Supplementary Material

Pd–H Elimination Reactions in Palladium(II) Allylic Complexes

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Contents:

Additional data for the decomposition reactions of allylic complexes.

Table 1. Decomposition data for the palladium cyclohexenyl complexes at 50 °C.[a]

Entry	**Complex**	**2h**						**1 day**					
		Pd-cpd	**8**	**9**	**10**	**11**	**12**	**Pd-cpd**	**8**	**9**	**10**	**11**	**12**
1	**3**							100					
2	**4**							100					
3	**1**							100					
4	**6**[b,c]							42	2	13	4		12
5	**7**							95			2		3
6	**5**[d]		30	31	31								
7	**2**[c]							79	1	2		9	

a) All the decomposition reactions were carried at 50 °C in $CDCl_3$ in an NMR tube. Percentages of products were determined by integration of signals in the ^{19}F spectra; they correspond to the percentage of C_6F_5 in the compound which is equivalent to the molar % except for the dimeric complex **1**. b) Complex **1** was also formed (18%). c) Several unidentified compounds were also formed (9% total). d) Several Pf-containing unidentified compounds were also formed (8% total). $C_6Cl_2F_3H$ (50%) and $[Pd(C_6Cl_2F_3)_2L_2]$ (50%, L = solvent or H_2O) were also formed.

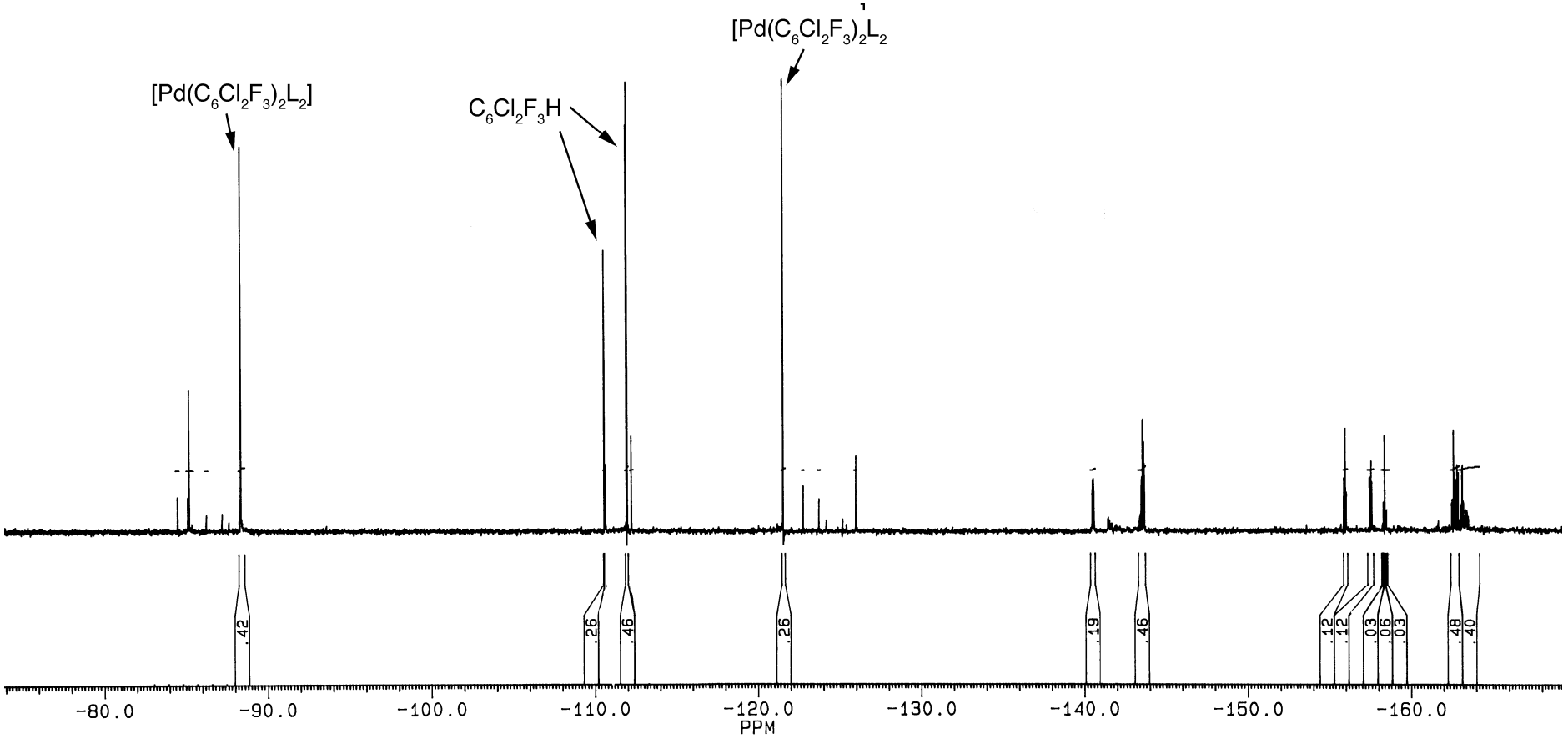
Table 2. Decomposition data for the complexes **1** and **4** at 100 °C.[a]

Entry	**Complex**	**2h**[b]						**1 day**					
		Pd-cpd	**8**	**9**	**10**	**11**	**12**	**Pd-cpd**	**8**	**9**	**10**	**11**	**12**
1	**1**	100						50	8	11	9	22	
2	**4**[c]	100							6	12	22		38

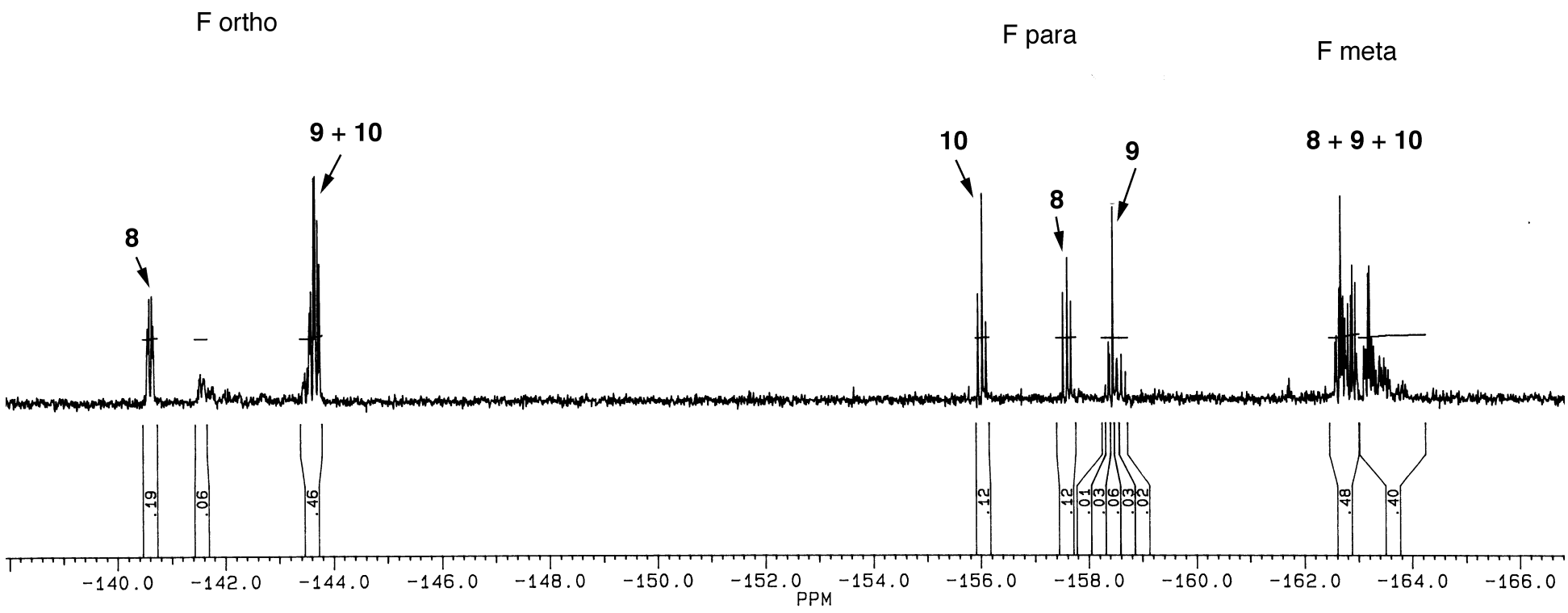
a) Decomposition reactions were carried at 100 °C in $CDCl_2CDCl_2$ in an NMR tube. Percentages of products were determined by integration of signals in the ^{19}F spectra; they correspond to the percentage of C_6F_5 in the compound which is equivalent to the molar % except for the dimeric complex **1**. b) The same results are obtained after 3.5 h. c) Several unidentified compounds were also formed.

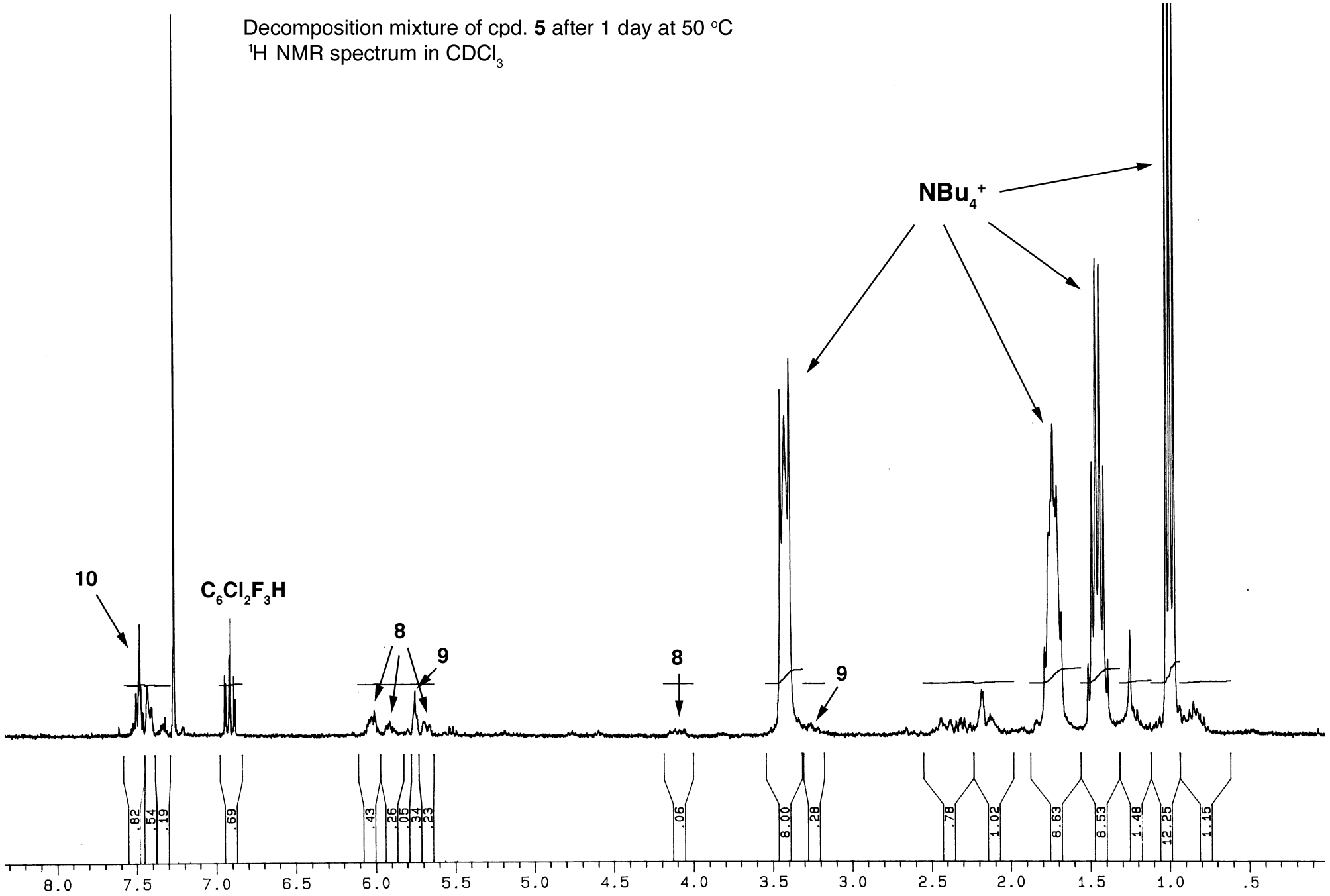
NMR spectra of decomposition mixtures for complexes **5** and **6**.

Decomposition mixture of cpd. **5** after 1 day at 50 °C
^{19}F NMR spectrum in $CDCl_3$

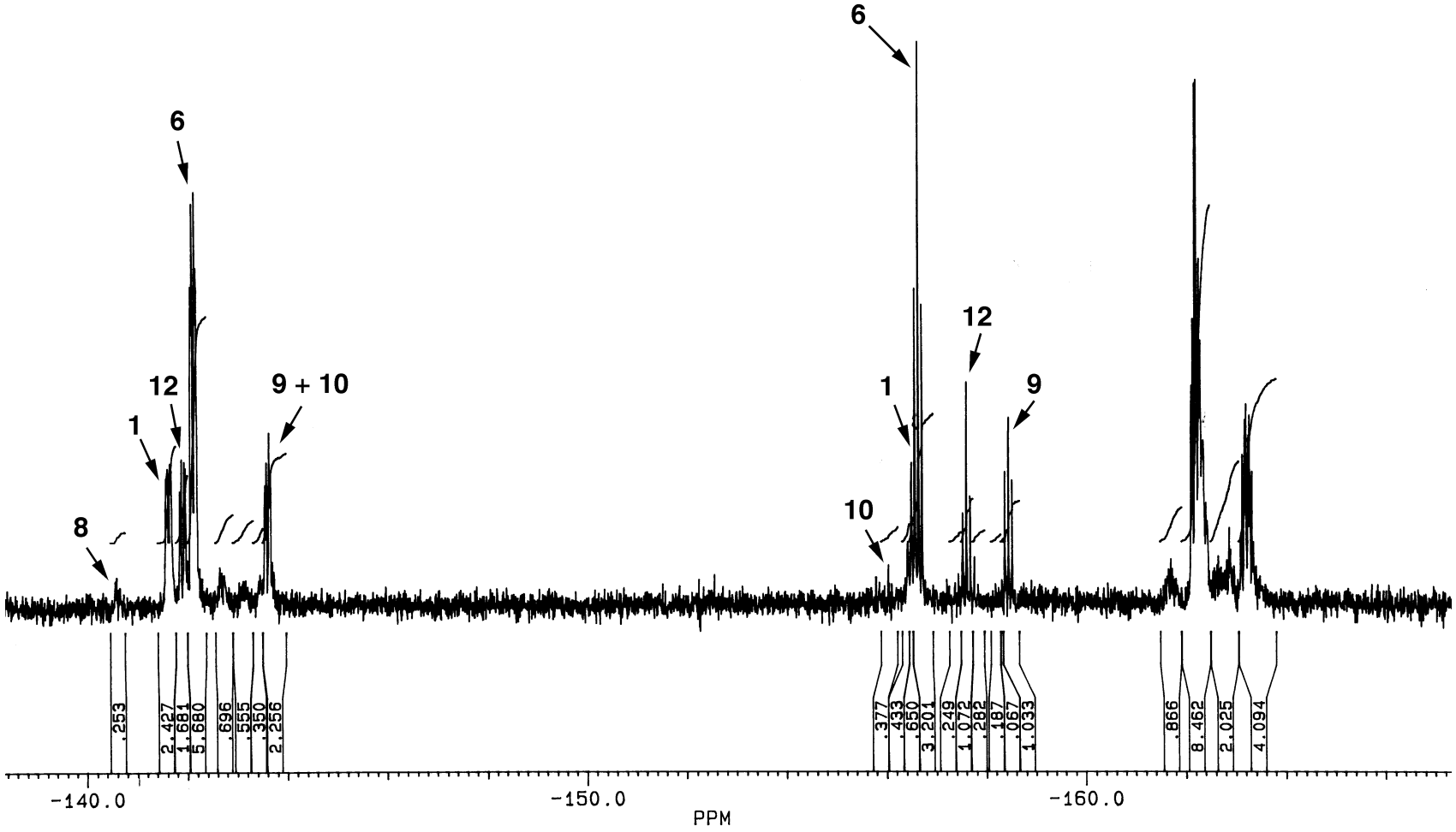


Decomposition mixture of cpd. **5** after 1 day at 50 °C
^{19}F NMR spectrum (C_6F_5 region) in $CDCl_3$




Decomposition mixture of cpd. 5 after 1 day at 50 °C
¹H NMR spectrum in CDCl₃
NBu₄⁺
10
C₆Cl₂F₃H
8
9
8
9
.82
.54
.19
.69
.43
.26
.05
.34
.23
.06
8.00
.28
.78
1.02
8.63
8.53
1.48
12.25
1.15
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5

Decomposition mixture of cpd. **6** after 1 day at 50 °C
^{19}F NMR spectrum in $CDCl_3$



Decomposition mixture of cpd. **6** after 1 day at 50 °C
^{1}H NMR spectrum in $CDCl_3$