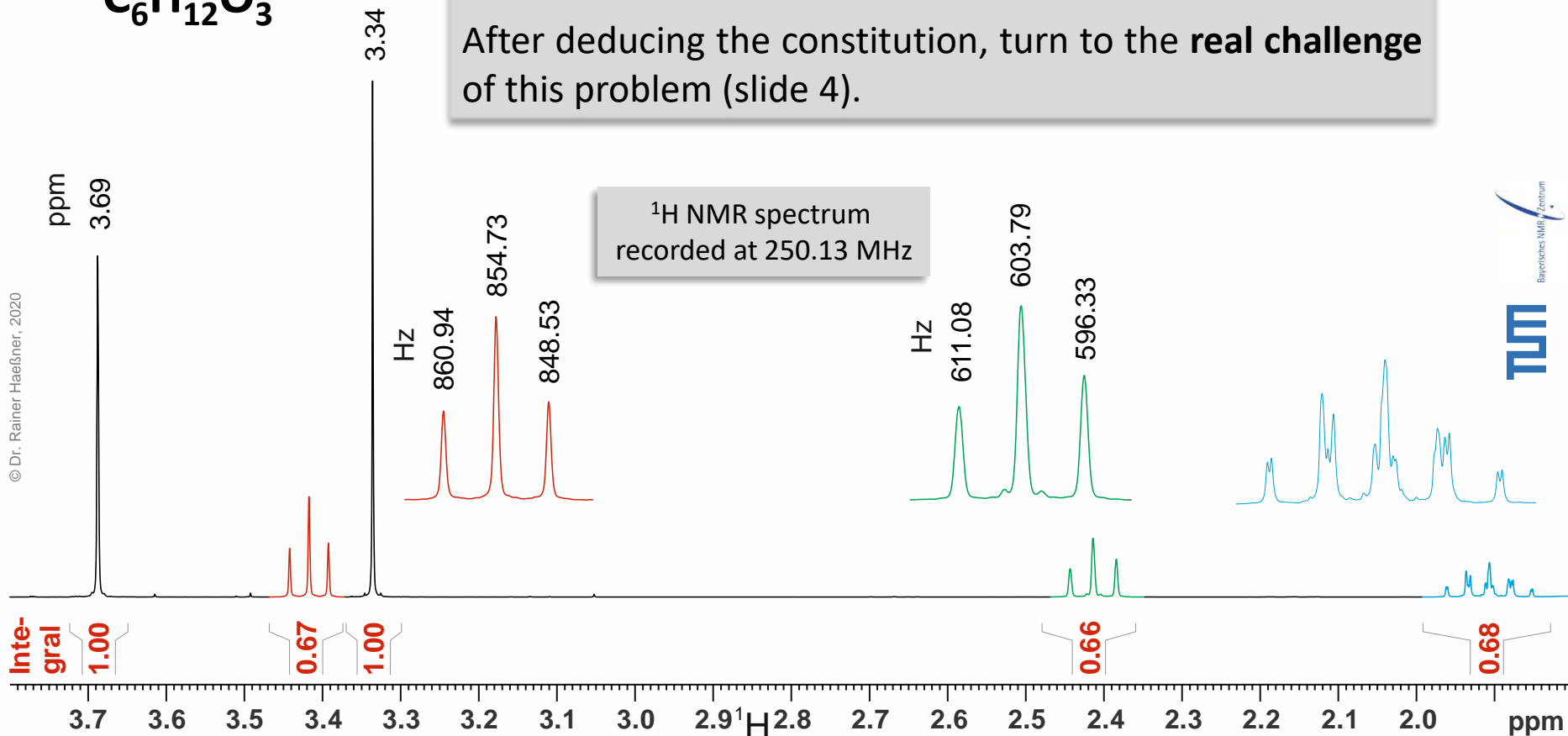
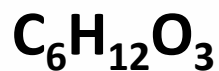


# Problem of the Month: February 2021

Deduce the constitution, assign all nuclei and work out two proton-proton coupling constants.

After deducing the constitution, turn to the **real challenge** of this problem (slide 4).



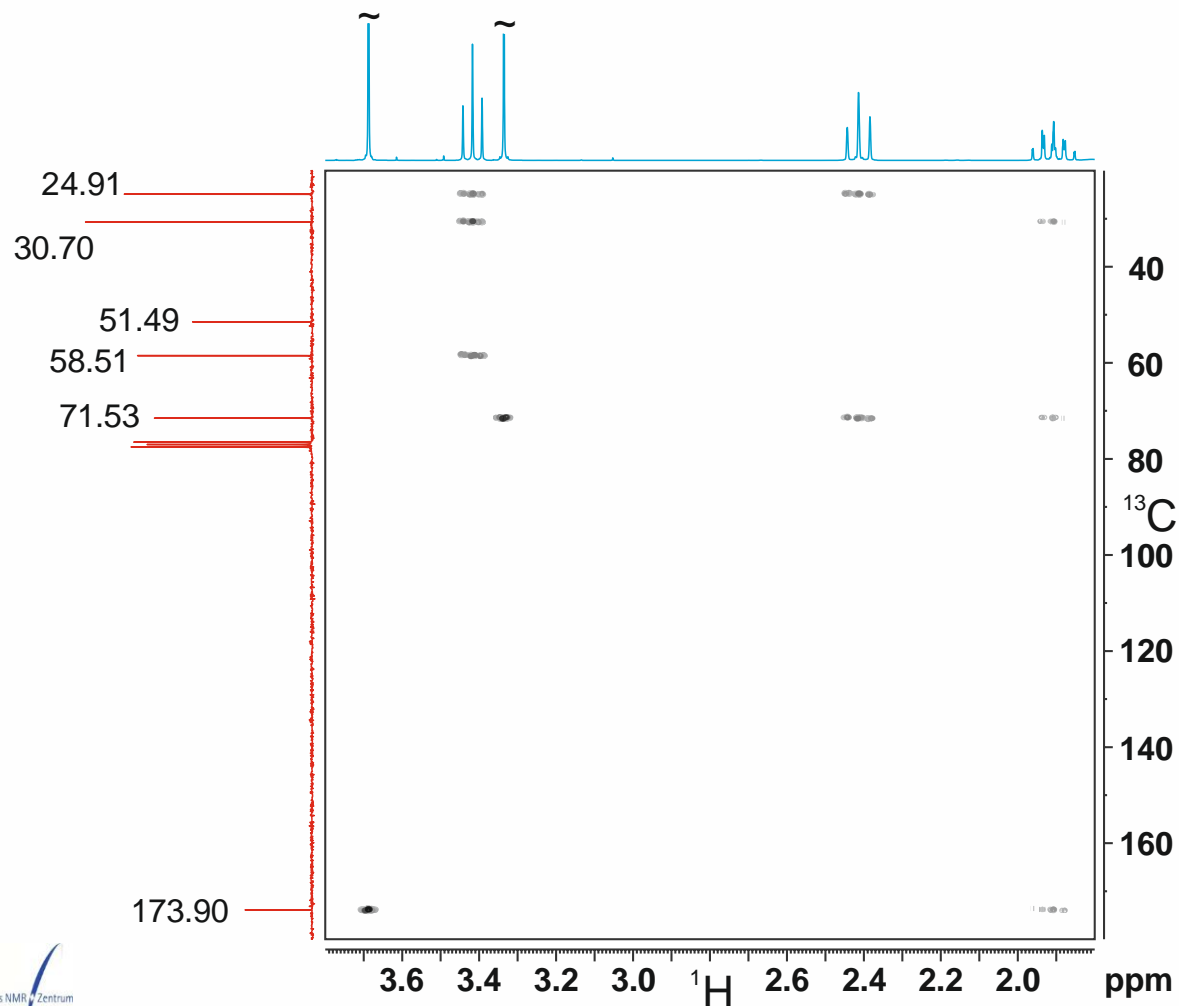
# Problem of the Month:

## February 2021

$^1\text{H}/^{13}\text{C}$ -HMBC  
recorded at 250.13/62.90 MHz

The  $f_1$  projection contains  
all six carbon signals of  
the compound.

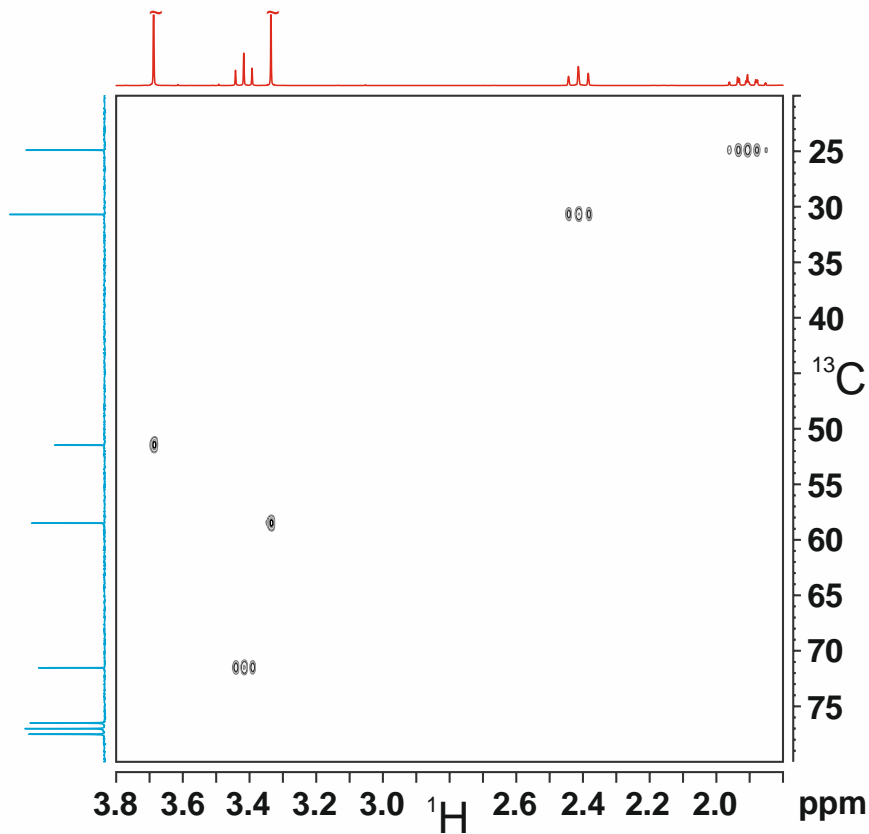
There is no separate one  
dimensional carbon  
spectrum given.



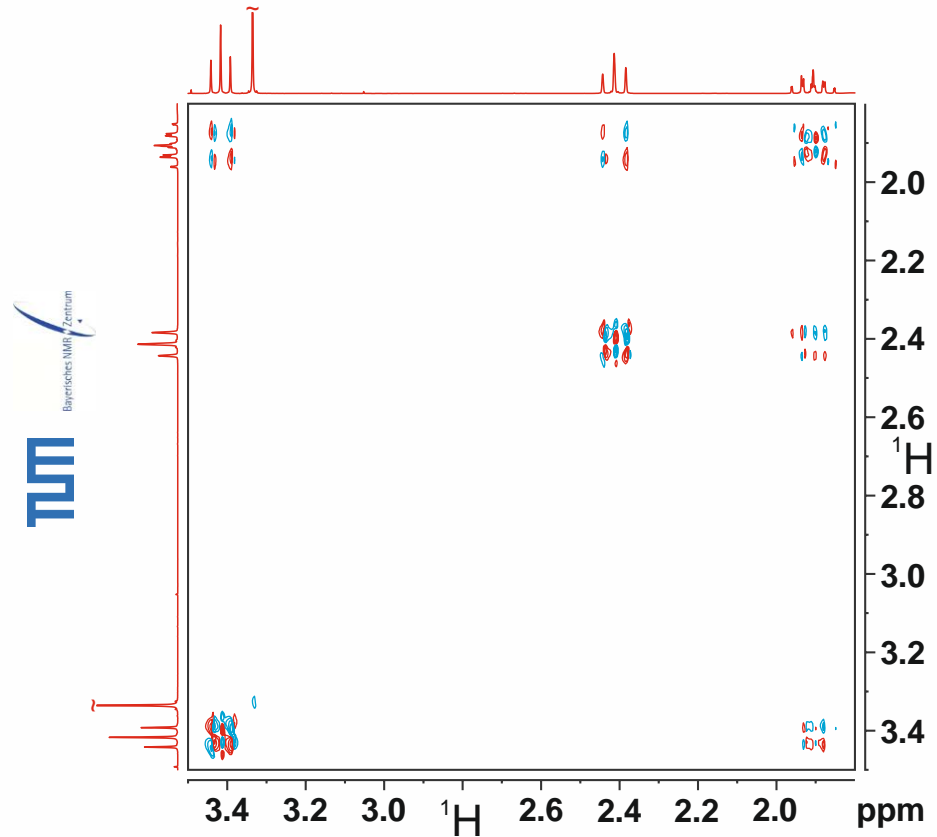
# Problem of the Month:

## February 2021

$^1\text{H}/^{13}\text{C}$ -HSQC  
recorded at 250.13/62.90 MHz



$^1\text{H}/^1\text{H}$ -DQF-COSY  
recorded at 250.13 MHz



# Problem of the Month:

February 2021

## And now the challenge

With three chemical shifts and two coupling constants, [you can simulate](#) the three multiplets in the proton spectrum.

The simulation for the multiplet at about 3.4 ppm will provide an almost perfect result, but in the case of the other two multiplets there are small but significant deviations: The multiplet at about 1.9 ppm looks a bit more complex than expected, although there exists a clear base structure. But the multiplet at about 2.4 ppm should be a pure triplet.

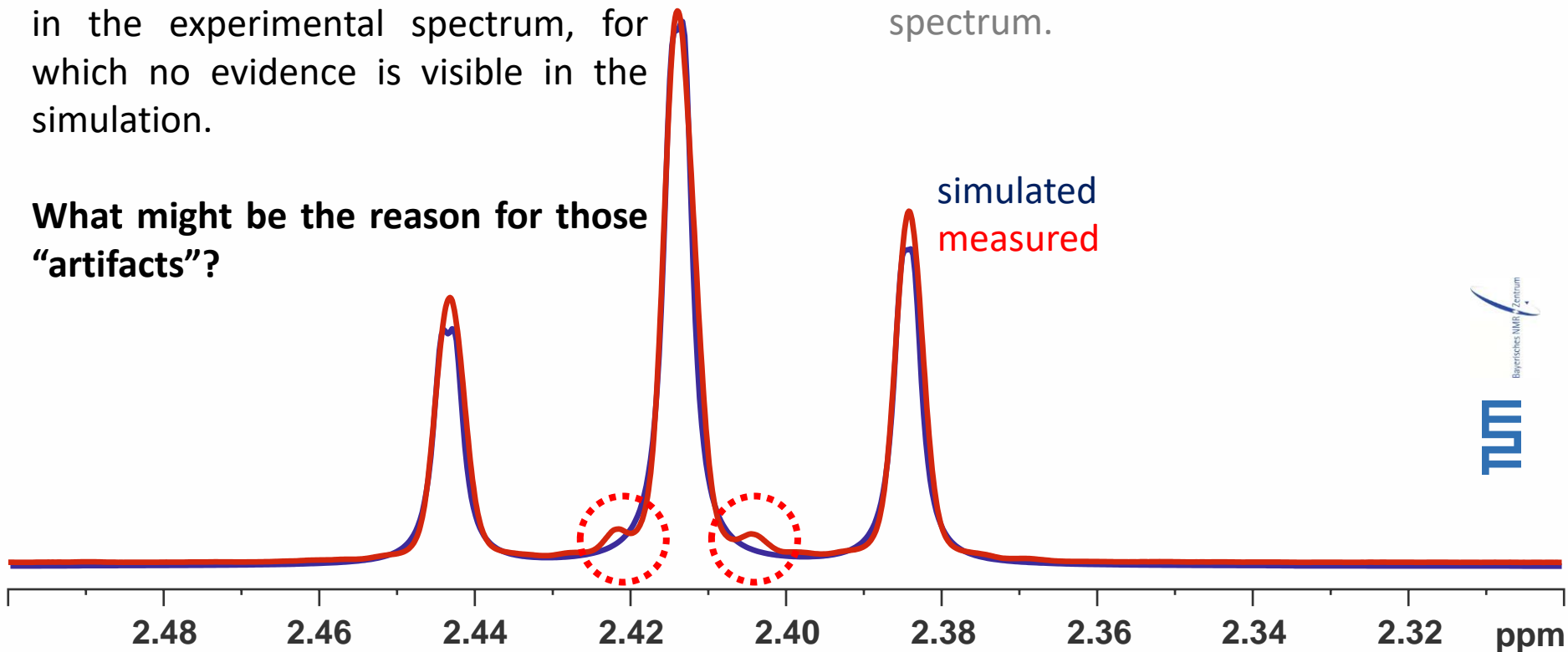
Because of the small difference in chemical shift between the multiplets at 1.9 ppm and 2.4 ppm, fine splitting is visible in the simulation for which the experimental resolution is insufficient.

But the real issue are the two "warts" in the experimental spectrum, for which no evidence is visible in the simulation.

**What might be the reason for those "artifacts"?**

**Hint:**

To answer this extremely difficult question, trawl through the literature for the proton spectrum of 1-bromo-2-chloroethane, marvel a little bit about what you find, and try to understand the theoretical explanation of this spectrum.



# Contributions

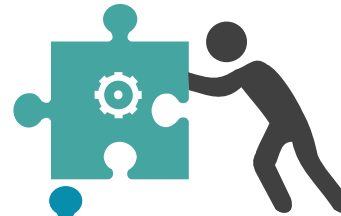
Spectrometer time

TU Munich



Measurements

Rainer Haeßner



Discussions and  
native English  
language support



Alan M. Kenwright  
Nils Schlörer

Compilation



Rainer Haeßner