Supplementary Material (ESI) for *PCCP*

Electronic Supplementary Information

GIPAW (*Gauge Including Projected Augmented Wave*) and local dynamics in ^{13}C and ^{29}Si solid state NMR: the study case of silsesquioxanes $(RSiO_{1.5})_8$

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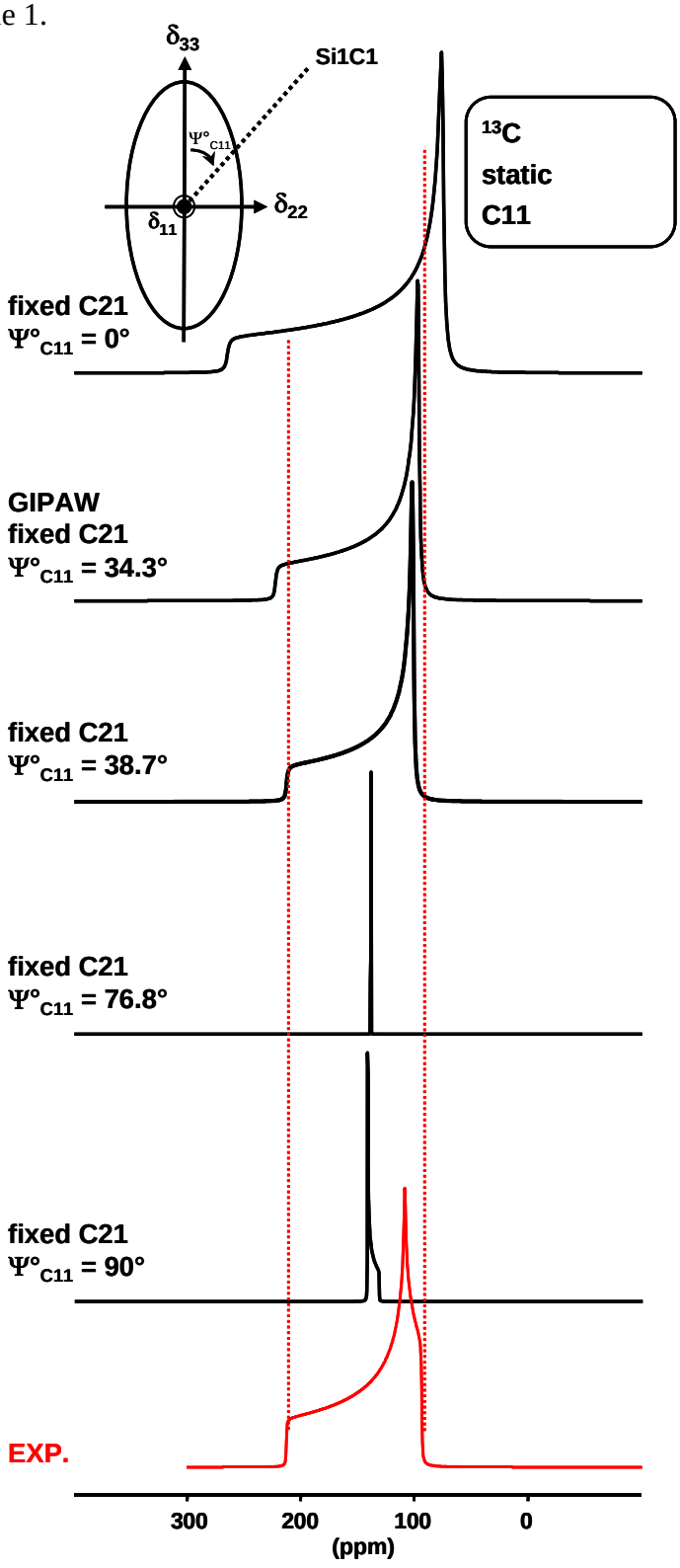
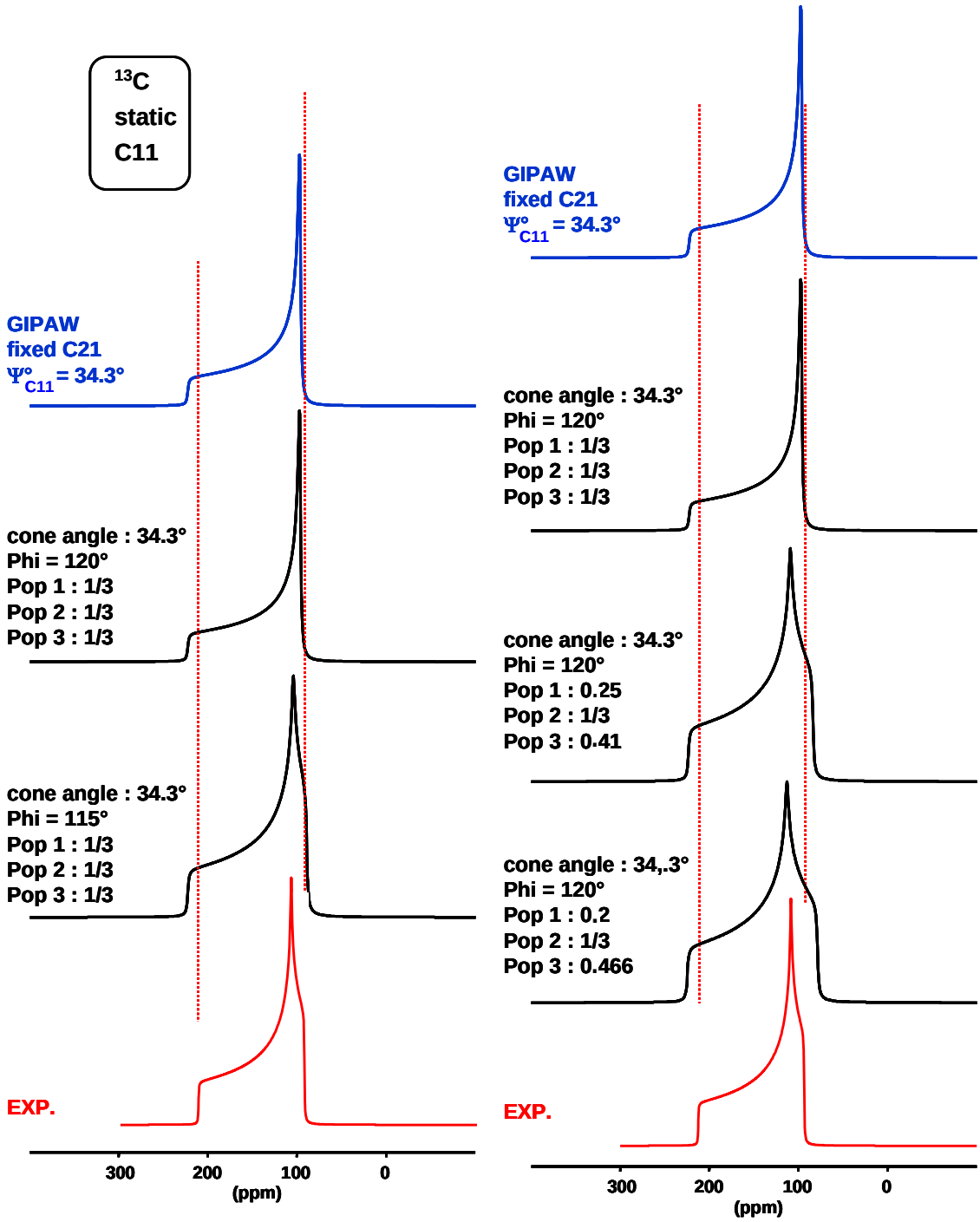
Bonhomme et al. ESI

Fig. S1. Averaged ^{13}C static spectra for C11 in T^{8v} (for fixed C21 position): influence of the cone angle ($\Psi°_{C11}$ or θ in the *NMR Weblab Software*)[37] on the CSA pattern. $\Psi°_{C11}$ = 34.3° corresponds to the GIPAW calculated angle. EXP corresponds to the *experimental* data reported in ref 27a for C11 and in Table 1.



Bonhomme et al. ESI

Fig. S2. Averaged ^{13}C static spectra for C11 in T^{8v} (for fixed C21 position): influence – of the jump angle φ in the *NMR Weblab Software*[37] on the CSA pattern (*left*). – of the populations p_j (*right*). $\Psi°_{C11}$ = 34.3° corresponds to the GIPAW calculated angle. EXP corresponds to the *experimental* data reported in ref 27a for C11 and in Table 1.



Bonhomme et al. ESI

Table S1. Fractional atomic coordinates of octameric silsesquioxanes $(RSiO_{1.5})_8$ structures after relaxation (R = H, CH_3). The lattice parameters were not relaxed; a = 12.498 Å, c = 13.087 Å for R = CH_3; a = 9.13100 Å, c = 15.35700 Å for R = H (see ref 31). The symmetry of the crystal was also constrained to be R-3.

	x/a	y/b	z/c
R=H			
H1	0.00000	0.00000	0.22687
H2	0.49016	0.31952	0.40932
O1	0.19417	0.11267	0.35772
O2	0.26511	-0.08242	0.17372
Si1	0.00000	0.00000	0.32241
Si2	0.31804	0.20799	0.44088
R=Me			
C1	0.00000	0.00000	0.15388
C2	0.01470	0.34306	0.37171
H1	0.00019	-0.08165	0.12359
H21	-0.06196	-0.30893	0.24949
H22	-0.06616	0.30873	0.32276
H23	0.04802	-0.23993	0.34621
Si1	0.00000	0.00000	0.29299
Si2	0.20721	0.20117	0.56854
O1	0.00619	0.12473	0.33513
O2	0.12812	0.24506	0.50054

	C21						C22						C23						C24					
	δiso	δ11	δ22	δ33	Δ_{CSA}	η_{CSA}	δiso	δ11	δ22	δ33	Δ_{CSA}	η_{CSA}	δiso	δ11	δ22	δ33	Δ_{CSA}	η_{CSA}	δiso	δ11	δ22	δ33	Δ_{CSA}	η_{CSA}
Si1	-80.5	-55.9	-79.5	-106.0	-25.6	0.9	-79.9	-54.7	-79.2	-105.7	-25.8	0.9	-79.7	-55.5	-78.7	-104.8	-25.2	0.9	-80.2	-55.3	-80.5	-104.7	-24.6	1.0
C1	123.4	231.7	133.2	5.2	-118.2	0.8	125.8	236.7	136.2	4.7	-121.2	0.8	127.1	239.3	137.3	4.9	-122.3	0.8	126.8	241.0	134.7	4.6	-122.2	0.9
C11-1	138.8	19.4	131.8	265.1	126.3	0.9	134.2	7.2	134.3	261.1	126.9	1.0	132.9	8.6	131.9	258.2	125.3	1.0	136.9	10.1	138.9	261.8	124.8	1.0
Si2	-79.1	-52.9	-79.1	-105.4	-26.2	1.0	-80.1	-104.6	-82.0	-53.6	26.5	0.9	-81.6	-60.5	-79.7	-104.7	-23.0	0.8	-80.0	-58.6	-76.4	-104.9	-25.0	0.7
C2	122.4	227.9	132.0	7.3	-115.1	0.8	127.2	237.9	137.2	6.3	-120.8	0.8	125.6	233.9	138.0	4.9	-120.7	0.8	128.3	241.4	140.3	3.2	-125.1	0.8
C2i	130.5	249.0	129.1	13.3	-117.2	1.0	137.2	263.5	136.9	11.1	-126.1	1.0	130.4	252.4	130.1	8.8	-121.7	1.0	137.5	265.6	138.6	8.3	-129.2	1.0
Si1	-80.5	-56.0	-79.4	-106.0	-25.6	0.9	-79.9	-54.8	-79.1	-105.7	-25.8	0.9	-79.7	-55.5	-78.6	-104.8	-25.2	0.9	-80.2	-55.4	-80.4	-104.7	-24.5	1.0
C1	123.4	231.7	133.3	5.1	-118.2	0.8	125.8	236.7	136.2	4.6	-121.2	0.8	127.1	239.3	137.4	4.8	-122.4	0.8	126.8	241.0	134.8	4.5	-122.3	0.9
C11-2	138.8	19.3	131.9	265.1	126.3	0.9	134.2	7.1	134.4	261.1	126.9	1.0	132.9	8.5	131.9	258.2	125.3	1.0	136.9	10.0	139.0	261.8	124.9	1.0
Si2	-79.7	-105.0	-80.6	-53.4	26.3	0.9	-80.6	-104.5	-83.5	-53.8	26.8	0.8	-81.7	-60.6	-79.7	-104.7	-23.1	0.8	-80.4	-59.6	-76.7	-105.0	-24.6	0.7
C2	123.2	229.9	134.0	5.6	-117.5	0.8	130.1	242.8	141.6	5.9	-124.2	0.8	125.0	233.2	135.8	5.8	-119.1	0.8	129.2	243.3	141.7	2.7	-126.6	0.8
C2i	125.9	244.6	124.4	8.6	-117.2	1.0	134.4	258.8	134.2	10.1	-124.3	1.0	131.0	253.0	130.4	9.5	-121.5	1.0	135.7	263.1	136.6	7.5	-128.2	1.0
Si1	-80.5	-55.9	-79.5	-106.0	-25.6	0.9	-79.9	-54.7	-79.3	-105.7	-25.8	1.0	-79.7	-55.4	-78.7	-104.8	-25.2	0.9	-80.2	-55.3	-80.5	-104.7	-24.6	1.0
C1	123.4	231.6	133.2	5.3	-118.1	0.8	125.8	236.6	136.2	4.7	-121.1	0.8	127.1	239.2	137.3	4.9	-122.3	0.8	126.8	241.0	134.7	4.6	-122.2	0.9
C11-3	138.8	19.4	131.8	265.1	126.3	0.9	134.2	7.3	134.3	261.1	126.9	1.0	132.9	8.7	131.8	258.2	125.3	1.0	136.9	10.2	138.9	261.8	124.8	1.0
Si2	-79.0	-53.0	-79.3	-104.8	-25.8	1.0	-79.9	-104.6	-82.6	-52.4	27.5	0.8	-81.3	-60.4	-79.3	-104.3	-23.0	0.8	-80.0	-59.1	-76.1	-104.9	-24.9	0.7
C2	122.0	227.6	131.3	7.0	-114.9	0.8	128.0	239.4	138.5	6.2	-121.8	0.8	124.8	232.6	136.2	5.7	-119.1	0.8	129.1	242.6	141.1	3.7	-125.4	0.8
C2i	128.3	247.3	127.2	10.3	-118.0	1.0	137.1	262.8	138.0	10.5	-126.6	1.0	131.0	252.9	131.3	8.6	-122.3	1.0	141.0	267.8	140.6	14.6	-126.4	1.0

Table S2: ^{13}C and ^{29}Si isotropic and anisotropic GIPAW calculated parameters (in ppm) for octavinylsilsesquioxane

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