Supporting Information for "Synthesis, Electrochemistry, Spectroelectrochemistry and Solid State Structures of Palladium Biferrocenylphosphines and Their Use in C,C Cross-Coupling Reactions"

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Table S1: Crystal and Intensity Collection Data for **15**, **16**, **21**, **23** and **25**.

	15	**16**	**21**	**23**	**25**
chemical formula	$C_{34}H_{31}Fe_2PSe$	$C_{28}H_{32}Fe_2O_2PSe$	$C_{44}H_{60}Fe_2P_2Se_2$	$C_{66}H_{58}Cl_6Fe_4P_2Pd$	$C_{172}H_{142}Cl_{16}Fe_{12}O_{12}P_6Pd_3$
fw	661.22	613.09	920.48	1455.56	4143.28
temperature [K]	105	105	100	100	105
cryst syst	monoclinic	monoclinic	triclinic	triclinic	triclinic
space group	P2(1)	P2(1)/c	P	P	P
a [Å]	12.0722(7)	15.7202(5)	8.1138(4)	9.8163(9)	10.7582(4)
b [Å]	7.45786(5)	11.3121(4)	9.2620(3)	11.2358(12)	15.150
c [Å]	15.2042(10)	14.7160(4)	13.9761(6)	14.9169(14)	26.4251(9)
V [Å^3]	826.81(16)	2361.88(13)	994.37(7)		
α [°]	90	90	91.239(3)	95.707(8)	103.956(3)
β [°]	92.184(5)	115.506(4)	92.001(4)	97.126(8)	92.056(3)
γ [°]	90	90	108.578(4)	113.675(9)	103.990(3)
Z	2	4	1	1	1
ρ_{calc} [g · cm^{-3}]	1.605	1.724	1.537	1.639	1.705
F(000)	672	1232	474	736	2082
crystal dimensions [mm^3]	0.25 · 0.1 ·0.1	0.4 · 0.4 · 0.06	0.4 · 0.2 · 0.09	0.38 · 0.30 ·0.30	0.35 · 0.15 · 0.08
diffractometer			Oxford Gemini S		
absorp coeff [mm^{-1}]	10.740	12.451	2.671	1.628	1.752
absorp correction			semiempiric		
max./min. transmn	-	10000 / 0.18468	10000 / 0.87968	10000 / 0.74925	10000 / 0.65526
θ scan range [°]	4.59 - 63.95	3.11 - 61.98	2.91 - 25.99	2.79 - 26.00	2.98 - 26.00
index range h, k, l	-13 ≤ h ≤ 13	-18 ≤ h ≤ 18	-9 ≤ h ≤ 9	-12 ≤ h ≤ 12	-12 ≤ h ≤ 13
total no. of reflns	9073	11000	9605	14551	33156
no. of unique reflns	4247	3672	3880	5747	15792
no of data/restraints/params	4247 / 1 / 343	3672 / 260 / 301	3880 / 0 / 226	5747/ 0 / 386	15792 / 0 / 997
R_{int}, Goodness-of-fit (*S*) on F^2	0.0599, 145	0.0408, 1.104	0.0293, 0.947	0.0275, 0.993	0.0372, 180
R_1, wR_2 [$I \geq 2\sigma(I)$]	0.0441, 0.1163	0.0384, 0.1056	0.0258, 0.0577	0.0283, 0.0661	0.0689, 0.1981
R_2, wR_2[a] (all data)	0.0451, 0.1172	0.0484, 0.1221	0.0337, 0.0587	0.0412, 0.0699	0.1026, 0.2079
max., min. peak in final Fourier map (e Å^{-3})	0.721/-0.746	0.755/-0.685	0.503/-0.338	0.679/-0.638	3.463/-1.313