

ORGANOMETALLICS

Supporting Information for *Organometallics*, 1994, 13(5), 2066-2074, DOI: [10.1021/om00017a073](https://doi.org/10.1021/om00017a073)

HAMPTON 2066-2074

Terms & Conditions

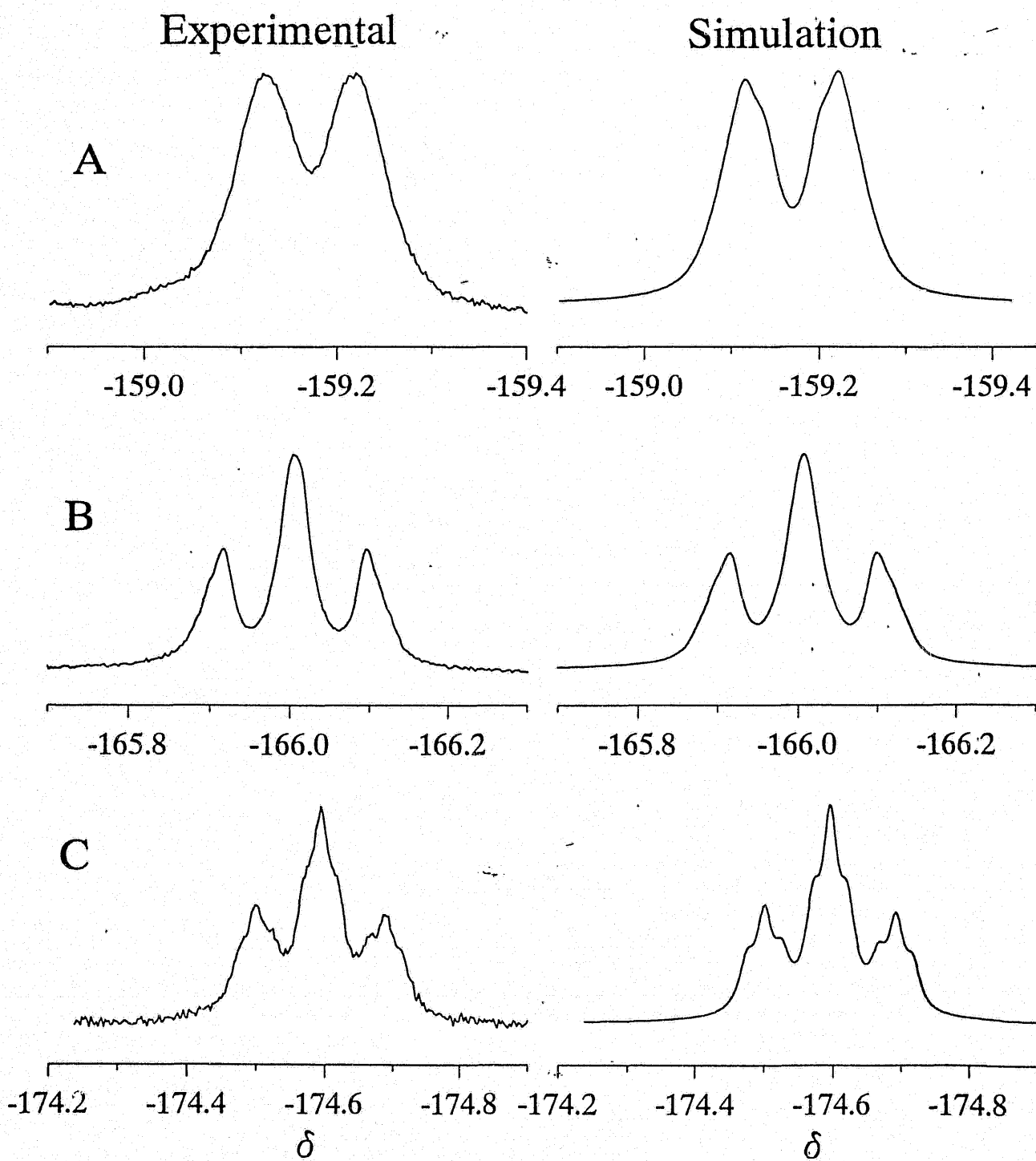
Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>.



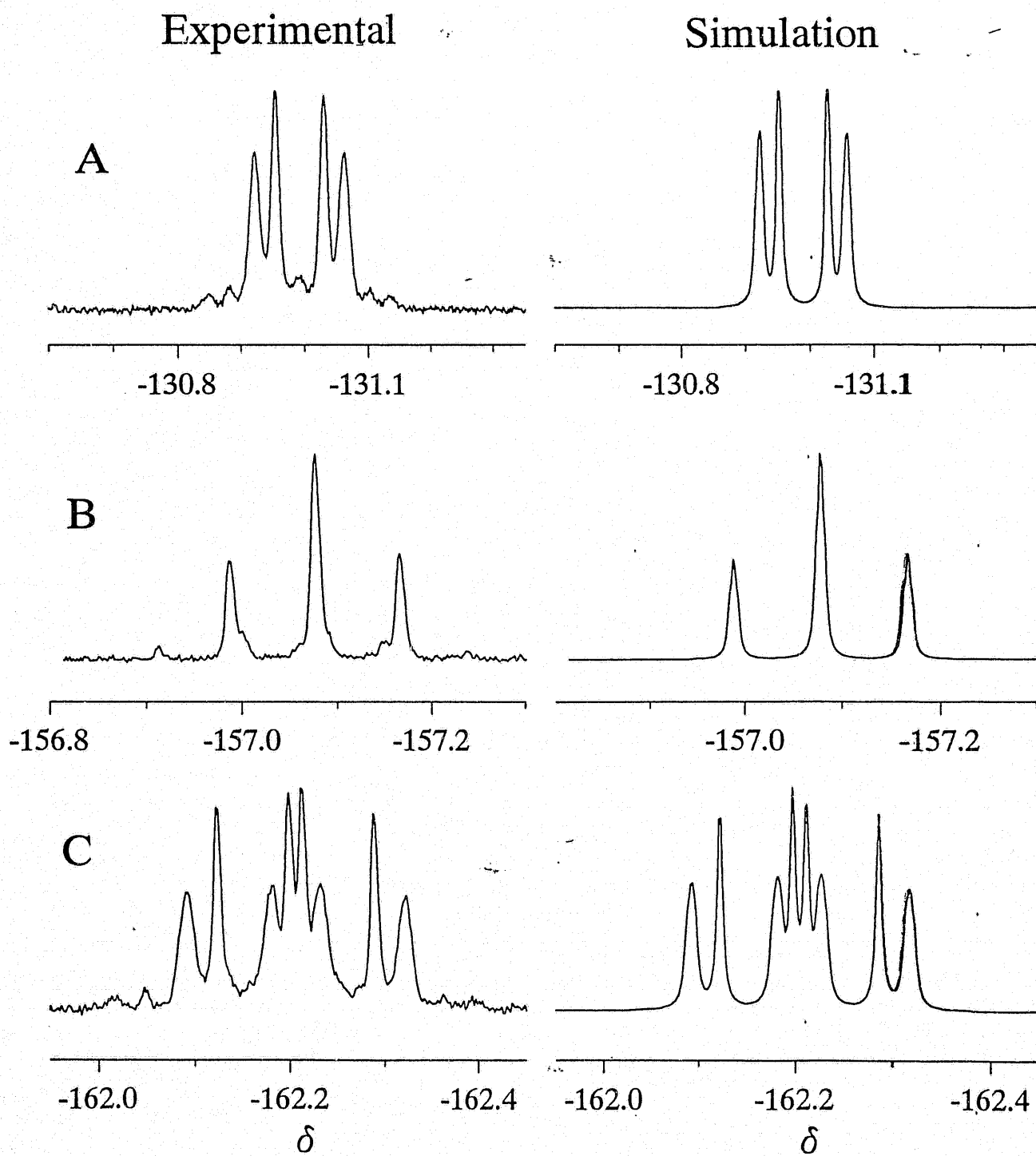
ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

2-2074-m1

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

L-2074-m2



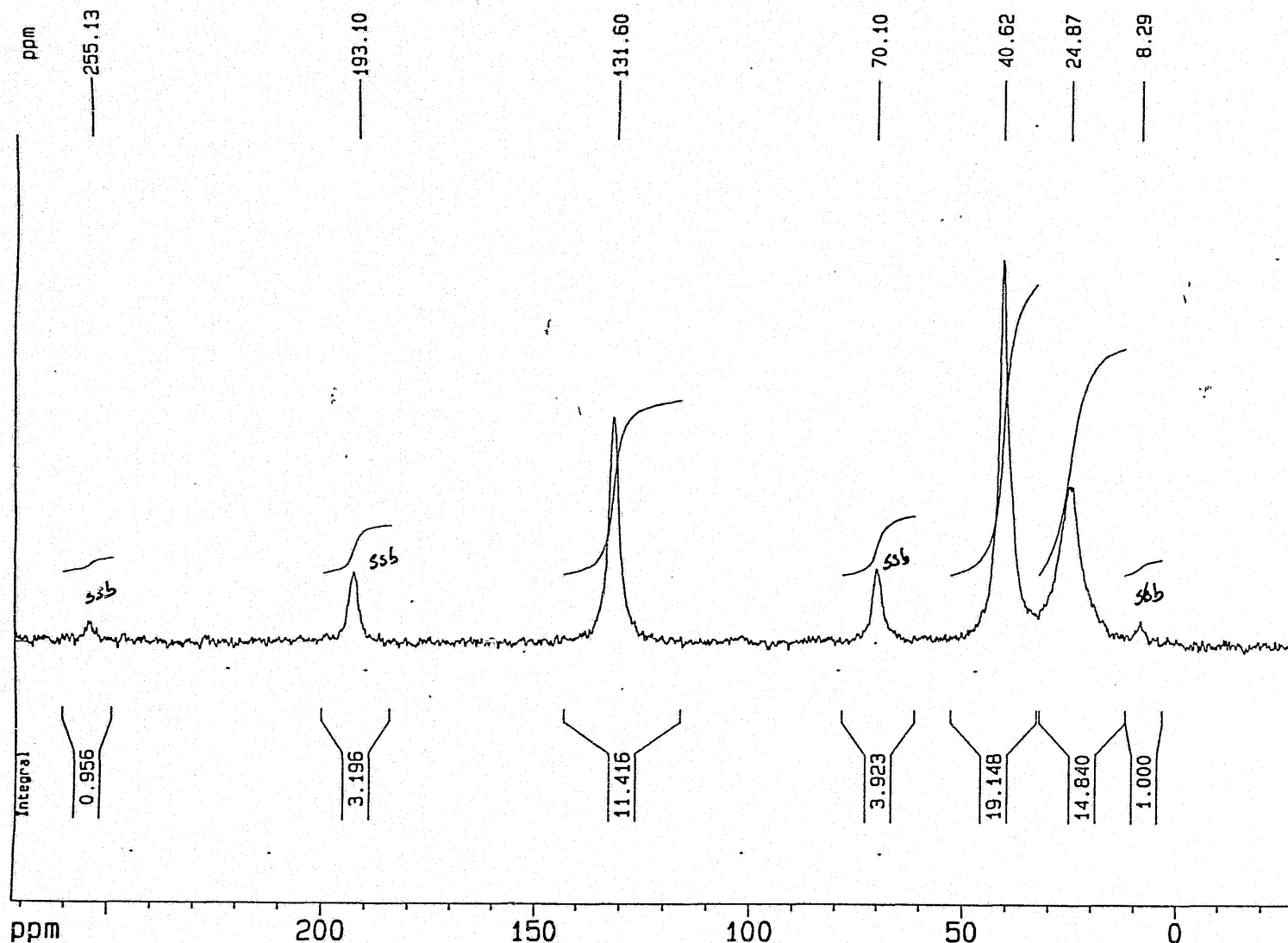
Simulation of ^{19}F NMR Spectra for Complex (8)

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 (± 0.2) ^a | -24.8 (± 0.1) ^a |
| AM' <i>para</i> | 25 | +5.5 (± 0.2) ^a | +7.1 (± 0.2) ^a |
| AA' <i>meta</i> | 26 | 4.0 (± 0.5) | 0.8 (± 0.2) |
| MM' <i>meta</i> | 35 | 3.5 (± 0.5) | 1.4 (± 0.2) |
| AX <i>meta</i> | 24 | 6.0 (± 0.2) | 1.0 (± 0.2) |
| MX <i>ortho</i> | 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 CDC13
 AQ 0.0338250 sec
 FIDRES 14.796402 Hz
 DW 16.5 usec
 RG 80
 NUCLEUS ^{13}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
 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

L-2074-mf