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ESI

Transition metal (Rh and Fe) complexes and main-group (Se and B) adducts with *N*,*N*'-Diphosphanyl NHC Ligands: a study of stereoelectronic properties†

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Table S1. Crystal data for compounds **$PC_{NHC}P$-RhCl**•$2CH_2Cl_2$, **PC_{NHC}-RhCO**, **$PC_{NHC}P$-Fe**, **$PC_{NHC}P$-Se**, **$PC_{NHC}P$-B-1**•THF and **$PC_{NHC}P$-B-2**•toluene.

	$PC_{NHC}P$-RhCl•$2CH_2Cl_2$	**$PC_{NHC}P$-RhCO**	**$PC_{NHC}P$-Fe**	**$PC_{NHC}P$-Se**	**$PC_{NHC}P$-B-1**•THF	**$PC_{NHC}P$-B-2**•toluene
Chemical formula	$C_{38}H_{76}ClN_4P_4Rh$•$2CH_2Cl_2$	$C_{24}H_{40}N_4O_2P_2Rh_2$	$C_{46}H_{92}Cl_6Fe_3N_4O_2P_4$	$C_{19}H_{38}N_2P_2Se_2$	$C_{37}H_{38}BF_{15}N_2P_2$•$C_4H_8O$	$C_{37}H_{38}B_3F_{15}N_2O_3P_2$•$C_7H_8$
CCDC Number	1449235	1449237	1449234	1449238	1449239	1449236
Formula Mass	1021.12	684.36	1237.36	435.41	940.55	1030.20
Crystal system	Triclinic	Orthorhombic	Trigonal	Orthorhombic	Monoclinic	Monoclinic
a/Å	14.6459(12)	15.9082(5)	23.440(3)	14.2413(17)	12.3210(5)	11.9249(6)
b/Å	15.1086(13)	14.5038(3)	23.440(3)	9.0598(11)	22.2071(10)	36.9050(17)
c/Å	15.8170(13)	25.3341(9)	32.519(5)	17.831(2)	16.3727(7)	13.6692(7)
α/°	88.107(2)	90	90	90	90	90
β/°	64.451(2)	90	90	90	105.5780(10)	102.6380(10)
γ/°	72.376(2)	90	120	90	90	90
Unit cell volume/Å^3	2990.1(4)	5845.3(3)	15473(5)	2300.6(5)	4315.2(3)	5869.9(5)
Temperature/K	173(2)	173(2)	173(2)	173(2)	173(2)	173(2)
Space group	*P-1*	*Pbca*	*R-3:H*	*Cmc21*	*P21/c*	*P21/c*
Formula units / cell, *Z*	2	8	9	4	4	4
Absorption coefficient, μ/mm^{-1}	0.643	1.265	0.983	1.775	0.201	0.156
No. of reflections measured	40535	34869	59437	5810	41879	58026
No. of independent reflections	14544	6627	8314	2220	10387	14178
R_{int}	0.0477	0.1222	0.2125	0.0407	0.0453	0.0427
Final R_1 values ($I > 2\,\sigma(I)$)	0.0699	0.1022	0.0897	0.0499	0.0499	0.0748
Final $wR(F^2)$ values ($I > 2\,\sigma(I)$)	0.1933	0.1914	0.1603	0.1166	0.1028	0.1998
Final R_1 values (all data)	0.1111	0.1534	0.1912	0.0707	0.0870	0.1126
Final $wR(F^2)$ values (all data)	0.2111	0.2130	0.1960	0.1285	0.1179	0.2152
Goodness of fit on F^2	1.060	1.289	1.016	1.030	1.019	1.050

The following special comments apply to the models of the structures:

For **$PC_{NHC}P$-RhCl**•$2CH_2Cl_2$, the asymmetric unit contains two half a molecule of the rhodium compound, one chloride and two molecules of CH_2Cl_2. The rhodium atoms are in special positions. A squeeze was used to eliminate residual density and this corresponds to one disordered molecule of pentane.

For **$PC_{NHC}P$-Fe**, the atom Fe2 is in special position (population 50%). The carbons C9, C10, C11 are disordered on two positions. A squeeze was made. The residual electron density was assigned to half a molecule of THF.

For **$PC_{NHC}P$-Se**, the atoms C1, C2, C3, N1, N2, P1, P2 and Se1 are in a special position (population 50%).

For **$PC_{NHC}P$-B-2**•toluene, the carbons C9, C10 and C11 are disordered on two positions. A squeeze was made. The residual electron density was assigned to two molecules of toluene.