1.11: Properties of Magnetic Nuclei of Interest to Organic Problems

Table 1-1 shows some of the magnetic properties of nuclei of particular interest to organic chemists. The comparison of relative sensitivities to detection of NMR signals for different nuclei is of particular importance. These sensitivities are computed for equal numbers of nuclei at a constant field strength, which normally is taken as high as practically possible within limitations of field homogeneity, stability, etc. The sensitivity figure given for deuterons must be corrected for their low natural abundance in order to have a measure of the relative ease of detecting deuterium NMR signals in material containing the natural proportions of the hydrogen isotopes. It is seen that protons and 19F are particularly favorable nuclei for observation. The precession frequencies of the nuclei are expressed in Table 1-1 in units of megacycles per 10,000 gauss and are seen to cover a very wide range of values. For high-resolution NMR spectroscopy, the rf oscillator must be extremely stable because oscillator stability is just as important to good resolution as is the homogeneity and stability of the magnetic field. As it is difficult to make a highly stable oscillator with a continuously variable frequency, customarily one uses separate fixed frequency units set at 3, 10, 20, 30, 40, and 60 Mc. The magnetic field is then adjusted to bring the nuclear precession frequencies to the appropriate oscillator frequency. In this way, one can cover a wide range of nuclei, keeping the magnetic field between 5,000 and 14,000 gauss. In general, the oscillator frequency is chosen which corresponds to the highest possible value of the field consistent with good homogeneity and stability because the sensitivity increases with field strength as does the separation between resonance lines corresponding to nuclei in different chemical environments.

Table 1-1. Magnetic properties of Representative Nuclei

Nucleus	Z	I	Mc/kgauss	% Natural abundance	Relative sensitivity*
1H	1	1/2	42.6	99.98	1.000
2H	1	1	6.5	0.016	0.0096
13C	6	1/2	10.7	1.11	0.016
14N	7	1	3.1	99.63	0.0010
15N	7	1/2	-4.3	0.37	0.0010
17O	8	5/2	-5.8	0.04	0.029
19F	9	1/2	40.1	100	0.834
31P	15	1/2	17.2	100	0.066

*For equal numbers of nuclei at constant field.

A more mathematical treatment of nuclear resonance absorption is presented in Appendix A for the purpose of elucidating the differences between the absorption and dispersion modes and the nature of certain probe adjustments which may influence the shapes of resonance signal curves.