

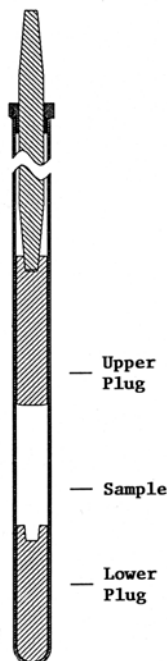
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Doty Susceptibility-Matched Sample Plugs for High-Resolution Liquids NMR

Triple the Sensitivity in Sample-Limited Applications
 Eliminate Convection Artifacts in Large-Sample NMR

Robust
 Low cost
 No bubbles
 No problems
 Easy to use

Wide selection for:
 All NMR tubes
 Low backgrounds
 Susceptibility match
 Chemical compatibility



HR-NMR has normally required a sample length three to five times that of the active coil length because it is generally impossible to shim out the effects of a magnetic susceptibility discontinuity at a material interface (air-sample, or glass-sample) that is not parallel to B_0 . The greater the susceptibility discontinuity, the further it must be from the sensitive region. Plugs matched to the solvent's susceptibility within 5% eliminate the need for 80% of the excess sample and allow sensitivity to be tripled (because of higher concentration) with no loss in resolution. Moreover, lineshape and resolution in older probes are dramatically improved.

Doty's design solves problems with: bubble removal, glass breakage, sample length adjustment, backgrounds, and VT.

An important, new application for these plugs occurs for large samples of low solubility. Thermal gradients as small as 0.2°C in larger non-spinning sample tubes (8 mm to 15 mm) can drive sample convection and may cause serious spectral artifacts.¹ Susceptibility-matched plugs eliminate these artifacts and permit VT HR-NMR on large, non-spinning samples.

Plug Materials: Susceptibility and Chemical Compatibility								
Select plug material with magnetic susceptibility similar to that of the sample solvent.								
Select Kel-F or zirconia when wide-line ^1H backgrounds would cause problems								
	Kel-F	(reference) Pyrex	PPS	Aurum	Ultem	Zirconia	GFP	G-10
$-\chi_{\text{VC}}$ (ppm, cgs)	0.92	0.86	0.73	0.71	0.71	0.70	0.52	~ 0.5
Wide-line NMR Backgrounds	F, Cl, C	Si, B, Al, Na	H, C, S	H, C, N	H, C, N	Zr	H, C, Al, Si, F	H, C, Al, Si, F
H ₂ O absorp. %	0.02	0.01	0.03	0.8	0.7	0.01	0.2	0.15
Density, g/cm ³	2.1	2.5	1.35	1.42	1.27	5.7	1.45	1.88
Max use T, °C	150	400	120	240	205	700	250	160
Color	clear	glass	ivory	black	amber	white	grey	green
Chemical Resistance: E- Excellent; G- Good, usually acceptable; F- Fair, sometimes acceptable; P- Poor								
Strong acids	E	E	G	G	G	E	P	F
Strong bases	E	E	E	G	G	E	G	E
Alcohols & Aliphatics	E	E	E	E	E	E	E	E
Aromatic H-C	E	E	E	E	G	E	E	E
Esters & Ketones	E	E	E	E	E	E	E	E
Chloro-solvents	E	E	E	G	F	E	G	G
Volumetric suscept. χ_{V} in S.I. is related to vol. suscept. χ_{VC} in cgs by: $\chi_{\text{V}} = 4\pi\chi_{\text{VC}}$								

Solvent	Suscept.
C ₃ H ₈ O ₃	0.779
C ₆ H ₅ Br	0.753
CHCl ₃	0.74
H ₂ O	0.719
D ₂ O	0.70
CS ₂	0.70
CCl ₄	0.691
C ₈ H ₁₆	0.684
C ₆ H ₁₂	0.627
C ₇ H ₈	0.618
C ₆ H ₆	0.611
C ₆ H ₅ NO	0.604
C ₃ H ₈ O	0.598
C ₂ H ₆ O	0.575
(C ₂ H ₅) ₂	0.534
CH ₄ O	0.53

¹ J. Lounila et al, *J. Magn. Reson. Ser. A*, **118**, 1996.

Abbreviations: Kel-F, p-chlorotrifluoroethylene; G-10, 60% e-glass epoxy composite; PPS, p-phenylene sulfide; Aurum, thermoplastic polyimide; Ultem, p-etherimide; GFP, glass-filled PEEK (p-etheretherketone); CPVC, chlorinated-p-vinylchloride.