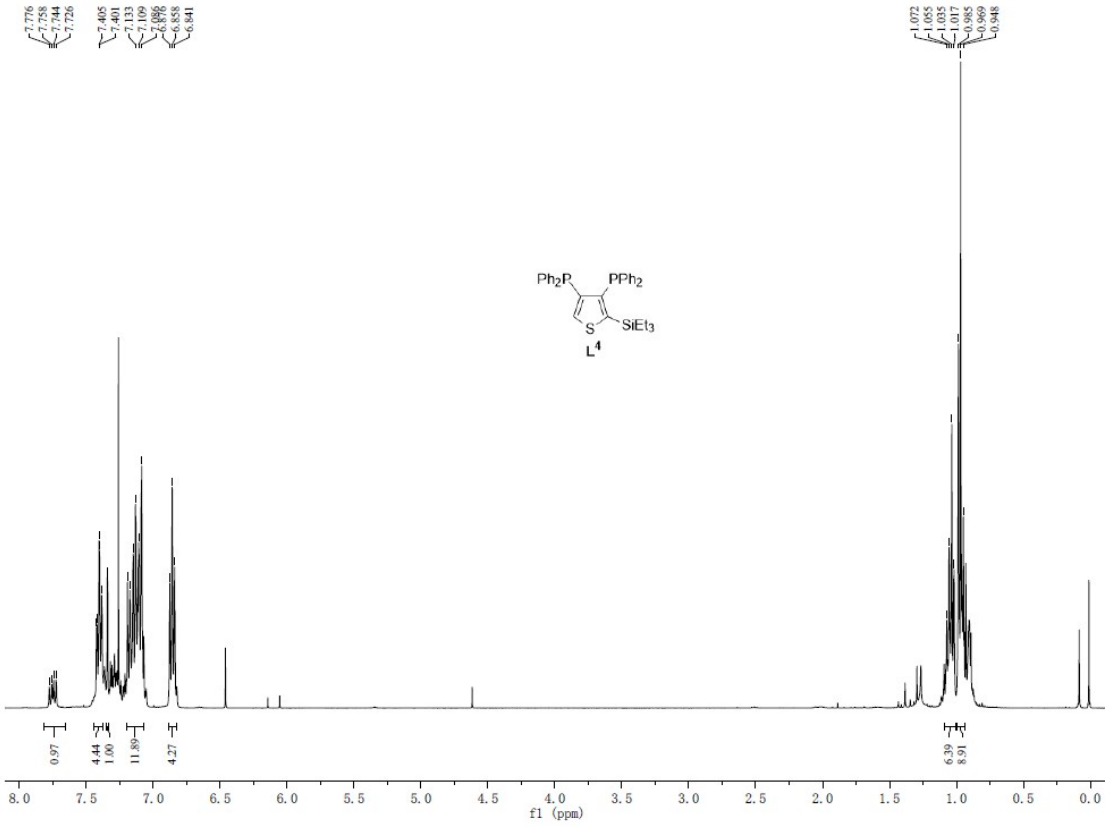
Electronic Supplementary Information for

Ethylene Tri-/Tetramerization Catalysts Supported by Diphosphinothiophene Ligands

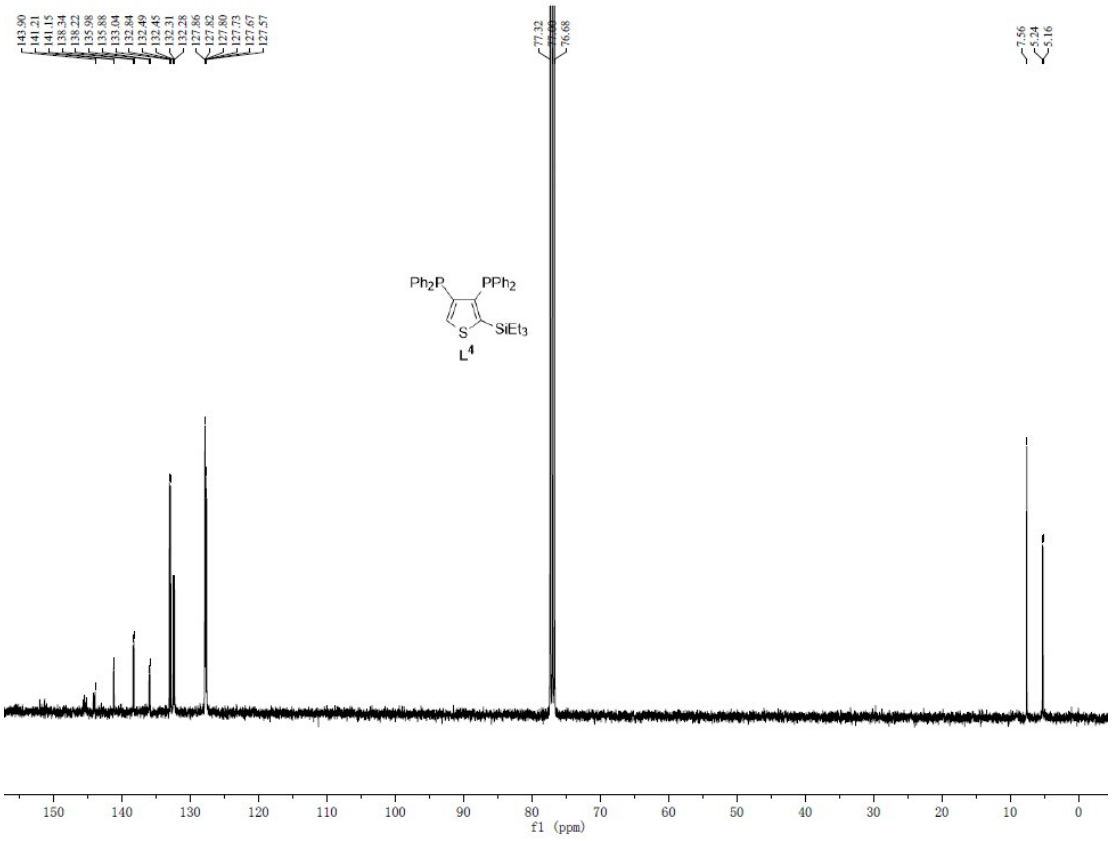
Chengye Zhang, Liubing Song, Hongfei Wu, Xiaoyu Ji, Jiajun Jiao, and Jun Zhang*

NMR Spectra:

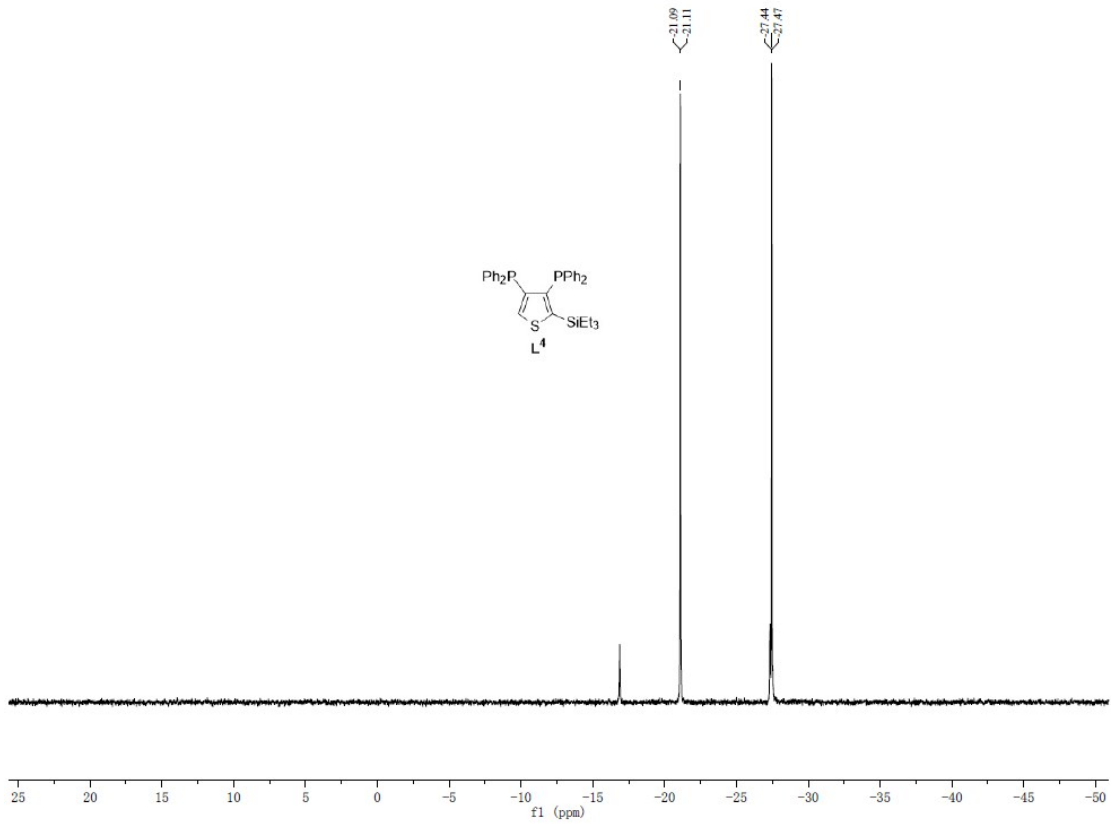
^{1}H NMR Spectrum of Ligand L^4



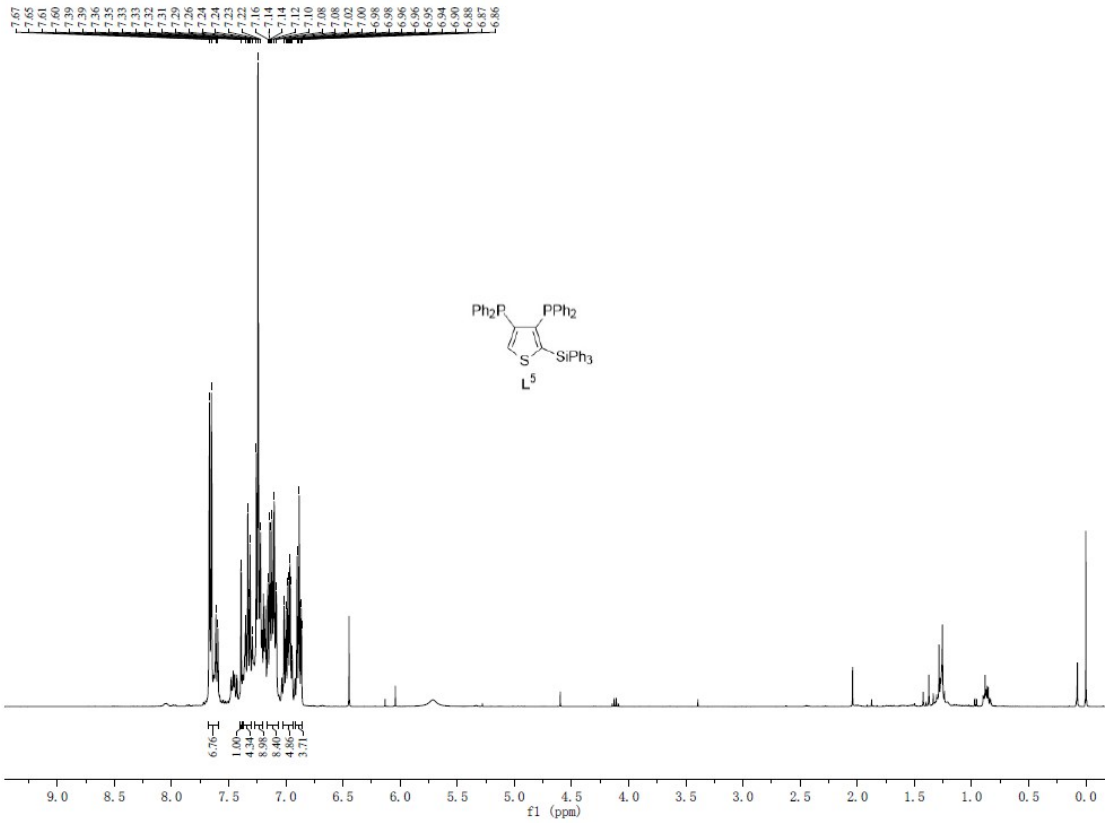
^{13}C NMR Spectrum of Ligand L^4



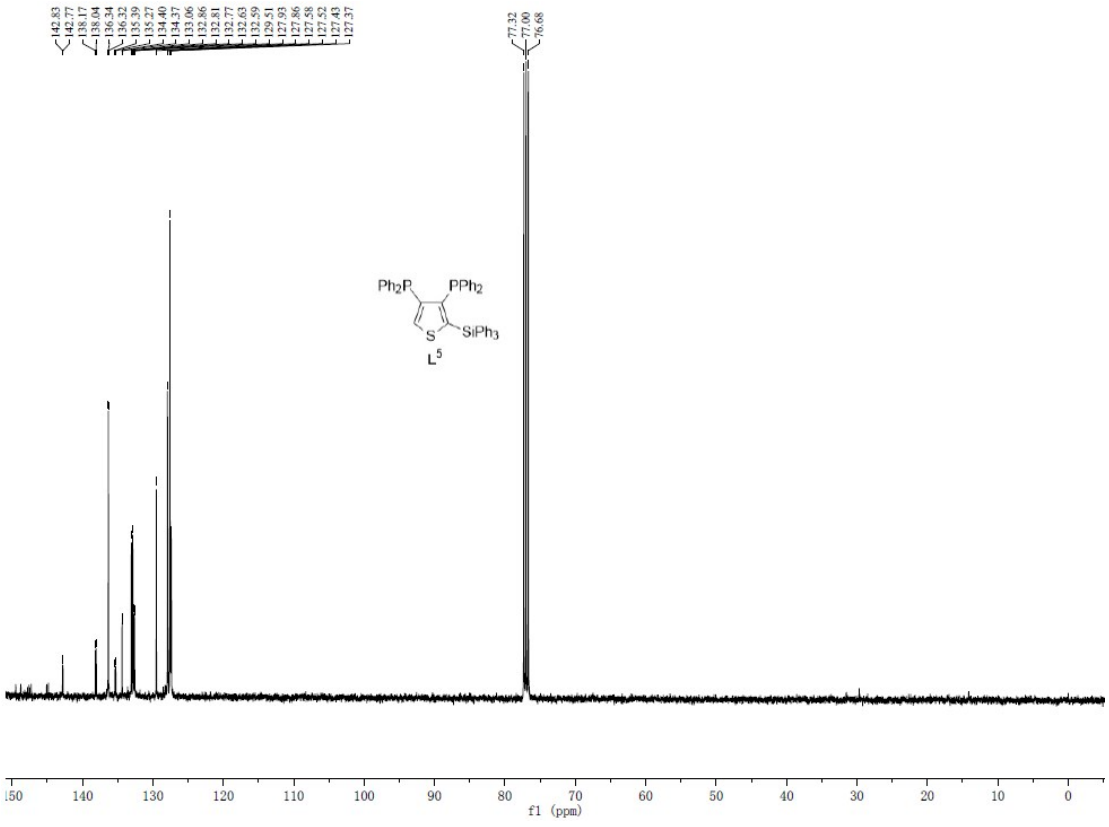
^{31}P NMR Spectrum of Ligand L^4



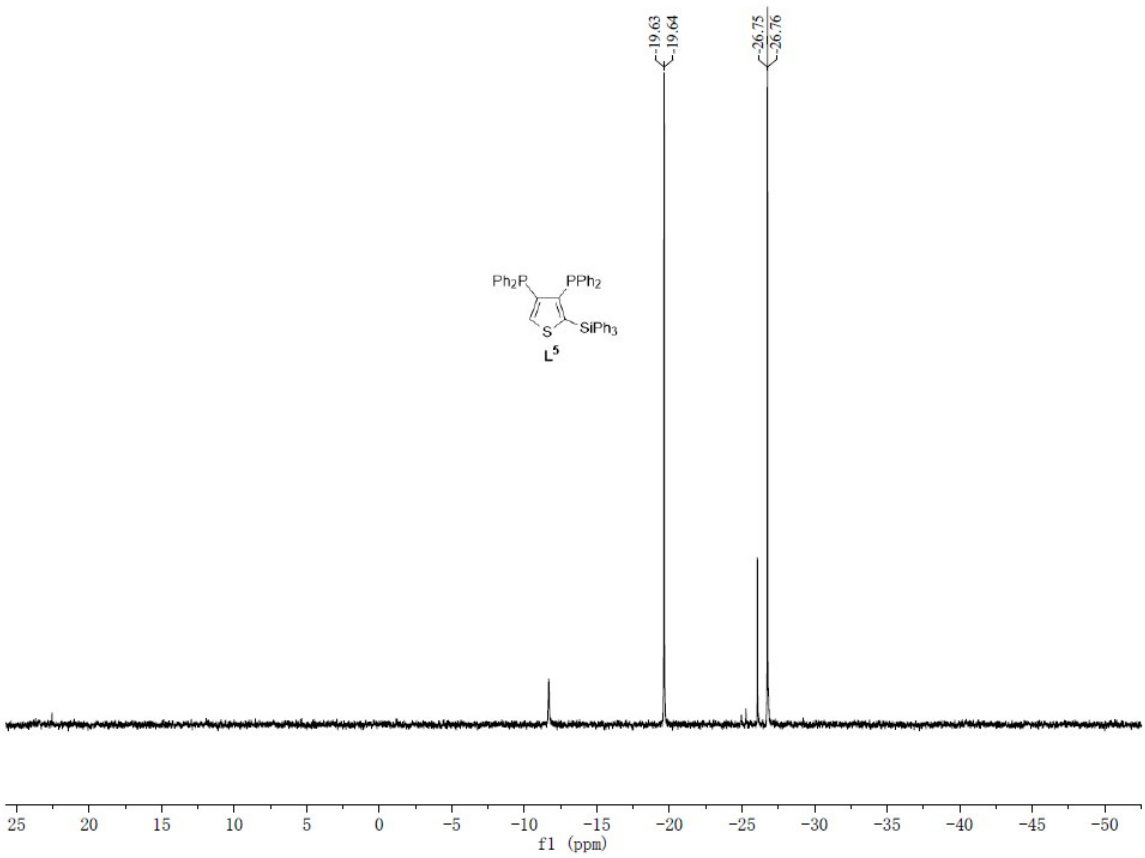
^{1}H NMR Spectrum of Ligand L^{5}



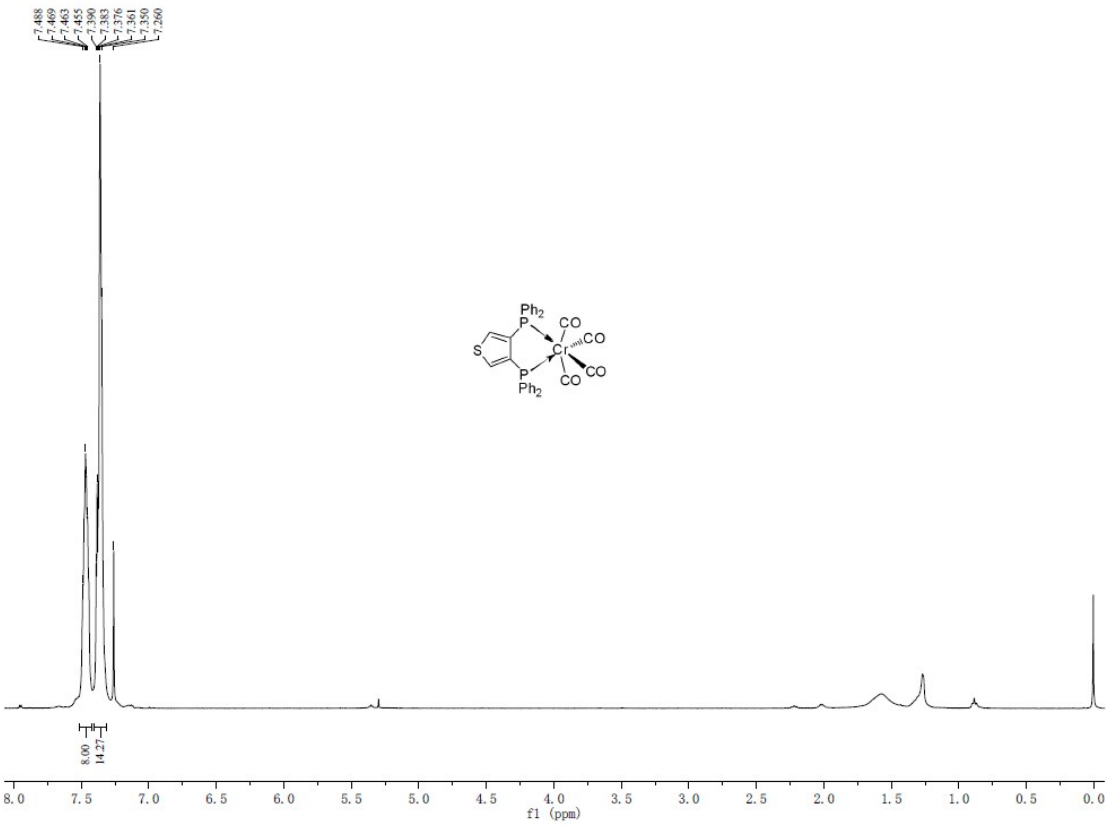
^{13}C NMR Spectrum of Ligand L^{5}



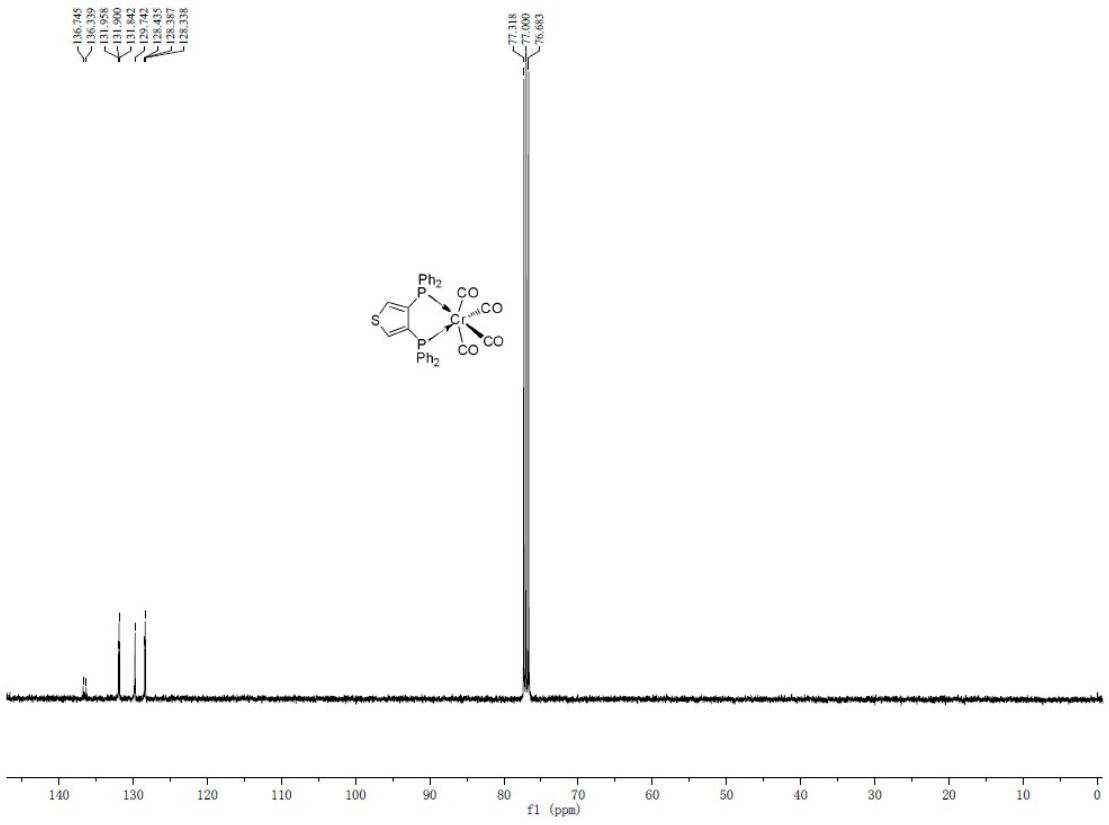
^{31}P NMR Spectrum of Ligand L^5



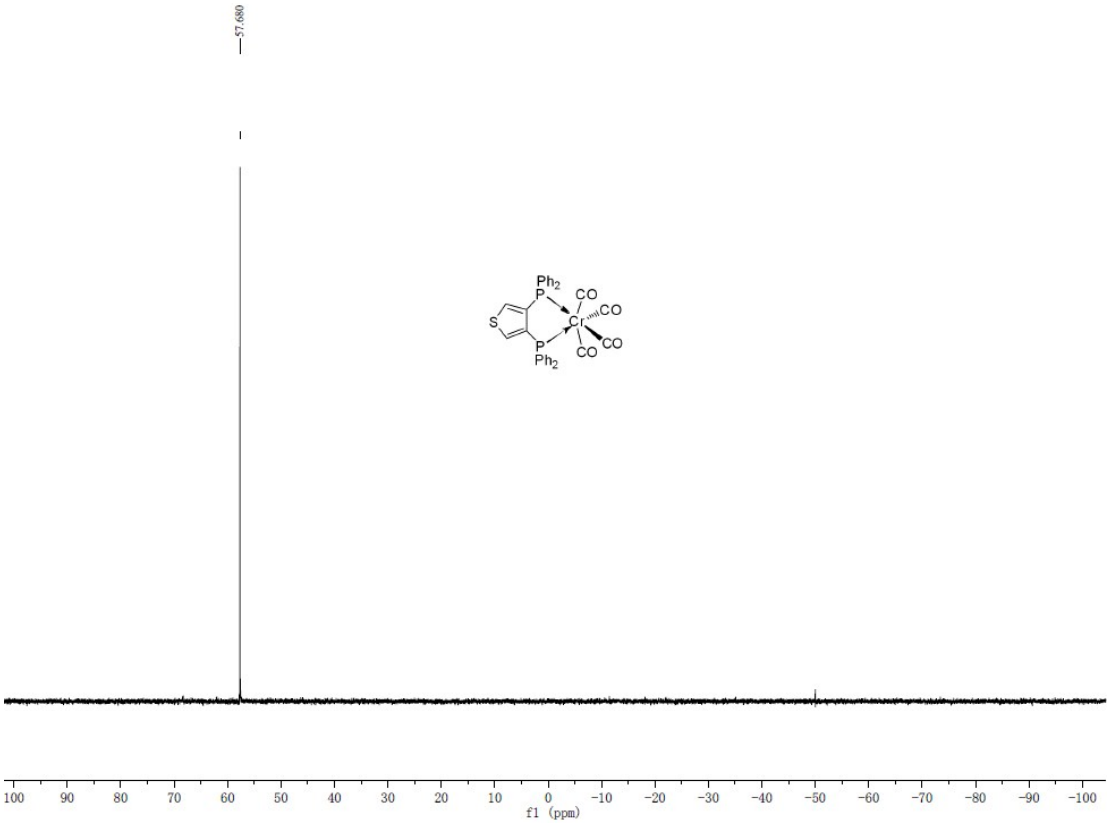
^{1}H NMR Spectrum of complex 1



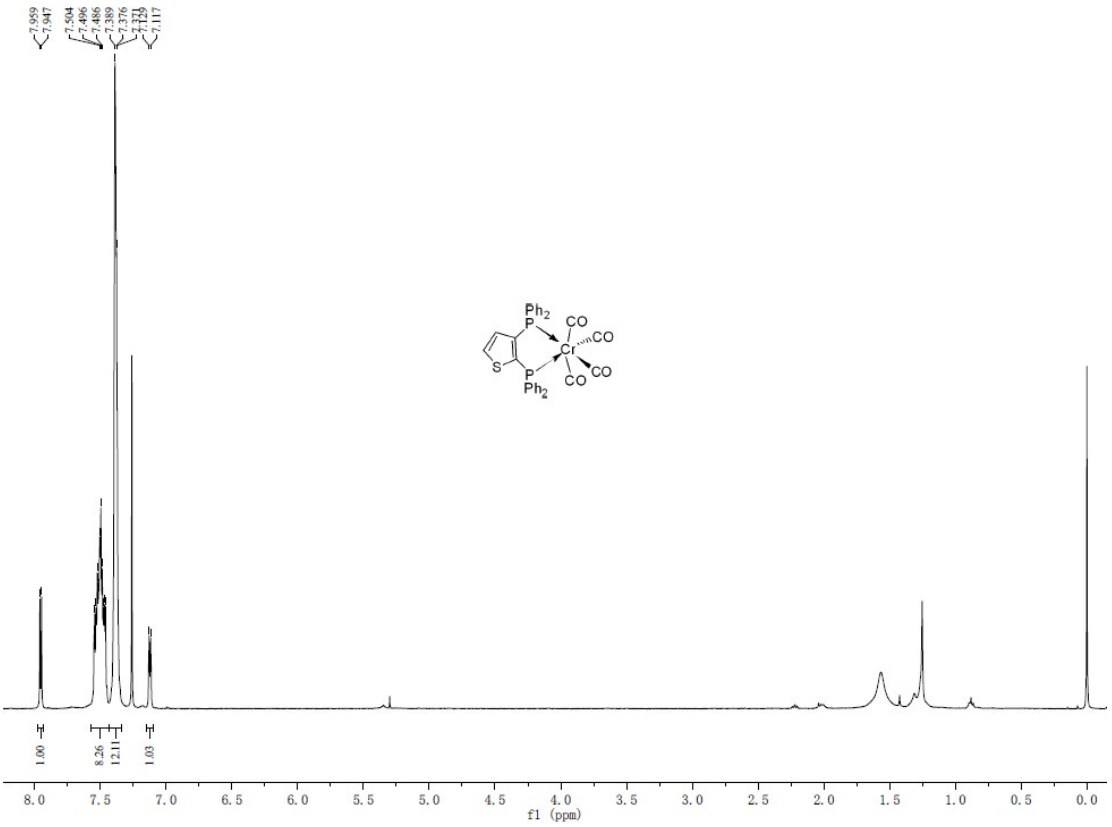
^{13}C NMR Spectrum of complex 1



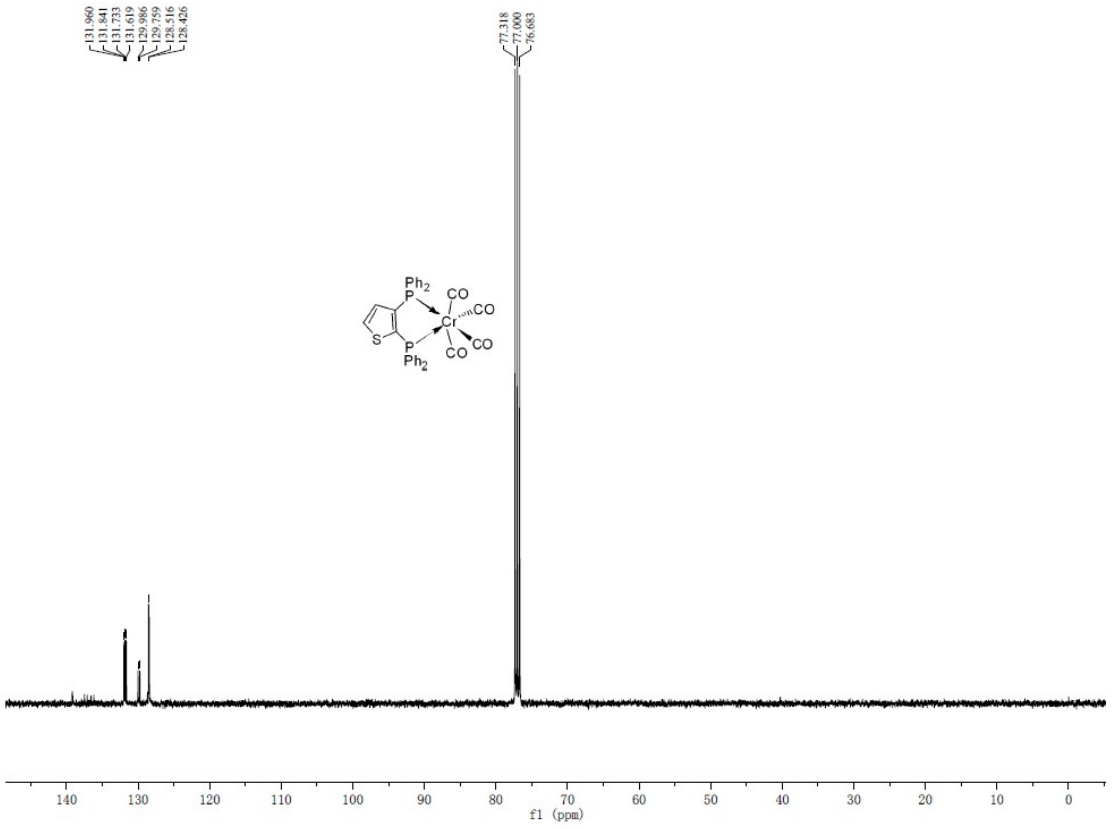
^{31}P NMR Spectrum of complex 1



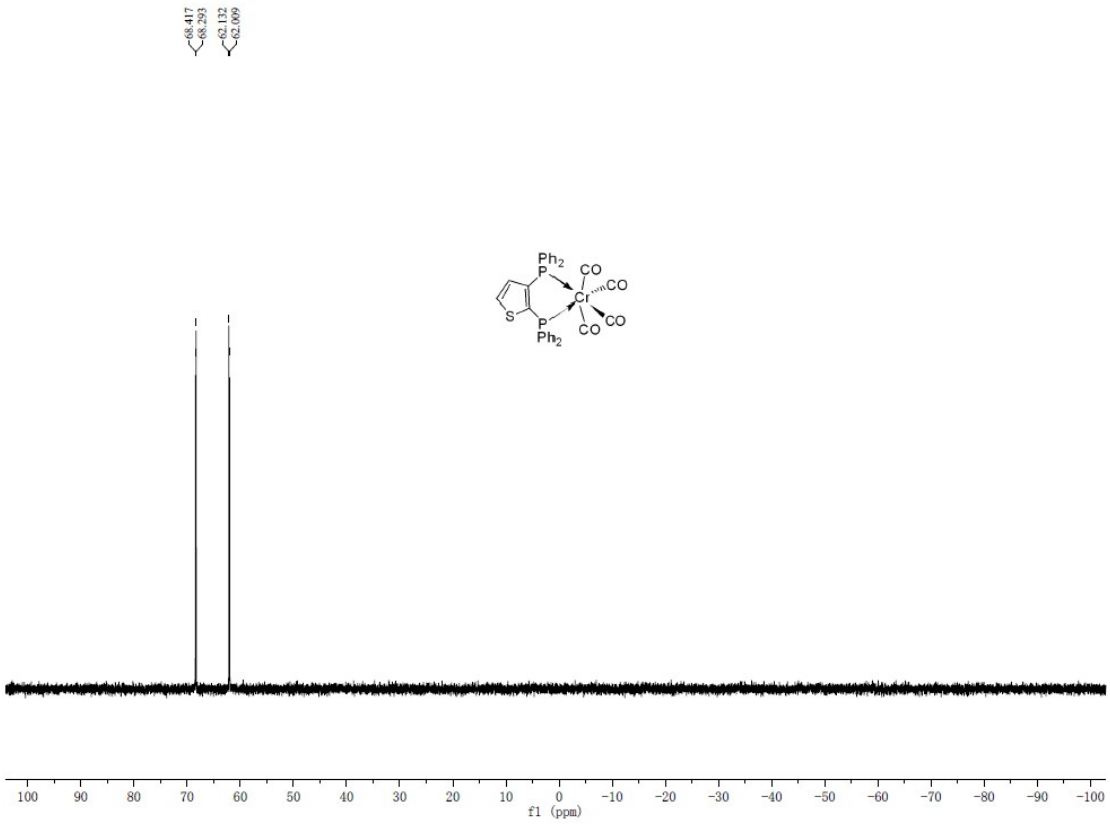
^{1}H NMR Spectrum of complex 2



^{13}C NMR Spectrum of complex 2



^{31}P NMR Spectrum of complex 2



X-Ray Crystallography. Each crystal was mounted on a glass fiber. Crystallographic measurements were made on a Bruker Smart Apex 100 CCD area detector using graphite monochromated Mo-Kαradiation ($\lambda_{\text{Mo-K}\alpha}$ = 0.71073 Å). The structures were solved by directed methods (SHELXS-97) and refined on F^2 by full-matrix least squares (SHELX-97) using all unique data. All the calculations were carried out with the SHELXTL18 program.

Key details of the crystal and structure refinement data are summarized in Table S1. Further crystallographic details may be found in the respective CIF files, which were deposited at the Cambridge Crystallographic Data Centre, Cambridge, UK [CCDC 1538907 (**1**) and 1538906 (**2**)].

Table S1. Crystal Data, Data Collection, and Structure Refinement for **1** and **2**

	1	**2**
Identification code	a60106c	mo_60325ba
CCDC No.	1538907	1538906
Formula	$C_{32}H_{22}Cr\ O_4P_2S$	$C_{32}H_{22}Cr\ O_4P_2S$
Formula weight	616.49	616.49
T, K	298(2) K	173(2) K
crystal system	Orthorhombic	Orthorhombic
space group	P n m a	Pnma
a, Å	16.801(7)	16.833(5)
b, Å	21.284(9)	21.330(6)
c, Å	7.993(4)	7.869(2)
α, deg	90°	90°
β, deg	90°	90°
γ, deg	90°	90°
Volume, Å ^{3}	2858 (2)	2825.3 (14)
Z	4	4
D_{calc}, Mg / m^3	1.433	1.449
absorption coefficient,	0.622	0.629
F(000)	1264	1264
crystal size, mm	0.250 x 0. 200 x 0.150	0.210 x 0.150 x 0.080
2θ range, deg	1.914 to 26.997°	1.909 to 27.070°.
reflections	10156	17126
data / restraints /	3150 / 0 / 190	3171/ 0 / 190
goodness of fit on F^2	0.830	1.008
final R indices [I >2σ(I)][a]	R1 = 0.0423, wR2 = 0.0782	R1 = 0.0443, wR2 = 0.0982
R indices (all data)	R1 = 0.0816, wR2 = 0.0829	R1 = 0.0833, wR2 = 0.1147
lgst diff peak and hole,	0.547 and -0.390	0.367 and -0.272