

Electron Spin Resonance

1. Introduction

Electron spin resonance (ESR) spectroscopy has been used for over 50 years to study a variety of paramagnetic species. Here, we will focus on the spectra of organic and organotransition metal radicals and coordination complexes. Although ESR spectroscopy is supposed to be a mature field with a fully developed theory [1], there have been some surprises as organometallic problems have explored new domains in ESR parameter space. We will start with a synopsis of the fundamentals of ESR spectroscopy. For further details on the theory and practice of ESR spectroscopy, refer to one of the excellent texts on ESR spectroscopy [2-9].

The electron spin resonance spectrum of a free radical or coordination complex with one unpaired electron is the simplest of all forms of spectroscopy. The degeneracy of the electron spin states characterized by the quantum number, $m_S = \pm 1/2$, is lifted by the application of a magnetic field and transitions between the spin levels are induced by radiation of the appropriate frequency, as shown in Figure 1.1. If unpaired electrons in radicals were indistinguishable from free electrons, the only information content of an ESR spectrum would be the integrated intensity, proportional to the radical concentration. Fortunately, an un-paired electron interacts with its environment, and the details of ESR spectra depend on the nature of those interactions.

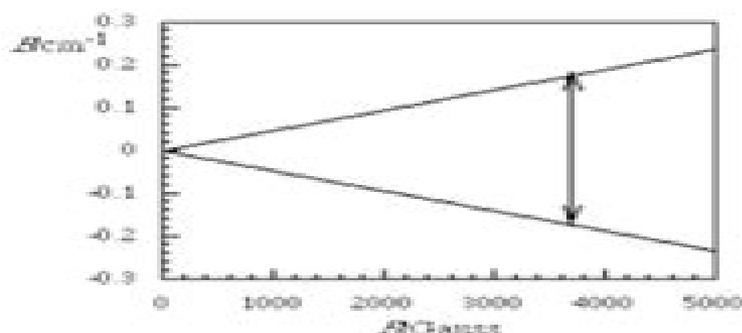


Figure 1.1. Energy levels of an electron placed in a magnetic field. The arrow shows the transitions induced by 0.315 cm^{-1} radiation.

There are two kinds of environmental interactions which are commonly important in the ESR spectrum of a free radical:

1. To the extent that the unpaired electron has unquenched orbital angular momentum, the total magnetic moment is different from the spin-only moment (either larger or smaller, depending on how the angular momentum vectors couple). It is customary to lump the orbital and spin angular

Electron Spin Resonance Of Metal Complex

Camilla Rothe



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