

Symmetrical molecule NMR challenge

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Accepted: 12 October 2022 / Published online: 4 January 2023
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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, symmetrical molecules 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

Structure elucidation of symmetrical molecules can often be accomplished using NMR with few such examples given in Fig. 1.

While symmetry dramatically simplifies the ¹H-NMR spectra of many molecules, it also introduces features that might not be trivial to inexperienced spectroscopists. As

an example, ¹H-NMR spectra of both *E* and *Z* isomers of symmetrical alkenes (Fig. 1) display a single signal corresponding to both *sp*² protons; however, its coupling pattern depends only on the substituent group R, and not on the coupling between the *sp*² protons. In addition, one cannot employ NOESY experiments to distinguish between the *E* and *Z* isomers because both *sp*² protons are chemically equivalent. Hence, one must resort to other approaches to interpret the NMR data.

The challenge

Figure 2 shows a ¹H-NMR spectrum of a mixture of *E* and *Z* isomers of an aliphatic amine hydrochloride whose structures are also shown in Fig. 2. The NMR spectrum was obtained using a routine 600-MHz NMR in DMSO-*d*₆ solvent.

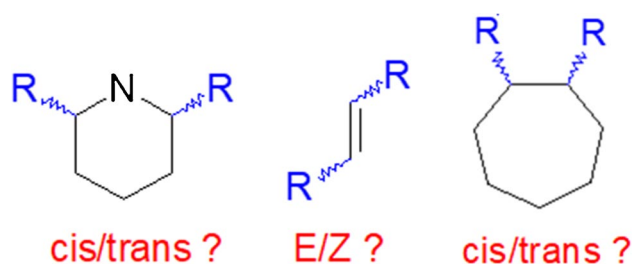


Fig. 1 Examples of symmetrical molecules whose structure can be elucidated using NMR

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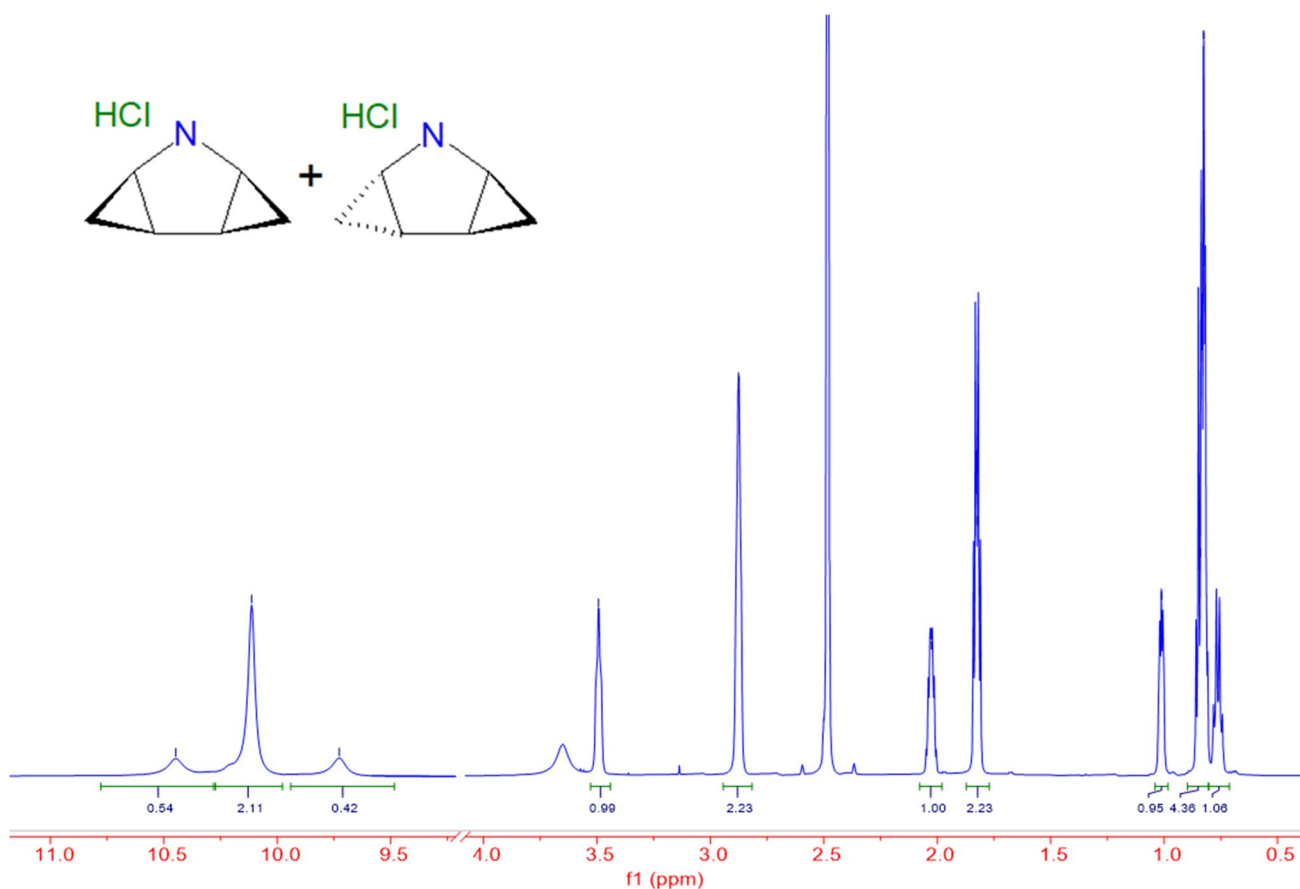


Fig. 2 ^1H -NMR spectrum (600 MHz in $\text{DMSO-}d_6$) for a mixture of *E* and *Z* isomers of an aliphatic amine hydrochloride

Can you determine the approximate composition of this mixture (for example, $E/Z = 1:1$, $10:1$)? Explain your reasoning.

Declarations

Conflict of interest The author declares no competing interests.

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 April 1, 2023. Make sure you enter “Symmetrical molecule 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 415/issue 16) where readers will find the solution and a short explanation.

The next Analytical Challenge will be published in 415/09, April 2023. If you have enjoyed solving this Analytical Challenge you are invited to try the previous puzzles on the ABC homepage.

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