Supplementary materials

REACTIONS OF POLYFUNCTIONAL (HALOGENMETHYL)SILANES WITH O-/N-TMS-CARBOXAMIDES AND RELATED COMPOUNDS

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Table 1S. The chemical shifts of N-TMS of amides and lactams **4-7** and intermediates of the transsilylation reaction **4a,c-7a,c**.

№	T, °C	^{1}H		^{13}C			^{39}Si	Ref.
		MeSi	CH_2Si	MeSi	CH_2Si	C=O		
4	25	0.25		-0.80		177.0	8.8	35
6	25	0.24		-0.22		177.0	8.8	35
7	25	0.22		0.16		183.1	8.8	35
4a	-70	0.33	3.06	-3.36	29.50	179.4	6.2	35
5a	-80	0.35	2.99				5.4	36
6a	-80	0.34	3.08	-3.47	30.45	177.6	5.3	35,36
7a	-90	0.34	3.07	-2.87	30.07	184.1	6.0	35,36
4c	-50	0.49	3.81	5.32	62.51	170.0	-51.4	35
6c	-40	0.55	3.82	5.42	61.98	172.9	-53.8	35, 36
7c	-40	0.60	3.88	5.74	63.17	178.9	-50.7	35, 36

Table 2S. Synthesis method, M.p. (B.p.), yield and NMR spectral data of N-(dimethylchlorosilylmethyl)carboxamides **3**, **4d**, **8-23**.

№	Method	M.p. °C (B.p. °C/Tprr)	Yield, %	NMR, δ, ppm ($CDCl_3$)				Ref.
				^1H		^{13}C	^{29}Si	
				Me_2Si	NCH_2Si	C=O		
3[a]	I	128-131	-	0.96	2.77			21
	IIb	113-116	92					64
4d[b]	I	64-66	56	0.76	2.57			21,23
4d[c]	I			0.56	2.73	174.4	-40.3	35
	IIb	96-99	85					54
	I	84-86	95					66
				0.37	2.65	173.2	-37.6	62
8[b]	IIa	67-68 (76-78/0.16)	-	0.70	2.42			21
	IIa	76-78 °C/0.16		0.48	2.53	163.5	-19.8	62
9[b]	IIa	(110/0.05)		0.78	2.91			21
				0.73	3.15	162.7	-9.5	62
10[b]	IIa	104-105		0.81	2.98			21
11[b]	IIa	113-114		0.76	2.90			21
12[b]	I	97-99	-	0.86	3.07			21
12	IIa	98-100		0.68	3.05	173.8	-34.1	62
	IIb		80					54
13	I	150-152	95	0.69	3.13	174.0	-34.5	63
14	IIa			0.64	3.07	173.6	-34.0	62
15	IIa	126.5-129		0.65	3.07	173.3	-30.7	62
	I	143-145	87	0.65	3.08	173.3	-31.8	63
16	IIa	141-144		0.65	3.06	173.2	-31.1	62
17	IIa	95-97		0.66	3.11	173.3	-29.0	62
18	IIa	152.5-154		0.67	3.12	173.0	-26.9	62
19	I	62-65	83	0.56	2.89	180.2	-44.2	60
	IIc		64					60
20[d]	IIa	(160-161/10)	95	0.33	2.94			65
21	I	150-152	87	0.79	3.41	171.3	-32.3	63
22	I	171-173	92	0.77	3.38	171.1	-33.3	61
	IIc		90					61
23	IIc	158-160	89	0.77	3.36	171.4	-30.3	61

The following solvents were used to obtain NMR spectra: [a]C_6H_6, [b]PhCl, [c]$CDCl_3/CH_2Cl_2$, [d]CCl_4

Table 3S. Synthesis method, M.p. (B.p.), yield and NMR spectral data of N-(dimethylchlorosilylmethyl)lactams **5d**-**7d**, **26**-**28**.

№	Method	M.p. °C (B.p. °C/Torr)	Yield, %	NMR, δ, ppm ($CDCl_3$)				Ref.
				^1H		^{13}C	^{29}Si	
				Me_2Si	NCH_2Si	C=O		
5d	I	84-86	76					54
	I	(93-95/0.5)	96	0.56	2.54			53
	IIa		72					53
	IIb		73					54
6d[a]	I			0.55	2.75	173.2	-41.8	35
	I	86-87	92	0.48	2.67			53
	IIb	(106-107/2)	76					54
7d[a]	I			0.60	2.92	178.8	-39.7	35
	I		84	0.51	2.74			53
	IIb	118-121	64					54
26	I	(164-165/0.5) 74-76	74	0.68	2.76	175.9		53
27	I	109-114	87	0.55	2.76			66
28	I		64	0.80	2.92	177.9		53

The following solvents were used to obtain NMR spectra: [a] $CDCl_3/CH_2Cl_2$

Table 4S. Synthesis method, M.p. (B.p.), yield and NMR spectral data of N-(dimethylchlorosilylmethyl)imides **29-32**.

№	Method	M.p. °C (B.p. °C/Torr)	Yield, %	NMR, δ, ppm ($CDCl_3$)				Ref.
				^1H		^{13}C,	^{29}Si	
				$SiMe_2$	NCH_2Si	C=O		
29	I	45-46	100	0.57	3.06	175.8	-24.2	67
30	I		83	0.55	3.14	177.2	25.4	68
31	I	55-56 (126-130/1)	77	0.51	3.04		6.1	68
	IIb	55-56 (130-132/1)	78					68
	I		90	0.54	3.18	173.8	7.2	69
32	I		80	0.56	3.20	173.8	-8.8	69

Table 5S. Synthesis method, M.p. (B.p.), yield and NMR spectral data of N-(dimethylchlorosilylmethyl)ureas **33-43**

№	Method	M.p. °C (B.p. °C/Torr)	Yield, %	NMR, δ, ppm ($CDCl_3$)				Ref.
				^1H		^{13}C, C=O	^{29}Si	
				$SiMe_2$	NCH_2Si ($ClCH_2Si$)			
33a	I			0.49	(2.95)		-2.5	70
34a	I			0.55	(2.94)	160.2	1.5	70
33b[a]	I	(191-192/7) 67-69	19	0.56	2.84		-22.8	70
33b[b]				0.70	3.06		-30.0	
34b[a]	I	(198/7), 45-47	26	0.56	2.84		-23.3	70
34b[b]				0.73	3.13		-32.7	
35	IIb		81	0.60	3.25	161.9	-39.6	71
36	I			0.67	3.26	161.5	-42.5	71
37	I			0.83	3.52	160.8	-19.5	71
38	I		93	0.59	2.85	160.6	-41.6	72
39	I	(203-205/1.5)	69	0.57	2.90	158.0	-6.7	73
40	I	147-149	83				10.6	74
41	I	(145/0.08)	59	0.40	2.95			75
	IIb	148-150	94	0.46	3.12	159.2	10.6	77
42	I	(136-140/0.08)	32					75
43	IIb	114-116	73	0.70	3.21	157.0	-32.8	77

The following solvents were used to obtain NMR spectra: [a]C_2HCl_3, [b]$PhNO_2$

Table 6S. Yield, NMR spectral data of N-(dimethylchlorosilylmethyl)heterocycles **45-64**

№	M.p. °C (B.p. °C/Torr)	Yield, %	NMR, δ, ppm ($CDCl_3$)				Ref.
			^{1}H		^{13}C, C=O	^{29}Si	
			$SiMe_2$	NCH_2Si			
45	91-94	87	0.64	3.70	160.1	-41.1	79
46	99–104	84	0.50	3.70	163.4	-24.7	79
47	99–101	85	0.67	3.70	164.2	-40.9	79
48[a]	96–99	88	0.62	3.70	157.6	-32.0	79
49[a]	96–100	77	0.50	3.70	156.6	-25,0	79
50[b]	99–106	88	0.46	4.00	160.9	-17.1	79
51	102–104	86	0.72	3.90	163.1	-18.4	79
52	108–111	87	0.45	3.70	163.7	-21.3	79
53	105–109	88	0.55	3.90	163.8	-27.4	79
54	105–108	90	0.73	4.20	154.9	-14.3	79
55[a]	110–112	90	0.76	3.90	157.0	-27.9	79
56	107–112	88	0.44	4.40	160.3	-12.7	79
57	(110/10)	85	0.79	2.50			80
58	111-114	82	0.47	2.80			80
59		89	0,75	3.65	163.4	-38.4	79
60		84	0.81	3.94	163.4	-28.9	79
61[c]	116-117	95	0.36	2.90	165.3	-3.17	81
62	84-86	95	0.65; 0.66	3.28; 3.55	164.6	13.7; -5.7	82
63[a]	235-238	95	0.53	3.07	167.8	2.3	82
63[d]					168.5	-32.4; 44.4	82
64	70-71	98	0.52	3.44	172.7	18.6	82

The following solvents were used to obtain NMR spectra: [a]CD_3CN, [b]CD_3OD, [c]$CDCl_3/CD_3OD$, [d]VACP-MAS (solid state)

Table 7S. Synthesis method, M.p. (B.p.), yield and NMR spectral data of compounds **65-84**

№	Method	M. p. °C	Yield, %	NMR, δ, ppm ($CDCl_3$)				Ref.
				^1H		^{13}C	^{29}Si	
				SiMe	NCH_2Si	C=O		
65	I	62-67	41					23
	IIb	59-64	60					83
	I	64-66	91	0.91	3.01	173.5	-48.5	87
66	III	69-73	70	0.91	3.07			36,
	IIb	67-72	92					36
	III	69-73	78	0.95	3.12		-46.8	84
67	III	120-122	69					36, 83
68	III	113-116	77		3.18			36, 83
69	I	155-156	58	1.04	3.32	174.3	-46.4	87
70	I	140-143	70	1.03	3.31	174.5	-43.6	87
71	I			0.98	3.38	160.8	-52.3	88
72	I				3.13	160.6	-87.9	88
73	I		96		2.96	159.8	-13.1	85
74[a]	I	107-111	88	0.95	3.90	162.2	-52.5	88
75	I	115–117	90	0.98	3.80	163.3	-52.3	88
76	I	108-111	98	0.92	3.20	156.4	-50.0	88
77	I	114–119	91	0.97	3.80	161.1	-50.2	88
78[a]	I	125–130	92		4.10	160.8	-77.7	88
79[b]	I	129–136	91		4.00	162.1	-89.7	88
80	I	131–134	90		4.00	162.5	-85.6	88
81[c]	I	93-95	70	0.36	2.90	165.3	-47.0	81
82	I	102-106	96	0.99, 1.03	3.45, 3.71	164.7	13.9, -20.8	82
83[c]	I	174-178	94	0.88	3.27	166.7	-18.3	82
84	I	57-60	90	0.94[d]	3.65[d]	172.3[d]	15.8[d]	82
				0.85, 0.94[e]	3.59, 3.65[e]	172.2, 173.6[e]	14.6, 21.8[e]	

The following solvents were used to obtain NMR spectra: [a]$CDCl_3/CD_3CN$; [b]CD_3CN; [c]$CDCl_3/CD_3OD$; [d]mj,[e]min

Table 8S. Synthesis method, M.p. (B.p.), yield and NMR spectral data of compounds **85-103.**

№	Method	M.p. °C (B.p. °C/Torr)	Yield, %	NMR, δ, ppm ($CDCl_3$)				Ref.
				^1H		^{13}C	^{29}Si	
				Me-Si	NCH_2Si	C=O		
85	I	66-67	79	0.56	2.72	174.2	-39.6	46
86	I			0.26	2.83	172.3	-55.1	46
87	I				3.06	174.1	-105.1	46
88	I	57-58	79	0.31	2.48	172.7	-56.5	46
	I	57-58	97	0.31	2.50	172.8	-55.8	92
89	I	72-73	59		2.60	174.9	-103.1	46
90	I	150-152	90	0.69	3.13	174.0	-34.5	64
91	I	143-145	84	0.65	3.08	173.3	-31.8	64
92	I	150-152	62	0.79	3.41	171.3	-32.3	64
93	I		92	0.35	2.78	171.4	–11.5	91
94	IIc	100—101	50	0.45	3.11	170.7	-7.0	91
95	I	157-158	87	0.53	3.13	172.8	–52.1	92
96	I		69	0.51	3.17	151.1	-30.4	92
97	I	105—106	90	0.42	2.85	173.3	-52.5	91
98	I	134–135	70		3.00	174.9	– 102.1	93
99	IIc	192–194	93		3.25	171.69	–103.4	93
100	I	73-74	87	0.42	2.80	173.7	-31.4	92
101	I	109-110	87	0.24	2.40	163.8	-48.6	92
102	I	84-85	59	0.51	2.74	175.5	-26.2	94
103	I	134-136	70	0.55	3.03	170.4	-24.7	94

Table 9S. Yield, M.p. (B.p.), yield and NMR spectral data of compounds **104**-**123**.

№	M.p. °C (B.p. °C/Torr)	Yield, %[a]	NMR, δ, ppm ($CDCl_3$)				Ref.
			^1H		^{13}C	^{29}Si	
			Me-Si	NCH_2Si	C=O		
104	(99-100/1)	71	0.44	2.52		-18.0	53,36
105	(154-156/1)	72	0.49	2.65	177.1	-14.3	53,36
106	(125-129/1)	68	0.33	2.64	172.8	-42.0	53,36
107	(145-147/2)	47	0.35	2.77		-41.6	53,36
108	(175-177/1)	69	0.45	2.85		-18.2	53,36
109			0.51	2.72	177.2	-14.6	53,36
110	(204-205/1)	65	0.38	2.86	173.0	-38.2	53,36
111	(225-227/1)	76	0.39	2.94		-36.7	53,36
112	(218-220/0.5)	78	0.45			-18.4	53,36
113	(260-263/3)	89	0.29	2.80		-33.9	53,36
114	(240-245/0.5)	72	0.29	2.90		-32.8	53,36
115	(169-171/12)	71	0.31	2.57		7.1	53,36
116		99	0.34	2.80	173.3	-37.4	95
116[b]			0.26	2.74	174.5	-37.5	95
117	(165-167/3)	76	0.36	2.68	172.2	-29.9	96
118	(188-190/2)	67	0.69	3.13	173.3	-26.2	96
119	(170-175/2)	64	0.45	3.18	172.1	-23.7	96
120		90	0.52	2.73	173.0	-19.1	97
121		94	0.43	2.82	172.9	-16.8	97
122		69		2.48	173.3	-100.3	97
123	72–74	49	0.58	2.91	173.9	-65.4	98

[a] The synthesis of compounds **104-123** was carried out using method **I**; [b]NMR in CD_3CN

Table 10S. Synthesis method, M.p. (B.p.), yield and NMR spectral data of compounds **124-132**.

№	Method	M.p., °C	Yield, %	NMR, δ, ppm ($CDCl_3$)					Ref.
				^1H			^{13}C	^{29}Si	
				Me-Si	H-Si	NCH_2Si	C=O		
124	IIa	116–124	77	0.83		3.10	173.6	-49.6	99
125	I	174–176	64			3.19	173.6	-62.6	100
126a	IIa	137–141	80	0.90		2.64, 3.05	173.2	-53.8	99
126b				0.83		2.76, 2.92		-54.3	99
127	I	139–141	86	0.78		2.98, 3.49	173.3	-47.2	99
128	I	115 разл.	93	0.62	5.21	2.75, 2.92	174.2	-64.7	100
129	I	157 разл.	87		5.72	2.95, 3.01	173.1	-74.6	100
130	I	53 разл.	60	0.64	5.23	2.74, 2.80	173.7	-64.1	101
131	I	89-92	87		5.74	2.93, 2.97	173.4	-74.4	101
132	I	59-61	87		5.42	2.59, 2.66	173.1	-66.4	101
132[a]					6.10	2.86, 3.05			

[a]NMR in C_6D_6