Electronic Supplementary Material (ESI) for Green Chemistry

Supporting information for:

Direct, One-Pot Synthesis of POCOP-Type Pincer Complexes from Metallic Nickel

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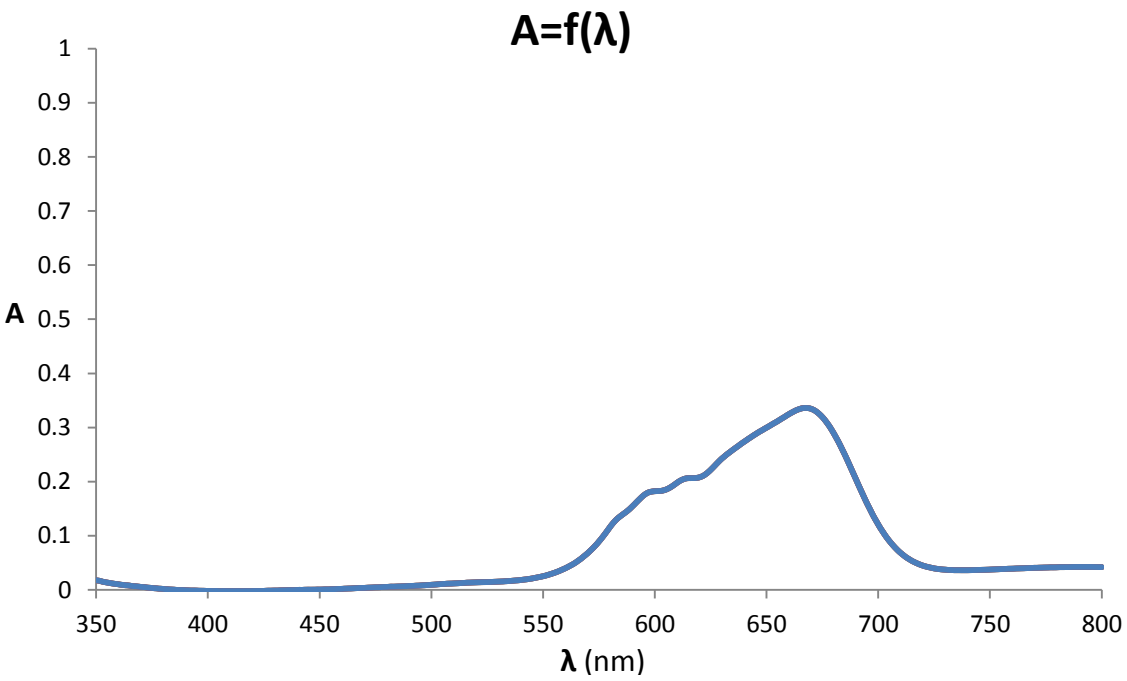
Table 1 : Crystal Data Collection and Refinement Parameters for Compound **2, 3** and **4**

Compound	**2**	**3**	**4**
chemical formula	$C_{19}H_{33}ClNiO_3P_2$	$C_{20}H_{33}ClNiO_4P_2$	$C_{26}H_{47}ClNiO_2P_2$
Fw	465.55	493.56	547.74
T (K)	100	150	200
wavelength (Å)	1.54178	1.54178	1.54178
space group	C2/c	P2(1)/c	P2(1)/n
a (Å)	18.8143(2)	15.9080 (12)	10.4275(4)
b (Å)	18.2714(2)	13.0746 (10)	14.0330(5)
c (Å)	14.9031(2)	11.1340 (8)	20.5730(7)
α (deg)	90	90	90.00
β (deg)	117.8053(4)	91.464	101.1800(10)
γ (deg)	90	90	90.00
Z	8	4	4
V (Å^3)	4531.62(9)	2315.0 (3)	2953.30(18)
ρcalcd (g cm^{-3})	1.365	1.416	1.232
μ (mm-1)	3.778	3.766	2.944
θ range (deg)	3.59 - 71.18	2.78 - 69.76	3.84 - 72.53
R_1[a] [I > 2ó(I)]	0.0253	0.0304	0.0448
wR_2[b] [I > 2ó(I)]	0.0951	0.0844	0.1176
R_1 [all data]	0.0265	0.0305	0.0464
wR_2 [all data]	0.0984	0.0845	0.1192
GOF	0.918	1.004	1.074

[a] $R_1=\Sigma(||F_o|-|F_c||)/\Sigma|F_o|$ [b] $wR_2=\{\Sigma[w(F_o^2-Fc^2)^2]/\Sigma[w(F_o^2)^2]\}^{½}$



Spectre 1 : UV-vis spectra (CH_2Cl_2, r.t.) of a sample of Co (0) one pot reaction.