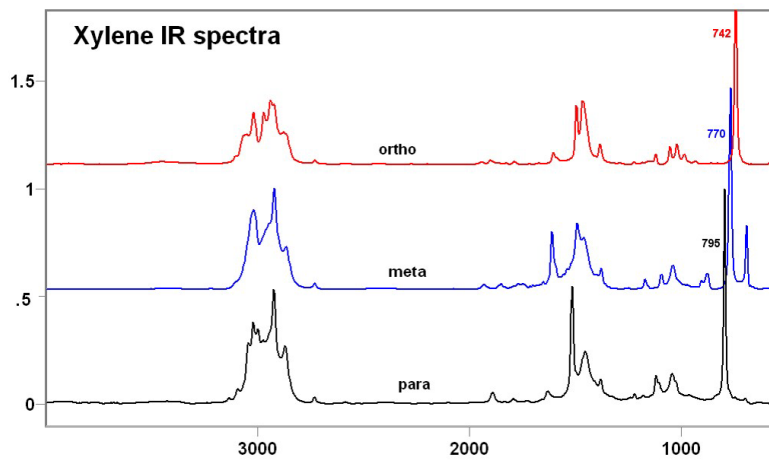
IR spectra provide valuable information about local configurations of atoms in molecules. This note demonstrates one specific case, how two sets of IR bands show the relative positions of the substituents on a disubstituted benzene ring. The three possible isomers are easy to differentiate by IR. Our examples are:

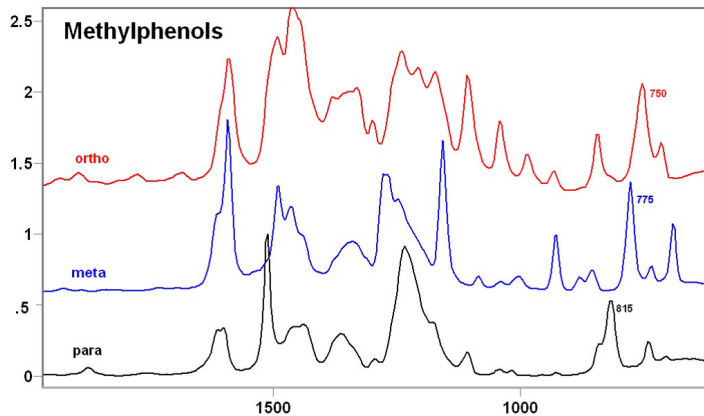
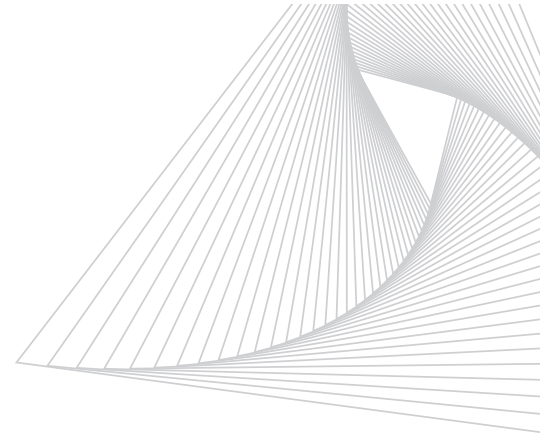
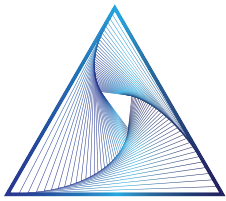




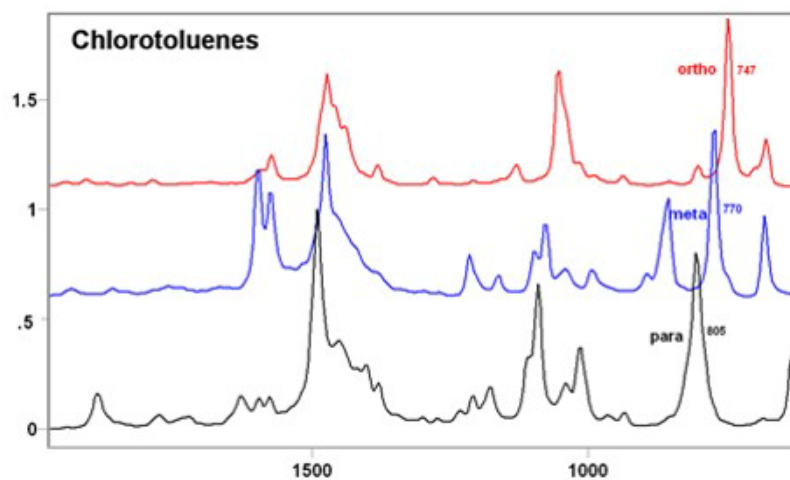
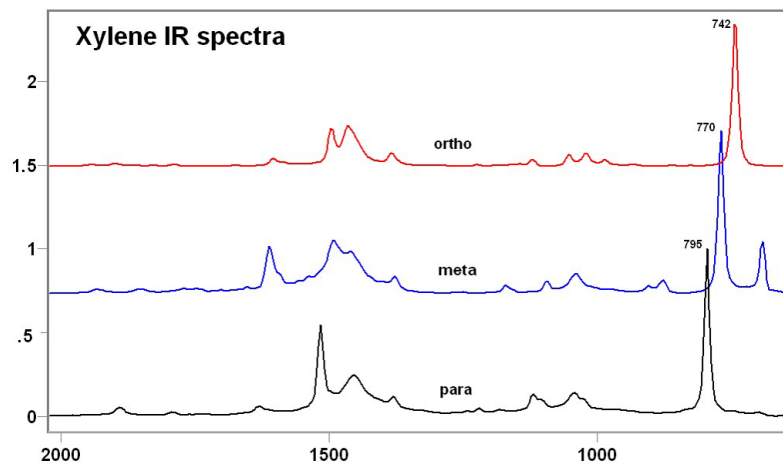
The full IR spectra are shown on this page, with an expanded view of the fingerprint region on the following page. Note the strong bands in the 740-830 cm^{-1} range, due to bending of the aromatic ring.

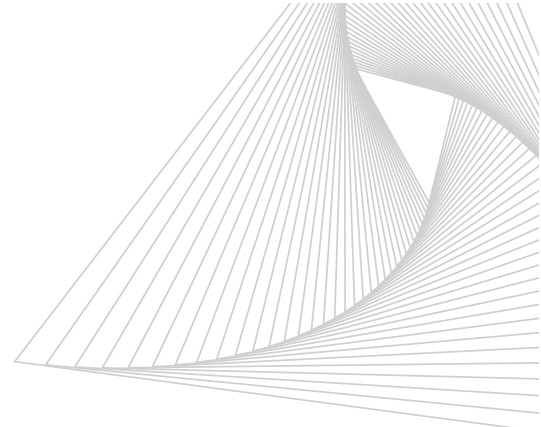
This band differentiates the isomers: ~ 750 for ortho, ~ 775 for meta, and ~ 800 for para.



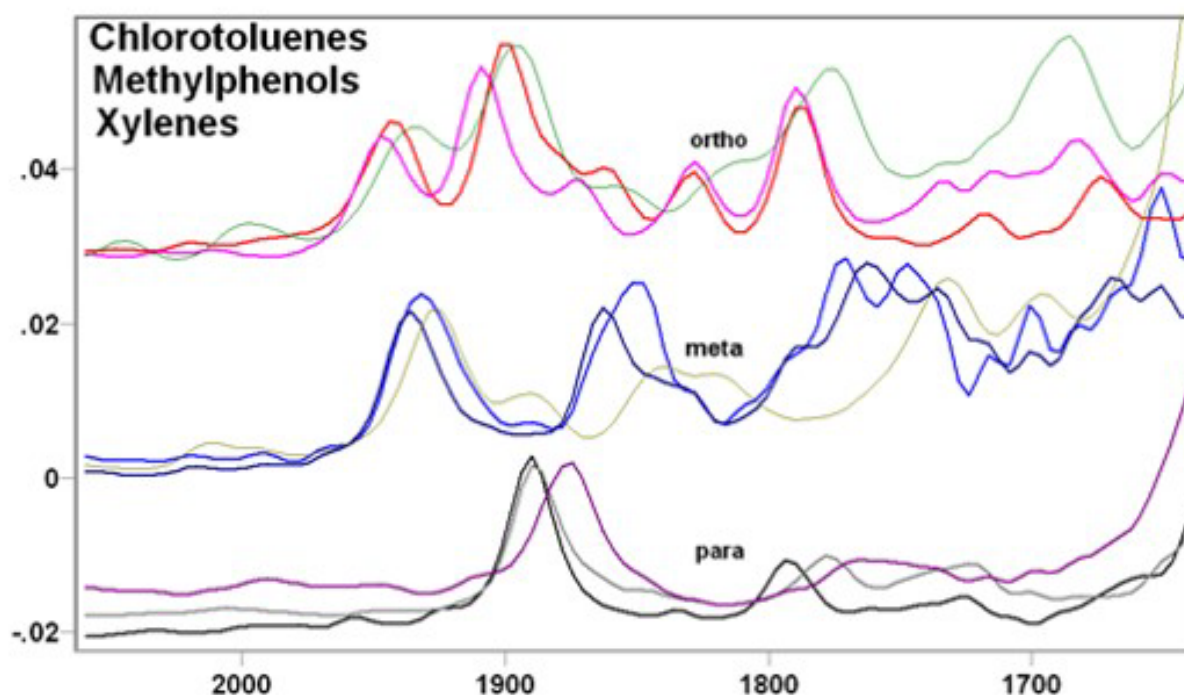


We show a more detailed view of the 740-830 region in these expanded spectra. Also note the weak overtone bands in the 1800-2000 cm⁻¹ range, which are expanded on the following page.





The spectral region between 1800 and 2000 cm^{-2} seldom contains any primary vibrational bands, so the weak combination-overtone bands which appear here, due to aromatic rings, can usually be seen without interference. The general shape of these overtones is distinctive and characteristic of the substitution pattern on the rings. From our example of the three sets of di-substituted benzenes, we overlay them by substitution pattern. These patterns can be used to determine or confirm the ortho, meta, or para configuration.



Concluding remarks

The IR spectrum provides specific information about the local bonding environment in a molecule, and many configurations have been correlated with specific IR bands. We have focused on only one example, that of the correlation of the 740-830 cm^{-1} band and the overtone region at 1800-2000 cm^{-1} to the configuration of di-substituted benzene rings to demonstrate the power of the IR spectrum.