Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2018

Phosphine-assisted C-H Bond Activation in Schiff Base and Formation of Novel

Organo Cobalt Complexes Bearing Schiff Base Ligand

Hua Zhang,^{*a*} Junyang Xing,^{*a*} Yanhong Dong,^{*a*} Shangqing Xie,^{*a*} Shishuai Ren,^{*a*} Xinghao Qi,^{*a*} Hongjian Sun,^{*a*} Xiaoyan Li,^{*a*,*} Olaf Fuhr,^{*b*} Dieter Fenske^{*b*}

SI The table of selected crystallographic data	S2
SII IR, ¹ H, ³¹ P{H} and ¹³ C{H} NMR spectra of complexes 3 - 8	S3
SIII EPR spectra of complexes 5 and 6	S12

Complex	4	5	7	8
Formula	$C_{31}H_{37}CoNP_3$	$C_{35}H_{40}CoNP_3$	$C_{35}H_{38}CoINP_3\\$	$C_{136}H_{120}Co_4N_4O_8P_8$
Mz	575.45	626.52	751.40	2422.01
crystal system	monoclinic	monoclinic	monoclinic	monoclinic
space group	C2/c	$P2_1/n$	$P2_1/n$	P21/c
a [Å]	40.6142(16)	8.7562(3)	8.8680(3)	10.289(2)
<i>b</i> [Å]	9.1256(3)	16.0052(4)	15.5580(5)	15.896(3)
<i>c</i> [Å]	15.9365(6)	23.0007(9)	23.3260(6)	18.982(4)
α [°]	90	90	90	90
β [°]	105.127(5)	99.977(3)	100.659(2)	104.414(2)
γ [°]	90	90	90	90
V [Å ³]	5701.9(4)	3174.68(19)	3162.72(17)	3006.6(10)
T [K]	174.15	173.15	153.15	296.15
Ζ	8	4	4	1
μ[mm-1]	0.791	0.717	1.697	1.3376
total reflns	44518	26537	24228	21174
unique reflns	6894	7685	6901	6896
Rint	0.0487	0.0206	0.0242	0.0699
R1[I>2σ(I)]	0.0382	0.0265	0.0228	0.0483
$wR(F2)[I>2\sigma(I)]$	0.0935	0.0684	0.0510	0.1696
R1(all data)	0.0516	0.0317	0.0303	0.1045
wR(F2) (all	0.0997	0.0717	0.0530	0.1048
data)				
GOF on F2	1.024	1.027	0.973	1.043

SI The table of selected crystallographic data



SII IR, ¹H, ³¹P{H} and ¹³C{H} NMR spectra of complexes 3 - 8

¹H NMR spectrum of complex **3**



³¹P{H} NMR spectrum of complex **3**



 $^{13}C\{H\}$ NMR spectrum of complex 3



¹H NMR spectrum of complex 4







IR spectrum of complex 6



¹H NMR spectrum of complex 7



S8



 $^{31}P\{H\}$ NMR spectrum of complex 7



 $^{13}C\{H\}$ NMR spectrum of complex 7







¹³C{H} NMR spectrum of complex 8

SIII EPR spectra of complexes 5 and 6



EPR spectrum of complex 5 recorded in solid state.



EPR spectrum of complex 6 recorded in solid state.