

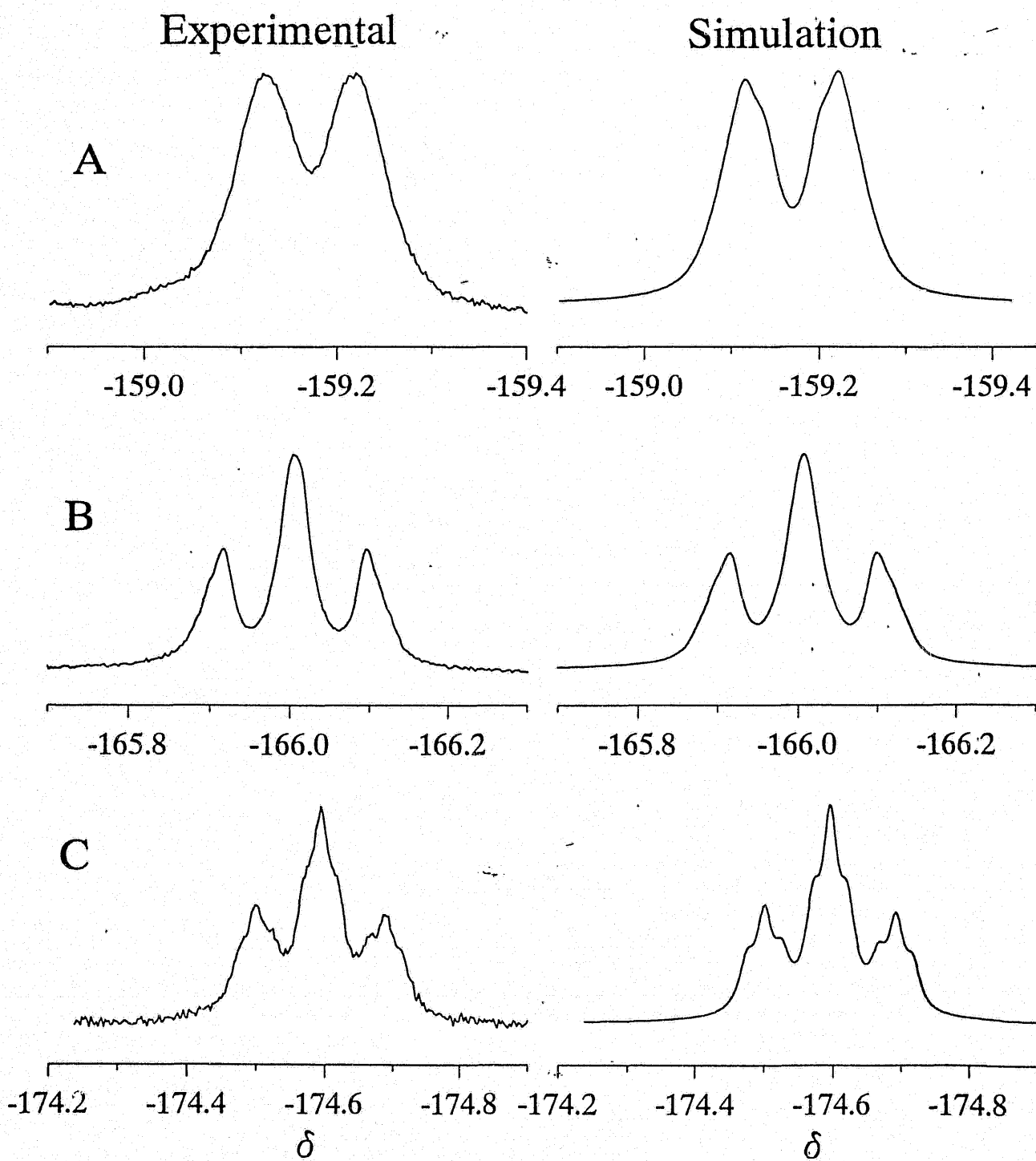
# HAMPTON 2066-2074

## Terms & Conditions

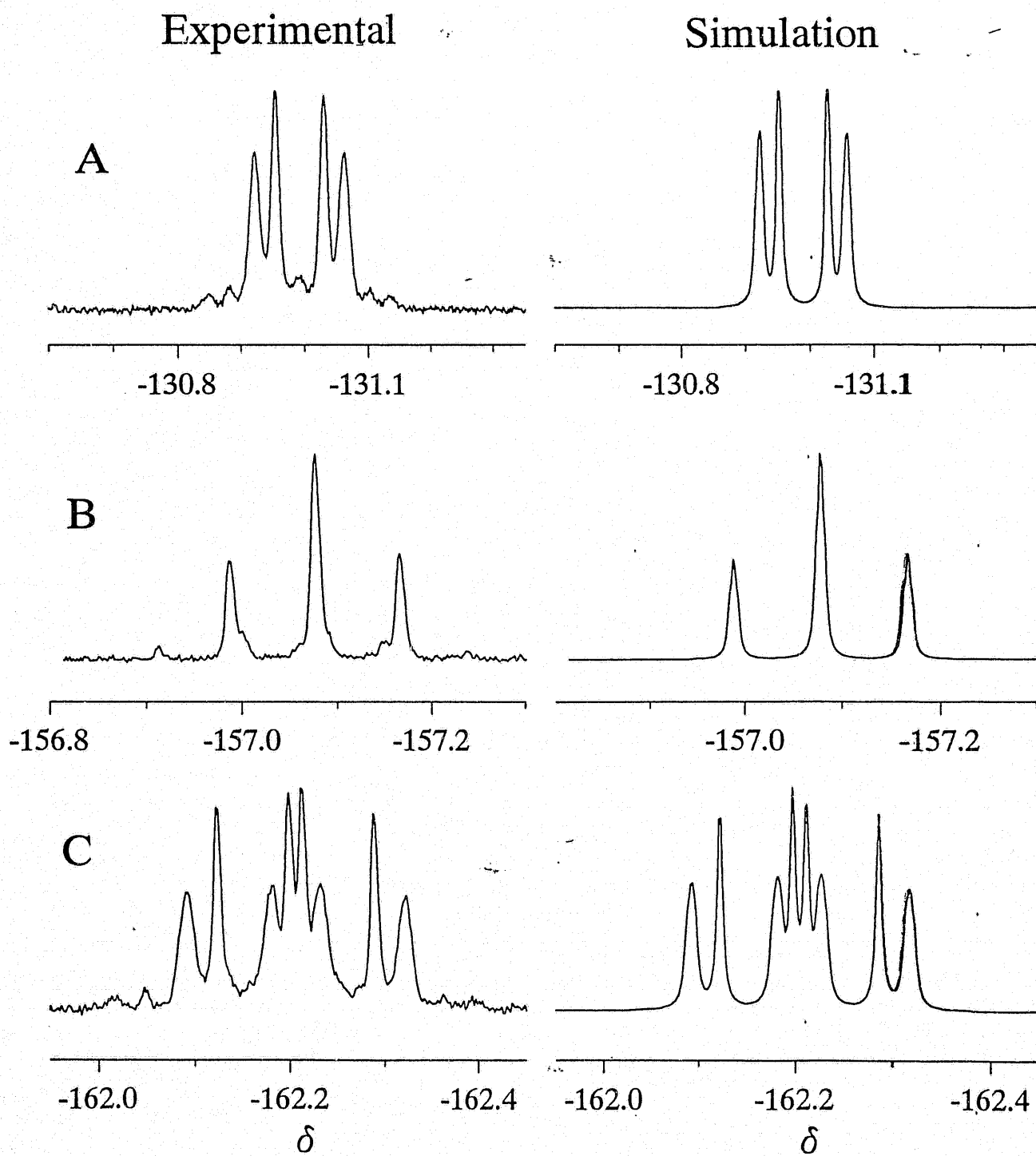
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2-2074-m1

Simulation of  $^{19}\text{F}$  NMR Spectra for Complex (5)

L-2074-m2



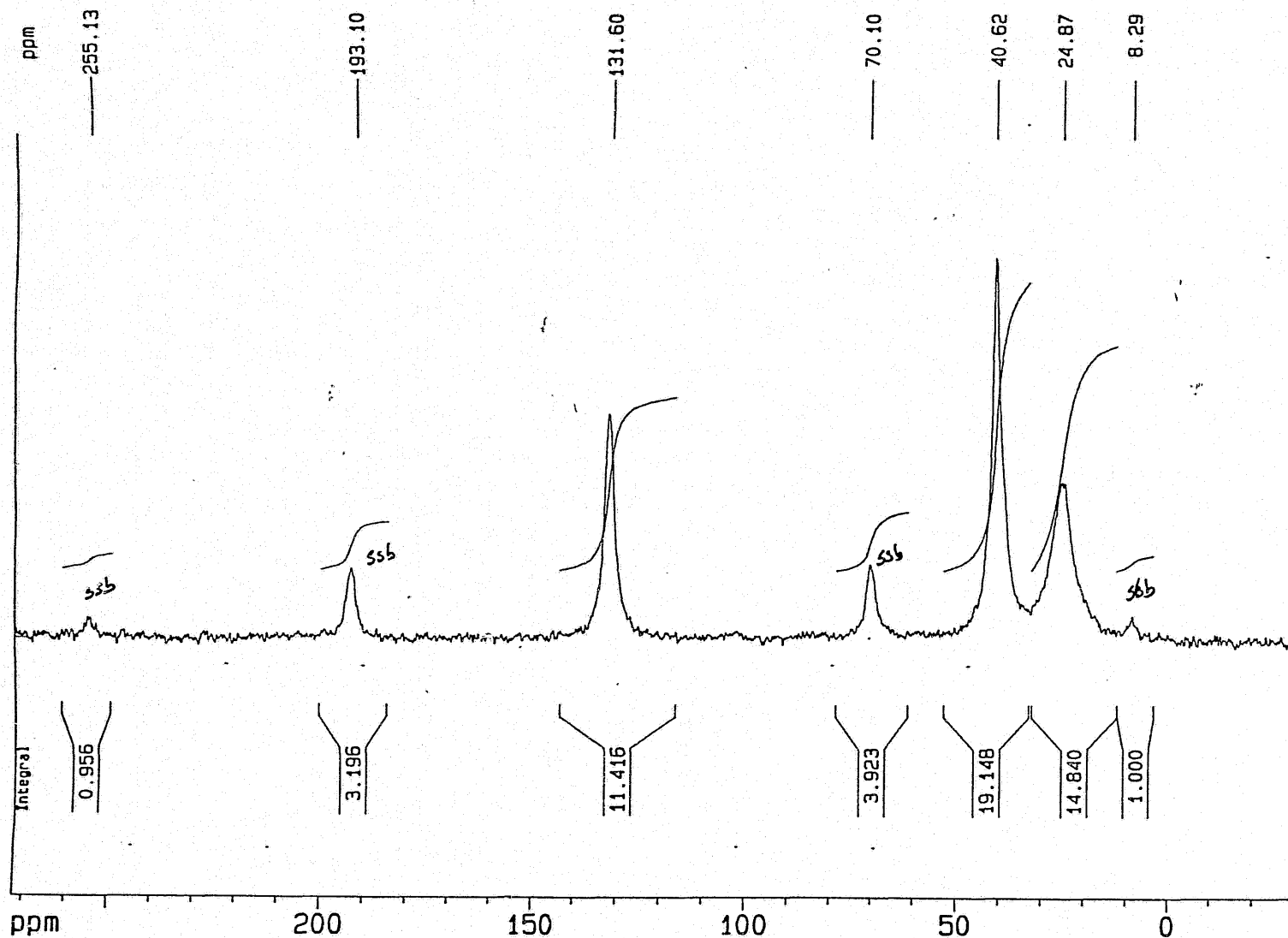
Simulation of  $^{19}\text{F}$  NMR Spectra for Complex (8)

**Table 1.** Coupling constants for pentafluorophenoxide (5) and pentafluorothiophenoxide (8) complexes.

Type	<i>ij</i>	Coupling (Hz)	
		(5)	(8)
AM <i>ortho</i>	23	-25.0 ( $\pm 0.2$ ) <sup>a</sup>	-24.8 ( $\pm 0.1$ ) <sup>a</sup>
AM' <i>para</i>	25	+5.5 ( $\pm 0.2$ ) <sup>a</sup>	+7.1 ( $\pm 0.2$ ) <sup>a</sup>
AA' <i>meta</i>	26	4.0 ( $\pm 0.5$ )	0.8 ( $\pm 0.2$ )
MM' <i>meta</i>	35	3.5 ( $\pm 0.5$ )	1.4 ( $\pm 0.2$ )
AX <i>meta</i>	24	6.0 ( $\pm 0.2$ )	1.0 ( $\pm 0.2$ )
MX <i>ortho</i>	34	-22.5 ( $\pm 0.2$ ) <sup>a</sup>	-21.0 ( $\pm 0.1$ ) <sup>a</sup>

<sup>a</sup> From analysis of the AA'MM'X spectra the relative sign of these  $J_{FF}$  couplings was obtained. Only the magnitude of the remaining  $J_{FF}$  couplings is reported.

Figure 3: Solid State CPMAS  $^{13}\text{C}$ -NMR Spectrum of Poly(1,3-Cyclohexadiene) Derived from Initiator 5



Current Data Parameters  
 NAME p14  
 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters  
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 Time 11.19  
 PULPROG cpmas  
 SOLVENT CDC13  
 AQ 0.0338250 sec  
 FIDRES 14.796402 Hz  
 DW 16.5 usec  
 RG 80  
 NUCLEUS  $^{13}\text{C}$   
 P3 4.0 usec  
 P17 1.5 usec  
 HL1 1 dB  
 D1 4.0000000 sec  
 TL0 16.00 dB  
 DL0 12.00 dB  
 P90 5.5 usec  
 SF02 400.1380650 MHz  
 P15 1000.0 usec  
 DE 20.6 usec  
 SF01 100.6264511 MHz  
 SWH 30303.03 Hz  
 TD 2048  
 NS 256  
 DS 0

F2 - Processing parameters  
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 WDW EM  
 SSB 0  
 LB 20.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
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 F1P 272.185 ppm  
 F1 27385.71 Hz  
 F2P -28.995 ppm  
 F2 -2917.32 Hz  
 PPMCM 15.13469 ppm/cm  
 HZCM 1522.76538 Hz/cm

L-2074-mf