

Reactivity of Waterlogged Archeological Elm Wood with Organosilicon Compounds Applied as Wood Consolidants: 2D ^1H - ^{13}C Solution-State NMR Studies

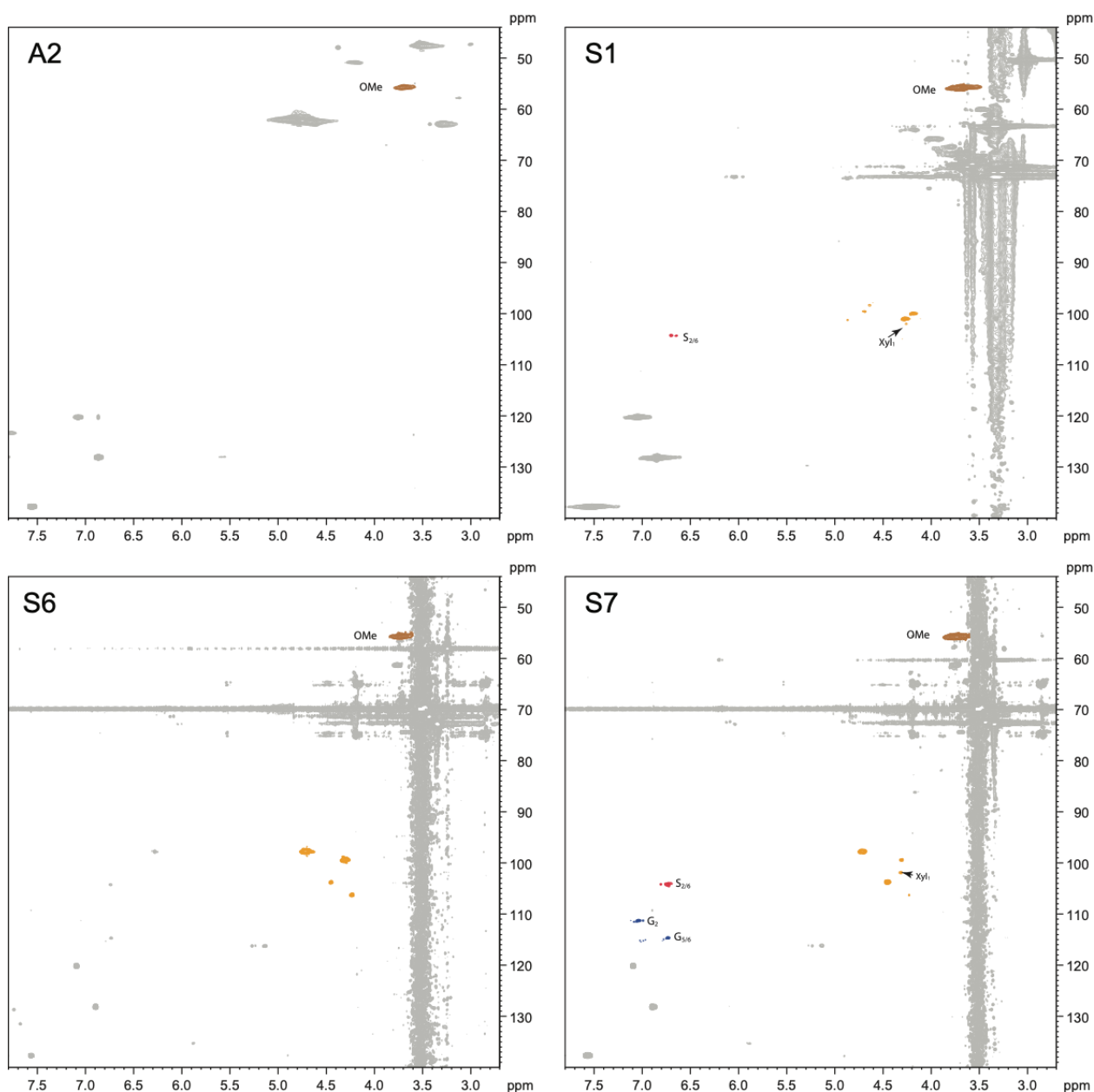


Figure S1. Partial 2D NMR spectra of organosilicon-treated wood showing 1-[3-(trimethoxysilyl)propyl]pyridinium chloride (A2), 1,3-bis(3-glycidyloxypropyl)-1,1,3,3-tetramethyldisiloxane (S1), 1,3,5,7-tetrakis(3-polyethoxypropyl)-1,3,5,7-tetramethyltetracyclosiloxane methoxy terminated (S6), 3-[3-(hydroxy)(polyethoxypropyl)]1,1,1,3,5,5,5-heptamethyltrisiloxane (S7). The colored contours and labels correspond to the chemical structures shown in Figure 3.

Table S1. Chemical shifts of functional groups present in selected organosilicon compounds used in this study.

Organo-silicon applied	Functional group	^1H δ (ppm)	^{13}C δ (ppm)	Reference
A1	methoxyl	3.558	45	[1]
	methyl	0.124	-10	
	methoxyl	3.558	45	
				[1,2]
				[3]
				(^1H NMR (CDCl_3) δ in ppm: 8.90 (s, 1H, OH); 8.60 (d, 1H, $\text{H}_{\text{py}2}$); 8.05 (d, 1H, $\text{H}_{\text{py}6}$); 7.95 (d, 1H, $\text{H}_{\text{py}4}$); 7.30 (t, 1H, $\text{H}_{\text{py}5}$); 3.96 (t, $\text{CH}_2\text{-Cl}$); 3.57 (s, 9H, CH_3); 3.00 (t, 2H, CH_2); 2.20 (q, 2H, CH_2); 1.65 (t, 2H, CH_2); 1.55 (t, 2H, CH_2); 1.4-1.15 (m, 16H, CH_2); 0.87 (t, 3H, CH_3), 0.65 (t, 2H, CH_2)
A2	A, B, C/2, 3, 4 (pyridinium chloride ring)	8.847, 8.671, 8.157	147.61, 146.59, 128.90	[4]
				^{13}C NMR (CDCl_3) δ in ppm: 156.5 (oxime $\text{C}=\text{N}$), 147.5 ($\text{C}_{\text{py}2}$), 144.6 ($\text{C}_{\text{py}6}$), 137.7 ($\text{C}_{\text{py}4}$), 134.3 ($\text{C}_{\text{py}5}$), 123.9 ($\text{C}_{\text{py}3}$), 52.7 ($\text{CH}_3\text{-O}$); 48.6 ($\text{CH}_2\text{-N}^+$), 41.8 ($\text{CH}_2\text{-C}=\text{O}$), 32.3 (CH_2), 31.2 (CH_2), 29.6 (CH_2), 29.5 (CH_2), 29.4 (CH_2), 29.3 (CH_2), 24.5 (CH_2), 23.6 (CH_2), 18.5 (CH_2), 13.8 (CH_3); 10.7 (CH_2), 7.9 ($\text{CH}_2\text{-Si}$) [4]
A3	3B, 2C, (D), 4E	2.537, 1.72, (1.356) HS, 0.76	27.54 (2,3), 8.27	[5,6]
	methoxyl	3.569	50.52	
A4	methoxyl	3.558	45	[1]
S1	1, 2, 3, 4, 5, 6, 7	na	73.58, 71.46, 50.89, 50.51, 44.27, 22.89, 5.32	[7,8]
S2	-Si-CH ₃ , -Si-CH ₂ -, -Si-CH ₂ -CH ₂ -, H	0.06, 0.52, 1.44, 0	0.00, 14.73, 27.02 - C4 (44.72)	[9]
	-NH ₂	1.14	na	
S6	O-Si(CH ₃)-O, Si-CH ₂ , Si-CH ₂ -CH ₂ , Si-CH ₂ -CH ₂ -CH ₂ , Si-CH ₂ -CH ₂ -CH ₂ -O-CH ₂ /CH ₂	-0.1, 0.4, 1.5, 3.4, 3.55	3, -1, 14, 24, 62, 70	[10]
	OH	3.55	na	
S7	-Si-CH ₃ , O-Si(CH ₃)-O, Si-CH ₂ , Si-CH ₂ -	0, -0.1, 0.4, 1.5, 3.4, 3.55	3, -1, 14, 24, 62, 70	[10]

CH₂, Si-CH₂-
CH₂-CH₂, Si-
CH₂-CH₂-CH₂-
O-CH₂/_CH₂

na = not available.

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