From bis(imidazole-2-thion-4-yl)phosphane to a flexible P-bridged bis(NHC) ligand and its silver complex

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Table S1. Crystal data and structure refinement for **3**

Device Type	Bruker X8-KappaApexII	
Empirical formula	$C_{22}H_{31}N_4OPS_2$	
Moiety formula	$C_{22}H_{31}N_4OPS_2$	
Formula weight	462.60	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P\,2_1/c$	
Unit cell dimensions	a = 11.2305(9) Å	α = 90°
	b = 19.7226(17) Å	β = 104.669(3)°
	c = 11.1563(10) Å	γ = 90°
Volume, Z	2390.5(4) Å^3, 4	
Calculated density	1.285 mg/m^3	
Absorption coefficient	0.311 mm^{-1}	
F(000)	984	
Crystal size	0.09 × 0.06 × 0.02 mm	
Theta range for data collection	3.78 to 28.00°	
Limiting indices	$-14 \le h \le 11$, $-25 \le k \le 23$, $-10 \le l \le 14$	
Reflections collected / unique	12276 / 5725 [R(int) = 0.0430]	
Completeness to theta = 28.00	99.1 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9938 and 0.9726	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5725 / 0 / 279	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2sigma(I)]	R_1 = 0.0421, wR_2 = 0.0884	
R indices (all data)	R_1 = 0.0774, wR_2 = 0.0999	
Largest diff. peak and hole	0.509 and -0.382 e.Å^{-3}	