For Supporting Information: "Reversible Haptotropic Shift in Zirconocene-Hexapentaene Complexes" by Noriyuki Suzuki et al.

Table S. Crystal data and structure refinement for **5b**, **6b**, **8** and **9**.

Complex	**5b**	**6b**	**8**	**9**
Empirical Formula	$C_{32}H_{46}Zr$	$C_{35}H_{55}PZr$	$C_{42}H_{64}N_2Zr$	$C_{37}H_{55}NZr$
Formula Weight	521.94	598.01	688.20	605.07
Crystal Color, Habit	yellow, block	yellow, needle	yellow, needle	yellow, block
Crystal Dimensions	0.15 × 0.10 × 0.05 mm	0.48 × 0.03 × 0.01 mm	0.10 × 0.02 × 0.02 mm	0.45 × 0.15 × 0.14 mm
Crystal System	monoclinic	orthorhombic	triclinic	monoclinic
Lattice Type	C-centered	Primitive	Primitive	Primitive
Space Group	*C2/c* (#15)	$P2_12_12_1$ (#19)	*P–1* (#2)	$P2_1/c$ (#14)
Lattice Parameters	*a* = 24.592(12) Å	*a* = 8.306(2) Å	*a* = 8.161(3) Å	*a* = 10.6733(9) Å
	b = 8.945(3) Å	*b* = 18.527(5) Å	*b* = 22.558(6) Å	*b* = 21.1693(19) Å
	c = 15.421(7) Å	*c* = 21.323(5) Å	*c* = 23.013(4) Å	*c* = 16.3627(16) Å
			α = 110.75(4)	
	β = 123.972(8) °		β = 96.16(4)	β = 107.8940(16) °
			γ = 96.57(5)	
	V = 2813(2) Å^3	*V* = 3281.4(14) Å^3	*V* = 3885.3(18) Å^3	*V* = 3518.3(6) Å^3
Z value	4	4	4	4
Absorption coefficient	4.074 cm^{-1}	4.041 cm^{-1}	3.120 cm^{-1}	3.351 cm^{-1}
Radiation	MoKα (λ = 0.71073 Å) graphite monochromated	MoKα (λ = 0.71073 Å) graphite monochromated	Synchrotron (λ = 0.800 Å) Si(111) monochromated on SPring-8 BL26B1	MoKα (λ = 0.71073 Å) Graphite monochromated
Temperature	90 K	90 K	90 K	90 K
No. of Reflections Measured	Total: 8759 Unique: 3211 (R_{int} = 0.058)	Total: 17159 Unique: 9185 (R_{int} = 0.033)	Total: 20664 Unique: 10538 (R_{int} = 0.082)	Total: 90364 Unique: 10266 (R_{int} = 0.038)
Corrections	Lorentz-polarization Absorption(trans. factors: 0.867 - 0.980)	Lorentz-polarization Absorption (trans. factors: 0.807 - 0.996)	Lorentz-polarization Absorption (trans. factors: 0.492 - 0.940)	Lorentz-polarization Absorption (trans. factors: 0.839 - 0.954)
No. of Reflections	3211	9185	10538	10240
No. Variables	171	375	866	573
Reflection/Parameter Ratio	18.78	24.49	12.17	17.81
Residuals: *R*; *wR* (All data)	0.0625; 0.0960	0.0521	0.161; 0.355	0.0462; 0.1001
Residuals: R_1	0.0497	0.0433	0.114	0.0430
No. of Reflections to	2743	8213	7846	9603