Relevant distances (pm) and angles (°) obtained for the optimized models.

	A1	**A2**	**B1**	**B2**	**C1**	**C2**	**D1**	**D2**	**HA1**	**HA2**	**HB1**	**HB2**	**HC1**	**HC2**	**HD1**	**HD2**
Sn-O1	208	211	212	218	208	211	213	218	221	247	253	244	212	218	256	227
Sn-O2	206	209	-	-	206	208	-	-	211	207	-	-	217	211	-	-
Sn-O8	-	-	205	207	-	-	206	207	-	-	205	205	-	-	206	236
Sn-C (Me)[a]	215	216	216	215	218	218	217	217	220	220	218	216	221	220	220	221
Sn-C(Me')[a]	216	216	216	216	218	218	218	218	219	219	217	218	220	219	219	220
C(Me´)-H8[b]	-	-	241	225	-	-	251	224	-	-	207	209	-	-	192	179
Sn-O[c]	249	261	264	260	251	259	267	262	203	203	206	211	206	207	206	207
Sn-O(W')	-	261	-	278	-	264	-	287	-	426	-	342	-	-	-	240
O1-Sn-O2	80.9°	78.0°	-	-	81.2°	78.0°	-	-	76.1°	75.3°	-	-	75.7°	75.6°	-	-
O1-Sn-O8	-	-	116.8°	113.8°	-	-	118.9°	112.1°	-	-	107.1°	102.8°	-	-	116.9°	120.1°
C(Me)-Sn-C(Me´)	124.7°	131.8°	132.3°	144.9°	122.7°	132.1°	134.1°	141.7°	110.2°	107.9°	145.2°	142.9°	115.8°	111.3°	152.0°	169.2°
O[c]-Sn-O(W´)	-	150.9°	-	110.7°	-	151.3°	-	120.2°	-	-	-	-	-	-	-	85.9°
H3a-C3-C4-H4	175.1°	175.4°	174.8°	174.6°	175.4°	176.1°	174.9°	174.5°	173.5°	174.8°	173.4°	172.8°	178.0°	174.2°	174.4°	174.5°
H3e-C3-C4-H4	57.5°	57.8°	54.9°	54.9°	56.7°	58.6°	55.1°	54.7°	56.1°	66.7°	53.9°	53.3°	58.8°	56.7°	54.7°	54.8°
H4-C4-C5-H5	179.4°	179.3°	169.1°	169.5°	177.5°	175.1°	169.4°	169.3°	171.5°	157.1°	169.2°	168.6°	174.1°	169.3°	168.3°	168.3°
H5-C5-C6-H6	174.9°	176.5°	169.1°	169.6°	177.7°	177.7°	169.4°	169.6°	179.8°	111.4°	172.8°	173.0°	177.0°	175.1°	169.3°	168.4°
Oe[d]-C3-C4-C6	2.7°	2.6°	1.4°	1.3°	1.6°	1.2°	1.2°	1.6°	4.2°	25.1°	3.5°	4.1°	1.0°	2.8°	1.8°	1.1°

[a] In (**3**) Me refers to the α-CH_2 group of the butyl chain;
[b] Minimum averaged CH3-**H8** or α-CH_2 –**H8** proton distances in (**2**) and (**3**), respectively;
[c] O refers to H_2O or OH ligands;
[d] Oe = endociclyc oxygen.

Table 5 Calculated ^{119}Sn and ^{13}C NMR cs (ppm) for non-hydrolyzed and hydrolyzed $Bu_2SnNANA$ (**3**).

	Sn	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C_α[a,b]	C_β[a,b]	C_γ[a,b]	Me[a]/C_δ[a,b]
Exp.	**-**	**181.0**	**99.7**	**42.9**	**70.1**	**55.3**	**72.7**	**71.2**	**73.1**	**65.7**	**177.6**	**24.8**	**26.5**	**28.9**	**28.6**	**15.5**
Non-hydrolyzed																
$Bu_2SnNANA$ (3)																
C1	-89	164.7	101.7	45.5	72.4	56.8	71.3	72.2	77.5	67.4	161.0	23.7	23.2	30.1	30.0	16.5
C2	-203	164.4	100.8	42.7	73.0	62.8	69.4	73.8	76.8	67.3	165.1	23.0	22.8	30.6	30.8	15.3
D1	-149	164.2	97.5	40.9	72.4	57.7	74.2	76.3	76.7	73.6	165.3	23.9	26.3	31.5	31.8	16.9
D2	-169	165.3	97.2	41.0	72.7	57.6	73.7	76.6	76.0	73.4	165.1	24.0	27.5	31.1	31.2	17.0
Hydrolyzed																
$Bu_2SnNANA$ (3)																
HC1	-197	167.9	101.8	48.0	73.4	58.8	69.2	72.8	77.0	68.7	160.3	24.2	22.3	31.9	31.1	17.4
HC2	-194	165.7	100.9	42.8	73.2	64.9	67.7	74.5	76.8	68.3	162.9	23.5	28.9	30.0	31.3	15.8
HD1	-194	165.2	97.4	42.5	74.7	58.5	73.2	79.4	73.3	74.3	162.0	24.3	27.3	31.7	31.6	17.7
HD2	-368	165.0	97.7	42.9	74.0	58.3	74.0	79.8	71.9	75.2	162.1	24.2	30.5	32.6	32.0	17.6

[a] C_α, C_β, C_γ, C_δ = butyl groups carbons of $Bu_2Sn(IV)^{2+}$
[b] Average of the calculate values for the two R groups in the $Bu_2Sn(IV)^{2+}$ moiety