Electronic Supplementary Material (ESI) for New Journal of Chemistry
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Supporting information for New Journal of Chemistry

Palladium(II) complexes with planar chiral ferrocenyl phosphane/ (benz)imidazol-2-ylidene ligands

Pauline Loxq,[a,b] Nathalie Debono,[a,b] Süleyman Gülcemal,[c] Jean-Claude Daran,[a,b] Eric Manoury,[a,b] Rinaldo Poli,[a,b] Bekir Çetinkaya [c] and Agnès Labande* [a,b]

[a] *CNRS, LCC (Laboratoire de Chimie de Coordination), 205 route de Narbonne, BP 44099, F-31077 Toulouse Cedex 4, France. Fax: (+33) 561553003. E-mail: agnes.labande@lcc-toulouse.fr*
[b] *Université de Toulouse, UPS, INPT, F-31077 Toulouse Cedex 4, France*
[c] *Department of Chemistry, Ege University, 35100 Bornova-Izmir, Turkey*
[d] *Institut Universitaire de France, 103 bd Saint-Michel, F-75005 Paris, France*

Figure S1. ORTEP representation of imidazolium salt *rac*-**2a**.[1] Ellipsoids are shown at the 50% level. All hydrogens are omitted for clarity. Selected bond lengths (Å) and bond angles (°) : C(11)-P(1) 1.792(3), C(1)-N(11) 1.317(3), C(1)-N(12) 1.309(4), C(3)-C(4) 1.333(5); N(11)-C(1)-N(12) 109.7(3); C(21)-P(2) 1.801(3), C(6)-N(21) 1.316(3), C(6)-N(22) 1.323(3), C(7)-C(8) 1.344(4); N(21)-C(6)-N(22) 109.4(3).

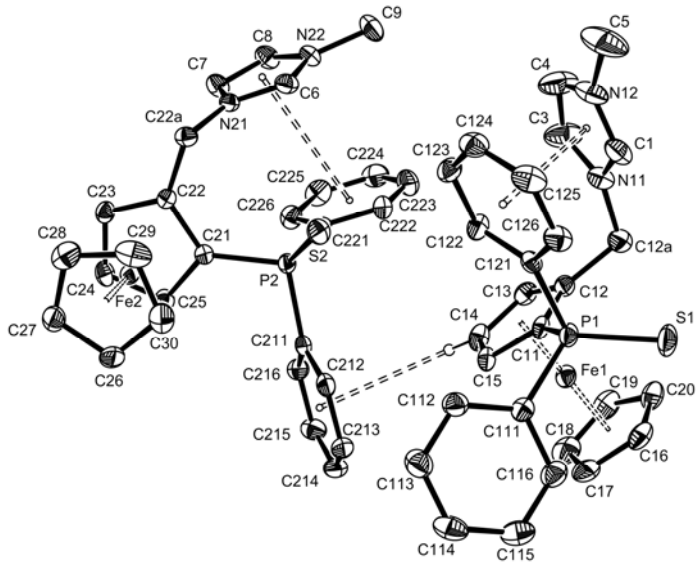

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Figure S2. ORTEP representation of complex *rac*-**4a**.[2] Ellipsoids are shown at the 30% level. All hydrogens are omitted for clarity. Selected bonds (Å) and angles (°) : C(22)-Pd(1) = 1.991(3), P(1)-Pd(1) = 2.2444(8), Cl(1)-Pd(1) = 2.3614(9), Cl(2)-Pd(1) = 2.3397(8), C(22)-Pd(1)-P(1) = 84.95(9), C(22)-Pd(1)-Cl(1) = 88.24(9), P(1)-Pd(1)-Cl(2) = 95.06(3).

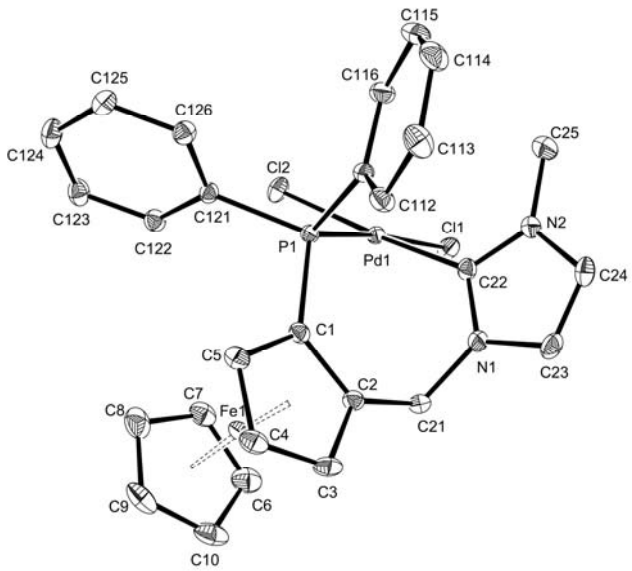

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Table S1. Crystal data and refinement parameters for **2c** and **2d**.

Identification code	*rac*-**2c**	*rac*-**2d**
Empirical formula	$C_{33}H_{32}FeN_2PS \cdot BF_4$	$C_{42}H_{42}FeN_2PS \cdot BF_4$, $0.5CH_2Cl_2$, $0.5C_4H_{10}O$
Formula weight	662.30	859.99
Temperature, K	180(2)	180(2)
Wavelength, Å	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/n$	C2/c
a, Å	10.8546 (5)	25.6211 (11)
b, Å	7.6314 (4)	9.1000 (4)
c, Å	36.279 (3)	34.9740 (13)
α, °	90.0	90.0
β, °	95.896 (5)	98.942 (2)
γ, °	90.0	90.0
Volume, $Å^3$	2989.3 (3)	8055.2 (6)
Z	4	8
Density (calc), Mg/m^3	1.472	1.418
Abs. coefficient, mm^{-1}	0.68	0.588
F(000)	1368	3584
Crystal size, mm^3	0.54 × 0.40 × 0.18	0.36 × 0.11 × 0.08
Theta range, °	2.8–28.6	2.4–30.9
Reflections collected	27251	42944
Indpt reflections (R_{int})	4694 (0.079)	8245 (0.033)
Completeness, %	99.9	1.0
Absorption correction	Multi-scan	Multi-scan
Max. / min. transmission	1.0 / 0.843	0.957 / 0.916
Refinement method	F^2	F^2
Data /restraints/parameters	5462 / 21 / 418	8245 / 0 / 474
Goodness-of-fit on F^2	1.24	1.08
R1, wR2 [I>2σ(I)]	0.0818, 0.1730	0.0389, 0.0988
R1, wR2 (all data)	0.0893, 0.1766	0.0471, 0.1029
Flack's parameter		
Residual density, $e.Å^{-3}$	0.78 and -0.78	0.35 / -0.32

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Table S2. Crystal data and refinement parameters for **4b-d**.

Identification code	(*S*)-**4b**	(*S*)-**4c**	*rac*-**4d**
Empirical formula	$C_{36}H_{31}Cl_2FeN_2PPd$, $1.5CH_2Cl_2$, $0.5\ C_4H_{10}O$	2($C_{33}H_{31}Cl_2FeN_2PPd$), $0.5C_3H_6O$	$C_{42}H_{41}Cl_2FeN_2PPd$, $0.5CH_4O$
Formula weight	924.23	1468.47	853.91
Temperature, K	180(2)	180(2)	180(2)
Wavelength, Å	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	C2	$P2_1$	P-1
a, Å	31.0431 (10)	11.8749 (3)	10.6863 (8)
b, Å	9.7619 (3)	15.7967 (4)	13.7235 (9)
c, Å	12.6606 (4)	16.9843 (4)	13.9621 (9)
α, °	90.0	90.0	75.975 (6)
β, °	95.076 (2)	100.01	77.655
γ, °	90.0	90.0	70.728
Volume, $Å^3$	3821.6 (2)	3137.49 (13)	1855.1 (2)
Z	4	2	2
Density (calc), Mg/m^3	1.606	1.554	1.529
Abs. coefficient, mm^{-1}	1.276	1.284	1.098
F(000)	1880	1488	874
Crystal size, mm^3	0.28 × 0.09 × 0.06	0.32 × 0.26 × 0.17	0.11 × 0.09 × 0.05
Theta range, °	2.2–30.7	2.9–28.5	3.7–29.2
Reflections collected	32604	22084	11701
Indpt reflections (R_{int})	11489 (0.023)	13118 (0.032)	5892 (0.068)
Completeness, %	99.5	99.4	90.0
Absorption correction	Multi-scan	Multi-scan	Multi-scan
Max. / min. transmission	0.746 / 0.640	1.0 / 0.811	1.0 / 0.808
Refinement method	F^2	F^2	F^2
Data /restraints/parameters	8095 / 1 / 418	13118 / 1 / 727	5892 / 0 / 447
Goodness-of-fit on F^2	1.05	1.07	1.01
R1, wR2 [I>2σ(I)]	0.0286, 0.0732	0.0294, 0.0702	0.0594, 0.1160
R1, wR2 (all data)	0.0326, 0.0749	0.0339, 0.0727	0.0910, 0.1271
Flack's parameter	-0.012(12)	0.001(12)	
Residual density, $e.Å^{-3}$	0.57 / -0.40	0.45 / -0.62	0.62 / -0.51

[1] A. Labande, J.-C. Daran, E. Manoury and R. Poli, *Eur. J. Inorg. Chem.*, 2007, 1205.
[2] N. Debono, A. Labande, E. Manoury, J.-C. Daran and R. Poli, *Organometallics*, 2010, **29**, 1879.