Electronic Supplementary Information

for

Nickel Complexes Incorporating an Amido Phosphine Chelate with a Pendant Amine Arm: Synthesis, Structure, and Catalytic Kumada Coupling

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Table S1. Crystal data and structure refinement for $\{Li[PNN]\}_2$.

Identification code	a7162	
Empirical formula	C44 H48 Li2 N4 P2	
Formula weight	708.68	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 16.1085(4) Å	α= 90°.
	b = 14.1250(5) Å	β= 109.3690(10)°.
	c = 18.6374(6) Å	γ = 90°.
Volume	4000.6(2) $Å^3$	
Z	4	
Density (calculated)	1.177 Mg/m^3	
Absorption coefficient	0.144 mm^{-1}	
F(000)	1504	
Crystal size	0.35 x 0.32 x 0.1 mm^3	
Theta range for data collection	1.97 to 25.02°.	
Index ranges	-18<=h<=19, -16<=k<=16, -22<=l<=22	
Reflections collected	26529	
Independent reflections	7006 [R(int) = 0.0486]	
Completeness to theta = 25.02°	99.2 %	
Absorption correction	multiscan	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7006 / 0 / 469	
Goodness-of-fit on F^2	0.629	
Final R indices [I>2sigma(I)]	R1 = 0.0449, wR2 = 0.1229	
R indices (all data)	R1 = 0.0671, wR2 = 0.1512	
Largest diff. peak and hole	0.398 and -0.349 $e.Å^{-3}$	

Table S2. Crystal data and structure refinement for [PNN]NiCl.

Identification code	a7129	
Empirical formula	C22 H24 Cl N2 Ni P	
Formula weight	441.56	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 10.034(3) Å	α= 90°.
	b = 10.622(3) Å	β= 100.008(13)°.
	c = 19.542(5) Å	γ = 90°.
Volume	2051.2(10) $Å^3$	
Z	4	
Density (calculated)	1.430 Mg/m^3	
Absorption coefficient	1.163 mm^{-1}	
F(000)	920	
Crystal size	0.2 x 0.1 x 0.05 mm^3	
Theta range for data collection	2.12 to 20.11°.	
Index ranges	-9<=h<=8, -10<=k<=10, -18<=l<=18	
Reflections collected	10908	
Independent reflections	1943 [R(int) = 0.1551]	
Completeness to theta = 20.11°	99.5 %	
Absorption correction	multiscan	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1943 / 0 / 238	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R1 = 0.0583, wR2 = 0.1052	
R indices (all data)	R1 = 0.1238, wR2 = 0.1240	
Largest diff. peak and hole	0.533 and -0.371 $e.Å^{-3}$	

Table S3. Crystal data and structure refinement for [PNN]NiBr.

Identification code	8776	
Empirical formula	C22 H24 Br N2 Ni P	
Formula weight	486.02	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 9.1844(4) Å	α= 90°.
	b = 11.8541(5) Å	β= 91.546(2)°.
	c = 18.9047(10) Å	γ = 90°.
Volume	2057.46(17) $Å^3$	
Z	4	
Density (calculated)	1.569 Mg/m^3	
Absorption coefficient	2.972 mm^{-1}	
F(000)	992	
Crystal size	0.14 x 0.11 x 0.03 mm^3	
Theta range for data collection	2.16 to 25.04°.	
Index ranges	-10<=h<=10, -13<=k<=14, -22<=l<=22	
Reflections collected	13481	
Independent reflections	3619 [R(int) = 0.1238]	
Completeness to theta = 25.04°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8354 and 0.6856	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3619 / 0 / 245	
Goodness-of-fit on F^2	1.093	
Final R indices [I>2sigma(I)]	R1 = 0.0758, wR2 = 0.1742	
R indices (all data)	R1 = 0.1434, wR2 = 0.2308	
Extinction coefficient	0.0182(19)	
Largest diff. peak and hole	1.298 and -1.145 $e.Å^{-3}$	

Table S4. Crystal data and structure refinement for [PNN]NiMe.

Identification code	3145	
Empirical formula	C23 H27 N2 Ni P	
Formula weight	421.15	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.3899(3) Å	α= 102.5040(10)°.
	b = 10.5707(3) Å	β= 92.234(2)°.
	c = 11.3703(5) Å	γ = 117.474(2)°.
Volume	1067.67(6) $Å^3$	
Z	2	
Density (calculated)	1.310 Mg/m^3	
Absorption coefficient	0.993 mm^{-1}	
F(000)	444	
Crystal size	0.14 x 0.06 x 0.06 mm^3	
Theta range for data collection	2.24 to 24.98°.	
Index ranges	-11<=h<=12, -12<=k<=12, -13<=l<=11	
Reflections collected	10003	
Independent reflections	3727 [R(int) = 0.0625]	
Completeness to theta = 24.98°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9428 and 0.8735	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3727 / 0 / 245	
Goodness-of-fit on F^2	1.117	
Final R indices [I>2sigma(I)]	R1 = 0.0520, wR2 = 0.1295	
R indices (all data)	R1 = 0.1004, wR2 = 0.1883	
Largest diff. peak and hole	0.589 and -0.932 $e.Å^{-3}$	

Table S5. Crystal data and structure refinement for [PNN]NiEt.

Identification code	3374	
Empirical formula	C24 H29 N2 Ni O P	
Formula weight	451.17	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 15.2700(2) Å	α= 90°.
	b = 9.27600(10) Å	β= 99.7350(10)°.
	c = 32.8820(4) Å	γ = 90°.
Volume	4590.49(10) $Å^3$	
Z	8	
Density (calculated)	1.306 Mg/m^3	
Absorption coefficient	0.932 mm^{-1}	
F(000)	1904	
Crystal size	0.6 x 0.48 x 0.22 mm^3	
Theta range for data collection	2.13 to 25.02°.	
Index ranges	-18<=h<=17, -10<=k<=10, -39<=l<=39	
Reflections collected	31891	
Independent reflections	8024 [R(int) = 0.0696]	
Completeness to theta = 25.02°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8161 and 0.5925	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8024 / 0 / 554	
Goodness-of-fit on F^2	0.890	
Final R indices [I>2sigma(I)]	R1 = 0.0496, wR2 = 0.1432	
R indices (all data)	R1 = 0.0630, wR2 = 0.1675	
Extinction coefficient	0.0304(15)	
Largest diff. peak and hole	0.892 and -1.283 $e.Å^{-3}$	

Table S6. Crystal data and structure refinement for [PNN]Ni(*n*-hexyl).

Identification code	8383	
Empirical formula	C28 H37 N2 Ni P	
Formula weight	491.28	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.7598(3) Å	α= 68.739(2)°.
	b = 10.5483(2) Å	β= 73.9460(10)°.
	c = 14.2416(4) Å	γ = 89.1460(10)°.
Volume	1307.11(6) $Å^3$	
Z	2	
Density (calculated)	1.248 Mg/m^3	
Absorption coefficient	0.821 mm^{-1}	
F(000)	524	
Crystal size	0.34 x 0.11 x 0.05 mm^3	
Theta range for data collection	2.08 to 25.42°.	
Index ranges	-11<=h<=11, -12<=k<=12, -16<=l<=17	
Reflections collected	16017	
Independent reflections	4792 [R(int) = 0.0608]	
Completeness to theta = 25.42°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9291 and 0.8183	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4792 / 0 / 284	
Goodness-of-fit on F^2	1.145	
Final R indices [I>2sigma(I)]	R1 = 0.0669, wR2 = 0.1673	
R indices (all data)	R1 = 0.0983, wR2 = 0.2051	
Extinction coefficient	0.085(8)	
Largest diff. peak and hole	0.891 and -0.962 $e.Å^{-3}$	