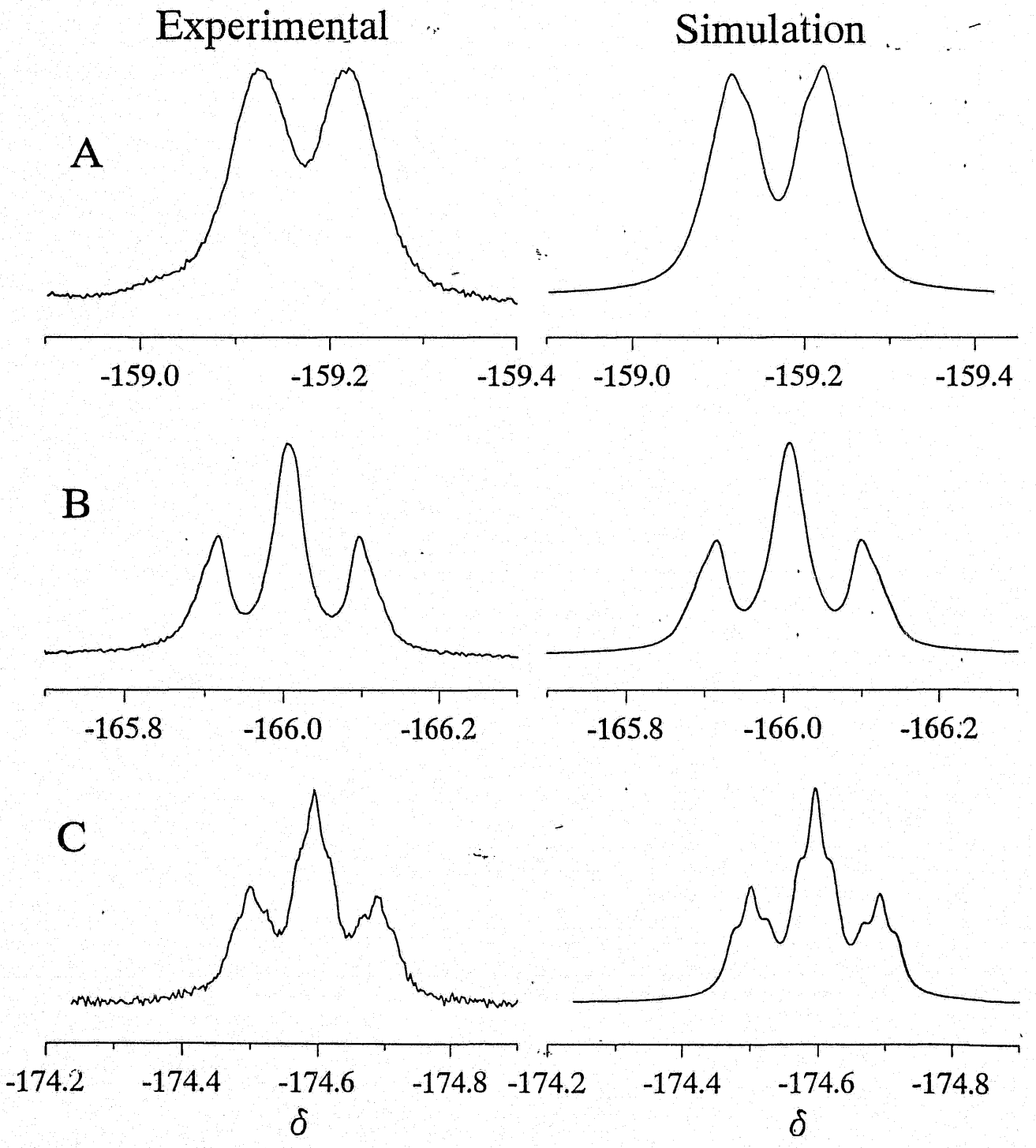
ORGANOMETALLICS

Supporting Information for *Organometallics*, **1994**, 13(5), 2066-2074, DOI: 10.1021/om00017a073

HAMPTON
2066-2074

Figure 1

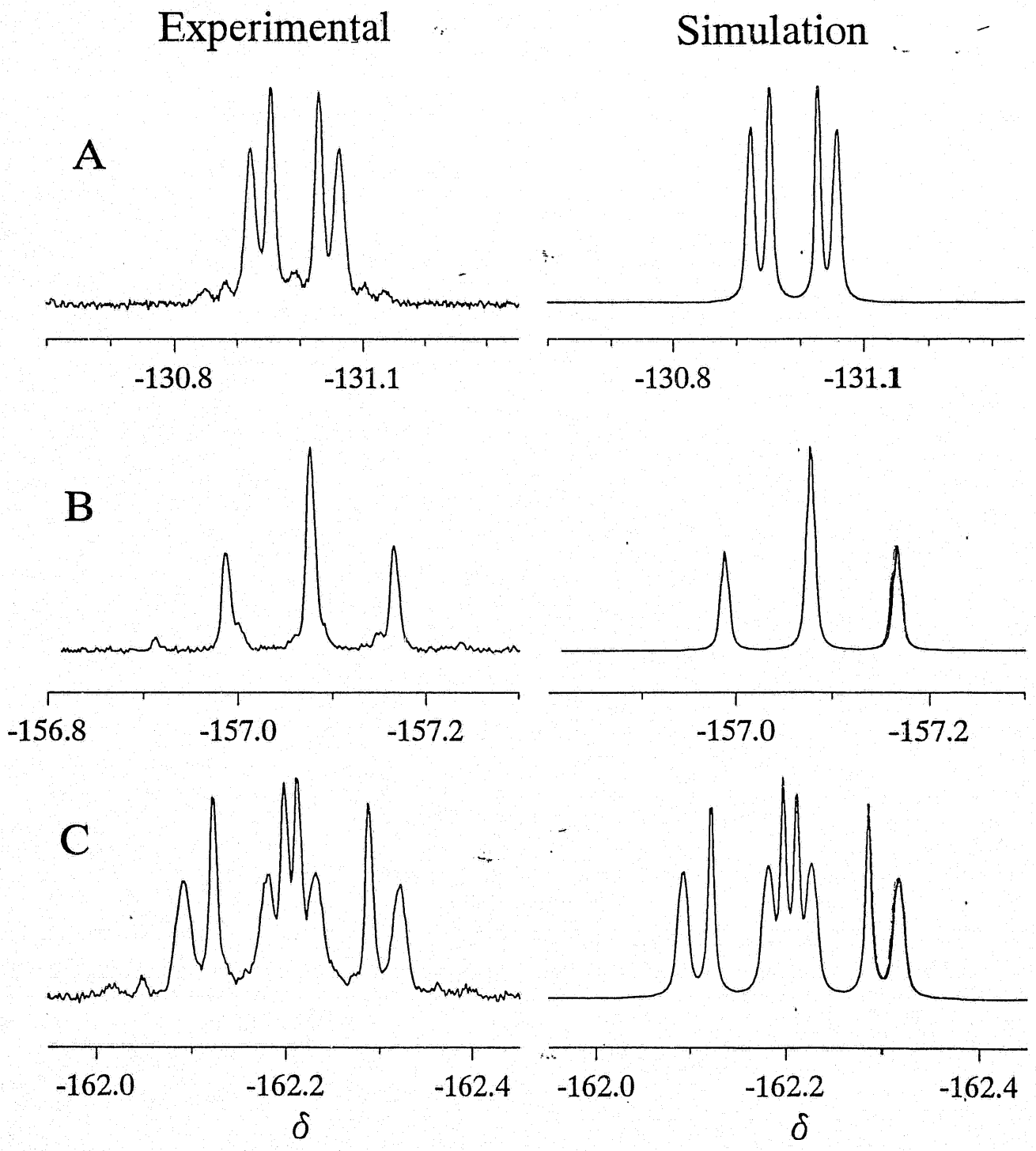
L-2074-M1



Simulation of ^{19}F NMR Spectra for Complex (**5**)

Figure 2

L-2074-M2



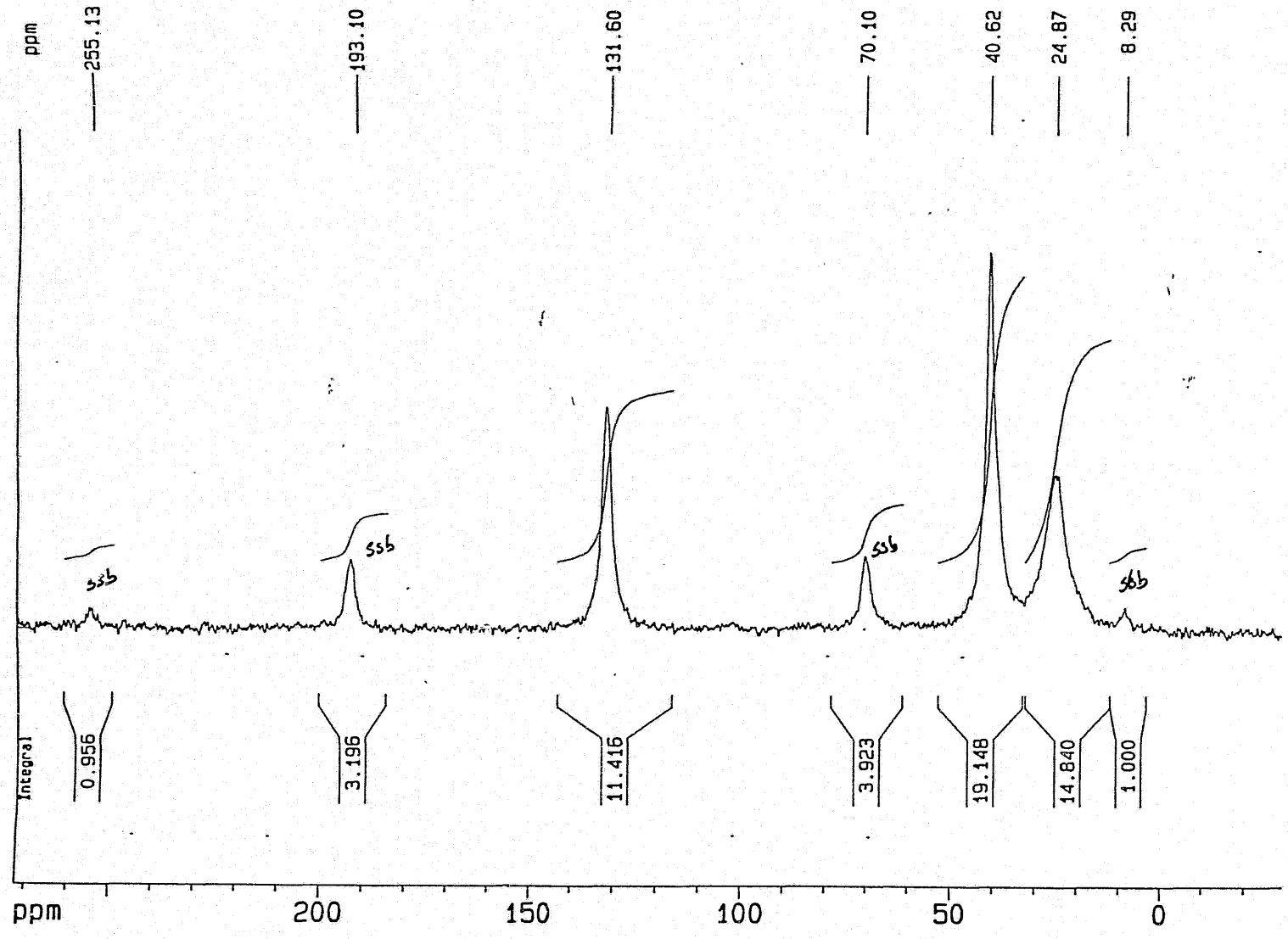
Simulation of ^{19}F NMR Spectra for Complex **(8)**

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

		Coupling (Hz)	
Type	*ij*	**(5)**	**(8)**
AM *ortho*	23	-25.0 (±0.2)[a]	-24.8 (±0.1)[a]
AM' *para*	25	+5.5 (±0.2)[a]	+7.1 (±0.2)[a]
AA' *meta*	26	4.0 (±0.5)	0.8 (±0.2)
MM' *meta*	35	3.5 (±0.5)	1.4 (±0.2)
AX *meta*	24	6.0 (±0.2)	1.0 (±0.2)
MX *ortho*	34	-22.5 (±0.2)[a]	- 21.0 (±0.1)[a]

[a] 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}C-NMR Spectrum of Poly(1,3-Cyclohexadiene) Derived from Initiator **5**



Current Data Parameters

NAME	p14
EXPNO	7
PROCNO	1

F2 - Acquisition Parameters

Date	930526
Time	11.19
PULPROG	cpmas
SOLVENT	CDCl3
AQ	0.0338250 sec
FIDRES	14.796402 Hz
DW	16.5 usec
RG	80
NUCLEUS	13C
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
SFO2	400.1380650 MHz
P15	1000.0 usec
DE	20.6 usec
SFO1	100.6264511 MHz
SWH	30303.03 Hz
TD	2048
NS	256
DS	0

F2 - Processing parameters

SI	4096
SF	100.6142169 MHz
WDW	EM
SSB	0
LB	20.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	19.90 cm
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