Solution to Phosphine NMR challenge

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The winner of the Phosphine NMR challenge (published in volume 412 issue 25) is:

Andreu Tortajada Navarro, Catalan Institute of Chemical Research, Tarragona, Spain

The award entitles the winner to select a Springer book of his choice up to a value of €100,-.

Our Congratulations!

This Analytical Challenge [1] invites you to explore the effects of isotopic substitution on the NMR spectra for PH_3 and PD_3 . For PH_3 , containing three equivalent ^1H atoms with nuclear spin $I = 1/2$, a binomial quartet with intensity ratios of 1:3:3:1 is observed in the ^{31}P NMR spectrum (Fig. 1).

For PD_3 , containing three equivalent ^2H atoms with nuclear spin $I = 1$, a more complex non-binomial septet with intensity

ratios of 1:3:6:7:6:3:1 is observed in the ^{31}P NMR spectrum (Fig. 2).

For a given pair of elements, the scalar coupling constant is proportional to the product of the gyromagnetic ratios of the nuclei provided all other factors remain the same. Given that the $^1J_{\text{P-H}}$ coupling constant in PH_3 is $^1J_{\text{P-H}} = 187.8 \text{ Hz}$, the $^1J_{\text{P-D}}$ coupling constant in PD_3 can be obtained. The gyromagnetic ratio of ^1H is $\gamma(^1\text{H}) = 26.75 \times 10^7 \text{ rad T}^{-1} \text{ s}^{-1}$ and for ^2H is $\gamma(^2\text{H}) = 4.107 \times 10^7 \text{ rad T}^{-1} \text{ s}^{-1}$, thus giving a ratio $\gamma(^1\text{H})/\gamma(^2\text{H}) = 6.5$. Dividing the $^1J_{\text{P-H}}$ coupling constant in PH_3 by this ratio gives a predicted $^1J_{\text{P-D}}$ coupling constant of $^1J_{\text{P-D}} = 28.8 \text{ Hz}$ for PD_3 which compares well with the experimentally measured value of 29.3 Hz [2].

This article is the solution to the Analytical Challenge to be found at
<https://doi.org/10.1007/s00216-020-02880-6>

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Fig. 1 ^{31}P NMR spectrum of PH_3 , showing a quartet whose intensities can be viewed as binomial coefficients of $(1+x)^3$ expansion: $1x^0 + 3x^1 + 3x^2 + 1x^3$

Fig. 2 ^{31}P NMR spectrum of PD_3 , showing a septet whose intensities can be viewed as trinomial coefficients of $(1+x+x^2)^3$ expansion: $1x^0 + 3x^1 + 6x^2 + 7x^3 + 6x^4 + 3x^5 + 1x^6$

Declarations

Conflict of interest The author declares no competing interests.

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