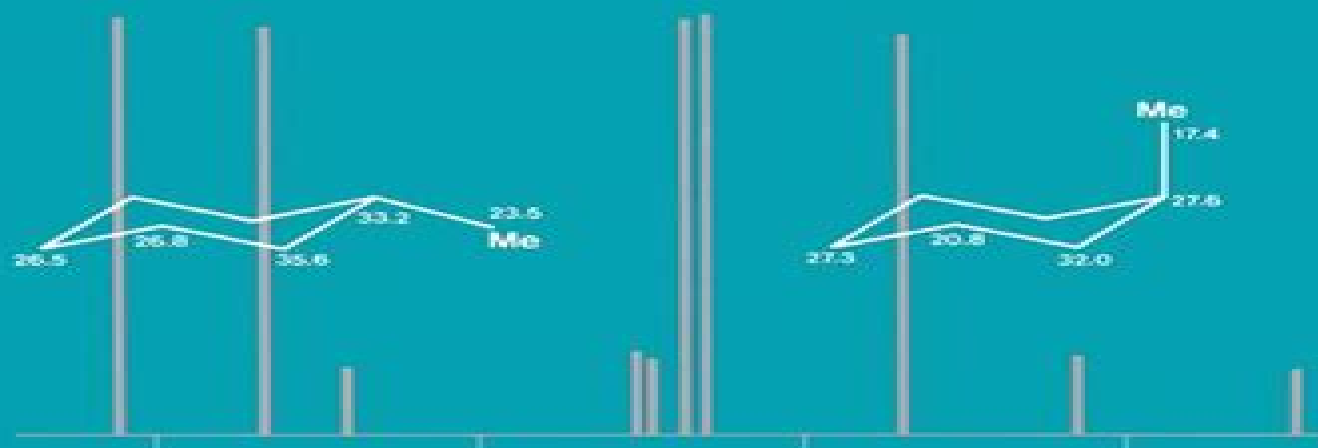


# Stereochemical Analysis of Alicyclic Compounds by C-13 NMR Spectroscopy

James K. Whitesell and  
Mark A. Minton



# Stereochemical Analysis Of Alicyclic Compounds By C 13 Nmr Spectroscopy

**Marcel A. Müller**



## **Stereochemical Analysis Of Alicyclic Compounds By C 13 Nmr Spectroscopy:**

**Stereochemical Analysis of Alicyclic Compounds by C-13 NMR Spectroscopy** J. A. Whitesell, 2012-12-06 Through numerous conversations with other synthetic chemists it became apparent that the great power of carbon nuclear magnetic resonance was being significantly underutilized In our own work we have found that <sup>13</sup>C spectroscopy is a more powerful tool than <sup>1</sup>H NMR spectroscopy especially for probing subtle stereochemical questions in complicated systems This is especially true in five membered ring compounds where <sup>1</sup>H NMR is at a particular disadvantage The two techniques can be used independently to solve the same question that of stereochemistry but they do so in different ways Advantage can be taken in <sup>1</sup>H NMR of a relatively consistent relationship between stereochemical orientation and coupling constants between vicinal protons while in <sup>13</sup>C NMR it is the correlation between spatial relationships of non hydrogen y substituents and their effect on chemical shift that can be used to assign stereochemistry It was also clear that the use of <sup>13</sup>C NMR required a different approach to problem solving than that typically used with <sup>1</sup>H NMR While the latter technique could be employed with a very general approach e g the Karplus equation <sup>13</sup>C NMR would at least for the immediate future require a relatively extensive set of model systems from which the consequences of stereochemical changes could be derived for any given carbon framework

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Through numerous conversations with other synthetic chemists it became apparent that the great power of carbon nuclear magnetic resonance was being significantly underutilized In our own work we have found that <sup>13</sup>C spectroscopy is a more powerful tool than <sup>1</sup>H NMR spectroscopy especially for probing subtle stereochemical questions in complicated systems This is especially true in five membered ring compounds where <sup>1</sup>H NMR is at a particular disadvantage The two techniques can be used independently to solve the same question that of stereochemistry but they do so in different ways Advantage can be taken in <sup>1</sup>H NMR of a relatively consistent relationship between stereochemical orientation and coupling constants between vicinal protons while in <sup>13</sup>C NMR it is the correlation between spatial relationships of non hydrogen y substituents and their effect on chemical shift that can be used to assign stereochemistry It was also clear that the use of <sup>13</sup>C NMR required a different approach to problem solving than that typically used with <sup>1</sup>H NMR While the latter technique could be employed with a very general approach e g the Karplus equation <sup>13</sup>C NMR would at least for the immediate future require a relatively extensive set of model systems from which the consequences of stereochemical changes could be derived for any given carbon framework

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Carbon-13 NMR Chemical Shifts in Structural and Stereochemical Analysis Kalevi Pihlaja, Erich Kleinpeter, 1994 A review of recent research on strategies and applications of the C 13 chemical shift a method for determining configuration of organic compounds Introduces C 13 NMR spectroscopy and describes conditions for collecting the FID for data handling and for obtaining a well resolved C 13 NMR spectrum as well as various substituent effect correlations their derivations and the origin of the effects Also discusses the use of multidimensional NMR methods For organic physical and natural products chemists Includes bandw diagrams Annotation copyright by Book News Inc Portland OR

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Tables of Spectral Data for Structure Determination of Organic Compounds Ernő Pretsch, Thomas Clerc, Joseph Seibl, Wilhelm Simon, 2013-03-09 Although numerical data are in principle universal the compilations presented in this book are extensively annotated and interleaved with text This translation of the second German edition has been prepared to facilitate the use of this work with all its valuable detail by the large community of English speaking scientists Translation has also provided an opportunity to correct and revise the text and to update the nomenclature Fortunately spectroscopic data and their relationship with structure do not change much with time so one can predict that this book will for a long period of time continue to be very useful to organic chemists involved in the identification of organic compounds or the elucidation of their structure Klaus Biemann Cambridge MA April 1983 Preface to the First German Edition Making use of the information provided by various spectroscopic techniques has become a matter of routine for the analytically oriented organic chemist Those who have graduated recently received extensive training in these techniques as part of the curriculum while their older colleagues learned to use these methods by necessity One can therefore assume that chemists are well versed in the proper choice of the methods suitable for the solution of a particular problem and to translate the experimental

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laboratory manual for organic chemistry students contains procedures for both miniscale also known as small scale and microscale users This lab manual gives students all the necessary background to enter the laboratory with the knowledge to perform the experiments with confidence For the microscale labs experiments were chosen to provide tangible quantities of material which can then be analyzed Chapters 1 2 introduce students to the equipment record keeping and safety of the laboratory Chapters 3 6 and 8 are designed to introduce students to laboratory techniques needed to perform all experiments In Chapters 7 and 9 through 20 students are required to use the techniques to synthesize compounds and analyze their properties In Chapter 21 students are introduced to multi step syntheses of organic compounds a practice well known in chemical industry In Chapter 23 students are asked to solve structures of unknown compounds The new chapter 24 introduces a meaningful experiment into the textbook that reflects the increasing emphasis on bioorganic chemistry in the sophomore level organic lecture course This experiment not only gives students the opportunity to accomplish a mechanistically interesting and synthetically important coupling of two amino acids to produce a dipeptide but also provides valuable experience regarding the role of protecting groups in effecting synthetic transformations with multiple functionalized molecules

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