

SUPPORTING INFORMATION for:

Synthesis and Characterization of Five-Coordinate, 16-Electron Ru^{II} Complexes Supported by Tridentate Bis(phosphino)silyl Ligation

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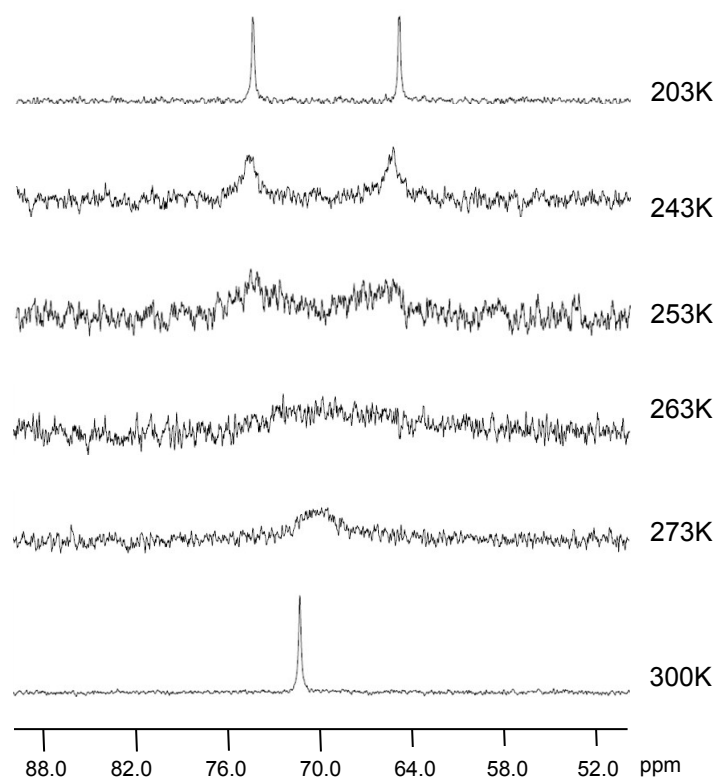


Figure S1. Variable-temperature $^{31}\text{P}\{^1\text{H}\}$ NMR spectra (toluene- d_8) of **9**.

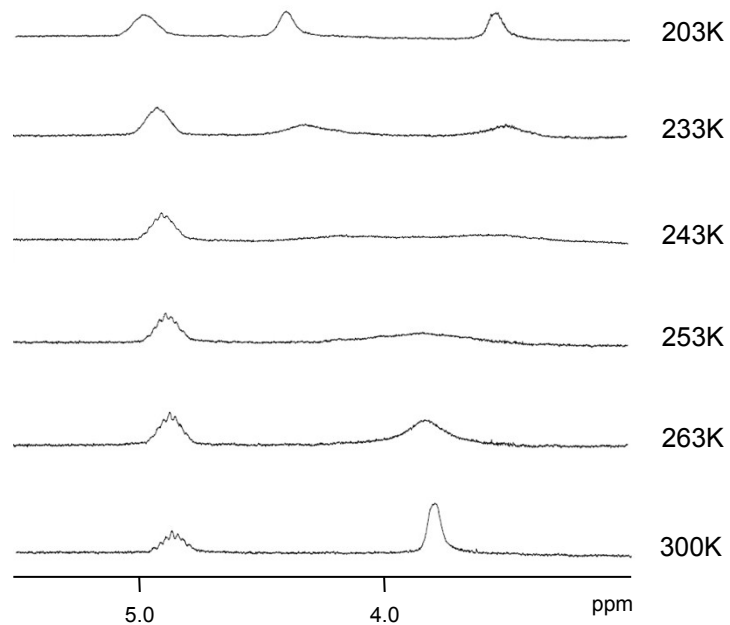


Figure S2. Variable-temperature ^1H NMR spectra (toluene- d_8) of **9**.

Table S1. Crystallographic data **3**, **4**, **5**, **9** and **11**.

	3	4	5	9	11
Empirical formula	C ₄₀ H ₆₄ ClP ₃ RuSi	C ₄₀ H ₆₁ P ₃ RuSi	C ₄₀ H ₆₅ P ₃ RuSi·(C ₅ H ₁₂) _{0.875}	C ₄₀ H ₆₀ P ₂ RuSi	C ₄₀ H ₆₄ N ₃ P ₃ RuSi
Formula weight	802.43	763.96	831.12	731.98	809.01
Crystal dimensions	0.41 × 0.39 × 0.22	0.46 × 0.36 × 0.31	0.36 × 0.35 × 0.05	0.37 × 0.36 × 0.12	0.44 × 0.38 × 0.04
Crystal system	triclinic	triclinic	tetragonal	triclinic	triclinic
Space group	<i>P</i>	<i>P</i>	<i>I</i> <i>2m</i>	<i>P</i>	<i>P</i>
<i>a</i> (Å)	10.3409 (5)	10.5218 (5)	22.5341 (9)	9.8037 (3)	10.3984 (4)
<i>b</i> (Å)	10.5020 (5)	12.5407 (6)	22.5341 (9)	10.8919 (3)	10.5102 (4)
<i>c</i> (Å)	18.9852 (9)	15.2414 (7)	17.3711 (7)	18.5073 (5)	19.0001 (8)
α (deg)	95.6088 (5)	87.6054 (5)	90	73.1497 (3)	95.6660 (5)
β (deg)	92.0827 (5)	70.3495 (5)	90	92.4226 (3)	92.3748 (5)
γ (deg)	101.5544 (5)	89.9268 (5)	90	79.5330 (3)	102.1706 (5)
<i>V</i> (Å ³)	2007.03 (17)	1892.16 (15)	8820.8 (6)	1858.13 (9)	2015.78 (14)
<i>Z</i>	2	2	8	2	2
ρ_{calcd} (g cm ⁻³)	1.328	1.341	1.252	1.308	1.333
μ (mm ⁻¹)	0.634	0.600	0.520	0.567	0.569
Range of transmission	0.8706–0.7803	0.8367–0.7686	0.9724–0.8344	0.9330–0.8185	0.9787–0.7878
2 θ limit (deg)	55.30	55.08	52.90	55.12	55.08
	-13 ≤ <i>h</i> ≤ 13	-13 ≤ <i>h</i> ≤ 13	-28 ≤ <i>h</i> ≤ 28	-12 ≤ <i>h</i> ≤ 12	-13 ≤ <i>h</i> ≤ 13
	-13 ≤ <i>k</i> ≤ 13	-16 ≤ <i>k</i> ≤ 16	-28 ≤ <i>k</i> ≤ 28	-14 ≤ <i>k</i> ≤ 14	-13 ≤ <i>k</i> ≤ 13
	-24 ≤ <i>l</i> ≤ 24	-19 ≤ <i>l</i> ≤ 19	-21 ≤ <i>l</i> ≤ 21	-23 ≤ <i>l</i> ≤ 24	-24 ≤ <i>l</i> ≤ 24
Total data collected	17730	16781	35591	16463	17901
Independent reflections	9159	8620	4722	8480	9205
<i>R</i> _{int}	0.0112	0.0121	0.0447	0.0100	0.0184
Data/restraints/parameters	9159 / 0 / 415	8620 / 0 / 410	4722 / 0 / 233	8480 / 0 / 398	9205 / 0 / 433
Goodness-of-fit	1.041	1.071	1.058	1.121	1.041
<i>R</i> ₁ [<i>F</i> _o ² ≥ 2σ(<i>F</i> _o ²)]	0.0211	0.0225	0.0251	0.0202	0.0252
<i>wR</i> ₂ [<i>F</i> _o ² ≥ -3σ(<i>F</i> _o ²)]	0.0549	0.0647	0.0619	0.0626	0.0650
Largest peak, hole (eÅ ⁻³)	0.504, -0.343	0.880, -0.477	0.990 and -0.202	0.361, -0.401	0.475, -0.444