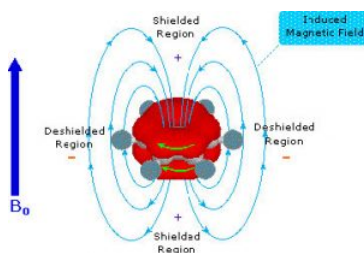
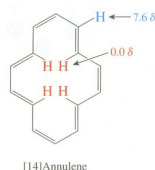


8.9: Spectroscopy of Aromatic Compounds-

As you might expect, both the ^{13}C and the ^1H NMR spectrum of benzene show only one peak (H-NMR 7.3 ppm and C-NMR 128 ppm) meaning that there is only one type of carbon and one type of hydrogen present in the molecule. However, these single peaks appear at lower field strengths relative to those found in alkenes or even conjugated alkenes (which normally appear between 5 and 6 ppm in the H-NMR). This low field absorption is caused by a phenomenon that occurs when the cyclic electron cloud in the ring is placed into an external magnetic field. The ring of electron density begins to cycle, producing a ring current and an induced magnetic field; the resulting intrinsic field reinforces the external field. The result is that the external field does not need to be very high to bring the carbon or hydrogen nuclei to resonance. In effect, the aromatic carbons and hydrogens are deshielded and appear at low field.



Interestingly, the induced field opposes the external field in the center of the ring, and, in fact, there are cyclic aromatic polyenes where (because of structural constraints) some of the hydrogens do point to the center of the ring. There is a marked difference between the inner and outer hydrogen resonances in these compounds because the hydrogens are in different areas of the induced magnetic field. This effect is called diamagnetic anisotropy.



The IR spectra of aromatic compounds typically show a $\text{C}-\text{H}$ stretch above $3,000\text{ cm}^{-1}$, and a $\text{C}-\text{C}$ bend around 1600 cm^{-1} , but these signals are often mixed in with others and, in general, IR is not very useful for identifying aromatic compounds. On the other hand, UV-VIS spectroscopy is often used to identify the aromatic chromophore. Benzene itself has a broad absorption around 254 nm and, as we will see, this absorption changes depending on the electron withdrawing and donating properties of groups on the ring itself.

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