chemistry proceedings

Supplementary Material

Cyclopalladated Compounds with Bulky Phosphine (dppm): Synthesis, Characterization, and X-ray Diffraction †

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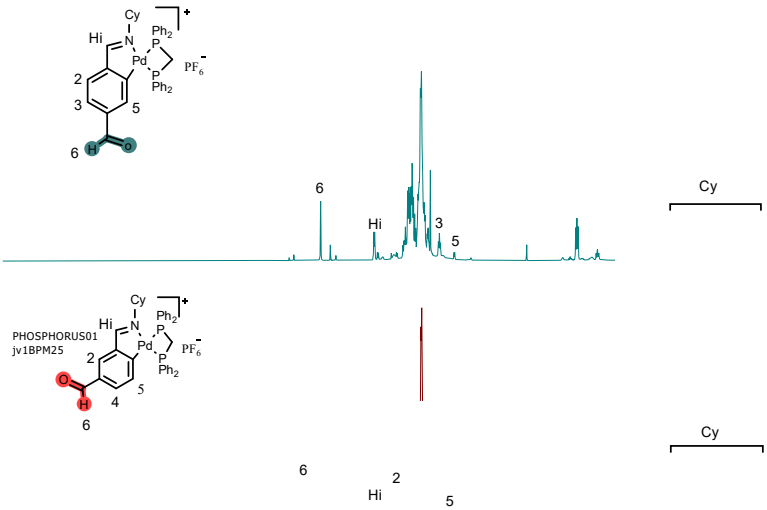

Figure S1. ^{1}H NMR of compounds 1a and 1b in $CDCl_3$.

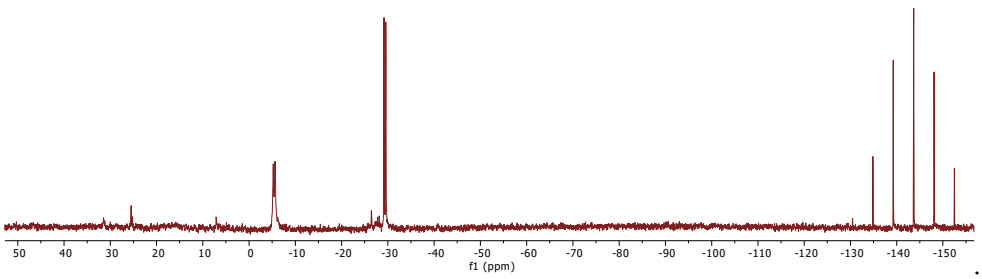

Figure S2. ^{31}P {^{1}H}NMR of compound 1a in $CDCl_3$.

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Table S1. Crystal data and structure refinement for 1b.

Molecular formula.	**$C_{39}H_{38}F_6NOP_3Pd$..**
Formula weight.	850.01..
Temperature/K.	100.00..
Crystal system.	monoclinic..
Space group.	$P2_1/n$..
a/Å.	10.0932(6)..
b/Å.	33.4658(18)..
c/Å.	11.4492(6)..
α/°.	90..
β/°.	110.580(2)..
γ/°.	90..
Volume/$Å^{3.}$	3620.5(3)..
Z.	4..
ϱ_{calc}g/$cm^{3.}$	1.559..
μ/$mm^{-1.}$	0.710..
F(000).	1728.0..
Crystal size/$mm^{3.}$	0.9 × 0.07 × 0.04..
Radiation.	MoKα (λ = 0.71073)..
θ range for data collection/°.	4.48 to 56.554..
Index ranges.	$-13 \leq h \leq 13$, $-44 \leq k \leq 44$, $-15 \leq l \leq 15$..
Reflections collected.	149704..
Independent reflections.	8997 [R_{int} = 0.0551, R_{sigma} = 0.0214]..
Data/restraints/parameters.	8997/0/461..
Goodness-of-fit on $F^{2.}$	1.194..
Final R indexes [I>=2σ (I)].	R_1 = 0.0595, wR_2 = 0.1224..
Final R indexes [all data].	R_1 = 0.0661, wR_2 = 0.1255..
Largest diff. peak/hole / e $Å^{-3.}$	2.50/–1.83..