

Supporting Information for
Refined High-Pressure Tube Design for Improved Resolution in
High-Pressure NMR Spectroscopy

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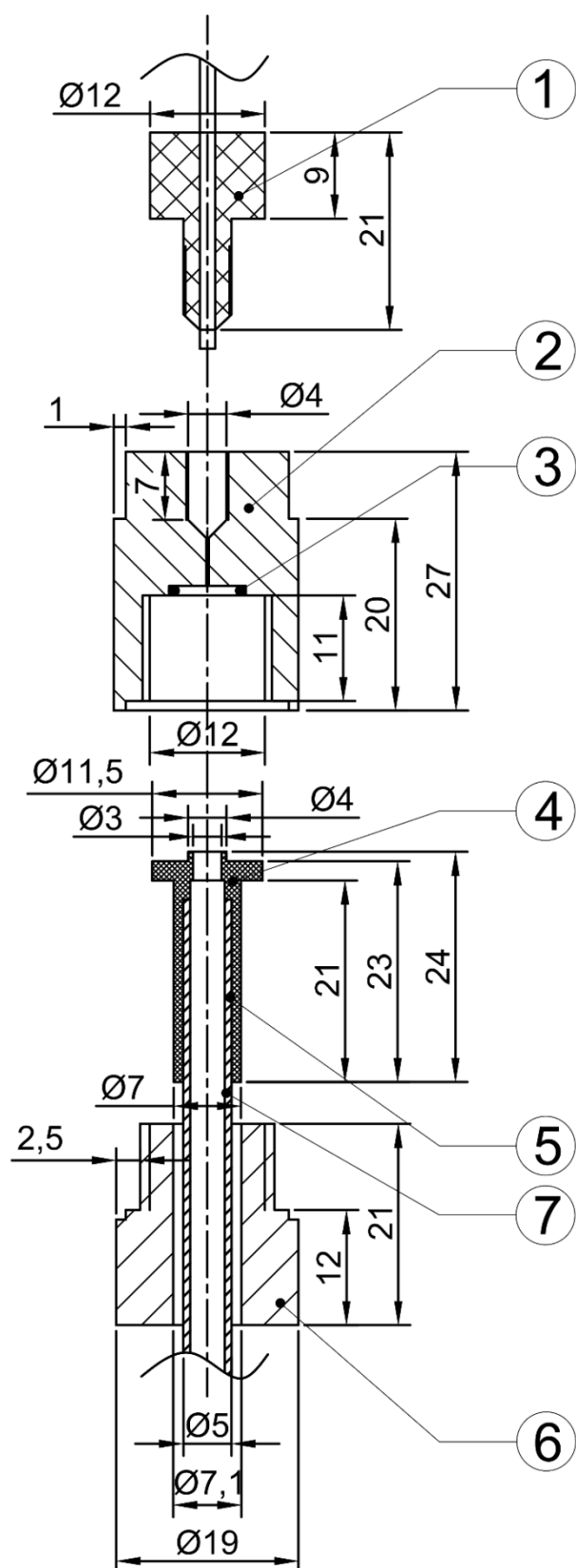


Figure S11: Technical drawing of the novel HP tube (1 - HPLC PEEK capillary fitting; 2 - PEEK top part; 3 - O-ring seal; 4 - titanium sleeve; 5 - epoxy glue; 6 – PEEK bottom part; 7 - sapphire tube).

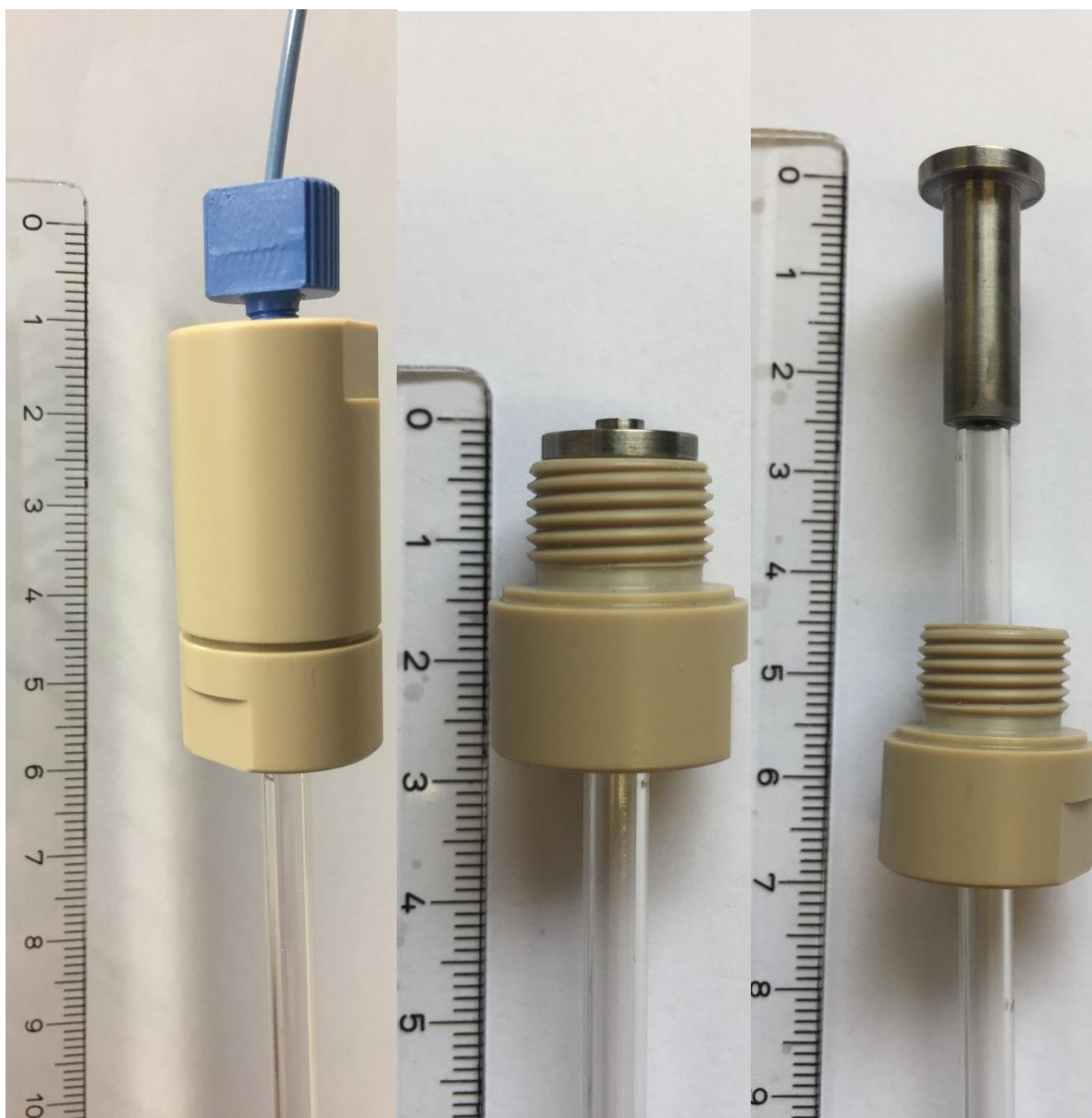


Figure SI2: Detailed photographs of the PEEK attachment for the sapphire tube. Left: Full assembly ready to use with the attachment machined from a PEEK rod (beige) and the PEEK HPLC capillary and fitting (blue). Middle: Top PEEK part deattached. Right: The bottom PEEK part is removable from the titanium sleeve glued to the sapphire tube.



Figure SI3: Detailed photographs of the PEEK attachment for the sapphire tube. Top: PEEK attachment connected (left) and unscrewed (right). Bottom: inside of the top attachment with the rubber O-ring in place.

Table SI1: Quantitative comparison of the methane and ethane peaks in ^1H NMR spectra measured at 200 bar with the previous ¹ and the improved tube design.

methane	previous design	improved design	change [%]
signal-to-noise ratio (4 scans)	19,895.70	36,061.72	+81.25
linewidth at 50% height [Hz]	1.11	1.02	-8.11
linewidth at 0.55% height [Hz]	45.64	19.00	-58.37
ethane			
signal-to-noise ratio (4 scans)	2,712.53	4,655.63	+71.63
linewidth at 50% height [Hz]	0.95	0.90	-5.26
linewidth at 0.55% height [Hz]	46.78*	19.30	-60.43

*number corresponds to 2x the half peak width of the side not overlapping with methane

Table SI2: Quantitative comparison of the methane and ethane peaks in ^1H NMR spectra of a 3-component mixture with methane (~91 mol%), ethane (~7 mol%), and propane (~3 mol%) at 200 bar with the previous ¹ and the improved tube design.

methane	previous design	improved design	change [%]
signal-to-noise ratio (4 scans)	11,062.78	35,735.67	+223.03
linewidth at 50% height [Hz]	2.05	1.12	-45.37
linewidth at 0.55% height [Hz]	99.12*	19.67	-80.16
ethane/propane cluster			
signal-to-noise ratio (4 scans)	1,309.57	4,007.03	+205.98
linewidth at 50% height [Hz]	2.22	1.0	-54.96
linewidth at 0.55% height [Hz]	165.74*	39.26	-76.31

*number corresponds to 2x the half peak width of the side not overlapping with the other signal

References

- [1] A. Duchowny, P. M. Dupuy, H. C. Widerøe, O. J. Berg, A. Faanes, A. Paulsen, H. Thern, O. Mohnke, M. Küppers, B. Blümich and A. Adams, *Journal of magnetic resonance (San Diego, Calif. : 1997)*, 2021, **329**, 107025,