

A passing spaceship NMR challenge

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We would like to invite you to participate in the Analytical Challenge, a series of puzzles to entertain and challenge our readers. This special feature of “Analytical and Bioanalytical Chemistry” has established itself as a truly unique quiz series, with a new scientific puzzle published every three months. Readers can access the complete collection of published problems with their solutions on the ABC homepage at <http://www.springer.com/abc>. Test your knowledge and tease your wits in diverse areas of analytical and bioanalytical chemistry by viewing this collection.

In the present challenge, NMR spectroscopy is the topic. And please note that there is a prize to be won (a Springer book of your choice up to a value of €100, given to one winner selected randomly). Please read on...

Meet the challenge

According to Douglas Adams’s *The Hitchhiker’s Guide to the Galaxy*, a person will die while hurdling through space approximately after 30 s, unless a passing spaceship happens to intercept him. But the chance of this happening is only 1 in $2^{276,709}$. Against these odds, though, Arthur Dent and Ford Prefect were both saved by the *Heart of Gold*, a spaceship that uses an infinite improbability drive by manipulating the laws of improbability [1]. Coincidentally, 227–6709 was also a telephone number of a flat in Islington where Arthur once went to a party [1].

This is a very explicit type of coincidence, a serendipity, and such coincidences can be found throughout the history of invention and scientific discoveries. Well-known examples of this are the discovery of guncotton by the German-Swiss chemist Christian Friedrich Schönbein in 1845, the

laminated safety-glass by the French chemist Edouard Benedictus in 1903, the penicillin by Sir Alexander Fleming in 1928, and the microwave oven by the American scientist Percy Spencer in 1945.

The challenge

Even spectroscopy has coincidences. Unfortunately, they are not always good news. Although we know the influencing factors for spectroscopic processes, we cannot always fully control them and the resulting spectra can be more or less unpredictable and random. A typical example of this is the chemical shift of the signals in NMR spectra. Nuclei in different chemical environments induce NMR signals with different chemical shifts. However, this *Analytical Challenge* explores situations where chemically non-equivalent nuclei (or groups of nuclei) give NMR signals with same chemical shift, always. Now, the challenge is to propose a name for this phenomenon of identical chemical shifts from non-equivalent nuclei.

Two examples are given, both from daily routine work and none being created artificially. In Fig. 1, the ¹H-NMR spectrum of 3-ethyl-3-(chloromethyl)-oxetane is shown. The proton signals of the ethyl group (at 0.9 ppm and 1.85 ppm) and of the chloromethyl group (at 3.79 ppm) can be easily identified. But only a single peak is observed at 4.42 ppm for the four non-equivalent ring methylene protons. Why?

In the ¹H-NMR spectrum of the 3-methylpentan-3-ol (Fig. 2), only three signals are visible. Both ethyl groups are enantiotopic and not distinguishable by NMR spectroscopy in an achiral medium. This explains a single triplet at 0.88 ppm for both methyl groups. And how can we explain the strange multiplet at 1.47 ppm from five hydrogen atoms?

However unlikely are such coincidences in ¹H-NMR spectroscopy, their probability is still not as low as encountering

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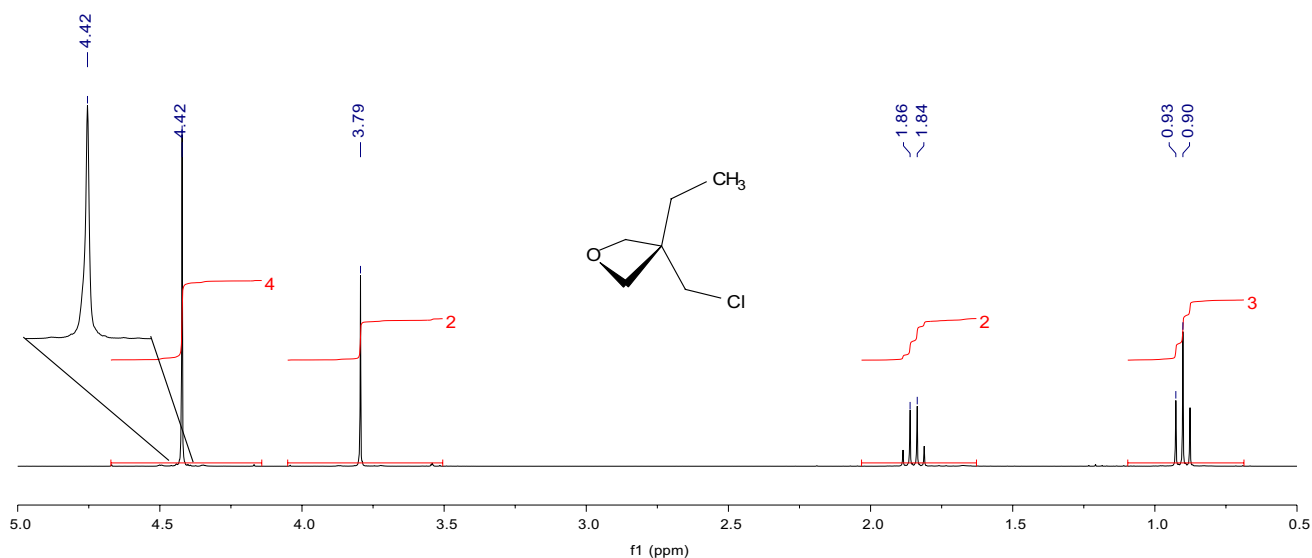


Fig. 1 500 MHz ^1H -NMR spectrum of 3-ethyl-3-(chloromethyl)-oxetane, measured in CDCl_3 . Only the region from 0.5 to 5.0 ppm, with all signals from this substance, is shown

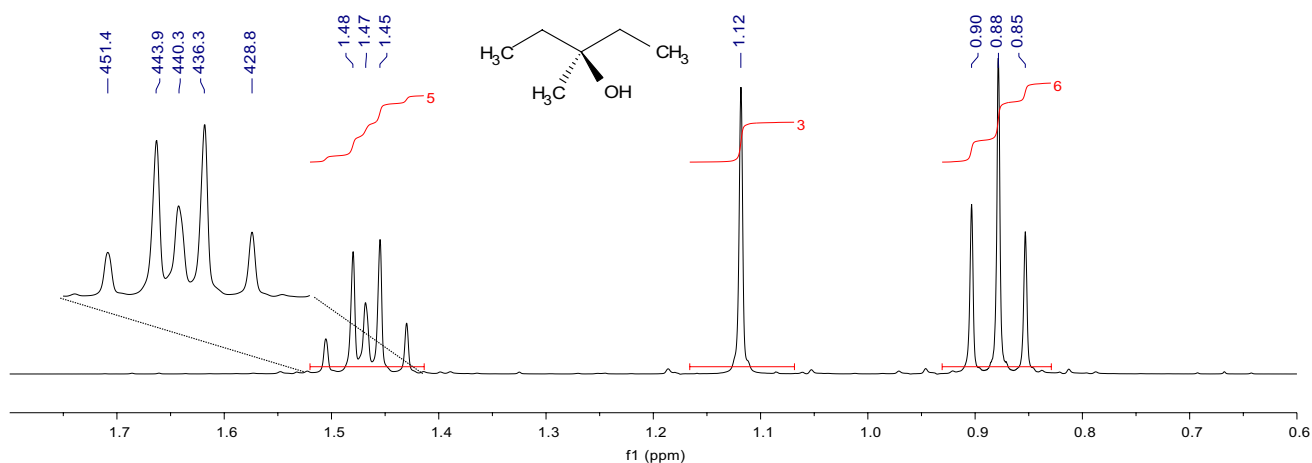


Fig. 2 300 MHz ^1H -NMR spectrum of 3-methylpentan-3-ol, measured in CDCl_3 . Only the region from 0.6 to 1.8 ppm, with all signals from this substance, is shown

a passing spaceship in space. *What is the correct name for this phenomenon in spectroscopy?*

Declarations

Conflict of interest The author declares no competing interests.

Reference

- Adams D (1979) *The Hitchhiker's guide to the galaxy*, Pan Books, UK, ISBN 0-330-25864-8

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We invite our readers to participate in the Analytical Challenge by solving the puzzle above. Please send the correct solution to abc@springer.com by July 1, 2024. Make sure you enter "A passing spaceship NMR challenge" in the subject line of your e-mail. The winner will be notified by e-mail and their name will be published on the "Analytical and Bioanalytical Chemistry" homepage at <http://www.springer.com/abc> and in the journal (volume 416/issue 24) where readers will find the solution and a short explanation.

The next Analytical Challenge will be published in 416/16, July 2024. If you have enjoyed solving this Analytical Challenge you are invited to try the previous puzzles on the ABC homepage.