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Influence of substituents in the pyrazole pre-ligands on their reaction products with (Phen)Pd(OAc)$_2$

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Table S1. Crystal data and structure refinement parameters for **1-3**

Parameters	**1**	**2**	**3**
Empirical formula	$C_{22}H_{10}F_{12}N_6Pd$	$C_{22}H_{16}F_6N_6Pd$	$C_{36}H_{44}N_{10}O_4Pd_2$
Formula weight (g mol^{-1})	692.76	585.2	893.61
Crystal system	monoclinic	monoclinic	triclinic
Space group	$P2_1/n$	$C2/c$	P-1
a (Å)	9.2257(12)	31.339(2)	10.4370(2)
b (Å)	15.6123(19)	31.339(2)	13.6164(3)
c (Å)	16.004(2)	25.5616(18)	14.1746(3)
β (°)	91.722(2)	127.458(2)	72.7524(19)
V (Å^3)	2304.1(5)	4281.8(5)	1812.89(7)
Z	4	4	2
D_{calc} (g cm^3)	1.997	1.814	1.637
μ(Mo-Kα) (mm^{-1})	0.930	0.943	1.047
$2\theta_{max}$, deg.	55	60	60
F(000)	1352.0	2320.0	908.0
R_{int}	0.0823	0.0577	0.0388
Reflections collected	16748	24085	29696
Independent reflections	5288	6245	8337
Parameters	389	318	483
GooF	1.131	1.013	1.063
R_1, wR_2 ($I > 2\sigma(I)$)	0.0823, 0.0627	0.0360, 0.0704	0.0290, 0.0684
$\Delta\rho_{max}$, ρ_{min} (e/Å^3)	1.07/-0.83	1.00/-0.60	1.12/-0.84

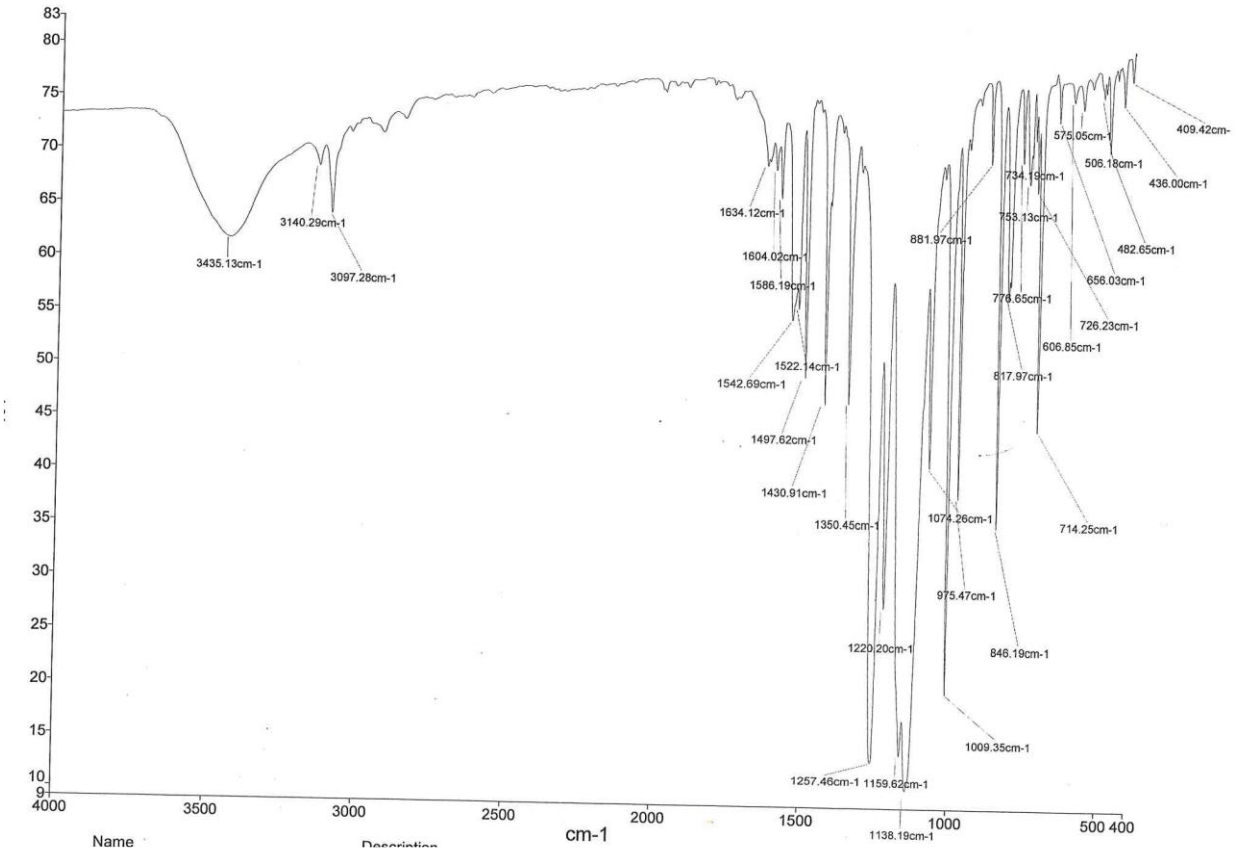
Table S2. Selected bond lengths(Å) and angles (°) for **1**–**3**

	1	**2**	**3**
Pd–N (phen)	2.033(3), 2.035(3)Å	2.034(2), 2.039(19)	2.047(2), 2.038(2)Å
Pd–N (pz)	2.007(3), 2.012(3)Å).	1.993(2), 1.985(2)	2.007(2)-2.032(2)
N-Pd-N (phen)	81.61(13)	81.39(8)	81.32(9)
N-Pd-N (pz)	92.42(13)	91.33(8)	86.72(9) (Pd2) 88.87(9), 90.58(9) (Pd1)

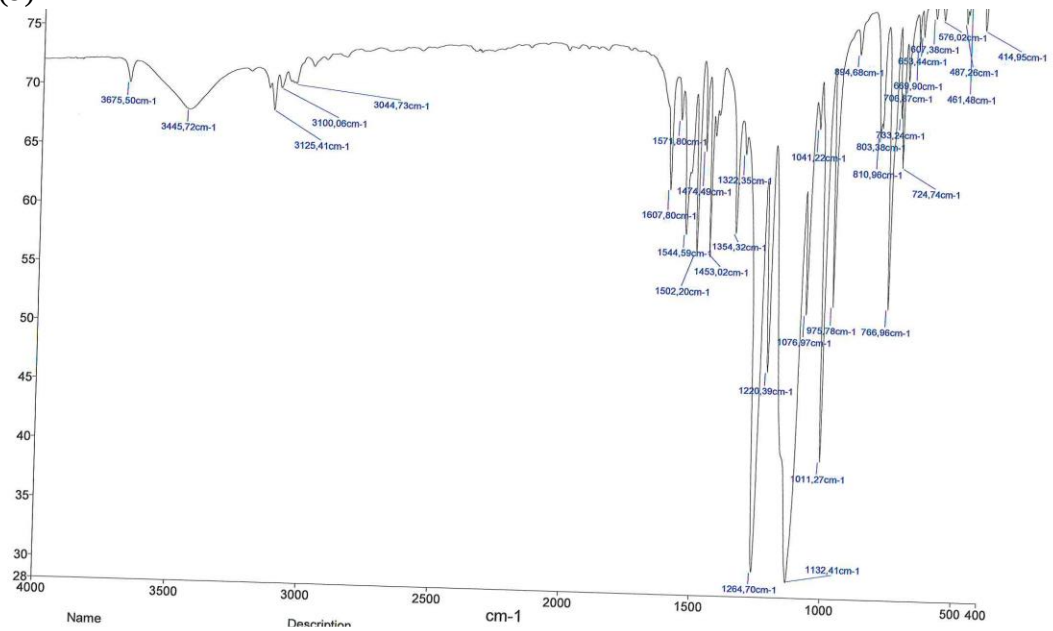
Experimental section

The yield of **1** was 0.11 g (62%). Anal. calc. $PdC_{22}H_{10}N_6F_{12}$: C 38.14, H 1.45, N 12.13. Found: C 38.34, H 1.58, N 12.29. FT-IR (ATR, ν/cm^{-1}): 3435 w, 3140 w, 3097 m, 1634s, 1604 w,1586 m, 1543 m, 1522 m, 1498 m, 1431 m, 1350 m, 1257 s, 1220 s, 1138 s, 1074 m, 1009 s., 975 m., 882 w., 846 s, 818 m, 776 m, 753 w, 714 m, 656 w, 609 w, 575 w, 506 m, 436 w, 409,4 w.
The yield of **2** was 0.1 g (70%) Anal. calc. $PdC_{22}H_{16}N_6F_6$: C 45.18, H 2.76, N 14.37. Found: C 45.24, H 2.87, N 14.11. FT-IR (ATR, ν/cm^{-1}): 3432 w, 3044 w, 1607 w, 1571 w, 1544 m, 1474 m, 1453 m,1354 w, 1322 m, 1264 s, 1220 s, 1132 m, 10769 s, 10116 w, 975 m, 766 s , 724 w, 706 s, 655 w, 464 w.
The yield of **3** was 0.08 g (35%). Anal. calc. $C_{36}H_{44}N_{10}O_4Pd_2$: C 48.38, H 5.20, N 15.67. Found: C 48.14, H 5.37, N 15,71. FT-IR (ATR, ν/cm^{-1}): 3419 s, 2920 m, 1629 m, 1524 s, 1582 s, 1492 m, 1473 m, 1426 s, 1415 s, 1352 m, 1340 m, 1313 s, 1221 s, 1199 w, 1163 s, 1058 m, 1032 s, 948 m, 866 s, 802 m, 787 s, 720 s, 660 m, 557 m, 437 m.
IR spectra were recorded on a Perkin Elmer Spectrum 65 spectrophotometer equipped with a Quest ATR Accessory (Specac) by the attenuated total reflectance (ATR) in the range of 400—4000 cm^{-1}. Microprobe analyses were carried out using a Carlo Erba EA 1108 Series CHNS Elemental Analyzer.

(*a*)



(*b*)



(*c*)

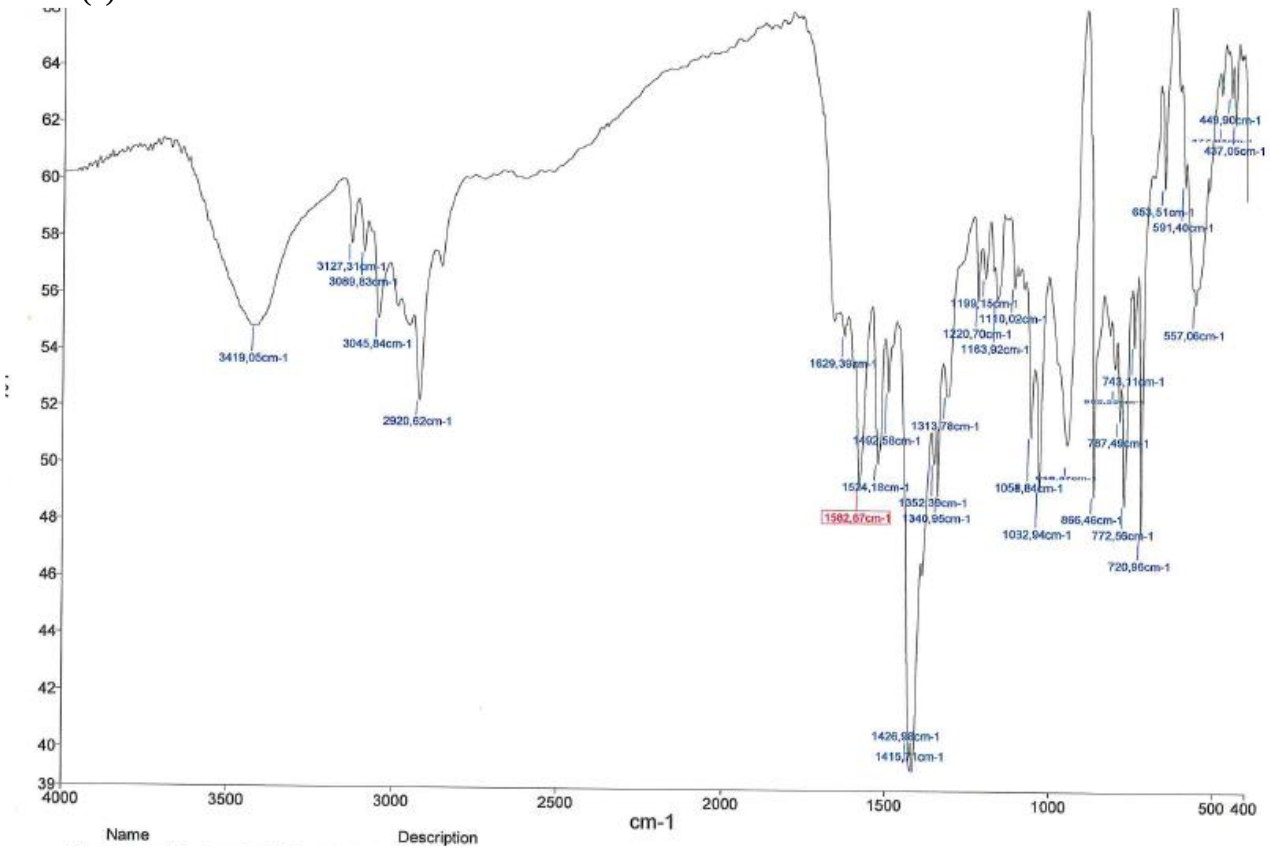


Figure S1. FT-IR spectra of complexes and (*a*) (Phen)Pd[$(CF_3)_2$pz]$_2$ **1**, (*b*) (Phen)Pd($MeCF_3$pz)$_2$ **2**, (*c*) [(Phen)Pd_2(μ-dmpz)$_2$(dmpz)(Hdmpz)]$(OAc)_2$H **3**.