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Supporting Information for

Synthesis and Oxygen to Iron Methyl Migration Reaction of the Heterodinuclear
Methoxycarbyne Complex $\text{Cp}(\text{CO})\text{Fe}(\mu\text{-COCH}_3)(\mu\text{-CO})\text{Cr}(\text{CO})(\eta^6\text{-C}_6\text{H}_6)$

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Variable temperature NMR data^a

cmpd (cis:trans)	¹ H	¹³ C	solvent	T (°C)	$\nu_{1/2}$ (Hz) ^b	k^c (s ⁻¹)
6-Na ⁺ (63:37)	x		CD ₃ CN	-50	1.9	14±2
	x			-40	1.3	55±5
	x			-20	3.8	500±50
	x			0	3.8	4000±1000
	x			22	1.1	>5000
6-Na ⁺ (63:37)		x	CD ₃ CN	-50	2.77	12±2
		x		22	2.77	≥15000
7 (82:18)	x		CD ₂ Cl ₂	-20	1.5	0.6 ± 0.4
	x			-10	1.5	2±1
	x			22	1.5	25±5
7 (75:25)		x	CD ₂ Cl ₂	-20	2.9	<1
		x		22	3.37	55±5
7d 59:41	x		toluene-d ₈	-20	1.5	2.0±0.5
55:45	x			-10	1.5	3±1
52:48	x			0	1.5	20±5
47:53	x			20	1.5	180±40
42:58	x			40	1.5	700±200

^aChemical shifts are those reported in the Experimental Section at the lowest temperature except as noted. ^bPeak width of non-exchanging peak (solvent). ^cAll rate constants are for cis to trans isomerization. ^cChemical shifts are extrapolated from the three lowest temperatures as described in the text; values used (in ppm) are as follows:

T (°C)	trans benzene	trans Cp	cis benzene	cis Cp	cis MeO	trans MeO
-20.000	4.587	4.578	4.450	4.317	4.212	4.191
-10.000	4.595	4.570	4.466	4.320	4.227	4.215
0.000	4.599	4.558	4.482	4.327	4.243	4.243
20.000	4.612	4.539	4.514	4.336	4.282	4.282
40.000	4.624	4.519	4.546	4.346	4.319	4.319