

Parahydrogen-induced polarization enables chemical reaction monitoring at zero magnetic field

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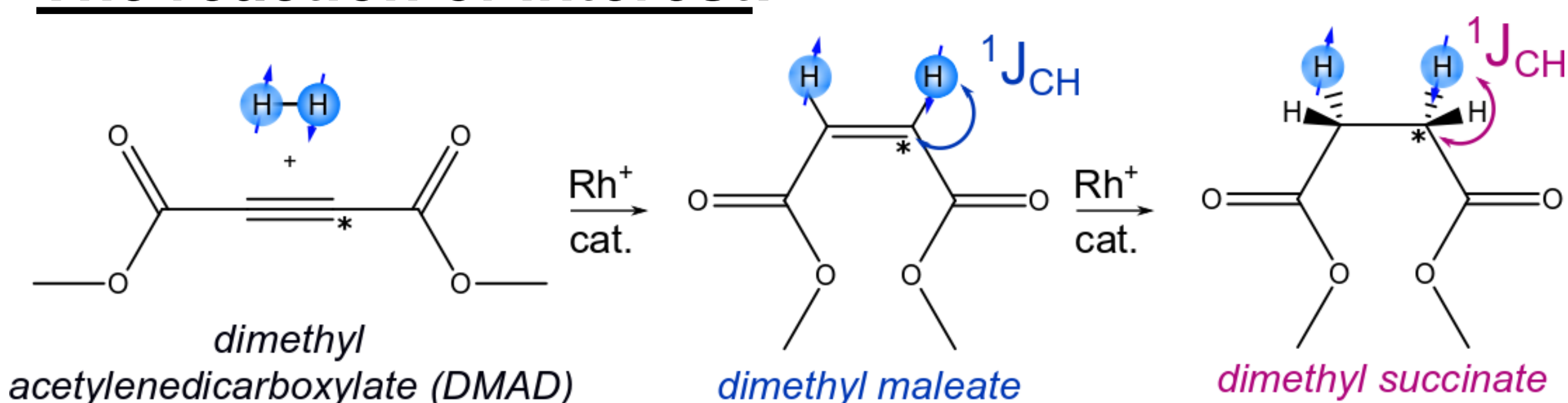
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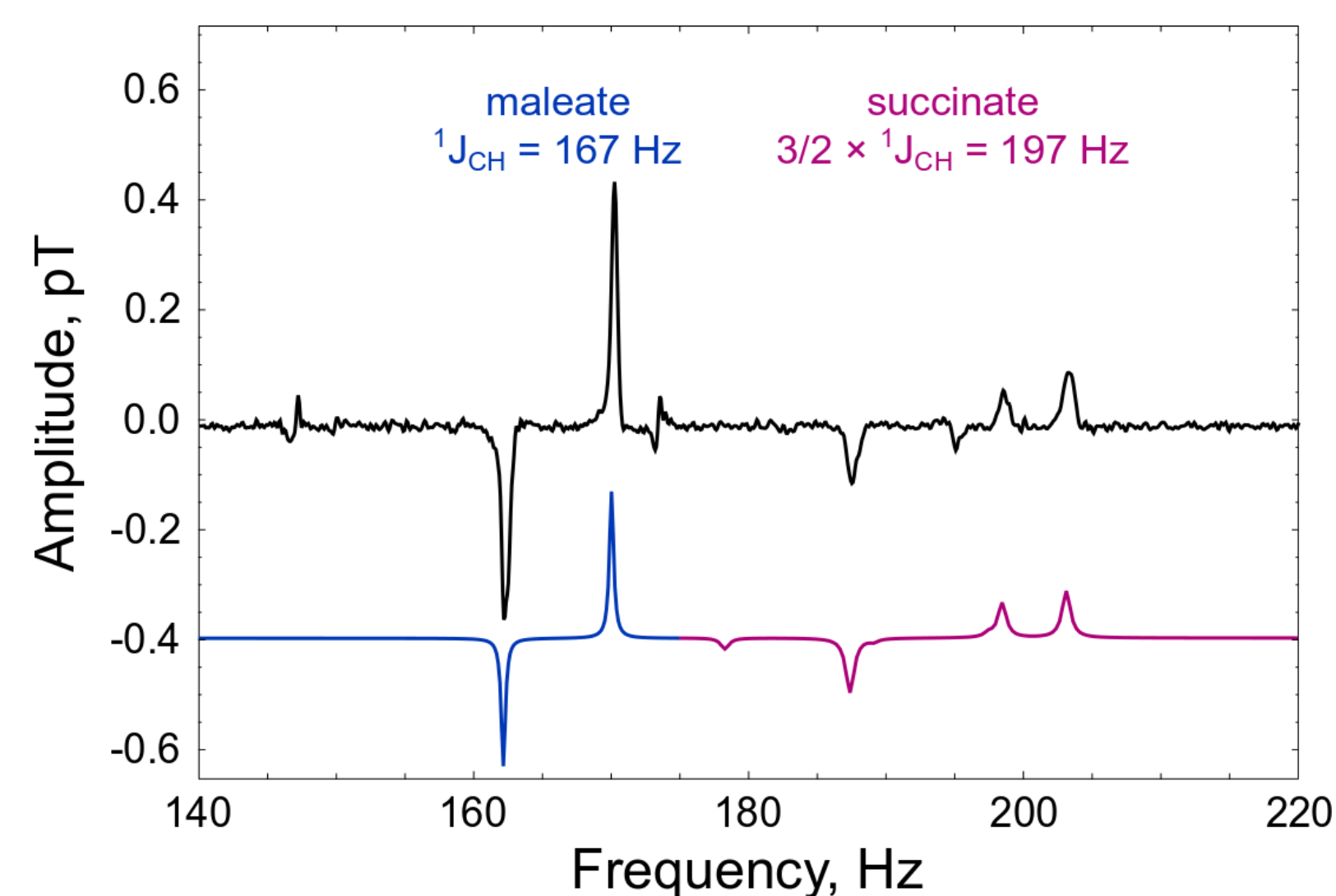
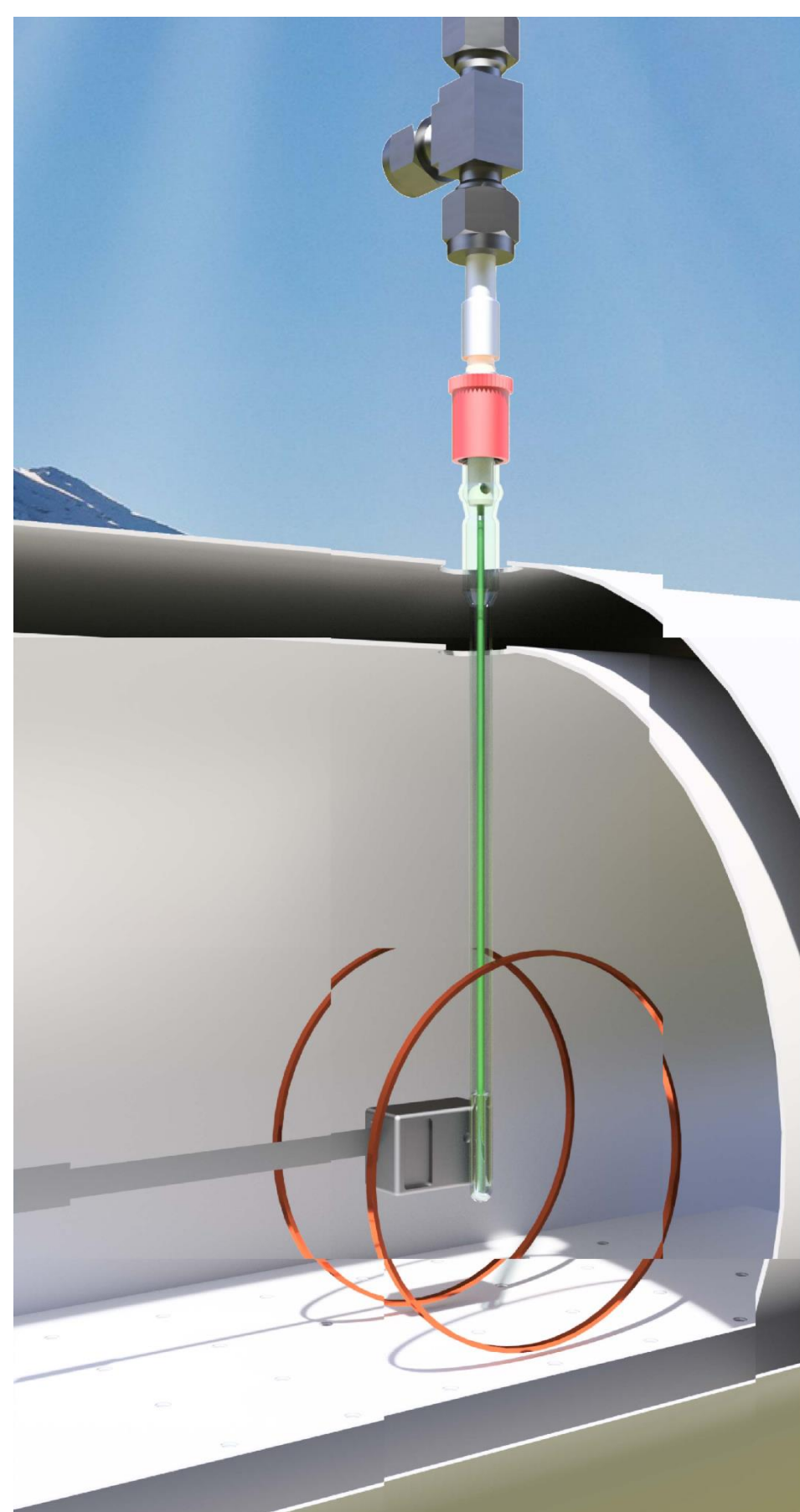
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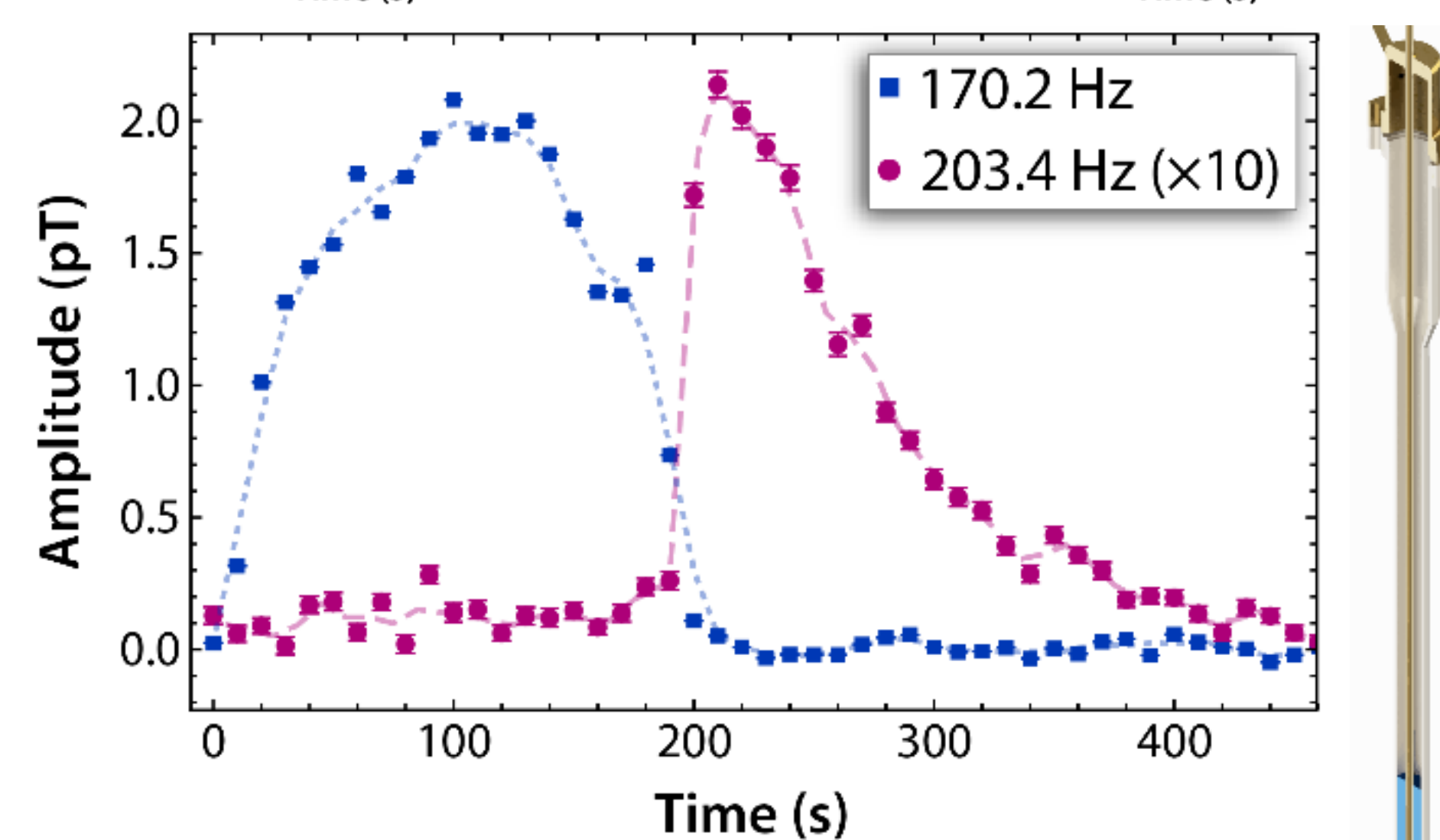
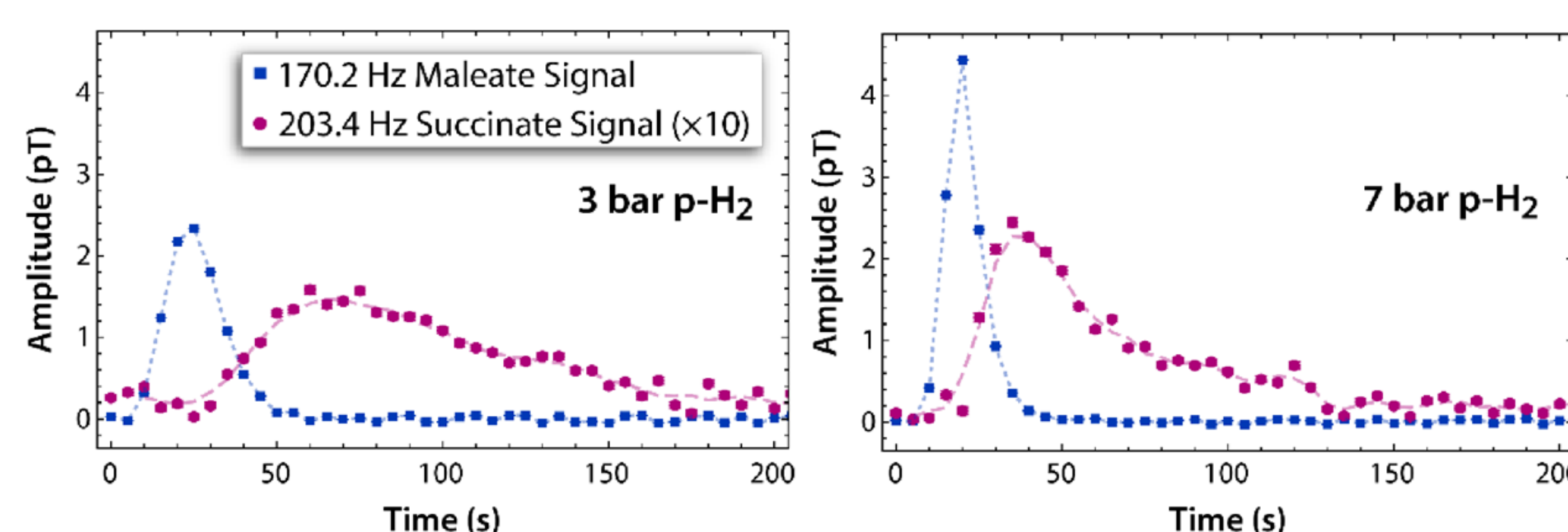
The reaction of interest:



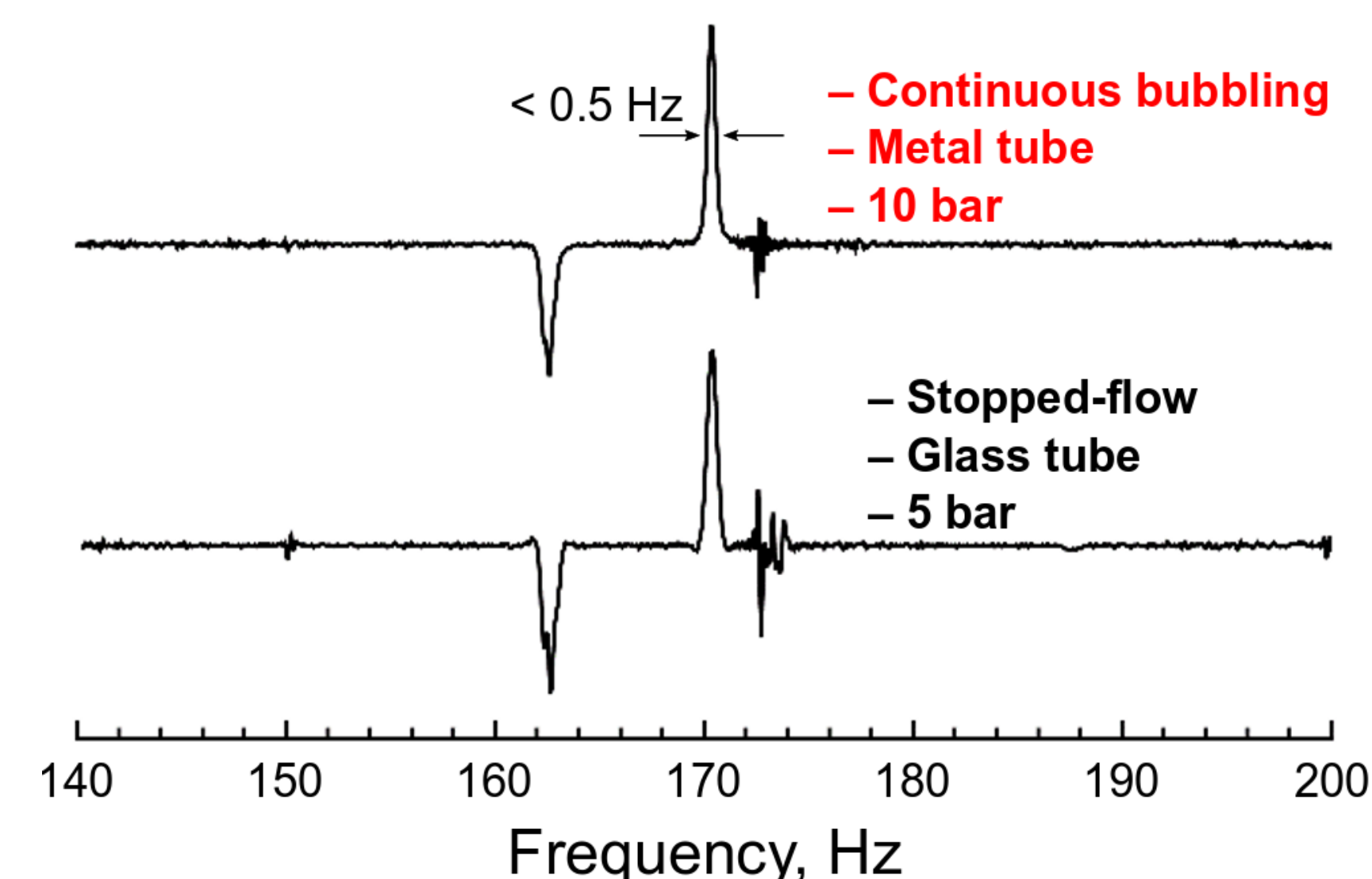
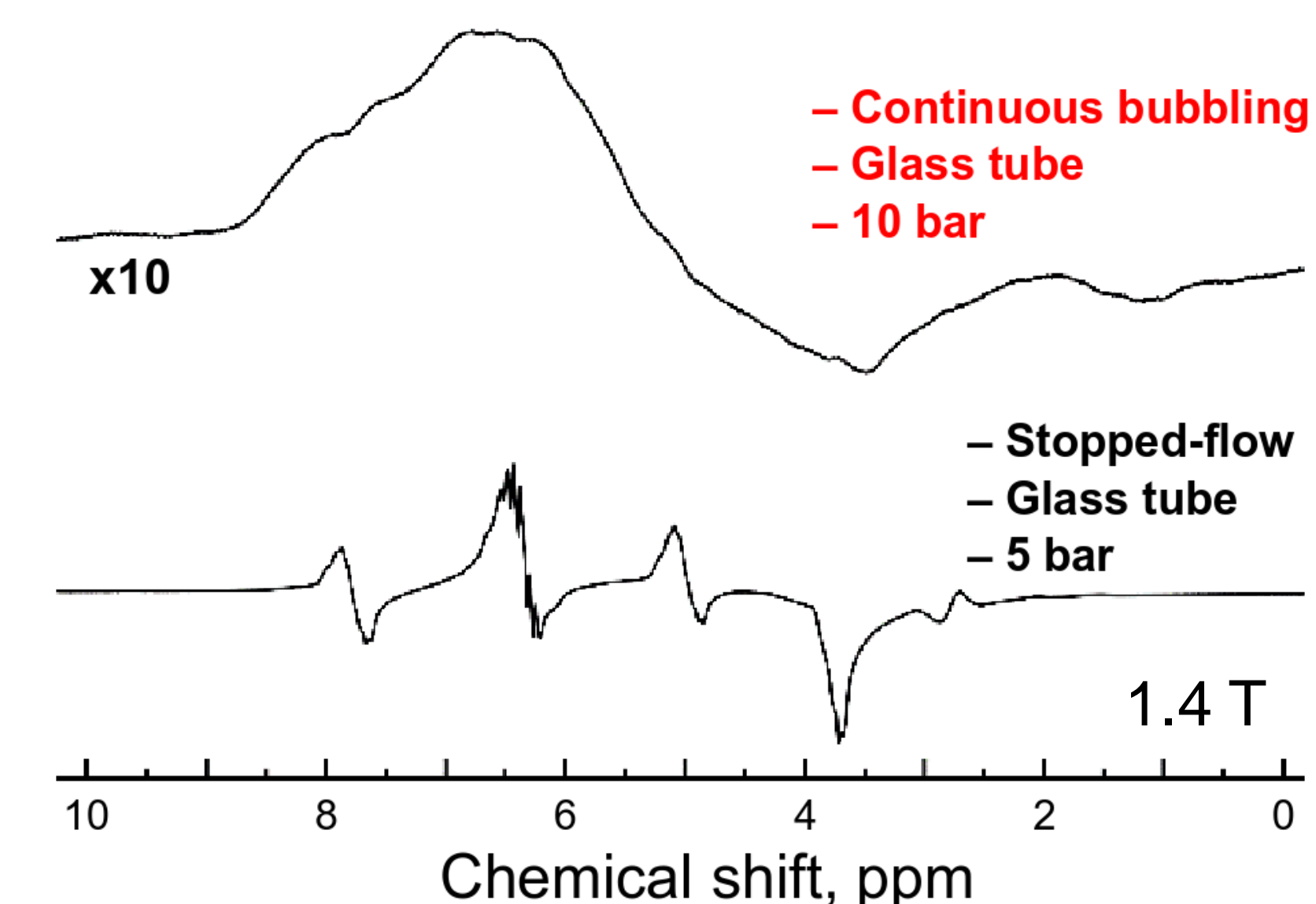
Zero-field NMR spectra:



The two-step hydrogenation of DMAD with parahydrogen was studied by ZULF NMR using a commercial atomic magnetometer.¹⁻² The hydrogenation reaction was monitored by observing the NMR signals of the hydrogenated products (dimethyl maleate and dimethyl succinate) over time.



- The reaction timescale depends measurably on the availability of H₂ in the system (at higher pressures it takes less time for the reaction to complete) – **oxidative addition of H₂ is the rate determining step**
- The stronger binding of alkyne to metal complex (compared to alkene) allows it to outcompete the alkene in binding to the catalyst, which results in **high selectivity toward alkene** production even at high alkyne conversions.



The figures above demonstrate that the sample heterogeneity induced by bubbling parahydrogen during signal acquisition practically **does not** affect the spectral resolution in ZULF NMR! Importantly, ZULF NMR spectra can be acquired even when it is carried out in a metal container.

¹<https://qusp.in.com>

²J. W. Blanchard, T. Wu, J. Eills, Y. Hu and D. Budker, *J. Magn. Reson.*, 2020, **314**, 106723 doi: [10.1016/j.jmr.2020.106723](https://doi.org/10.1016/j.jmr.2020.106723)

The results are published in ACIE:

<https://onlinelibrary.wiley.com/doi/abs/10.1002/anie.202006266>