

Electronic supporting information (ESI)

Well-defined palladium(0) complexes bearing *N*-heterocyclic carbene and phosphine moieties:

efficient catalytic applications in Mizoroki–Heck reaction and direct C–H functionalization

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Table S1 Crystallographic data

	2aa	2ba	2ca	2da
empirical formula	C ₂₈ H ₂₄ FN ₂ O ₄ PPd· C ₄ H ₈ O	C ₂₉ H ₂₇ N ₂ O ₄ PPd	C ₂₈ H ₂₅ N ₂ O ₃ PPd· 0.5C ₄ H ₈ O	C ₃₀ H ₂₉ N ₂ O ₃ PPd· 0.5H ₂ O
formula weight	664.96	604.89	610.92	611.93
crystal system	triclinic	monoclinic	triclinic	triclinic
space group	<i>P</i> $\bar{1}$	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
<i>a</i> , Å	10.723(2)	9.1522(5)	10.6104(6)	10.8121(3)
<i>b</i> , Å	12.725(3)	25.9604(14)	11.6829(6)	10.9909(3)
<i>c</i> , Å	22.555(5)	10.9541(6)	12.5519(6)	12.7110(3)
α , deg	76.391(6)	90	95.426(3)	84.157(2)
β , deg	79.537(6)	93.829(3)	93.106(3)	69.851(2)
γ , deg	86.496(6)	90	110.644(3)	71.348(2)
<i>V</i> , Å ³	2940.7(12)	2596.8(2)	1443.09(13)	1343.52(6)
<i>T</i> , K	150(2)	150(2)	150(2)	150(2)
<i>Z</i>	4	4	2	2
no. of unique data	12813	6708	5871	5780
no. of params refined	739	335	352	346
<i>R</i> ₁ ^a [<i>I</i> > 2σ(<i>I</i>)]	0.0499	0.0460	0.0871	0.0255
<i>wR</i> ₂ ^b (all data)	0.1100	0.1048	0.2466	0.0669

$$^a R_1 = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|. \quad ^b wR_2 = [\Sigma(|F_o|^2 - |F_c|^2)^2/\Sigma(F_o^2)]^{1/2}$$

Table S2 Crystallographic data of 4ea and 4eb

	4ea	4eb
empirical formula	C ₂₇ H ₂₃ N ₂ O ₃ PPd, 2(CHCl ₃)	C ₂₇ H ₃₅ N ₂ O ₃ PPd
formula weight	799.58	572.94
crystal system	triclinic	triclinic
space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
<i>a</i> , Å	10.4095(18)	9.2416(16)
<i>b</i> , Å	14.834(3)	9.8555(18)
<i>c</i> , Å	22.083(4)	14.849(3)
α , deg	87.766(12)	79.479(14)
β , deg	88.760(11)	82.978(13)
γ , deg	76.094(11)	86.719(13)
<i>V</i> , Å ³	3307.2(11)	1318.9(4)
<i>T</i> , K	150(2)	150(2)
<i>Z</i>	4	2
no. of unique data	12981	6809
no. of params refined	759	308
<i>R</i> ₁ ^a [<i>I</i> > 2σ <i>I</i>]	0.0966	0.0551
<i>wR</i> ₂ ^b (all data)	0.2863	0.1695

$$^a R_1 = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|. \quad ^b wR_2 = [\Sigma(|F_o|^2 - |F_c|^2)^2/\Sigma(F_o^2)]^{1/2}$$

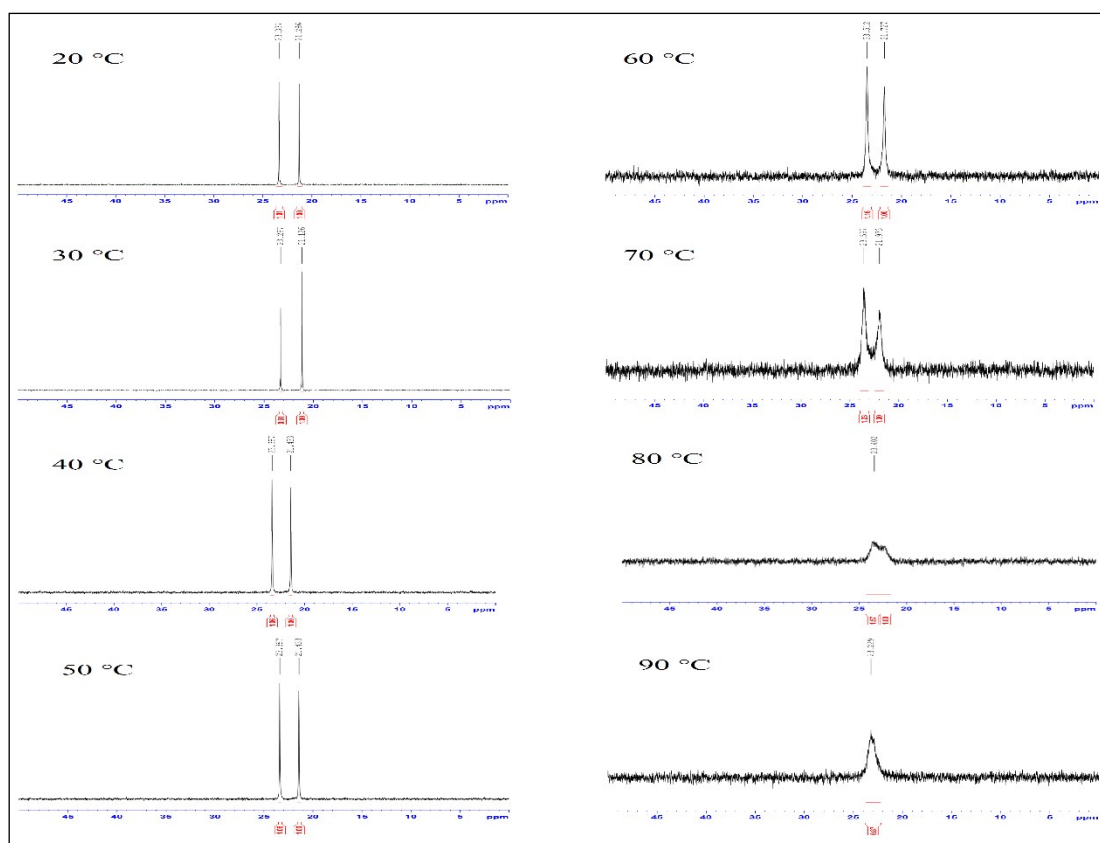


Fig. S1 Variable-temperature $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of 4eb.