

Abraham R J & Bernstein H J. The analysis of nuclear magnetic resonance spectra. V. The analysis of deceptively simple spectra. *Can. J. Chem.* **39**:216-30, 1961. [Div. Pure Chemistry, Natl. Research Council, Ottawa, Canada]

**The analyses of some types of nuclear magnetic resonance (NMR) spectra are discussed and the conditions under which the observed spectra give less than the theoretical number of transitions are derived. Examples of such spectra are given. [The *SCI*<sup>®</sup> indicates that this paper has been cited over 300 times since 1961.]**

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"Students of NMR have been taught for the past two decades, and are still being taught, that the observation of two 1:2:1 triplets in the NMR spectrum of two pairs of chemically equivalent nuclei (e.g.,  $XCH_2-CH_2Y$ ) means that there is one *and only one* coupling between them. This is the truth but not the whole truth. Two well-separated groups of nuclei with only one coupling between them (i.e., the  $A_2X_2$  system) can only produce such a spectrum. The problem lies in the converse: this is not the only condition which will produce such a spectrum.

"The paper cited arose from precisely the failure of such an explanation for the NMR spectrum of furan.

"At the time, I was a postdoctoral fellow with Harold Bernstein at the National

Research Council, Canada, engaged in analysing the NMR spectra which were then being produced on one of the first commercial high-resolution NMR spectrometers.

"We became dubious about the furan interpretation when we found that the proton-proton couplings in substituted furans differed greatly from those so obtained for furan.<sup>1</sup> We then found that if we input the couplings obtained from the substituted compounds into the analysis for furan a spectrum essentially identical to that observed was calculated. This paper detailed the conditions under which these 'deceptively simple' spectra are produced, i.e., in which the spectrometer limitations of resolution and sensitivity are such as to fail to differentiate between a number of possible solutions. These conditions were given for a number of simple spin systems capable of explicit solutions. Our interpretation for furan was confirmed by the better resolved spectra obtained by later workers.<sup>2</sup> However, the confusion caused by such deceptively simple spectra has been so widespread that this paper has been widely quoted. Later, much more refined examples have shown that even rigorous computer analysis of an NMR spectrum need not necessarily produce an unambiguous answer.<sup>3</sup>

"Basically, the spectrum contains less information than that required to solve for the unknown parameters (the chemical shifts and coupling constants). After all, the solution of  $N$  equations in  $N + 1$  unknowns has never been easy to solve!

"This problem was subsequently covered fully in a text devoted to the analysis of NMR spectra."<sup>4</sup>

1. Abraham R J & Bernstein H J. The proton resonance spectra of some substituted furans and pyrroles. *Can. J. Chem.* **39**:905-14, 1961.
2. Grant D M, Hint R C & Gutowitzky H S. Analysis of  $A_2B_2$  high-resolution NMR spectra. I. Furan, thiophene, and disubstituted benzenes. *J. Chem. Phys.* **38**:470-5, 1963.
3. Abraham R J & Castellano S. Uncertainties in the analysis of n.m.r. spectra. *J. Chem. Soc. B* **1**:49-53, 1970.  
Abraham R J. *The analysis of high resolution NMR spectra*. Amsterdam: Elsevier, 1971. 324 p.