Electronic Supplementary Information

Synthesis and Reductive Elimination of ArylPd(II) Trifluoromethyl Complexes: A Remarkable Concentration Effect on Chemoselectivity

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Contents

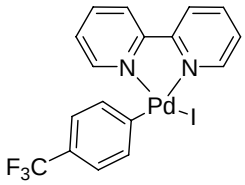
1. General experimental details

All chemicals were purchased commercially. The solvents were simply dried over Na_2SO_4 before use to extrude adventitious water. Other reactants were used as received without further purification. All the reactions were performed in a Schlenk tube under a N_2 atmosphere which was realized through evacuation/back-fill techniques after three times. ^1H NMR spectra were recorded on a 400 MHz spectrometer in deuterated $CDCl_3$ or DMSO-d_6 or CD_2Cl_2 solvent; ^{19}F NMR were recorded with 376 MHz; ^{31}P NMR were recorded with 162 MHz. All the NMR spectra were processed with MestReNova program. Chemical shifts are reported in ppm and referenced to residual solvent peaks. Coupling constants are reported in hertz for fine splitting of signals where applicable. HRMS data was obtained using MALDI SYNAPT Q-TOF MS spectrometer to determine the accurate molecular weight. UV-vis absorption and emission experiments were done on a fluorescence spectrometer TU-1901.

2. Synthesis and characterization of complexes 1a-c and 2a-c

2.1 Complexes 1a and 2a with bpy as the ancillary ligand

[(bpy)Pd(PhCF$_3$)I] (1a): Pd(dba)$_2$ (0.575g, 1.0 mmol) and 2,2′-bipyridine (0.31g, 2.0 mmol) were placed in an oven-dried 150-mL Schlenk tube equipped with a magnetic stir bar. The tube was sealed, evacuated and back-filled with nitrogen three times. A solution of 4-iodobenzotrifluoride (0.83g, 3.0 mmol) in THF (30mL) was then added by syringe. After stirring at 60 ºC for 8h, the reaction mixture was filtered through a pad of Celite. The filtrate was then evaporated under reduced pressure to remove the solvent. The resulting residue was purified by column chromatography on silica gel (eluent: first petroleum ether/ethyl acetate = 20:1~5:1 (v/v), then CH_2Cl_2/ethyl acetate = 1:1 (v/v)) to provide yellow solid **1a**. After dried under vacuum overnight, **1a** was obtained in a yield of 0.38g, 71%. (Note: toluene as reaction solvent in place of THF is also effective, with a little lower yield of 62%).



Complex **1a** (yellow solid). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.38 (s, 1H), 8.63 (d, J = 7.7 Hz, 2H), 8.27 (t, J = 7.2 Hz, 2H), 7.79 (s, 1H), 7.67 (s, 1H), 7.54 (d, J = 7.4 Hz, 2H), 7.44 (s, 1H), 7.31 (d, J = 7.5 Hz, 2H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -60.1.

Figure S1. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of (**1a**) (signals at 3.34 and 2.51 ppm are residual DMSO solvent peaks)

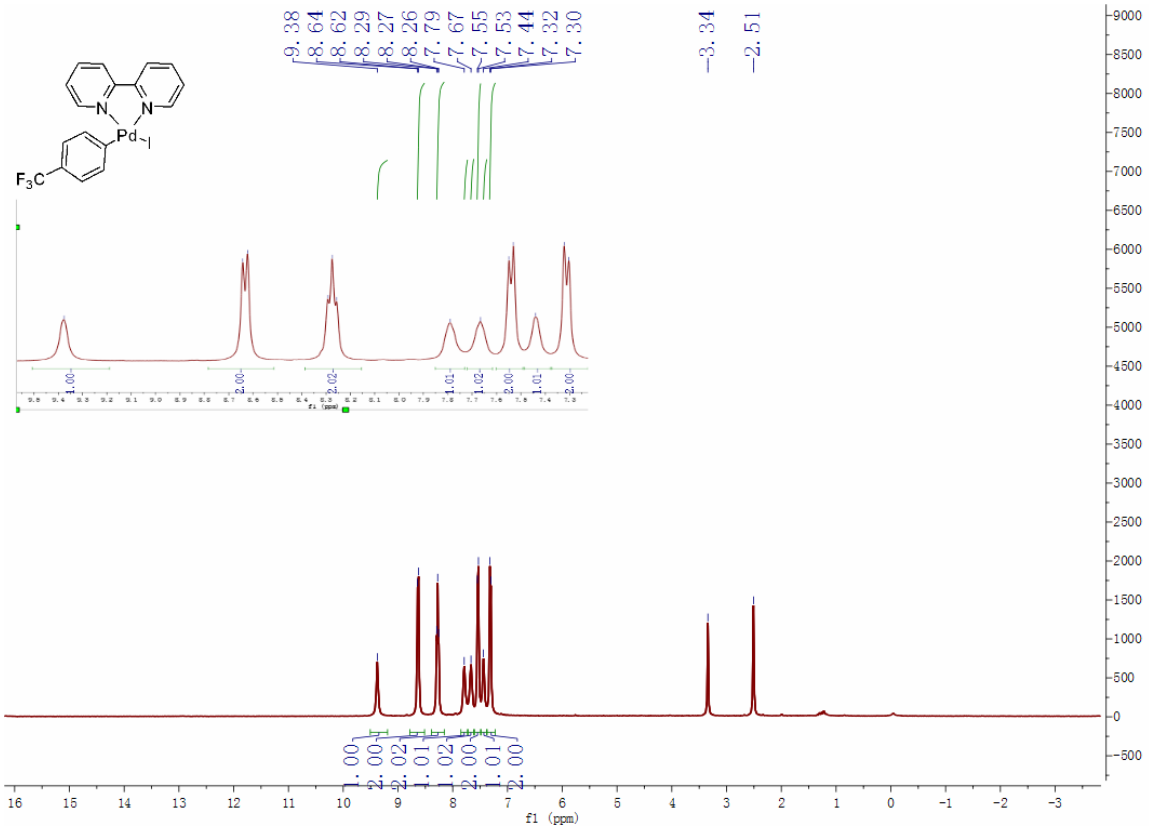
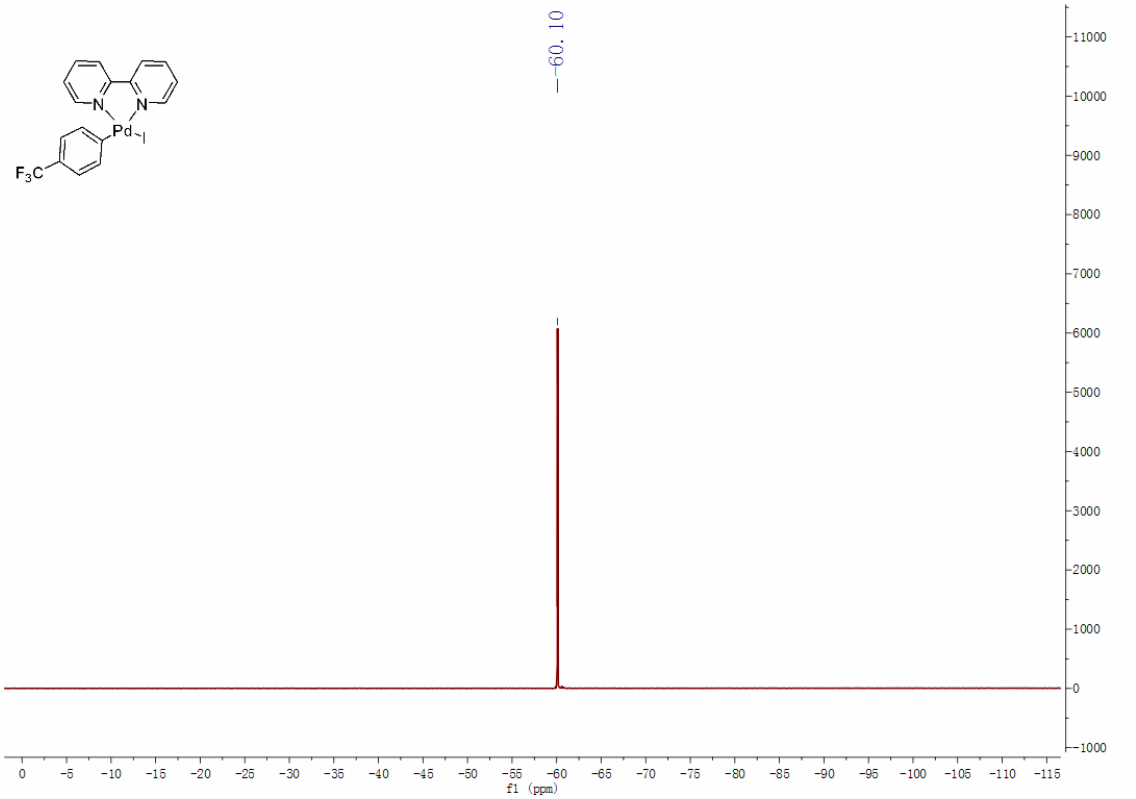
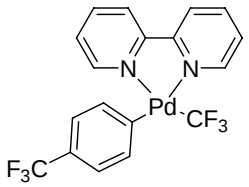


Figure S2. ^{19}F NMR (376 MHz, DMSO-d_6) spectrum of (**1a**)



[(bpy)Pd(PhCF$_3$)CF$_3$] (2a): 1a (0.267g, 0.50 mmol) and AgF (0.15g，1.2 mmol) were placed in an oven-dried 50-mL Schlenk tube equipped with a magnetic stir bar. The tube was sealed, evacuated and back-filled with nitrogen three times. A solution of CF_3SiMe_3 (0.5 mL, 3.4 mmol) in THF (8 mL) was added by syringe. After stirring at 25^{o}C for 3h, the reaction mixture was filtered through a pad of Celite. The filtrate was then evaporated under reduced pressure to remove the solvent. The resulting residue was purified by column chromatography on silica gel with eluent: petroleum ether/ethyl acetate = 20:1~5:1 (v/v), then CH_2Cl_2/ethyl acetate = 1:1 (v/v) to provide light yellow solid **2a**. After dried under vacuum overnight, **2a** was obtained in a yield of 0.165 g (69%).



2a (light yellow solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.17 – 8.05 (m, 3H), 8.02 – 7.95 (m, 1H), 7.78 (d, *J* = 7.7 Hz, 2H), 7.70 (d, *J* = 5.1 Hz, 1H), 7.65 – 7.56 (m, 1H), 7.43 – 7.27 (m, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -21.0 (s), -61.7 (s).

Figure S3. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of (**2a**)

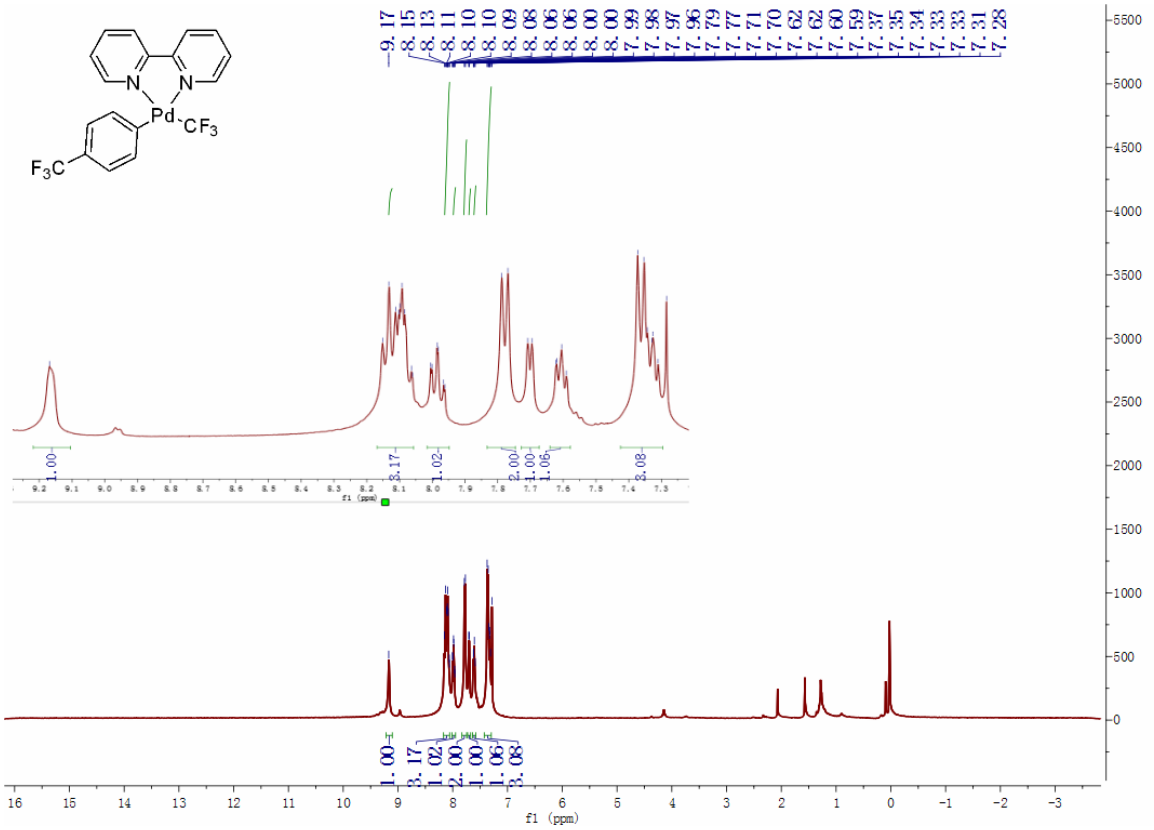
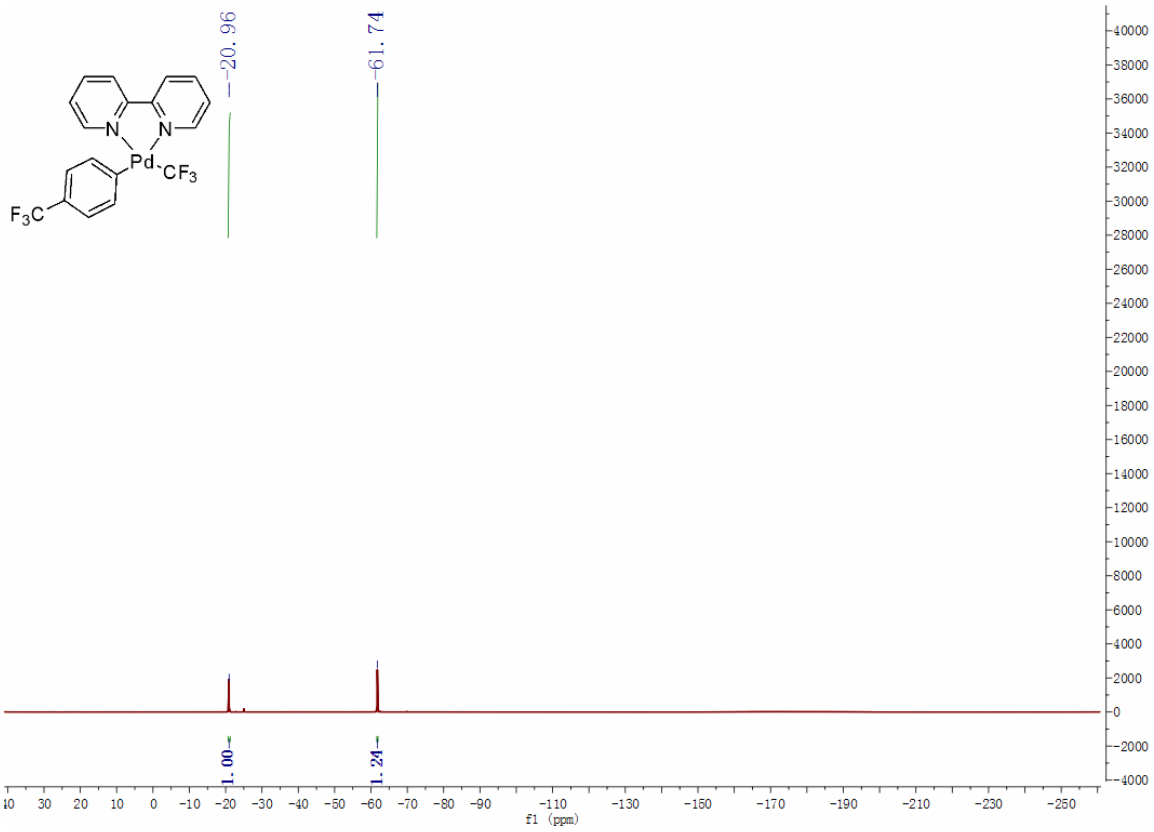
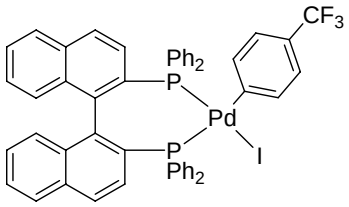


Figure S4. ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of (**2a**)



2.2 Complexes 1b and 2b with BINAP as the ancillary ligand

[(BINAP)Pd($PhCF_3$)I] (1b)：$Pd(dba)_2$ (0.575g, 1.0 mmol) and BINAP (1.25g, 2.0 mmol) were placed in a dry 150-mL Schlenk tube equipped with a magnetic stir bar. The tube was evacuated and back-filled with nitrogen three times. Under nitrogen, 4-Iodobenzotrifluoride (0.83g, 3.0 mmol) in toluene (30mL) was added. After stirring at 25ºC for 8h, the reaction mixture was filtered through a pad of Celite, and the solvent was removed under reduced pressure. The resulting residue was purified by column chromatography on silica geleluent: V(petroleum ether)/V(ethyl acetate) = 20:1~1:1 to provide yellow solid **1b**, and dried under vacuum overnight.



Complex **1b** (yellow solid, 0.52g, 52%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.95 (m, 1H), 7.82 – 7.74 (m, 3H), 7.68 – 7.49 (m, 9H), 7.43 – 7.30 (m, 5H), 7.21 – 7.06 (m, 5H), 7.04 – 6.89 (m, 6H), 6.80 – 6.64 (m, 4H), 6.60 – 6.48 (m, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.8 (s). ^{31}P NMR (162 MHz, $CDCl_3$) δ 22.09 (d, J = 39.9 Hz, 1P), 9.85 (d, J = 39.9 Hz, 1P).

Figure S5. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of (**1b**)

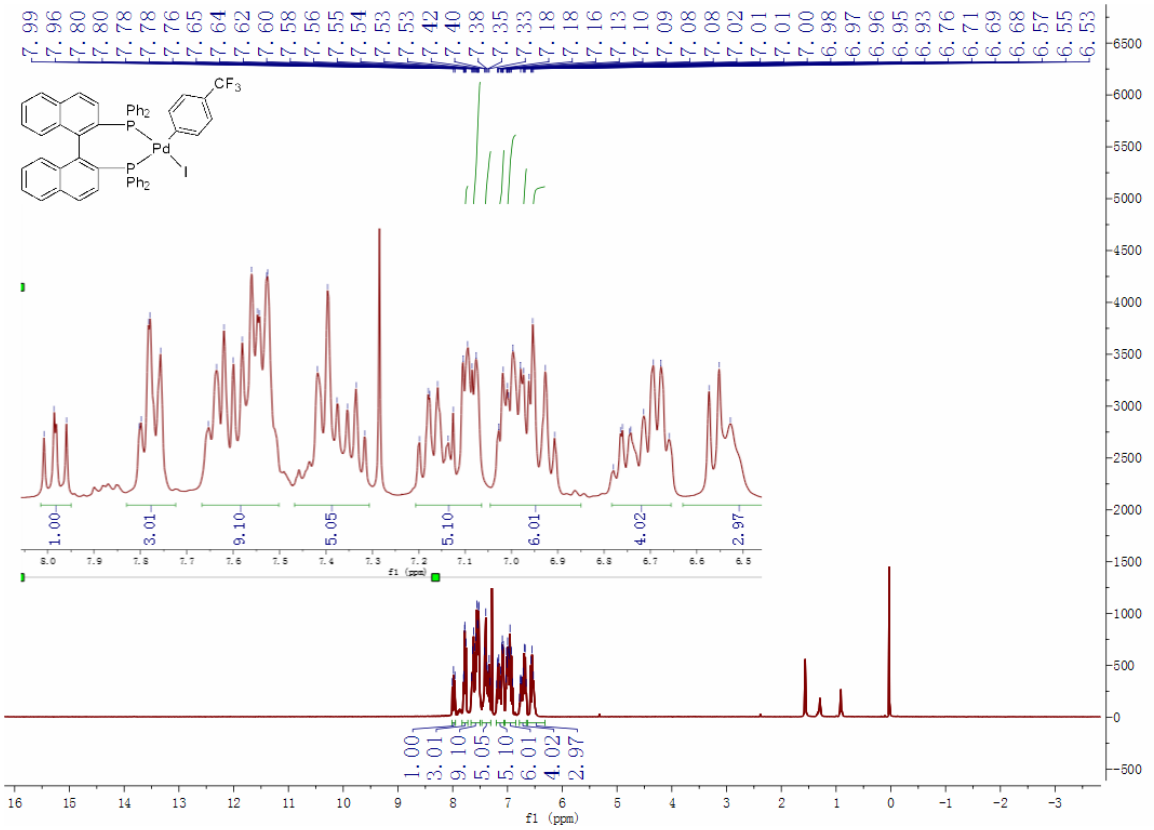


Figure S6. ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of (**1b**)

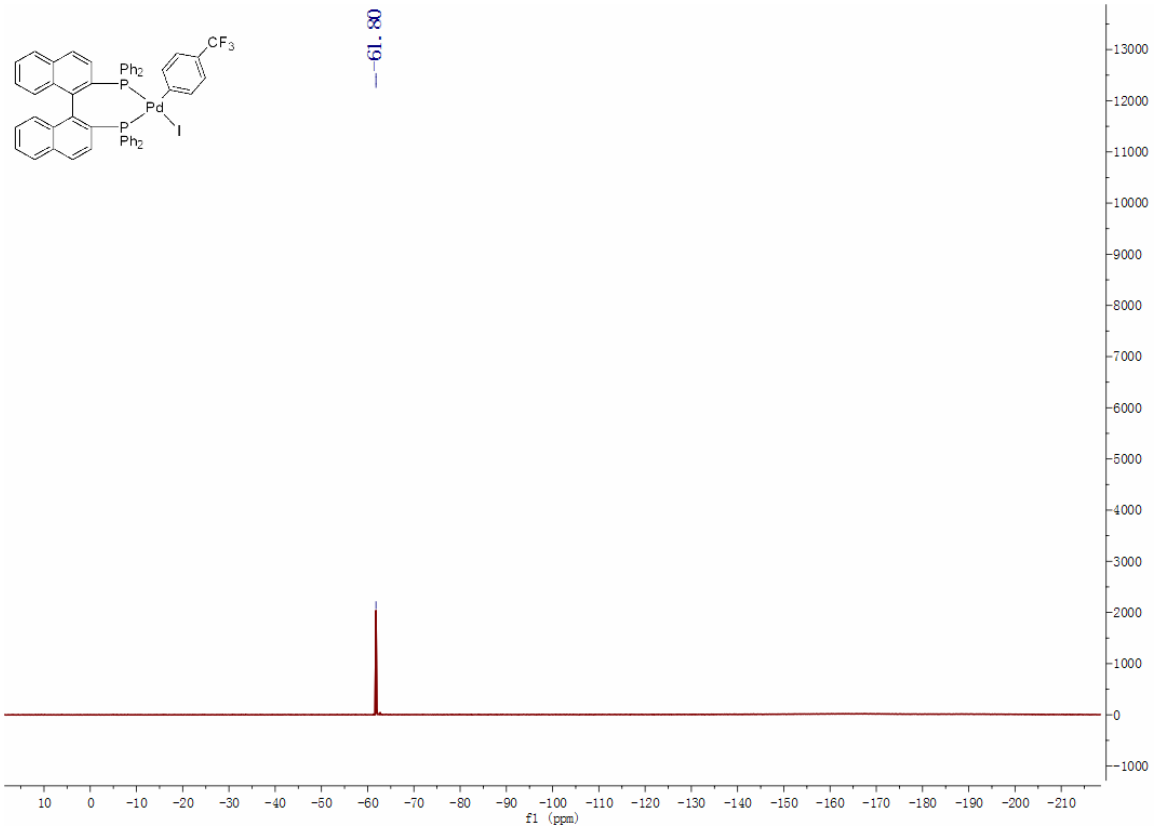
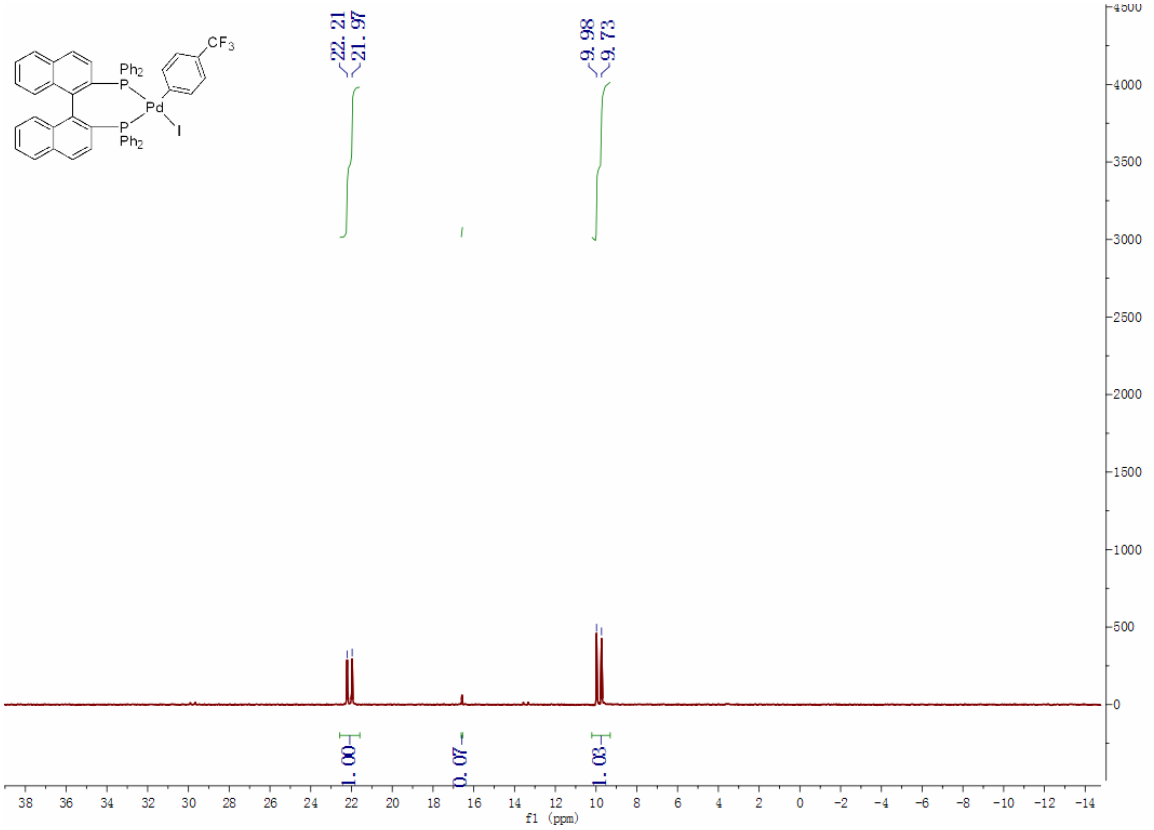
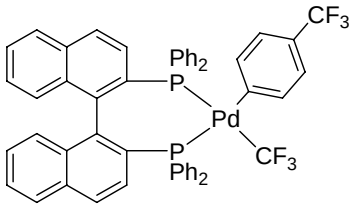


Figure S7. ^{31}P NMR (162 MHz, $CDCl_3$) spectrum of (**1b**)



[(BINAP)Pd(PhCF$_3$)CF$_3$] (2b): 1b (0.5g, 0.5 mmol) and AgF (0.15g，1.2mmol) were placed in a dry 50-mL Schlenk tube equipped with a magnetic stir bar. The tube was evacuated and back-filled with nitrogen three times. Under nitrogen, CF_3SiMe_3 (0.5mL, 3.4 mmol) in benzene (8mL) was added. After stirring at 25ºC for 5h, the reaction mixture was filtered through a pad of Celite and the volume of the filtrate reduced to a half. An equal amount of hexanes was added and the resulting solution was left overnight at *ca* 0°C to give a dark yellow solid **2b**, thoroughly washed with hexanes, and dried under vacuum overnight. The yield of **2b** was 0.34 g (72%).



Complex **2b** (dark yellow, 0.34g, 72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.82 (m, 4H), 7.74 (t, *J* = 6.0 Hz, 1H), 7.64 – 7.47 (m, 9H), 7.42 – 7.29 (m, 8H), 7.23 – 7.15 (m, 2H), 7.06 – 7.00 (m, 2H), 6.99 – 6.89 (m, 1H), 6.80 (t, *J* = 8.0 Hz, 2H), 6.75 – 6.61 (m, 4H), 6.57 (d, *J* = 8.6 Hz, 2H), 6.4-6.5 (br s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -19.65 (dd, *J* = 49.8, 17.2 Hz), -20.70 – -21.14 (m), -61.7 (s). ^{31}P NMR (162 MHz, $CDCl_3$) δ 21.44 (m 1P); 19.48 (m, 4P); 16.88 (m, 1P).

Figure S8. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of (**2b**)

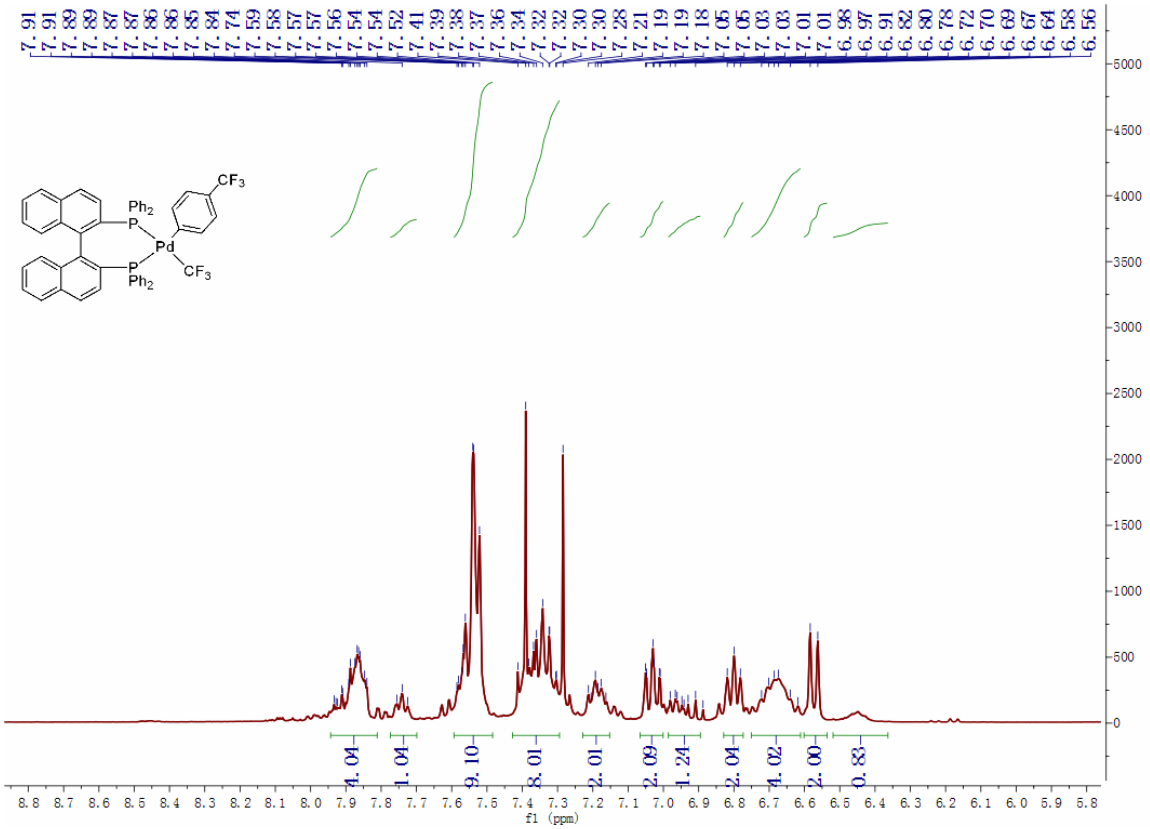


Figure S9. ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of (**2b**)

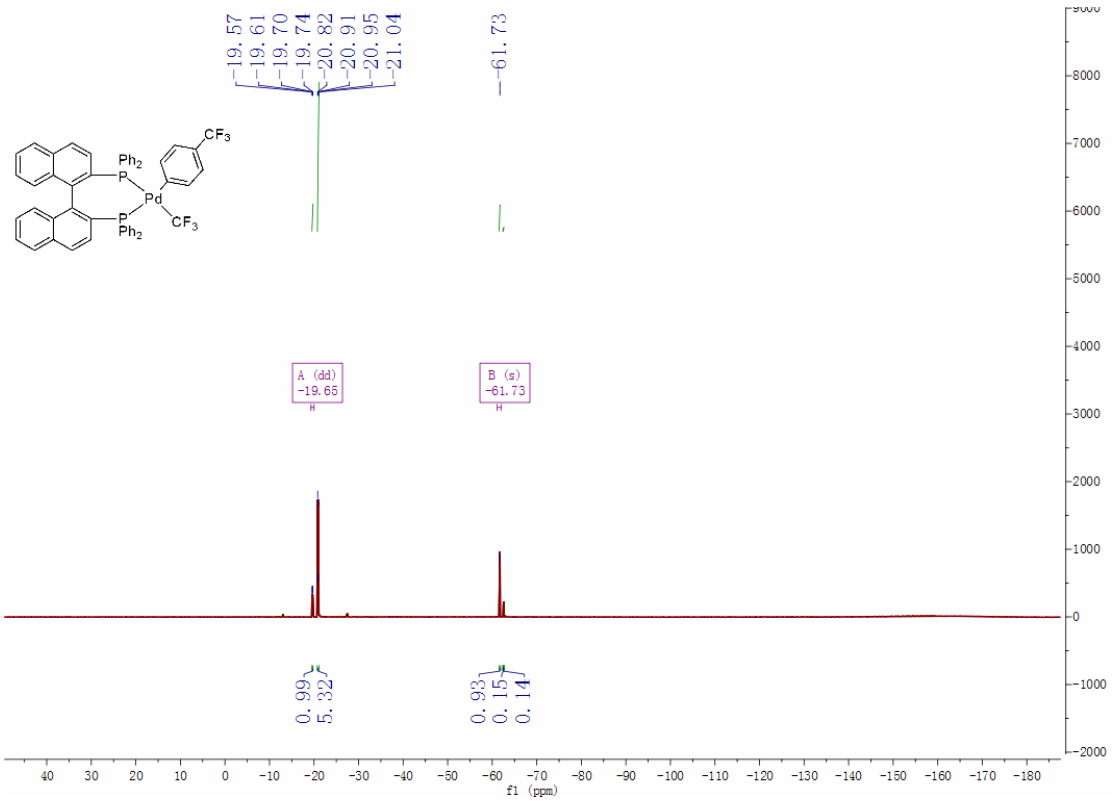
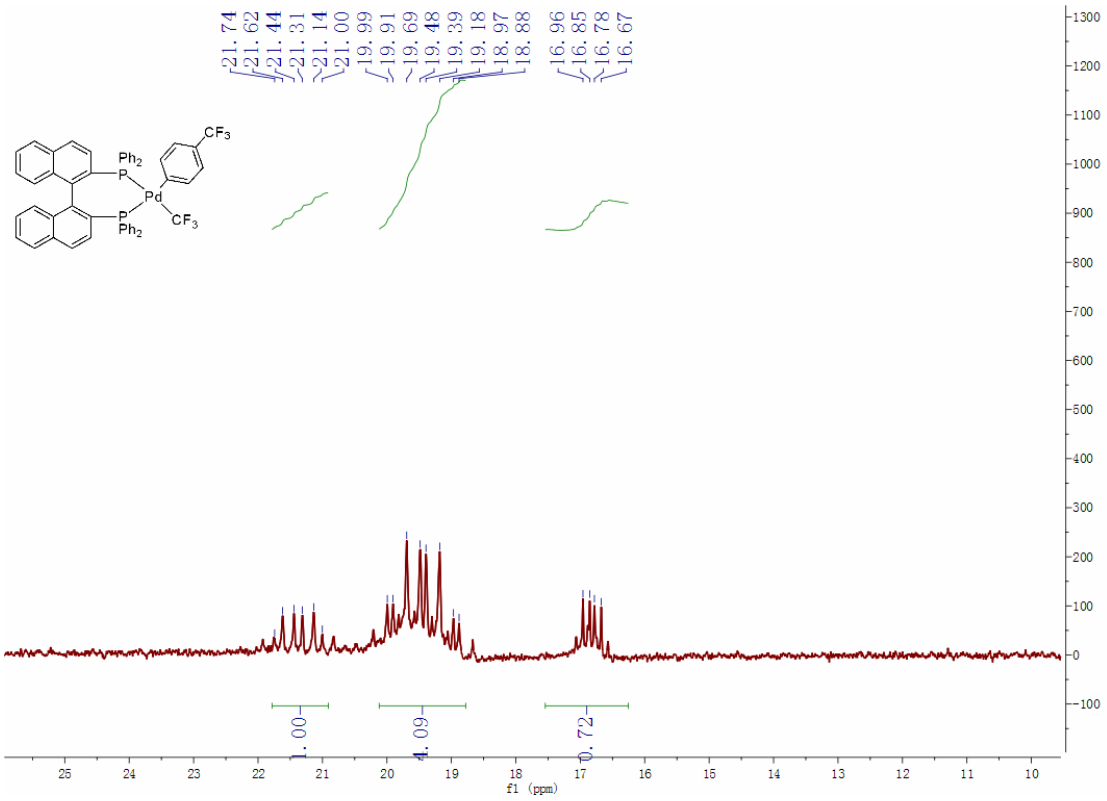
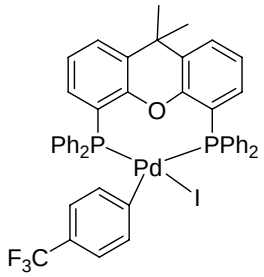


Figure S10. ^{31}P NMR (162 MHz, $CDCl_3$) spectrum of (**2b**)



2.3 Complexes 1c and 2c with Xantphos as the ancillary ligand

[(Xantphos)Pd(PhCF$_3$)I] (1c)： Pd(dba)$_2$ (0.575g, 1.0 mmol) and Xantphos (1.16g, 2.0 mmol) were placed in an oven-dried 150-mL Schlenk tube equipped with a magnetic stir bar. The tube was sealed, evacuated and back-filled with nitrogen three times. A solution of 4-iodobenzotrifluoride (0.83g, 3.0 mmol) in toluene (30mL) was then added by syringe. After stirring at 25ºC for 2h, the reaction mixture was filtered through a pad of Celite. The filtrate was then evaporated under reduced pressure to remove the solvent. The resulting residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 20:1~5:1 (v/v)) to provide yellow solid of **1c**. After dried under vacuum overnight, **1c** was obtained in a yield of 0.593 g, 62%.



Complex **1c** (yellow solid, *trans*-isomer, 0.593 g, 62% yield). ^{1}H NMR (400MHz, $CDCl_3$), δ 7.65 (dd, *J* = 7.6, 1.4 Hz, 2H), 7.48 – 7.08 (m, 24H), 6.65 (s, 2H), 6.34 (d, *J* = 7.9 Hz, 2H), 1.83 (s, 6H). ^{19}F NMR (376 MHz, CD_2Cl_2) δ -62.3(s). ^{31}P NMR (162 MHz, $CDCl_3$) δ 9.5 (s).

Figure S11. ^{1}H NMR spectrum of **(1c)**

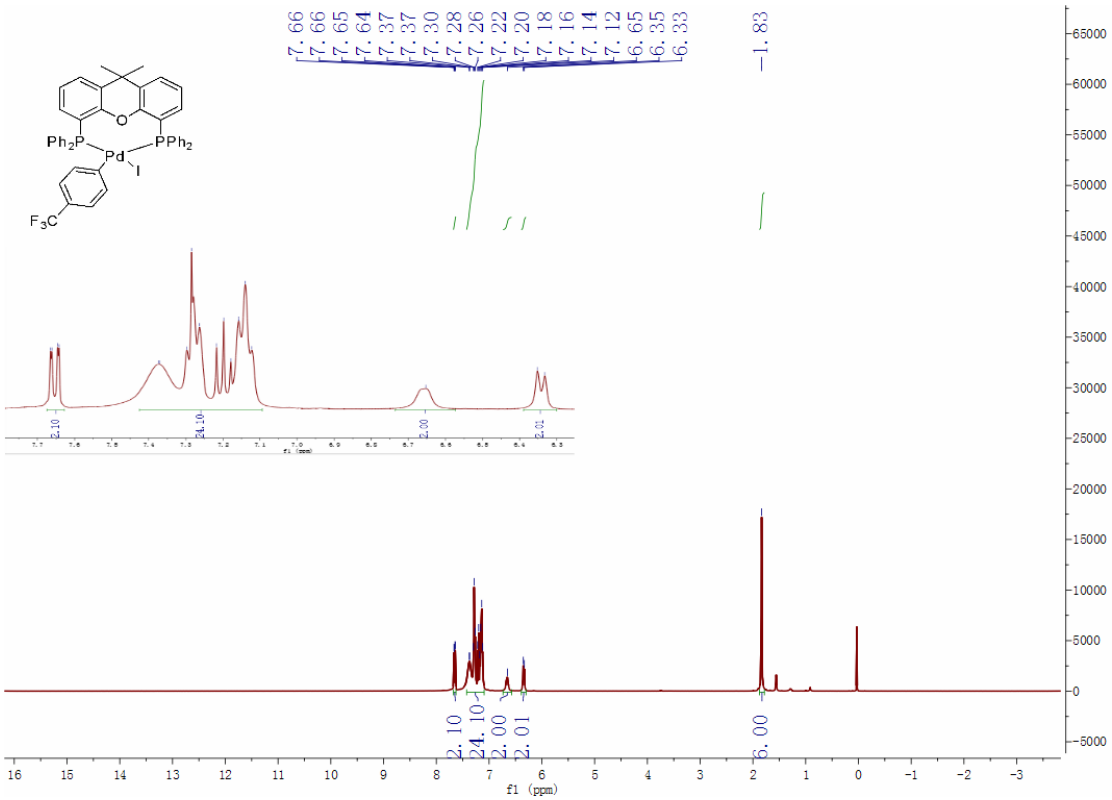


Figure S12. ^{19}F NMR spectrum of **(1c)**

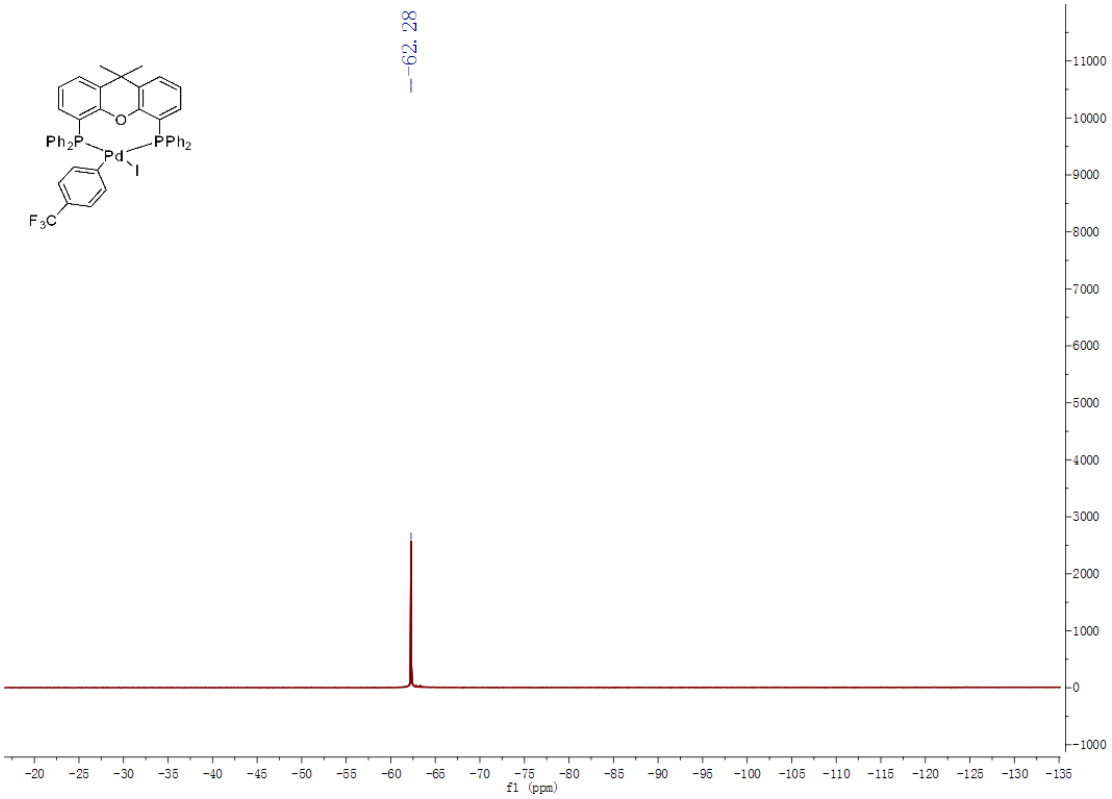
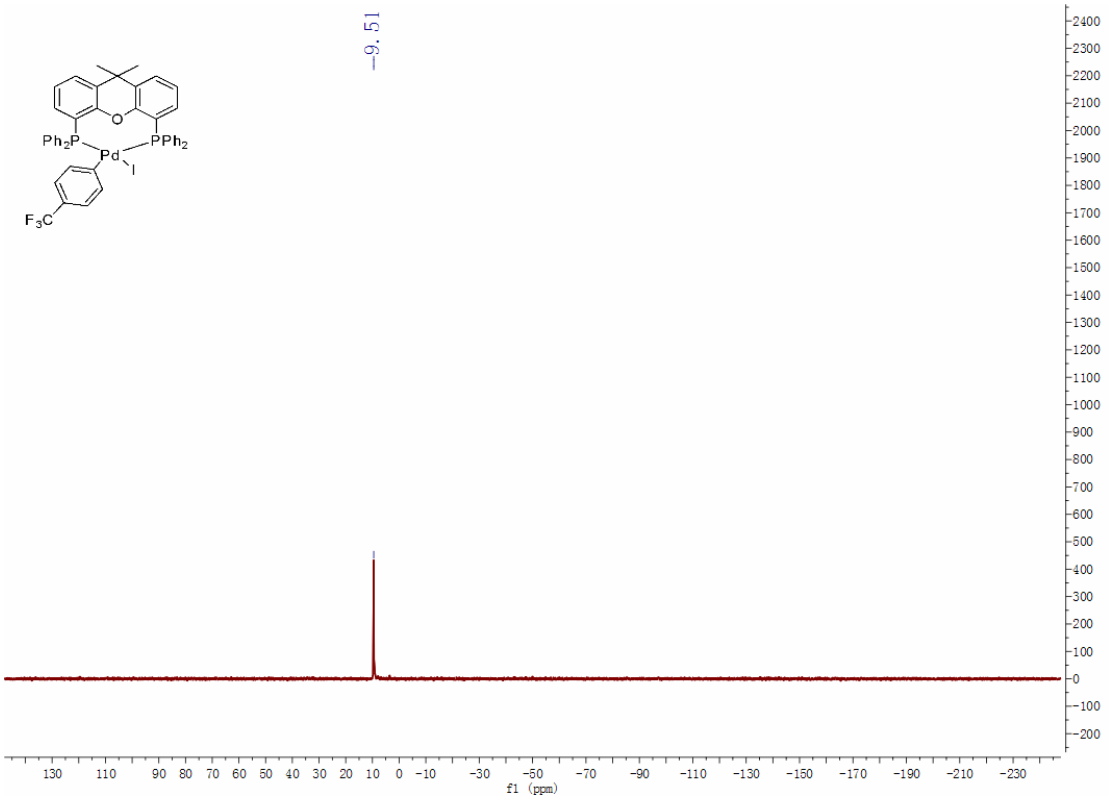
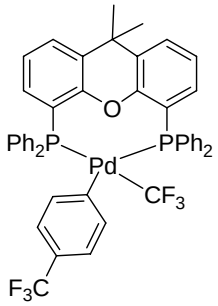


Figure S13. ^{31}P NMR spectrum of **(1c)**



[(Xantphos)Pd(PhCF$_3$)CF$_3$] (2c): 1c (0.478g, 0.5 mmol) and AgF (0.15g，1.2 mmol) were placed in an oven-dried 50-mL Schlenk tube equipped with a magnetic stir bar. The tube was sealed, evacuated and back-filled with nitrogen three times. A solution of CF_3SiMe_3 (0.5 mL, 3.4 mmol) in benzene (8 mL) was then added by syringe. After stirring at 25℃ for 3h, the reaction mixture was filtered through a pad of Celite. The filtrate was then evaporated under reduced pressure to remove the solvent. The resulting residue was dissolved in CH_2Cl_2, and hexanes (*ca* 15 mL) was added. Then, the solution was kept at +0^{o}C in the refrigerator for more than 12 hours. The yellow crystals of **2c** were separated, thoroughly washed with hexanes, and dried under vacuum overnight. The yield of **2c** was 0.30 g (67%).



Complex **2c** (yellow solid, a mixture of *cis* and *trans*-isomers in a ratio of *ca* 16:1 with ***cis*-isomer** dominant as determined by ^{19}F and ^{31}P NMR). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.00 – 7.50 (m, 4H), 7.48 – 6.76 (m, 26 H), 1.79 (s, 4H), 1.59 (s, 2H). ^{19}F NMR (376 MHz, CD_2Cl_2) -62.05 (s, aromatic CF_3), for *trans*-**2c**, δ -13.80 (t, J = 17.0 Hz, Pd-bound CF_3); for cis-**2c**, δ-15.63 (dd, J = 45.8, 17.0 Hz, Pd-bound CF_3). ^{31}P NMR (162 MHz, CD_2Cl_2) for *trans*-**2c**, δ 16.1 (q, J = 16.4 Hz, 2P); for *cis*-**2c**, δ: 4.2 (m, 16P); 8.4 (m, 16P). HRMS: m/z $(M\text{-}F)^+$ Calcd: 879.1213; Found: 879.1246.

Figure S14. ^{1}H NMR spectrum of **(2c)**

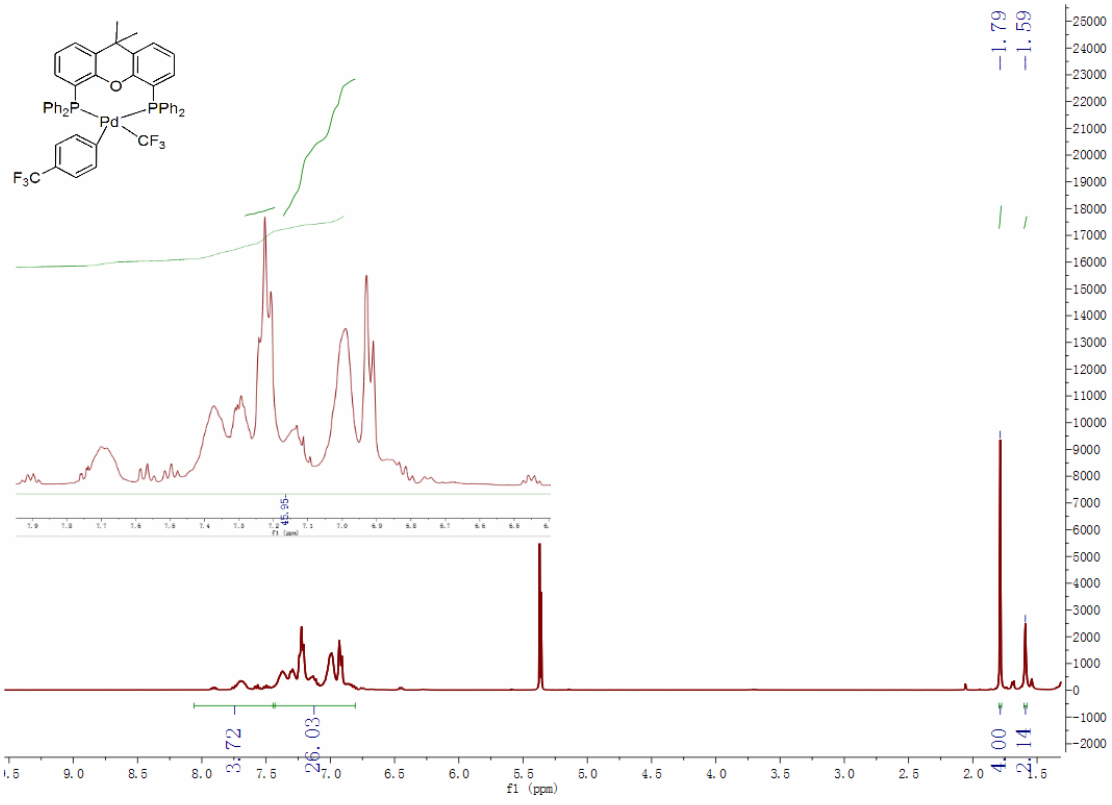


Figure S15. ^{19}F NMR spectrum of **(2c)** (the ratio of cis/trans isomers is *c*a 16:1)

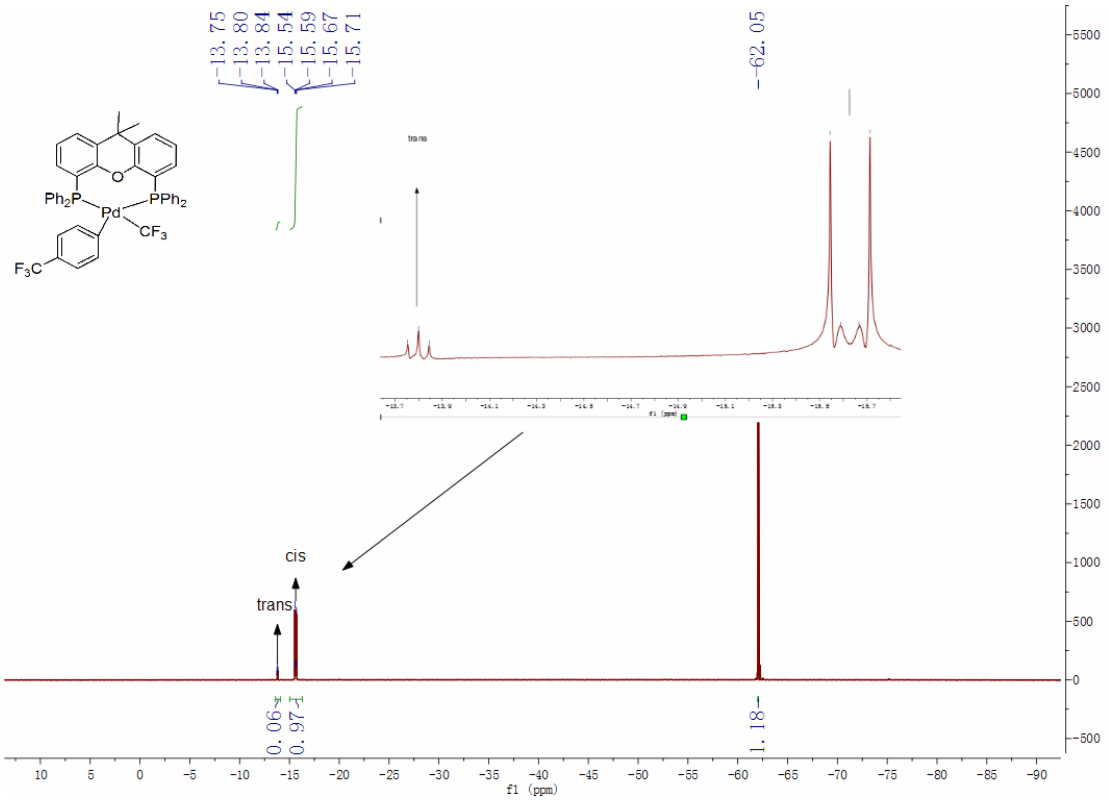
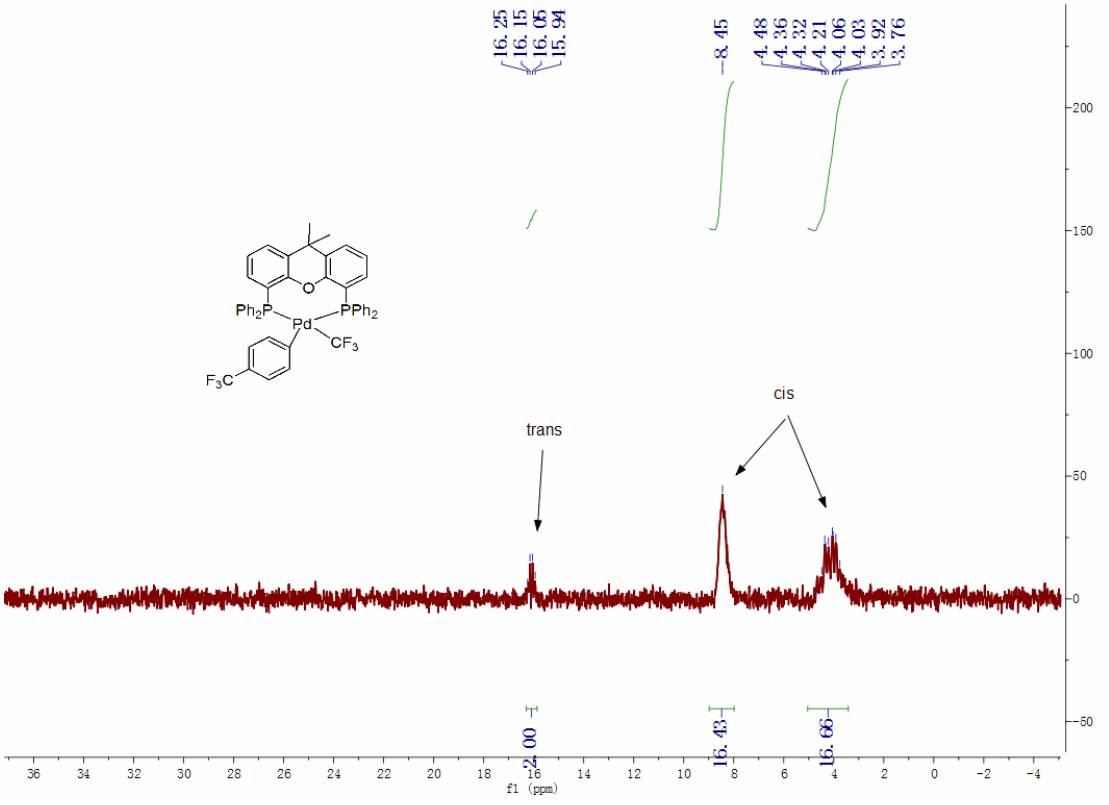
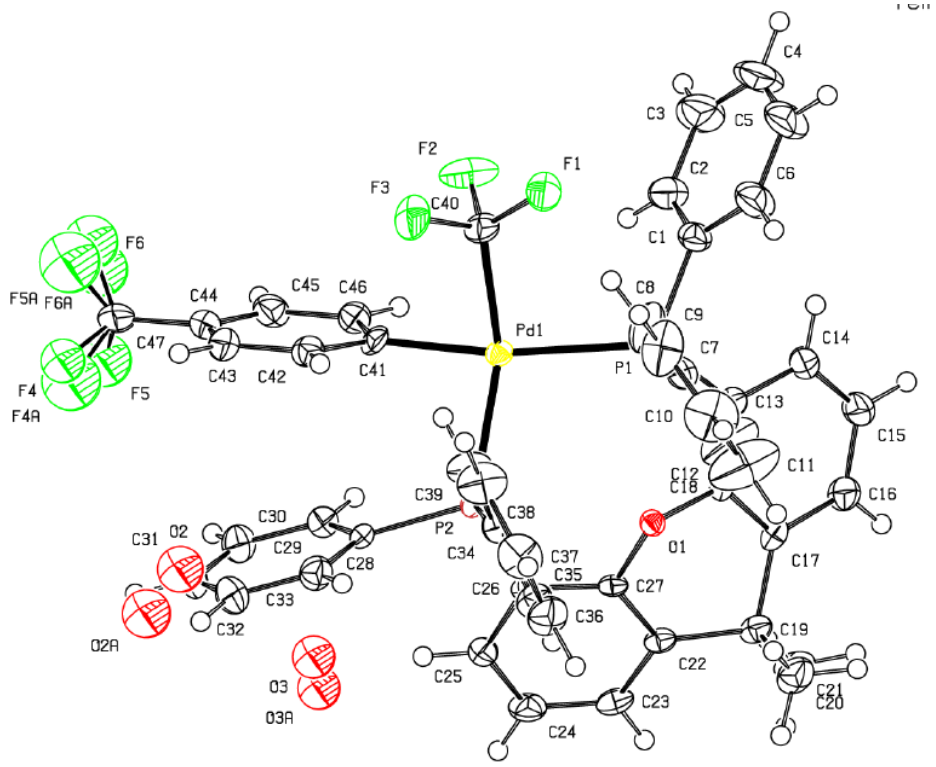


Figure S16. ^{31}P NMR spectrum of (**2c**)



3. X-ray crystallographic study of 2c

Crystals of complex **2c** suitable for X-ray crystallographic analyses were grown by dissolving **2c** in a mixed solvent of CH_2Cl_2/hexane and then stored in the refrigerator for more than 12 hours. CCDC 1446596 contains the detailed information about the crystallographic study and crystal structure of complex **2c**. The following sections show some key information.



Crystal data

$C_{47}H_{40}F_6O_3P_2Pd$	?
M_r = 935.13	D_x = 1.485 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: ? K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 17.5019 (10) Å	Cell parameters from 9799 reflections
b = 9.8634 (5) Å	θ = 2.4–28.1°

c = 25.5915 (15) Å	μ = 0.59 mm^{-1}
β = 108.725 (2)°	T = 153 K
V = 4184.0 (4) $Å^3$	Block, yellow
Z = 4	0.22 × 0.13 × 0.12 mm
$F(000)$ = 1904	

Data collection

Bruker APEX-II CCD diffractometer	7777 independent reflections
Radiation source: fine-focus sealed tube	6489 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.085
Detector resolution: ? pixels mm^{-1}	θ_{max} = 25.5°, θ_{min} = 2.2°
φ and ω scans	h = −21 21
Absorption correction: multi-scan Jacobson, R. (1998) Private communication	k = −11 11
T_{min} = 0.882, T_{max} = 0.933	l = −31 31
118559 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.071	H-atom parameters constrained
$wR(F^2)$ = 0.180	$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 34.5819P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.16	$(\Delta/\sigma)_{max}$ < 0.001
7777 reflections	$\Delta\rho_{max}$ = 2.08 e $Å^{-3}$
528 parameters	$\Delta\rho_{min}$ = −1.00 e $Å^{-3}$

0 restraints	Extinction correction: none
? constraints	Extinction coefficient: ?
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Pd1	0.50843 (3)	0.58869 (5)	0.256364 (18)	0.01830 (15)	
P1	0.44888 (9)	0.46911 (16)	0.16765 (6)	0.0190 (3)	
P2	0.52297 (8)	0.40948 (16)	0.32331 (6)	0.0175 (3)	
O1	0.4134 (2)	0.2588 (4)	0.23550 (16)	0.0174 (9)	
O2	0.9023 (8)	0.3979 (13)	0.4778 (5)	0.055 (3)*	0.50
O3	0.8396 (7)	0.1765 (13)	0.4362 (5)	0.047 (2)*	0.50
O2A	0.9310 (8)	0.3579 (14)	0.5104 (6)	0.061 (3)*	0.50
O3A	0.8133 (7)	0.1469 (13)	0.4470 (5)	0.047 (2)*	0.50
F1	0.5544 (3)	0.7225 (5)	0.16783 (16)	0.0402 (10)	
F2	0.5040 (3)	0.8624 (5)	0.2118 (2)	0.0522 (13)	
F3	0.6234 (3)	0.7878 (5)	0.24754 (17)	0.0453 (12)	
F4	0.6826 (7)	0.9446 (10)	0.4997 (4)	0.050 (2)*	0.50
F5	0.5607 (7)	0.9790 (13)	0.4884 (5)	0.073 (3)*	0.50
F6	0.6180 (8)	1.1117 (13)	0.4487 (5)	0.075 (3)*	0.50
F4A	0.6452 (10)	0.9335 (16)	0.5060 (6)	0.091 (4)*	0.50
F5A	0.6880 (9)	1.0634 (15)	0.4605 (6)	0.095 (4)*	0.50
F6A	0.5741 (8)	1.0932 (13)	0.4571 (5)	0.072 (3)*	0.50
C1	0.4177 (4)	0.5857 (7)	0.1091 (3)	0.0280 (14)	
C2	0.3755 (5)	0.7001 (8)	0.1146 (3)	0.0384 (17)	
H2	0.3664	0.7180	0.1486	0.046*	
C3	0.3463 (6)	0.7891 (10)	0.0705 (4)	0.056 (2)	

H3	0.3165	0.8671	0.0741	0.067*	
C4	0.3606 (6)	0.7638 (11)	0.0214 (4)	0.063 (3)	
H4	0.3420	0.8259	−0.0083	0.075*	
C5	0.4015 (6)	0.6498 (11)	0.0154 (3)	0.055 (2)	
H5	0.4102	0.6321	−0.0187	0.066*	
C6	0.4305 (5)	0.5600 (9)	0.0591 (3)	0.0430 (19)	
H6	0.4591	0.4811	0.0549	0.052*	
C7	0.5214 (4)	0.3533 (7)	0.1530 (3)	0.0247 (14)	
C8	0.5929 (4)	0.4049 (9)	0.1497 (3)	0.0432 (19)	
H8	0.6023	0.4998	0.1534	0.052*	
C9	0.6509 (5)	0.3224 (10)	0.1410 (4)	0.051 (2)	
H9	0.6990	0.3610	0.1378	0.061*	
C10	0.6401 (5)	0.1867 (10)	0.1369 (4)	0.056 (2)	
H10	0.6799	0.1299	0.1304	0.068*	
C11	0.5710 (7)	0.1316 (11)	0.1424 (6)	0.080 (4)	
H11	0.5637	0.0361	0.1412	0.096*	
C12	0.5120 (5)	0.2163 (9)	0.1497 (4)	0.058 (3)	
H12	0.4637	0.1777	0.1524	0.070*	
C13	0.3556 (3)	0.3674 (6)	0.1512 (2)	0.0197 (13)	
C14	0.2914 (4)	0.3821 (7)	0.1025 (3)	0.0291 (15)	
H14	0.2956	0.4435	0.0749	0.035*	
C15	0.2218 (4)	0.3074 (7)	0.0942 (3)	0.0338 (16)	
H15	0.1782	0.3186	0.0610	0.041*	
C16	0.2144 (4)	0.2164 (7)	0.1335 (3)	0.0304 (15)	
H16	0.1656	0.1672	0.1274	0.036*	
C17	0.2786 (4)	0.1969 (6)	0.1822 (3)	0.0217 (13)	
C18	0.3472 (3)	0.2738 (6)	0.1890 (2)	0.0157 (12)	
C19	0.2788 (3)	0.0931 (6)	0.2264 (3)	0.0231 (13)	

C20	0.3183 (4)	−0.0370 (7)	0.2145 (3)	0.0375 (17)	
H20A	0.3723	−0.0159	0.2129	0.056*	
H20B	0.2853	−0.0749	0.1790	0.056*	
H20C	0.3227	−0.1031	0.2438	0.056*	
C21	0.1927 (4)	0.0590 (7)	0.2259 (3)	0.0342 (17)	
H21A	0.1949	−0.0133	0.2526	0.051*	
H21B	0.1604	0.0286	0.1889	0.051*	
H21C	0.1679	0.1399	0.2358	0.051*	
C22	0.3296 (3)	0.1502 (6)	0.2817 (2)	0.0190 (12)	
C23	0.3164 (4)	0.1284 (7)	0.3317 (3)	0.0272 (15)	
H23	0.2718	0.0744	0.3326	0.033*	
C24	0.3668 (4)	0.1837 (7)	0.3801 (3)	0.0308 (15)	
H24	0.3573	0.1656	0.4140	0.037*	
C25	0.4305 (4)	0.2645 (6)	0.3799 (3)	0.0242 (14)	
H25	0.4643	0.3024	0.4135	0.029*	
C26	0.4464 (3)	0.2915 (6)	0.3308 (2)	0.0174 (12)	
C27	0.3949 (3)	0.2318 (6)	0.2831 (2)	0.0163 (12)	
C28	0.5694 (4)	0.4591 (6)	0.3957 (2)	0.0188 (12)	
C29	0.5274 (4)	0.5480 (7)	0.4188 (3)	0.0263 (14)	
H29	0.4756	0.5798	0.3973	0.032*	
C30	0.5605 (4)	0.5904 (8)	0.4729 (3)	0.0332 (16)	
H30	0.5316	0.6514	0.4883	0.040*	
C31	0.6351 (5)	0.5444 (8)	0.5042 (3)	0.0401 (19)	
H31	0.6582	0.5745	0.5412	0.048*	
C32	0.6765 (5)	0.4543 (8)	0.4819 (3)	0.0383 (18)	
H32	0.7276	0.4209	0.5039	0.046*	
C33	0.6437 (4)	0.4125 (7)	0.4276 (3)	0.0301 (15)	
H33	0.6728	0.3513	0.4124	0.036*	

C34	0.5994 (3)	0.3042 (6)	0.3097 (2)	0.0203 (13)	
C35	0.5995 (4)	0.1648 (7)	0.3120 (3)	0.0305 (15)	
H35	0.5569	0.1191	0.3202	0.037*	
C36	0.6607 (4)	0.0900 (8)	0.3025 (3)	0.0391 (17)	
H36	0.6600	−0.0062	0.3038	0.047*	
C37	0.7236 (5)	0.1577 (8)	0.2908 (3)	0.0411 (19)	
H37	0.7665	0.1076	0.2850	0.049*	
C38	0.7232 (5)	0.2961 (9)	0.2878 (4)	0.044 (2)	
H38	0.7654	0.3420	0.2792	0.052*	
C39	0.6613 (4)	0.3699 (8)	0.2972 (3)	0.0349 (17)	
H39	0.6615	0.4660	0.2951	0.042*	
C40	0.5470 (4)	0.7474 (7)	0.2185 (3)	0.0286 (15)	
C41	0.5483 (4)	0.7166 (6)	0.3217 (3)	0.0245 (14)	
C42	0.6277 (4)	0.7237 (7)	0.3564 (3)	0.0265 (14)	
H42	0.6676	0.6683	0.3491	0.032*	
C43	0.6499 (4)	0.8107 (7)	0.4016 (3)	0.0348 (17)	
H43	0.7043	0.8128	0.4253	0.042*	
C44	0.5930 (5)	0.8941 (7)	0.4122 (3)	0.0343 (17)	
C45	0.5140 (5)	0.8917 (7)	0.3770 (3)	0.0333 (16)	
H45	0.4748	0.9495	0.3837	0.040*	
C46	0.4925 (4)	0.8051 (7)	0.3321 (3)	0.0275 (14)	
H46	0.4385	0.8057	0.3079	0.033*	
C47	0.6171 (6)	0.9851 (8)	0.4603 (3)	0.054 (3)	

Geometric parameters (Å, °)

Pd1—C41	2.030 (6)	C17—C19	1.524 (9)
Pd1—C40	2.066 (6)	C19—C22	1.518 (9)

Pd1—P2	2.4175 (16)	C19—C20	1.534 (9)
Pd1—P1	2.4723 (16)	C19—C21	1.541 (8)
P1—C1	1.829 (7)	C20—H20A	0.9800
P1—C7	1.833 (6)	C20—H20B	0.9800
P1—C13	1.846 (6)	C20—H20C	0.9800
P2—C34	1.813 (6)	C21—H21A	0.9800
P2—C26	1.831 (6)	C21—H21B	0.9800
P2—C28	1.834 (6)	C21—H21C	0.9800
O1—C18	1.377 (7)	C22—C23	1.388 (9)
O1—C27	1.384 (7)	C22—C27	1.388 (8)
F1—C40	1.365 (8)	C23—C24	1.384 (10)
F2—C40	1.342 (8)	C23—H23	0.9500
F3—C40	1.364 (8)	C24—C25	1.372 (9)
F4—C47	1.322 (13)	C24—H24	0.9500
F5—C47	1.397 (15)	C25—C26	1.397 (8)
F6—C47	1.285 (15)	C25—H25	0.9500
F4A—C47	1.226 (16)	C26—C27	1.393 (8)
F5A—C47	1.460 (17)	C28—C33	1.374 (9)
F6A—C47	1.291 (15)	C28—C29	1.393 (9)
C1—C2	1.380 (10)	C29—C30	1.381 (9)
C1—C6	1.389 (10)	C29—H29	0.9500
C2—C3	1.391 (11)	C30—C31	1.371 (11)
C2—H2	0.9500	C30—H30	0.9500
C3—C4	1.379 (14)	C31—C32	1.381 (11)
C3—H3	0.9500	C31—H31	0.9500
C4—C5	1.368 (14)	C32—C33	1.385 (10)
C4—H4	0.9500	C32—H32	0.9500
C5—C6	1.389 (12)	C33—H33	0.9500

C5—H5	0.9500	C34—C35	1.377 (9)
C6—H6	0.9500	C34—C39	1.385 (9)
C7—C12	1.360 (11)	C35—C36	1.385 (10)
C7—C8	1.380 (9)	C35—H35	0.9500
C8—C9	1.373 (11)	C36—C37	1.399 (11)
C8—H8	0.9500	C36—H36	0.9500
C9—C10	1.351 (13)	C37—C38	1.367 (12)
C9—H9	0.9500	C37—H37	0.9500
C10—C11	1.373 (13)	C38—C39	1.388 (10)
C10—H10	0.9500	C38—H38	0.9500
C11—C12	1.387 (12)	C39—H39	0.9500
C11—H11	0.9500	C41—C42	1.390 (9)
C12—H12	0.9500	C41—C46	1.399 (9)
C13—C18	1.378 (8)	C42—C43	1.393 (10)
C13—C14	1.391 (9)	C42—H42	0.9500
C14—C15	1.382 (9)	C43—C44	1.383 (11)
C14—H14	0.9500	C43—H43	0.9500
C15—C16	1.384 (10)	C44—C45	1.387 (10)
C15—H15	0.9500	C44—C47	1.472 (11)
C16—C17	1.399 (9)	C45—C46	1.383 (10)
C16—H16	0.9500	C45—H45	0.9500
C17—C18	1.383 (8)	C46—H46	0.9500
C41—Pd1—C40	80.7 (3)	C24—C23—H23	119.4
C41—Pd1—P2	86.60 (19)	C22—C23—H23	119.4
C40—Pd1—P2	155.6 (2)	C25—C24—C23	120.7 (6)
C41—Pd1—P1	169.89 (19)	C25—C24—H24	119.6
C40—Pd1—P1	92.02 (19)	C23—C24—H24	119.6
P2—Pd1—P1	102.67 (5)	C24—C25—C26	120.8 (6)

C1—P1—C7	105.6 (3)	C24—C25—H25	119.6
C1—P1—C13	98.4 (3)	C26—C25—H25	119.6
C7—P1—C13	103.5 (3)	C27—C26—C25	116.6 (5)
C1—P1—Pd1	112.3 (2)	C27—C26—P2	117.8 (4)
C7—P1—Pd1	111.7 (2)	C25—C26—P2	125.4 (5)
C13—P1—Pd1	123.4 (2)	O1—C27—C22	120.7 (5)
C34—P2—C26	105.4 (3)	O1—C27—C26	114.9 (5)
C34—P2—C28	103.4 (3)	C22—C27—C26	124.3 (5)
C26—P2—C28	99.6 (3)	C33—C28—C29	119.0 (6)
C34—P2—Pd1	101.5 (2)	C33—C28—P2	122.6 (5)
C26—P2—Pd1	128.67 (19)	C29—C28—P2	118.3 (5)
C28—P2—Pd1	115.6 (2)	C30—C29—C28	120.5 (6)
C18—O1—C27	114.3 (4)	C30—C29—H29	119.7
C2—C1—C6	119.5 (7)	C28—C29—H29	119.7
C2—C1—P1	117.3 (5)	C31—C30—C29	119.9 (7)
C6—C1—P1	123.1 (6)	C31—C30—H30	120.0
C1—C2—C3	120.2 (8)	C29—C30—H30	120.0
C1—C2—H2	119.9	C30—C31—C32	120.0 (7)
C3—C2—H2	119.9	C30—C31—H31	120.0
C4—C3—C2	119.8 (9)	C32—C31—H31	120.0
C4—C3—H3	120.1	C31—C32—C33	120.2 (7)
C2—C3—H3	120.1	C31—C32—H32	119.9
C5—C4—C3	120.4 (8)	C33—C32—H32	119.9
C5—C4—H4	119.8	C28—C33—C32	120.4 (7)
C3—C4—H4	119.8	C28—C33—H33	119.8
C4—C5—C6	120.2 (8)	C32—C33—H33	119.8
C4—C5—H5	119.9	C35—C34—C39	119.1 (6)
C6—C5—H5	119.9	C35—C34—P2	123.7 (5)

C5—C6—C1	120.0 (8)	C39—C34—P2	117.2 (5)
C5—C6—H6	120.0	C34—C35—C36	121.0 (7)
C1—C6—H6	120.0	C34—C35—H35	119.5
C12—C7—C8	117.2 (7)	C36—C35—H35	119.5
C12—C7—P1	123.6 (5)	C35—C36—C37	119.3 (7)
C8—C7—P1	119.0 (6)	C35—C36—H36	120.3
C9—C8—C7	121.6 (8)	C37—C36—H36	120.3
C9—C8—H8	119.2	C38—C37—C36	119.8 (7)
C7—C8—H8	119.2	C38—C37—H37	120.1
C10—C9—C8	120.4 (8)	C36—C37—H37	120.1
C10—C9—H9	119.8	C37—C38—C39	120.3 (7)
C8—C9—H9	119.8	C37—C38—H38	119.8
C9—C10—C11	119.5 (8)	C39—C38—H38	119.8
C9—C10—H10	120.3	C34—C39—C38	120.4 (7)
C11—C10—H10	120.3	C34—C39—H39	119.8
C10—C11—C12	119.5 (9)	C38—C39—H39	119.8
C10—C11—H11	120.2	F2—C40—F3	103.6 (6)
C12—C11—H11	120.2	F2—C40—F1	104.5 (5)
C7—C12—C11	121.8 (8)	F3—C40—F1	101.3 (5)
C7—C12—H12	119.1	F2—C40—Pd1	116.4 (4)
C11—C12—H12	119.1	F3—C40—Pd1	112.1 (4)
C18—C13—C14	117.5 (5)	F1—C40—Pd1	117.0 (4)
C18—C13—P1	119.3 (4)	C42—C41—C46	117.5 (6)
C14—C13—P1	123.2 (5)	C42—C41—Pd1	124.5 (5)
C15—C14—C13	120.0 (6)	C46—C41—Pd1	117.9 (5)
C15—C14—H14	120.0	C41—C42—C43	121.2 (6)
C13—C14—H14	120.0	C41—C42—H42	119.4
C14—C15—C16	121.2 (6)	C43—C42—H42	119.4

C14—C15—H15	119.4	C44—C43—C42	120.1 (7)
C16—C15—H15	119.4	C44—C43—H43	119.9
C15—C16—C17	120.1 (6)	C42—C43—H43	119.9
C15—C16—H16	120.0	C43—C44—C45	119.6 (6)
C17—C16—H16	120.0	C43—C44—C47	119.7 (7)
C18—C17—C16	116.9 (6)	C45—C44—C47	120.7 (7)
C18—C17—C19	118.7 (5)	C46—C45—C44	119.9 (7)
C16—C17—C19	124.3 (6)	C46—C45—H45	120.0
O1—C18—C13	115.4 (5)	C44—C45—H45	120.0
O1—C18—C17	120.3 (5)	C45—C46—C41	121.5 (6)
C13—C18—C17	124.3 (5)	C45—C46—H46	119.2
C22—C19—C17	107.6 (5)	C41—C46—H46	119.2
C22—C19—C20	109.2 (5)	F4A—C47—F6	126.3 (12)
C17—C19—C20	108.0 (5)	F4A—C47—F6A	116.8 (12)
C22—C19—C21	111.6 (5)	F6—C47—F6A	39.9 (7)
C17—C19—C21	111.8 (5)	F4A—C47—F4	33.0 (8)
C20—C19—C21	108.6 (6)	F6—C47—F4	113.4 (10)
C19—C20—H20A	109.5	F6A—C47—F4	129.9 (10)
C19—C20—H20B	109.5	F4A—C47—F5	67.9 (10)
H20A—C20—H20B	109.5	F6—C47—F5	102.9 (11)
C19—C20—H20C	109.5	F6A—C47—F5	64.9 (9)
H20A—C20—H20C	109.5	F4—C47—F5	100.1 (9)
H20B—C20—H20C	109.5	F4A—C47—F5A	97.7 (12)
C19—C21—H21A	109.5	F6—C47—F5A	54.1 (8)
C19—C21—H21B	109.5	F6A—C47—F5A	92.3 (9)
H21A—C21—H21B	109.5	F4—C47—F5A	68.2 (9)
C19—C21—H21C	109.5	F5—C47—F5A	139.4 (10)
H21A—C21—H21C	109.5	F4A—C47—C44	117.8 (10)

H21B—C21—H21C	109.5	F6—C47—C44	115.0 (9)
C23—C22—C27	116.4 (6)	F6A—C47—C44	116.5 (9)
C23—C22—C19	125.4 (5)	F4—C47—C44	113.5 (8)
C27—C22—C19	118.1 (5)	F5—C47—C44	110.3 (9)
C24—C23—C22	121.2 (6)	F5A—C47—C44	109.9 (9)

4. Thermal decomposition study

A typical procedure for thermal decomposition of ***2c:*** In an oven-dried Schlenk tube equipped with a magnetic stir bar were added **2c** (85 mg, 0.1 mmol) (and equal molecular of Xantphos for entries 2,4 in Table 1). The tube was then sealed, evacuated and back-filled with nitrogen three times. Under nitrogen, benzene (1 mL) was added by syringe. The contents in the tube were then vigorously stirred at 80 ºC for 2 hours. The reaction mixture was cooled to room temperature. After filtration, the filtrate was subjected to ^{19}F NMR spectroscopy using 4,4-difluorobiphenyl as the internal standard to determine the NMR yield. Alternatively, the solvents in the filtrate were removed under reduced pressure to get crude product residuals. Ar-CF_3 (**A**) and Ar-Ar (**B**) in the residuals were further separated by column chromatography on silical gel using petroleum ether as the eluent. Figures S17-S20 shows the NMR spectra of isolated Ar-CF_3 (**A**) and Ar-Ar (**B**).

Figure S17. ^1H NMR (400 MHz, $CDCl_3$) of Ar-CF_3 (**A**)

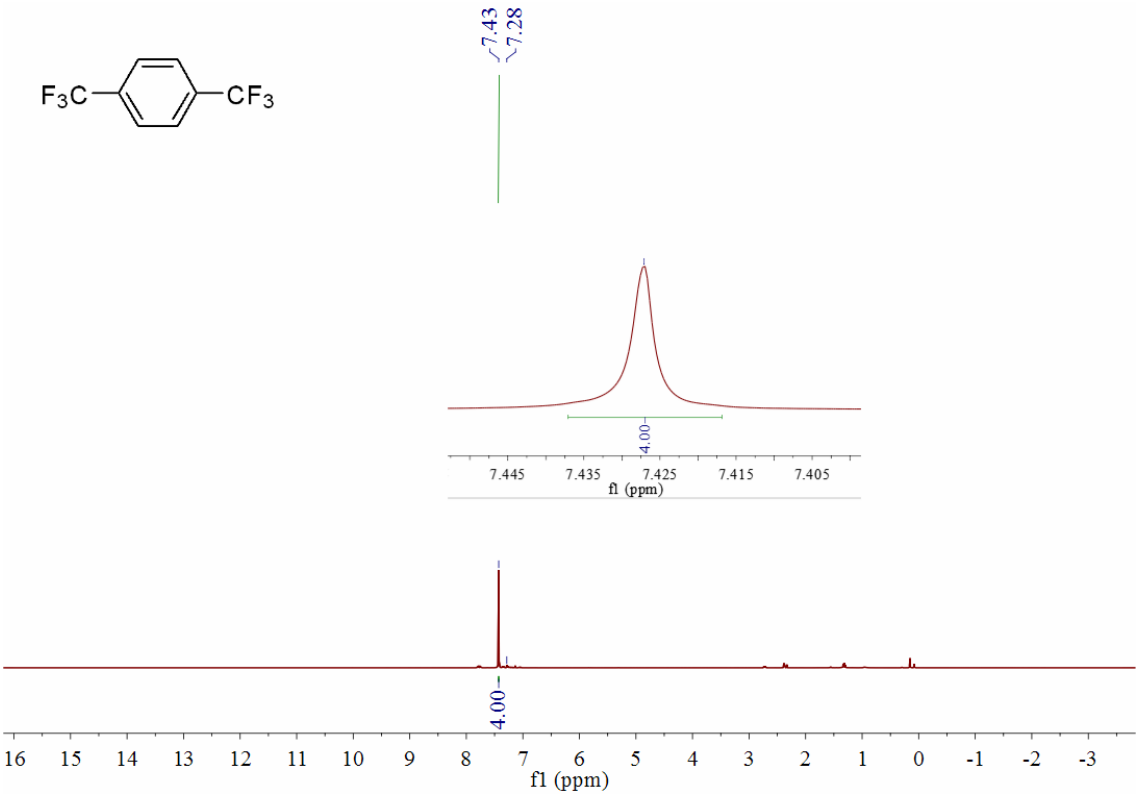


Figure S18. ^{19}F NMR (376 MHz, $CDCl_3$) of Ar-CF_3 (**A**)

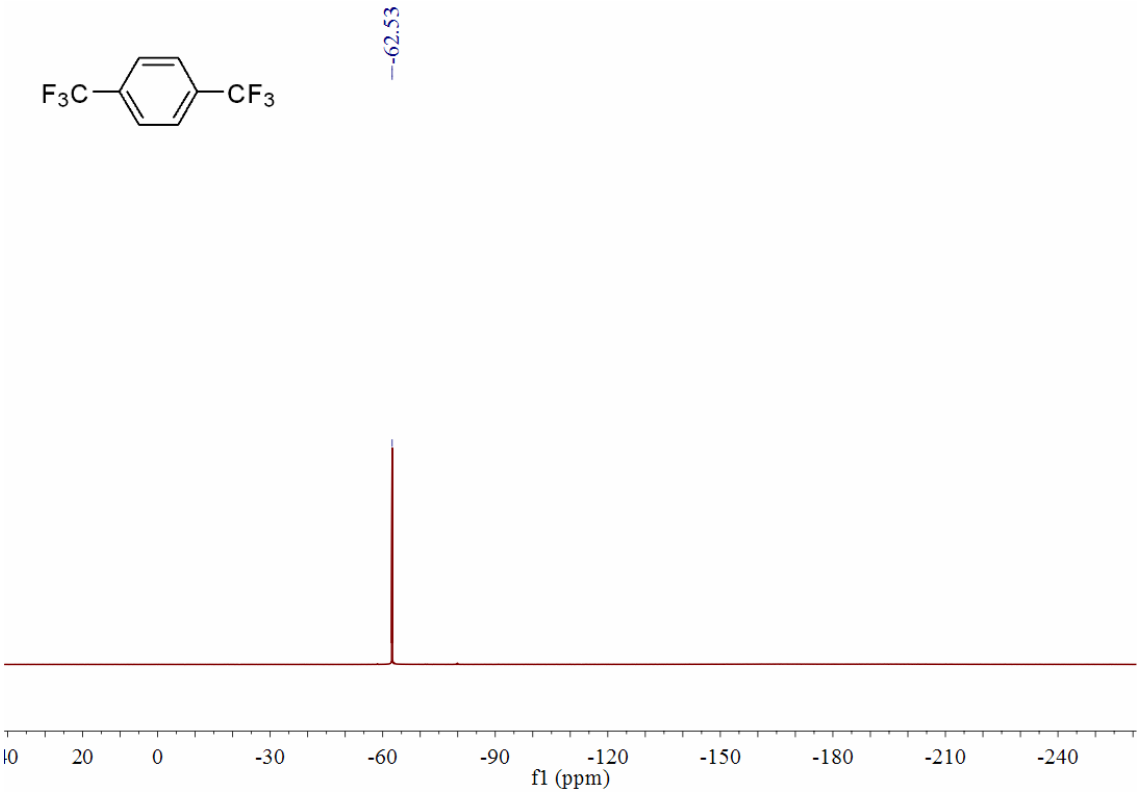


Figure S19. ^{1}H NMR (400 MHz, $CDCl_3$) of Ar-Ar (**B**)

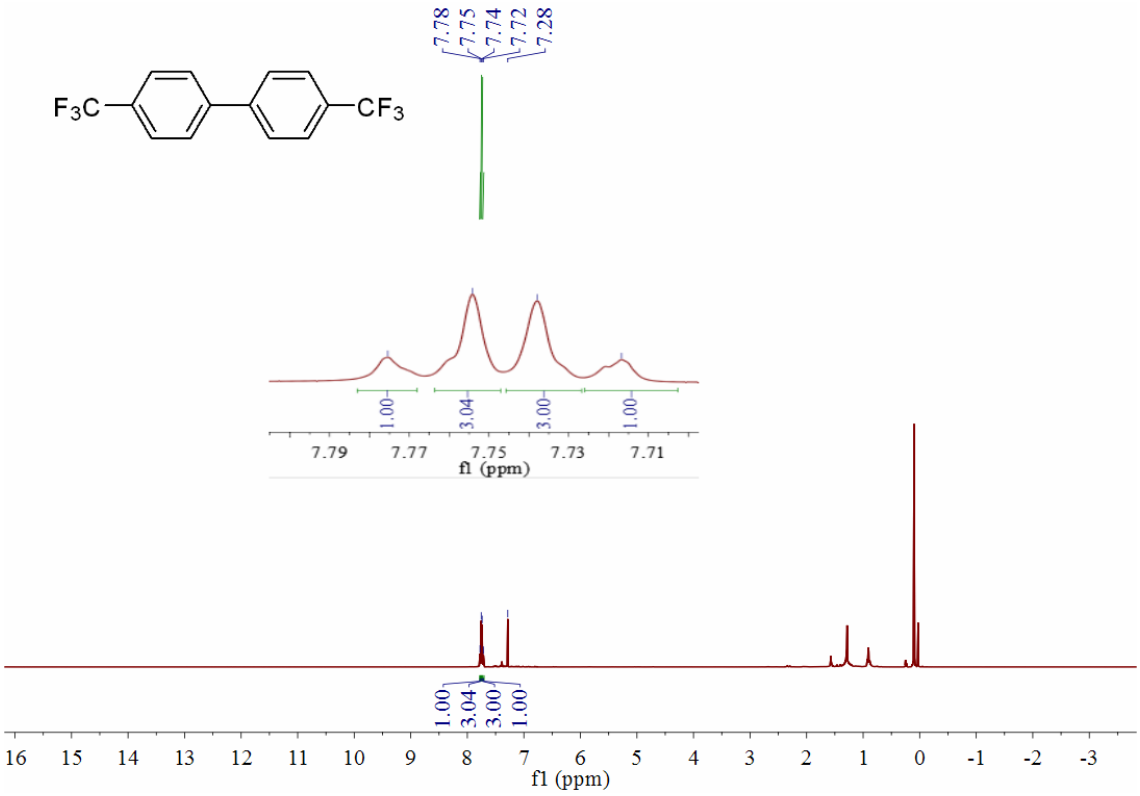
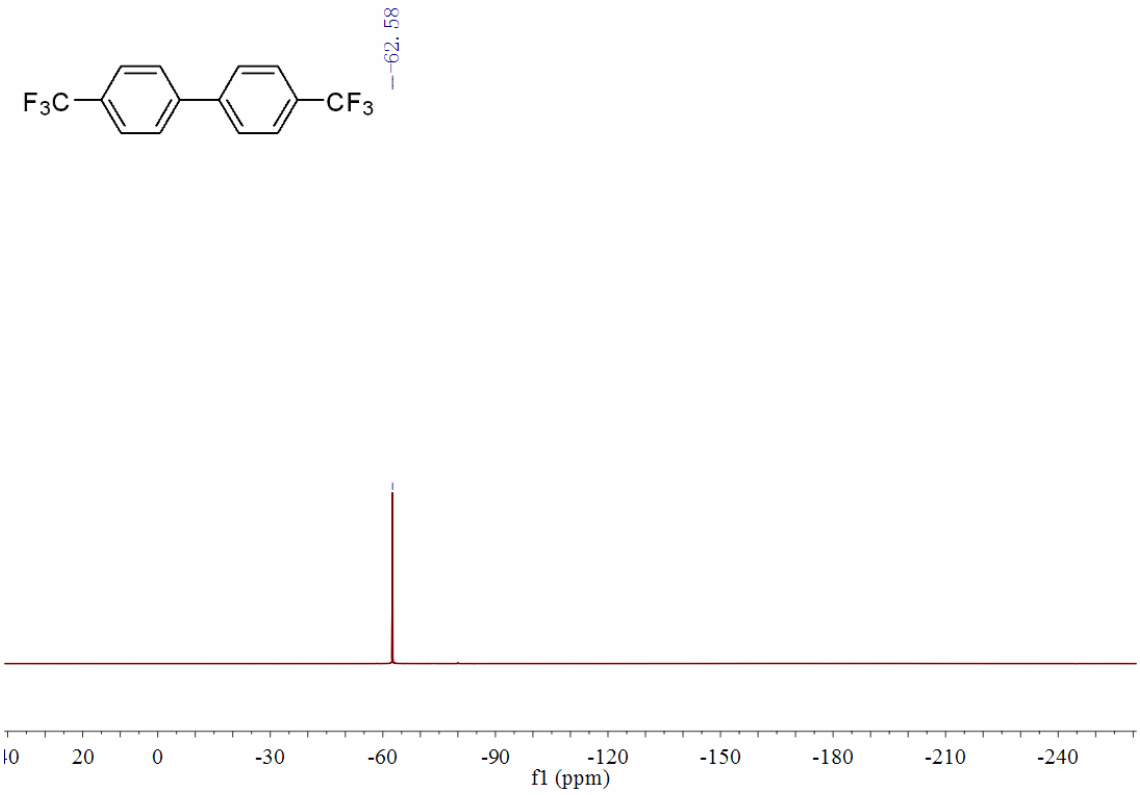


Figure S20. ^{19}F NMR (376 MHz, $CDCl_3$) of Ar-Ar (**B**)



5. DFT computational study

5.1 Computational methods and model reactions

All calculations were performed with Gaussian 09.[1] B3LYP method[2] was used for geometry optimization calculations with a combined basis set where Pd and P were described by LANL2DZ basis set and effective core potential implemented;[3] the other atoms were described by standard Pople all-electron basis set 6-31G(d). Frequency analyses were conducted at the same level of theory for geometry optimization, aiming to verify the stationary points to be real minima or saddle points, and to get thermodynamic energy correction items. For each saddle point, the intrinsic reaction coordinate (IRC) analysis[4] was carried out to confirm that it connected the correct reactant and product on the potential energy surface. Single-point energy calculations were performed by using B97D functional[5] on the B3LYP-optimized gas-phase stationary points with a larger basis set, *i.e.*, SDD[6] for Pd and 6−311+G(d, p) for the other elements. Solvation effects were taken into account by using self-consistent reaction field (SCRF) method[7] with SMD solvation model[8] in toluene. For each stationary point, its energy was calculated by the solution-phase single-point energy corrected by Gibbs free energy correction item throughout the study. Noteworthy, the B97D/SDD-6-311+g(d,p)//B3LYP/LANL2DZ-6-31g(d) methodology combination used in this study has been demonstrated to be a reliable method for treating Pd fluoro-containing systems by our previous systematic benchmark study.[9] The model reactions studied are shown in Scheme 1 in the main text.

References:

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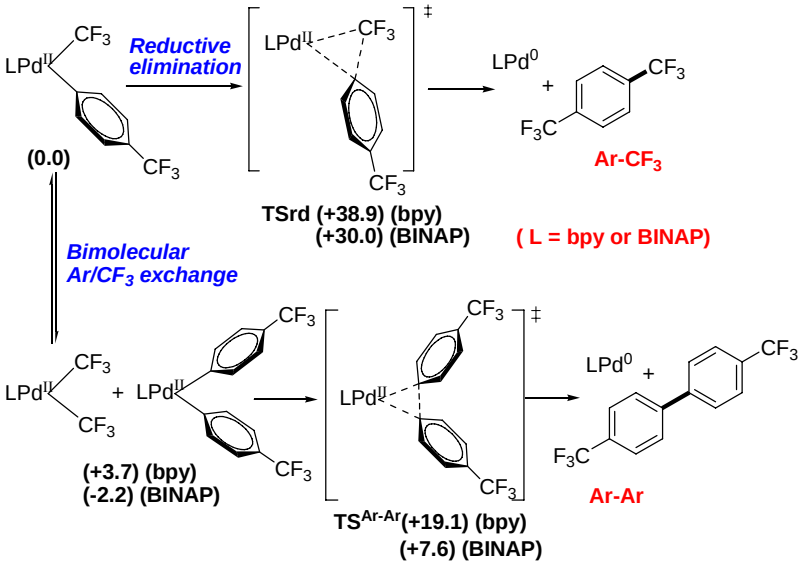
5.2 Additional computational results

Scheme S1. Computational results for **2a** and **2b** with bpy and BINAP ligands



5.3 Cartesian coordinates for the optimized stationary points

(Xantphos)Pd(Ar)(CF_3) (2c):
SCF Done: E(RB3LYP) = -2626.65333952 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.364993	0.643820	-1.651809
2	6	0	-2.508375	1.052566	-0.621127
3	6	0	-3.085825	1.598833	0.537380
4	6	0	-4.472269	1.694869	0.681358
5	6	0	-5.310552	1.251742	-0.344258
6	6	0	-4.750645	0.731809	-1.514876
7	46	0	-0.483107	0.910728	-0.641582
8	6	0	-0.520030	2.491810	-1.910205
9	9	0	-1.508142	2.552991	-2.835531
10	15	0	2.037204	1.572037	0.136406
11	6	0	3.499767	0.706218	-0.677895
12	6	0	3.378338	-0.678796	-0.870964
13	6	0	4.376968	-1.463057	-1.448640
14	6	0	5.538403	-0.793829	-1.864350
15	6	0	5.685463	0.581478	-1.703729
16	6	0	4.669303	1.332613	-1.104931
17	6	0	4.224815	-2.981311	-1.593024
18	6	0	2.834532	-3.428350	-1.119764
19	6	0	1.899210	-2.522219	-0.602703
20	8	0	2.194963	-1.202480	-0.420772
21	6	0	0.597861	-2.897559	-0.233248
22	6	0	0.250319	-4.248324	-0.327422
23	6	0	1.172439	-5.185445	-0.792928
24	6	0	2.440058	-4.770081	-1.195313
25	6	0	4.406291	-3.376856	-3.081750
26	6	0	5.310401	-3.683405	-0.735316
27	15	0	-0.670854	-1.586872	0.284713
28	6	0	-0.864863	-1.857996	2.139746
29	6	0	-1.822382	-1.090506	2.821852
30	6	0	-2.000256	-1.245553	4.197352
31	6	0	-1.210955	-2.151347	4.910406
32	6	0	-0.247002	-2.903804	4.238976
33	6	0	-0.077184	-2.763321	2.859255
34	6	0	2.629784	3.369010	0.195172
35	6	0	2.582754	4.148493	-0.970634
36	6	0	3.023481	5.472446	-0.951730
37	6	0	3.501326	6.041051	0.230284
38	6	0	3.540506	5.274678	1.394977
39	6	0	3.112074	3.945203	1.378288
40	6	0	2.233215	1.049104	1.937637
41	6	0	1.133533	1.206818	2.790448
42	6	0	1.233190	0.876382	4.143046
43	6	0	2.431351	0.374680	4.653881
44	6	0	3.530041	0.209230	3.808320
45	6	0	3.433773	0.548610	2.457157
46	6	0	-2.209236	-2.409397	-0.446791
47	6	0	-3.265506	-2.898445	0.325972
48	6	0	-4.374912	-3.486650	-0.290323
49	6	0	-4.431589	-3.600162	-1.678576
50	6	0	-3.374905	-3.116657	-2.455022
51	6	0	-2.274768	-2.518366	-1.843529
52	9	0	0.644214	2.399161	-2.668691
53	9	0	-0.479871	3.719266	-1.326010
54	1	0	0.896963	-6.233865	-0.857947
55	6	0	-6.797267	1.400349	-0.216584
56	1	0	3.139303	-5.507599	-1.578818
57	1	0	-2.957272	0.248362	-2.575580
58	1	0	-5.398490	0.390877	-2.316906
59	1	0	-4.899537	2.115710	1.586941
60	1	0	-2.454713	1.965657	1.343775
61	1	0	-0.749884	-4.564014	-0.050087

62	1	0	4.787854	2.402594	-0.971969
63	1	0	6.595962	1.071208	-2.036531
64	1	0	6.345225	-1.361870	-2.318941
65	1	0	-3.233108	-2.825128	1.407734
66	1	0	-5.192476	-3.858102	0.321725
67	1	0	-5.293819	-4.059021	-2.154645
68	1	0	-3.410899	-3.197476	-3.538225
69	1	0	-1.463636	-2.134031	-2.456953
70	1	0	-2.437403	-0.378247	2.278426
71	1	0	-2.755560	-0.656037	4.710548
72	1	0	-1.347454	-2.269093	5.982101
73	1	0	0.373411	-3.608965	4.785881
74	1	0	0.669938	-3.362058	2.348560
75	1	0	0.194844	1.585353	2.394408
76	1	0	0.369687	0.995100	4.790728
77	1	0	2.507715	0.111081	5.705397
78	1	0	4.466397	-0.180071	4.199959
79	1	0	4.296905	0.427795	1.809656
80	1	0	3.155819	3.363602	2.292132
81	1	0	3.907474	5.707009	2.322286
82	1	0	3.835456	7.075130	0.244156
83	1	0	2.979773	6.062206	-1.863445
84	1	0	2.188808	3.731349	-1.888381
85	1	0	5.394127	-3.079265	-3.448250
86	1	0	4.318388	-4.460127	-3.214685
87	1	0	3.650321	-2.892923	-3.708220
88	1	0	6.313988	-3.384974	-1.057035
89	1	0	5.200434	-3.423436	0.322522
90	1	0	5.239009	-4.772621	-0.828158
91	9	0	-7.467992	0.459380	-0.923137
92	9	0	-7.209385	1.302400	1.071220
93	9	0	-7.234343	2.602637	-0.667227

TSrd:

SCF Done: E(RB3LYP) = -2626.62129500 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	2.930822	1.712717	-1.409349
4	6	0	4.263245	1.494431	-1.750376
5	6	0	5.204735	1.200536	-0.757961
6	6	0	4.797638	1.122492	0.579838
7	46	0	0.554477	0.933597	0.097316
8	15	0	-2.059013	1.384102	-0.055770
9	6	0	-2.928610	1.277775	1.615327
10	6	0	-4.161094	0.640117	1.795082
11	6	0	-4.753044	0.592780	3.060163
12	6	0	-4.126861	1.194055	4.152326
13	6	0	-2.899076	1.837296	3.977189
14	6	0	-2.297296	1.871238	2.718949
15	6	0	6.626585	0.939096	-1.148893
16	9	0	7.069278	1.814771	-2.080973
17	15	0	0.706487	-1.583069	0.487159
18	6	0	-0.032579	-2.799181	-0.753898
19	6	0	-1.361073	-2.621885	-1.158512
20	6	0	-2.005809	-3.468226	-2.068229
21	6	0	-1.249429	-4.504700	-2.626459
22	6	0	0.082885	-4.696200	-2.260874
23	6	0	0.683519	-3.859519	-1.319460
24	8	0	-2.040132	-1.559470	-0.597805
25	6	0	-3.018031	-0.967243	-1.368023
26	6	0	-3.766547	-1.741212	-2.266233
27	6	0	-3.503467	-3.250900	-2.314168
28	6	0	-4.750261	-1.086965	-3.013886
29	6	0	-4.984512	0.278616	-2.852164

30	6	0	-4.224117	1.019577	-1.948786
31	6	0	-3.210712	0.409707	-1.199012
32	6	0	-3.966626	-3.876033	-3.641376
33	6	0	-4.287888	-3.920874	-1.148388
34	6	0	2.420330	-2.329430	0.734296
35	6	0	2.715258	-3.231956	1.764682
36	6	0	4.001476	-3.761318	1.890696
37	6	0	5.002892	-3.396863	0.988741
38	6	0	4.717248	-2.495333	-0.038497
39	6	0	3.433311	-1.960252	-0.160642
40	6	0	-0.177461	-2.061979	2.083025
41	6	0	-0.183995	-1.134366	3.131718
42	6	0	-0.795083	-1.444786	4.347662
43	6	0	-1.414327	-2.683263	4.523621
44	6	0	-1.418071	-3.610439	3.479695
45	6	0	-0.800482	-3.303374	2.265272
46	6	0	-2.473036	3.142866	-0.613252
47	6	0	-3.359010	3.977030	0.077952
48	6	0	-3.630328	5.264409	-0.394467
49	6	0	-3.028806	5.724836	-1.565903
50	6	0	-2.148245	4.894351	-2.263413
51	6	0	-1.867355	3.614696	-1.786108
52	9	0	7.473887	1.000761	-0.099110
53	9	0	6.784365	-0.299690	-1.701623
54	1	0	-5.761084	0.767204	-3.433726
55	1	0	-5.348824	-1.645046	-3.725922
56	1	0	-4.404862	2.082730	-1.838512
57	1	0	1.715705	-4.024677	-1.031665
58	1	0	0.653042	-5.509015	-2.701591
59	1	0	-1.701747	-5.177540	-3.346919
60	1	0	-3.839522	3.628431	0.986185
61	1	0	-4.316136	5.904163	0.154983
62	1	0	-3.241077	6.725683	-1.932357
63	1	0	-1.670075	5.246481	-3.173565
64	1	0	-1.166130	2.983740	-2.324716
65	1	0	-1.339772	2.365983	2.589661
66	1	0	-2.405517	2.311597	4.821674
67	1	0	-4.592029	1.162462	5.134076
68	1	0	-5.708527	0.090334	3.187289
69	1	0	-4.664965	0.181386	0.950090
70	1	0	0.278756	-0.161386	2.988512
71	1	0	-0.798762	-0.712759	5.150293
72	1	0	-1.896210	-2.923100	5.467756
73	1	0	-1.900509	-4.575928	3.609195
74	1	0	-0.805464	-4.032913	1.460906
75	1	0	1.944963	-3.524339	2.470538
76	1	0	4.218525	-4.458898	2.695663
77	1	0	6.004452	-3.806488	1.090665
78	1	0	5.495338	-2.179520	-0.725973
79	1	0	3.224371	-1.240838	-0.946999
80	1	0	-3.788786	-4.955590	-3.643409
81	1	0	-5.043239	-3.739425	-3.780929
82	1	0	-3.447691	-3.437992	-4.500570
83	1	0	-4.100079	-5.000799	-1.135205
84	1	0	-3.986066	-3.509527	-0.180178
85	1	0	-5.364710	-3.755522	-1.269856
86	1	0	2.222366	1.995879	-2.181285
87	1	0	4.578054	1.579907	-2.786614
88	1	0	5.526612	0.902342	1.352742
89	1	0	3.172071	1.286984	1.965522
90	6	0	1.347836	3.126916	0.355223
91	9	0	0.353261	3.363708	1.288910
92	9	0	2.374807	3.874115	0.835918
93	9	0	0.960781	3.732342	-0.794206

TSrd-prod:
SCF Done: E(RB3LYP) = -2626.70346003 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.610203	1.361588	-1.155943
2	6	0	2.807106	0.424865	-1.878489
3	6	0	2.736164	-0.935051	-1.427975
4	6	0	3.411012	-1.282733	-0.224190
5	6	0	4.116289	-0.335026	0.493346
6	6	0	4.233544	0.998258	0.014886
7	46	0	0.814753	0.002690	-0.830147
8	15	0	-0.346740	2.056991	0.079225
9	6	0	-0.205639	1.993358	1.960078
10	6	0	1.009552	1.552252	2.500478
11	6	0	1.194638	1.504949	3.882327
12	6	0	0.160813	1.888449	4.739588
13	6	0	-1.055056	2.321360	4.207894
14	6	0	-1.237817	2.378394	2.823324
15	6	0	2.534154	0.698390	-3.331693
16	9	0	2.225936	1.996060	-3.572063
17	6	0	-2.188099	2.384191	-0.195064
18	6	0	-3.097935	1.322044	-0.100180
19	6	0	-4.469052	1.464095	-0.350764
20	6	0	-4.927453	2.729840	-0.730885
21	6	0	-4.049246	3.808346	-0.831633
22	6	0	-2.692309	3.638664	-0.557360
23	8	0	-2.590582	0.091720	0.267315
24	6	0	-3.204472	-1.020251	-0.271567
25	6	0	-4.580530	-0.998734	-0.536385
26	6	0	-5.371914	0.246550	-0.120451
27	6	0	-5.146568	-2.146783	-1.100376
28	6	0	-4.369130	-3.274122	-1.365600
29	6	0	-3.005762	-3.271641	-1.072120
30	6	0	-2.395954	-2.136564	-0.524945
31	15	0	-0.545037	-2.029541	-0.173090
32	6	0	-0.441338	-2.516426	1.645328
33	6	0	0.697763	-2.121909	2.358551
34	6	0	0.853969	-2.479881	3.698240
35	6	0	-0.135228	-3.225092	4.342272
36	6	0	-1.280268	-3.610273	3.641140
37	6	0	-1.433279	-3.260677	2.297326
38	6	0	-6.704538	0.364047	-0.879834
39	6	0	-5.675953	0.144318	1.402733
40	6	0	0.079945	-3.576056	-1.060153
41	6	0	0.311269	-3.480386	-2.441901
42	6	0	0.797321	-4.575214	-3.157204
43	6	0	1.073907	-5.776192	-2.497991
44	6	0	0.856850	-5.875289	-1.123396
45	6	0	0.358328	-4.782599	-0.407090
46	6	0	0.379938	3.761488	-0.297301
47	6	0	0.550146	4.750378	0.680517
48	6	0	1.099083	5.989928	0.342335
49	6	0	1.475501	6.256327	-0.975376
50	6	0	1.305962	5.275421	-1.955064
51	6	0	0.766342	4.033195	-1.616403
52	9	0	1.521944	-0.055195	-3.827390
53	9	0	3.620962	0.422680	-4.098290
54	1	0	-4.423807	4.786181	-1.120866
55	6	0	4.684072	-0.693823	1.831637
56	1	0	-5.979929	2.883243	-0.943896
57	1	0	3.712155	2.370589	-1.542269
58	1	0	4.823635	1.719126	0.570073
59	1	0	3.375746	-2.311809	0.118885
60	1	0	2.436357	-1.726069	-2.107600
61	1	0	-2.017492	4.483349	-0.638381
62	1	0	-2.406913	-4.150973	-1.283807
63	1	0	-4.828017	-4.158349	-1.798849
64	1	0	-6.206217	-2.170512	-1.330825
65	1	0	0.258604	4.555681	1.707766
66	1	0	1.230561	6.747194	1.111081

67	1	0	1.902901	7.220950	-1.236434
68	1	0	1.602672	5.470765	-2.982216
69	1	0	0.661815	3.266888	-2.376406
70	1	0	1.811333	1.237048	1.839224
71	1	0	2.143451	1.156401	4.280269
72	1	0	0.300081	1.845445	5.816664
73	1	0	-1.864882	2.618342	4.869564
74	1	0	-2.184668	2.724346	2.419522
75	1	0	1.459632	-1.522537	1.871716
76	1	0	1.747013	-2.165185	4.230899
77	1	0	-0.018603	-3.500324	5.387261
78	1	0	-2.057046	-4.185035	4.139187
79	1	0	-2.326085	-3.566728	1.759871
80	1	0	0.188842	-4.873647	0.661088
81	1	0	1.073204	-6.804632	-0.602732
82	1	0	1.461559	-6.626452	-3.052736
83	1	0	0.968773	-4.486820	-4.226786
84	1	0	0.120036	-2.541679	-2.956703
85	1	0	-7.339900	-0.504780	-0.683326
86	1	0	-7.266448	1.240898	-0.544301
87	1	0	-6.551359	0.443841	-1.961342
88	1	0	-6.296911	-0.735435	1.607975
89	1	0	-4.754394	0.055533	1.986029
90	1	0	-6.212485	1.037392	1.743620
91	9	0	5.769336	0.043284	2.151373
92	9	0	3.769681	-0.477962	2.831796
93	9	0	5.032302	-1.995239	1.923125

(Xantphos)Pd(CF_3)$_2$

SCF Done: E(RB3LYP) = -2395.61097841 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.748539	-1.072474	-1.820396
2	6	0	3.674601	-0.603302	-0.502470
3	6	0	4.826561	-0.601651	0.291546
4	6	0	6.037305	-1.069511	-0.226286
5	6	0	6.106976	-1.533416	-1.540225
6	6	0	4.959994	-1.531121	-2.337060
7	15	0	2.008912	0.042183	0.110417
8	6	0	2.326714	0.369707	1.939757
9	6	0	2.419978	-0.734185	2.801148
10	6	0	2.677854	-0.544323	4.158964
11	6	0	2.822440	0.745843	4.674786
12	6	0	2.713946	1.845920	3.823935
13	6	0	2.473961	1.659992	2.460003
14	46	0	0.077522	-1.647620	-0.602774
15	15	0	-2.097007	-0.244028	0.144004
16	6	0	-1.847739	0.194564	1.957524
17	6	0	-1.234764	-0.759267	2.779642
18	6	0	-1.071108	-0.512686	4.143752
19	6	0	-1.507613	0.693108	4.694772
20	6	0	-2.114808	1.649410	3.878360
21	6	0	-2.289560	1.399990	2.515777
22	6	0	-1.072800	-2.802298	-1.806560
23	9	0	-2.034304	-3.535442	-1.191610
24	9	0	-0.425440	-3.650727	-2.637598
25	9	0	-1.738201	-1.925509	-2.650660
26	6	0	-2.509680	1.414689	-0.645386
27	6	0	-1.477977	2.352806	-0.767372
28	6	0	-1.642329	3.600308	-1.377540
29	6	0	-2.905718	3.886049	-1.909362
30	6	0	-3.953864	2.972158	-1.807239
31	6	0	-3.762459	1.746610	-1.167864
32	6	0	-0.476878	4.594665	-1.336741
33	6	0	0.834414	3.798686	-1.368389
34	6	0	0.874148	2.532871	-0.765517

35	8	0	-0.265583	1.984220	-0.224061
36	6	0	2.045408	1.770703	-0.662793
37	6	0	3.225849	2.320940	-1.176724
38	6	0	3.218146	3.570703	-1.792992
39	6	0	2.032164	4.296762	-1.891274
40	6	0	-0.555818	5.612196	-2.489834
41	6	0	-0.544051	5.363646	0.014765
42	6	0	-3.798521	-1.078777	0.189488
43	6	0	-4.341813	-1.615438	-0.987424
44	6	0	-5.601667	-2.215002	-0.973379
45	6	0	-6.329027	-2.302247	0.215017
46	6	0	-5.790233	-1.779469	1.390237
47	6	0	-4.534924	-1.166537	1.378280
48	1	0	4.139763	3.980290	-2.196068
49	1	0	2.048347	5.268678	-2.372406
50	1	0	4.151568	1.762099	-1.108678
51	1	0	-4.583203	1.042839	-1.087694
52	1	0	-4.927629	3.218929	-2.220338
53	1	0	-3.083022	4.836647	-2.400589
54	1	0	4.785555	-0.241533	1.314204
55	1	0	6.924826	-1.069443	0.401168
56	1	0	7.048754	-1.898826	-1.940911
57	1	0	5.002827	-1.898591	-3.358644
58	1	0	2.858350	-1.093438	-2.441628
59	1	0	2.301082	-1.738300	2.407646
60	1	0	2.762279	-1.407378	4.814285
61	1	0	3.018436	0.892003	5.733749
62	1	0	2.823953	2.853308	4.216984
63	1	0	2.407608	2.523000	1.805498
64	1	0	-0.886121	-1.696407	2.352317
65	1	0	-0.592448	-1.258781	4.771261
66	1	0	-1.374386	0.887467	5.755614
67	1	0	-2.458715	2.589515	4.302044
68	1	0	-2.776168	2.142123	1.890204
69	1	0	-4.136044	-0.759601	2.300432
70	1	0	-6.345320	-1.843276	2.322517
71	1	0	-7.305908	-2.778370	0.224998
72	1	0	-6.007028	-2.626181	-1.893997
73	1	0	-3.779257	-1.583294	-1.911582
74	1	0	-1.484206	6.188187	-2.436686
75	1	0	0.260133	6.338148	-2.427699
76	1	0	-0.508625	5.120332	-3.466981
77	1	0	-1.482595	5.925268	0.087611
78	1	0	-0.492308	4.674705	0.864080
79	1	0	0.291842	6.068324	0.094632
80	6	0	1.339502	-3.243020	-0.496396
81	9	0	2.252551	-3.060465	0.523073
82	9	0	0.681282	-4.386382	-0.164135
83	9	0	2.075978	-3.534767	-1.594933

(Xantphos)Pd(Ar)$_2$:

SCF Done: E(RB3LYP) = -2857.70117897 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.338331	-1.857549	-1.689460
2	6	0	2.058402	-1.464911	-0.368583
3	6	0	2.747952	-2.111832	0.667031
4	6	0	3.637416	-3.154726	0.403135
5	6	0	3.868132	-3.562561	-0.913492
6	6	0	3.223291	-2.900947	-1.963409
7	46	0	0.608175	-0.067565	-0.092186
8	15	0	-0.950987	2.087046	-0.178398
9	6	0	-0.027424	3.488165	-1.048287
10	6	0	0.321539	4.689115	-0.425040
11	6	0	1.015779	5.674926	-1.133963
12	6	0	1.352749	5.474910	-2.471842

13	6	0	0.997765	4.279353	-3.102375
14	6	0	0.320361	3.289662	-2.392624
15	6	0	4.729861	-4.753435	-1.201441
16	9	0	3.997185	-5.902911	-1.274361
17	6	0	2.272821	1.117956	-0.024729
18	6	0	2.925693	1.631489	-1.155310
19	6	0	4.024363	2.483436	-1.037918
20	6	0	4.508749	2.835086	0.225298
21	6	0	3.895463	2.310447	1.365477
22	6	0	2.798477	1.456089	1.234969
23	6	0	5.722250	3.706216	0.352370
24	9	0	6.874757	2.991438	0.319461
25	15	0	-1.168059	-1.920692	0.503090
26	6	0	-1.924475	-1.465867	2.169140
27	6	0	-1.169858	-0.671093	3.040132
28	6	0	-1.673134	-0.323423	4.295193
29	6	0	-2.937458	-0.764759	4.688116
30	6	0	-3.696425	-1.556090	3.822956
31	6	0	-3.192605	-1.907372	2.569038
32	6	0	-2.697005	-2.299659	-0.533638
33	6	0	-3.514225	-1.224061	-0.894838
34	6	0	-4.674892	-1.359775	-1.662178
35	6	0	-4.988701	-2.647419	-2.114061
36	6	0	-4.187875	-3.740824	-1.783524
37	6	0	-3.054834	-3.572920	-0.985232
38	6	0	-5.560515	-0.124881	-1.865192
39	6	0	-4.650496	1.109242	-1.925221
40	6	0	-3.466943	1.112013	-1.171473
41	8	0	-3.118606	0.010142	-0.426341
42	6	0	-2.594907	2.205741	-1.118309
43	6	0	-2.965256	3.365276	-1.811985
44	6	0	-4.138095	3.399327	-2.563341
45	6	0	-4.963034	2.276319	-2.628646
46	6	0	-6.436593	-0.251280	-3.124912
47	6	0	-6.487886	0.014585	-0.622987
48	6	0	-0.499355	-3.657605	0.814715
49	6	0	0.237783	-4.283508	-0.200453
50	6	0	0.767627	-5.559883	-0.008736
51	6	0	0.565270	-6.225493	1.202199
52	6	0	-0.168694	-5.609803	2.216508
53	6	0	-0.699646	-4.331479	2.025752
54	6	0	-1.386698	2.809073	1.509254
55	6	0	-0.356835	2.990004	2.445709
56	6	0	-0.638368	3.496378	3.715471
57	6	0	-1.952179	3.809902	4.071772
58	6	0	-2.980422	3.621693	3.148027
59	6	0	-2.700009	3.129718	1.870802
60	9	0	5.806892	4.612880	-0.651096
61	9	0	5.733855	4.397533	1.518010
62	9	0	5.375988	-4.647530	-2.385784
63	9	0	5.664797	-4.961060	-0.247572
64	1	0	-4.408486	4.302300	-3.102986
65	1	0	-5.866882	2.321179	-3.226627
66	1	0	2.578932	1.369186	-2.150393
67	1	0	4.502843	2.880903	-1.928259
68	1	0	4.275587	2.566406	2.350237
69	1	0	2.358264	1.041357	2.139336
70	1	0	-2.322851	4.237687	-1.779818
71	1	0	-2.444463	-4.429687	-0.722432
72	1	0	-4.454149	-4.731722	-2.139927
73	1	0	-5.872901	-2.807097	-2.721846
74	1	0	0.056879	4.865483	0.612048
75	1	0	1.287671	6.601382	-0.635291
76	1	0	1.890604	6.243088	-3.020657
77	1	0	1.256782	4.113552	-4.144786
78	1	0	0.056597	2.359052	-2.889151
79	1	0	0.667727	2.746650	2.180334
80	1	0	0.171043	3.644447	4.425686
81	1	0	-2.171663	4.199721	5.062162

82	1	0	-4.005681	3.863230	3.415941
83	1	0	-3.508879	2.998203	1.159629
84	1	0	-0.191458	-0.315067	2.727518
85	1	0	-1.082532	0.303811	4.956598
86	1	0	-3.332141	-0.490522	5.662838
87	1	0	-4.681860	-1.902664	4.123544
88	1	0	-3.787941	-2.526443	1.904206
89	1	0	-1.265394	-3.863534	2.823975
90	1	0	-0.328439	-6.120615	3.162589
91	1	0	0.987064	-7.215017	1.356893
92	1	0	1.371405	-6.012427	-0.789123
93	1	0	0.428211	-3.763434	-1.133134
94	1	0	-7.095119	-1.121937	-3.053701
95	1	0	-7.088796	0.619828	-3.236666
96	1	0	-5.830541	-0.349108	-4.031711
97	1	0	-7.136440	-0.864296	-0.531506
98	1	0	-5.904000	0.104781	0.298545
99	1	0	-7.118853	0.906065	-0.716843
100	1	0	2.589165	-1.812668	1.699594
101	1	0	4.150257	-3.653660	1.219940
102	1	0	3.418841	-3.197338	-2.990145
103	1	0	1.857407	-1.350509	-2.522787

$TS^{Ar\text{-}Ar}$:

SCF Done: E(RB3LYP) = -2857.69036667 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.716990	4.188940	2.077221
2	6	0	1.165763	3.523210	0.974167
3	6	0	0.335573	4.231095	0.094504
4	6	0	0.068075	5.585215	0.306750
5	6	0	0.622615	6.242220	1.406599
6	6	0	1.445092	5.542009	2.291249
7	15	0	1.490628	1.700062	0.611475
8	6	0	2.266782	1.090172	2.219347
9	6	0	1.445560	0.426167	3.138000
10	6	0	1.964669	-0.032477	4.350196
11	6	0	3.312475	0.165531	4.653805
12	6	0	4.139074	0.823376	3.740576
13	6	0	3.619506	1.284042	2.528989
14	46	0	-0.574183	0.271123	-0.024831
15	15	0	0.515686	-2.143338	-0.228237
16	6	0	2.087100	-2.573355	-1.194837
17	6	0	3.145777	-1.658346	-1.246602
18	6	0	4.284134	-1.844416	-2.044339
19	6	0	4.359228	-3.027675	-2.785284
20	6	0	3.345859	-3.984729	-2.717258
21	6	0	2.218540	-3.759227	-1.929333
22	6	0	5.392218	-0.783963	-1.996869
23	6	0	4.732366	0.579574	-1.754812
24	6	0	3.602688	0.627344	-0.931568
25	8	0	3.030905	-0.535708	-0.460730
26	6	0	2.998581	1.819728	-0.517762
27	6	0	3.537108	3.020522	-0.988993
28	6	0	4.636645	3.008443	-1.849402
29	6	0	5.230650	1.802028	-2.221269
30	6	0	6.244778	-0.789586	-3.278129
31	6	0	6.314043	-1.095432	-0.781905
32	6	0	-0.707376	-3.290493	-1.103807
33	6	0	-1.394731	-4.320700	-0.455931
34	6	0	-2.336940	-5.087076	-1.149177
35	6	0	-2.581143	-4.848004	-2.501008
36	6	0	-1.890304	-3.825802	-3.157771
37	6	0	-0.971448	-3.043392	-2.459906
38	6	0	0.795073	-2.988638	1.435233
39	6	0	1.963350	-3.695266	1.741327

40	6	0	2.128697	-4.272571	3.002865
41	6	0	1.124970	-4.161016	3.965592
42	6	0	-0.045670	-3.460444	3.665022
43	6	0	-0.206202	-2.868473	2.411374
44	1	0	3.432099	-4.905459	-3.287089
45	1	0	5.220358	-3.216120	-3.417538
46	1	0	1.424722	-4.497330	-1.903080
47	1	0	3.092436	3.963447	-0.689941
48	1	0	5.041673	3.945802	-2.219937
49	1	0	6.097826	1.820460	-2.872703
50	1	0	-1.206931	-4.528814	0.592011
51	1	0	-2.879781	-5.869304	-0.626510
52	1	0	-3.308366	-5.449822	-3.039359
53	1	0	-2.074774	-3.630214	-4.211037
54	1	0	-0.451218	-2.239775	-2.975588
55	1	0	-1.116580	-2.319944	2.186048
56	1	0	-0.835310	-3.371955	4.406838
57	1	0	1.252768	-4.617376	4.943601
58	1	0	3.042874	-4.815471	3.228589
59	1	0	2.747255	-3.798132	0.997968
60	1	0	0.400301	0.254981	2.895048
61	1	0	1.318171	-0.557377	5.047731
62	1	0	3.718575	-0.195442	5.595039
63	1	0	5.190183	0.979361	3.969732
64	1	0	4.270363	1.794451	1.825165
65	1	0	2.355954	3.655266	2.772836
66	1	0	1.876143	6.046663	3.152185
67	1	0	0.407172	7.293626	1.578264
68	1	0	-0.599805	6.109824	-0.369064
69	1	0	-0.119939	3.721563	-0.748776
70	1	0	7.039336	-0.040066	-3.217627
71	1	0	6.740586	-1.755509	-3.412429
72	1	0	5.640980	-0.583394	-4.168166
73	1	0	7.105813	-0.341589	-0.701070
74	1	0	5.747428	-1.096522	0.154556
75	1	0	6.780891	-2.080131	-0.900777
76	6	0	-2.114457	1.644802	-0.313729
77	6	0	-2.234160	2.084913	-1.651456
78	6	0	-2.793135	3.320633	-1.964484
79	6	0	-3.277032	4.150739	-0.946294
80	6	0	-3.188505	3.726276	0.383913
81	6	0	-2.618333	2.493822	0.691314
82	1	0	-1.889608	1.448459	-2.462061
83	1	0	-2.868344	3.636486	-3.001137
84	6	0	-3.824189	5.502654	-1.284761
85	1	0	-3.567605	4.361250	1.178657
86	1	0	-2.576192	2.185477	1.731808
87	6	0	-2.584522	-0.294536	-0.018625
88	6	0	-3.228887	-0.881219	-1.124432
89	6	0	-4.274422	-1.784480	-0.961332
90	6	0	-4.719818	-2.124300	0.320631
91	6	0	-4.122329	-1.526599	1.434534
92	6	0	-3.083162	-0.613911	1.263202
93	1	0	-2.911687	-0.630070	-2.131660
94	1	0	-4.742194	-2.234392	-1.831331
95	6	0	-5.770969	-3.177149	0.492309
96	1	0	-4.477271	-1.767604	2.432141
97	1	0	-2.656008	-0.139777	2.143212
98	9	0	-6.443504	-3.048899	1.659581
99	9	0	-6.684824	-3.157217	-0.505733
100	9	0	-5.237714	-4.429713	0.494021
101	9	0	-4.662060	5.974736	-0.335703
102	9	0	-2.836053	6.435989	-1.421342
103	9	0	-4.496879	5.503608	-2.458705

(bpy)Pd(Ar)(CF_3) (2a):

SCF Done: E(RB3LYP) = -1528.45853790 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.936582	3.305847	0.115960
2	6	0	-2.536771	1.965685	0.045475
3	7	0	-1.223034	1.637097	0.026099
4	6	0	-0.297782	2.605497	0.070215
5	6	0	-0.626504	3.957740	0.136794
6	6	0	-1.973347	4.310393	0.161903
7	6	0	-3.505235	0.837003	-0.007721
8	6	0	-4.890960	1.030713	-0.057970
9	6	0	-5.737516	-0.074157	-0.104640
10	6	0	-5.182567	-1.350923	-0.100874
11	6	0	-3.795191	-1.472664	-0.052738
12	7	0	-2.979008	-0.410477	-0.008318
13	1	0	-3.309539	-2.439639	-0.048435
14	1	0	-5.802095	-2.240700	-0.136098
15	1	0	-6.813727	0.065649	-0.144725
16	1	0	0.732747	2.268559	0.044922
17	1	0	0.158867	4.705266	0.170264
18	1	0	-2.275421	5.352027	0.217897
19	1	0	-5.311418	2.028988	-0.065751
20	1	0	-3.986868	3.569725	0.140319
21	46	0	-0.767346	-0.507099	0.001594
22	6	0	1.236173	-0.350611	-0.021238
23	6	0	-0.589059	-2.516369	0.005416
24	6	0	2.013554	-0.574483	1.129045
25	6	0	3.386559	-0.329575	1.134910
26	6	0	4.022371	0.132670	-0.022529
27	6	0	3.273318	0.341990	-1.182441
28	6	0	1.896095	0.103374	-1.176621
29	1	0	1.545831	-0.947073	2.036013
30	1	0	3.966076	-0.493720	2.038998
31	6	0	5.507510	0.342418	-0.028070
32	1	0	3.762893	0.694481	-2.085464
33	1	0	1.335290	0.276562	-2.092268
34	9	0	0.611116	-3.130448	0.079820
35	9	0	-1.324746	-3.030090	1.060976
36	9	0	-1.203493	-3.037737	-1.115343
37	9	0	5.894285	1.234778	-0.971405
38	9	0	5.959613	0.801146	1.164584
39	9	0	6.188246	-0.802893	-0.278934

TSrd (bpy)

SCF Done: E(RB3LYP) = -1528.40183384 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.844394	-0.802886	-1.215286
2	6	0	1.185309	-0.970794	0.028474
3	6	0	1.890610	-0.626759	1.205976
4	6	0	3.151241	-0.040152	1.135404
5	6	0	3.761614	0.175849	-0.105272
6	6	0	3.101327	-0.214961	-1.279203
7	46	0	-0.787979	-0.603410	0.036286
8	7	0	-3.057023	-0.431137	-0.029903
9	6	0	-3.577483	0.811970	-0.110030
10	6	0	-4.946169	1.009715	-0.337128
11	6	0	-5.785353	-0.094508	-0.462868
12	6	0	-5.239851	-1.373675	-0.367523
13	6	0	-3.867139	-1.490419	-0.156520
14	6	0	-2.617939	1.943317	0.041961
15	6	0	-3.034355	3.264659	0.253899
16	6	0	-2.078780	4.271189	0.372227
17	6	0	-0.728366	3.936982	0.283733
18	6	0	-0.392191	2.597784	0.091016
19	7	0	-1.307726	1.629515	-0.026744

20	6	0	5.086435	0.869246	-0.188258
21	9	0	5.824855	0.704087	0.933560
22	9	0	5.829886	0.429988	-1.230884
23	9	0	4.947638	2.211822	-0.360690
24	1	0	-3.382968	-2.459961	-0.089397
25	1	0	-5.855385	-2.262474	-0.460040
26	1	0	-6.847819	0.045047	-0.640139
27	1	0	0.643517	2.275184	0.029941
28	1	0	0.049826	4.688553	0.368173
29	1	0	-2.387156	5.299361	0.538020
30	1	0	-5.352106	2.010148	-0.434137
31	1	0	-4.087273	3.506348	0.344660
32	1	0	1.441212	-0.822819	2.174533
33	1	0	3.670417	0.239659	2.047054
34	1	0	3.583443	-0.069096	-2.241325
35	1	0	1.357789	-1.130470	-2.129456
36	6	0	0.298172	-2.641888	0.234159
37	9	0	1.397256	-3.406272	-0.004521
38	9	0	-0.043072	-2.898075	1.526053
39	9	0	-0.661237	-3.230363	-0.566749

(bpy)Pd(CF_3)$_2$

SCF Done: E(RB3LYP) = -1297.41213993 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.533768	-1.426490	-0.213100
2	6	0	2.336436	-0.722504	-0.036911
3	7	0	1.148231	-1.369675	0.027712
4	6	0	1.128480	-2.706973	-0.073832
5	6	0	2.282452	-3.469807	-0.242841
6	6	0	3.507908	-2.814691	-0.314771
7	6	0	2.297053	0.759085	0.067112
8	7	0	1.076898	1.337879	-0.014032
9	6	0	0.976538	2.673182	0.061177
10	6	0	2.084608	3.502238	0.223395
11	6	0	3.344052	2.917808	0.321384
12	6	0	3.451069	1.531879	0.244682
13	46	0	-0.652462	-0.051606	0.007116
14	1	0	-0.024178	3.076446	-0.007614
15	1	0	1.950088	4.577186	0.278238
16	1	0	4.232365	3.526621	0.461556
17	1	0	0.149583	-3.161375	-0.012018
18	1	0	2.208073	-4.549291	-0.319841
19	1	0	4.431024	-3.369245	-0.455244
20	1	0	4.422016	1.061078	0.339928
21	1	0	4.476765	-0.899080	-0.290437
22	6	0	-2.146991	-1.386619	0.255665
23	9	0	-3.091585	-1.016966	1.155395
24	9	0	-2.804296	-1.716486	-0.886153
25	9	0	-1.660583	-2.589957	0.747693
26	6	0	-2.058325	1.369183	-0.269781
27	9	0	-3.340059	1.041610	-0.519770
28	9	0	-2.089889	2.249131	0.787904
29	9	0	-1.661440	2.141153	-1.346261

(bpy)Pd(Ar)$_2$

SCF Done: E(RB3LYP) = -1759.50237678 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.275172	-2.717499	-0.008299
2	6	0	-0.638509	-3.912262	0.000506
3	6	0	-1.364718	-5.109517	0.017728
4	6	0	-2.756824	-5.068938	0.022727

5	6	0	-3.398281	-3.832579	0.009644
6	6	0	-2.614218	-2.680781	-0.004957
7	6	0	0.849340	-3.868924	-0.008979
8	7	0	1.415553	-2.639187	0.003298
9	6	0	2.750179	-2.524819	-0.002560
10	6	0	3.599677	-3.629204	-0.022381
11	6	0	3.031029	-4.900675	-0.037969
12	6	0	1.643630	-5.022028	-0.030878
13	46	0	0.018579	-0.927520	0.001833
14	6	0	-1.403284	0.496286	0.006394
15	6	0	-2.116301	0.792140	-1.170837
16	6	0	-3.203789	1.668852	-1.165880
17	6	0	-3.605059	2.277219	0.026414
18	6	0	-2.903556	2.008882	1.205952
19	6	0	-1.816564	1.133830	1.190414
20	6	0	-4.737723	3.260136	0.029029
21	9	0	-5.387562	3.285209	1.217592
22	9	0	-4.319156	4.528347	-0.205995
23	9	0	-5.659441	2.978354	-0.924052
24	1	0	3.131609	-1.509170	0.013901
25	1	0	4.675108	-3.486567	-0.026564
26	1	0	3.655128	-5.789257	-0.055655
27	1	0	-3.054068	-1.689011	-0.018550
28	1	0	-4.480189	-3.752621	0.011837
29	1	0	-3.328273	-5.992316	0.036674
30	1	0	1.191652	-6.006586	-0.044318
31	1	0	-0.856589	-6.066307	0.029020
32	1	0	-1.282139	0.951574	2.118943
33	1	0	-3.210621	2.481879	2.134251
34	1	0	-3.743171	1.876133	-2.085727
35	1	0	-1.825051	0.333671	-2.113349
36	6	0	1.351558	0.580250	0.005028
37	6	0	2.081229	0.876560	1.172115
38	6	0	3.110518	1.821022	1.170607
39	6	0	3.432188	2.501432	-0.006672
40	6	0	2.712078	2.233836	-1.175124
41	6	0	1.682819	1.291547	-1.162582
42	1	0	1.845291	0.369561	2.105228
43	1	0	3.655236	2.037910	2.085073
44	6	0	4.580776	3.465017	-0.030499
45	1	0	2.948283	2.772474	-2.088230
46	1	0	1.124807	1.118842	-2.078954
47	9	0	4.415520	4.437004	-0.957275
48	9	0	4.763538	4.074353	1.164586
49	9	0	5.755824	2.848822	-0.327782

$TS^{Ar\text{-}Ar}$(bpy)

SCF Done: E(RB3LYP) = -1759.47767884 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.260118	-2.757865	-0.025921
2	6	0	0.625886	-3.948950	-0.057677
3	6	0	1.343773	-5.144679	-0.194489
4	6	0	2.732822	-5.102335	-0.285954
5	6	0	3.377274	-3.867378	-0.242341
6	6	0	2.594998	-2.720752	-0.115064
7	6	0	-0.860654	-3.906216	0.053472
8	7	0	-1.425024	-2.680015	0.033656
9	6	0	-2.755656	-2.567202	0.124140
10	6	0	-3.602695	-3.668037	0.240958
11	6	0	-3.030567	-4.938453	0.271693
12	6	0	-1.646319	-5.059874	0.178781
13	46	0	-0.028305	-0.877395	0.007335
14	6	0	0.990446	0.906047	0.024152
15	6	0	1.607853	1.285216	1.240136
16	6	0	2.826637	1.956487	1.263857

17	6	0	3.474558	2.284891	0.067943
18	6	0	2.879615	1.936048	-1.150994
19	6	0	1.660118	1.267845	-1.170611
20	6	0	4.761683	3.051341	0.079241
21	9	0	5.594714	2.653787	-0.914465
22	9	0	4.572533	4.383189	-0.095064
23	9	0	5.432814	2.906278	1.246305
24	1	0	-3.143233	-1.552846	0.102648
25	1	0	-4.676211	-3.525759	0.309451
26	1	0	-3.650112	-5.825103	0.370099
27	1	0	3.039842	-1.730325	-0.084177
28	1	0	4.457274	-3.786685	-0.309291
29	1	0	3.300240	-6.022213	-0.393282
30	1	0	-1.189993	-6.042229	0.215236
31	1	0	0.831498	-6.098581	-0.241023
32	1	0	1.218603	1.018803	-2.131250
33	1	0	3.378507	2.182168	-2.084103
34	1	0	3.283013	2.219387	2.213269
35	1	0	1.125818	1.050209	2.184666
36	6	0	-0.921114	0.974508	-0.013919
37	6	0	-1.508249	1.394338	-1.231838
38	6	0	-2.673628	2.153837	-1.258393
39	6	0	-3.292223	2.539347	-0.063569
40	6	0	-2.724972	2.152637	1.156472
41	6	0	-1.559431	1.393570	1.178753
42	1	0	-1.041345	1.126259	-2.175133
43	1	0	-3.102498	2.456389	-2.209069
44	6	0	-4.582565	3.299349	-0.087731
45	1	0	-3.193543	2.454734	2.088609
46	1	0	-1.132596	1.124790	2.140649
47	9	0	-5.661283	2.471001	-0.068040
48	9	0	-4.714311	4.118259	0.982191
49	9	0	-4.708291	4.061580	-1.198809

(BINAP)Pd(Ar)(CF_3) (2b):

SCF Done: E(RB3LYP) = -2741.97695795 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.833069	-2.509159	-1.377700
2	6	0	-0.882020	-2.696062	-0.367589
3	6	0	-0.355414	-3.975807	-0.141590
4	6	0	-0.776944	-5.055245	-0.918656
5	6	0	-1.724881	-4.864532	-1.927011
6	6	0	-2.251778	-3.592640	-2.153831
7	15	0	-0.376452	-1.223574	0.682817
8	6	0	-1.267685	-1.513769	2.319409
9	6	0	-2.116595	-2.602563	2.540126
10	6	0	-2.803989	-2.724897	3.751716
11	6	0	-2.645512	-1.765726	4.751659
12	6	0	-1.797771	-0.675213	4.536625
13	6	0	-1.119121	-0.545836	3.325388
14	46	0	-0.996636	1.209909	0.205742
15	15	0	1.441194	1.781533	-0.268977
16	6	0	2.661134	1.932875	1.145531
17	6	0	2.159463	2.471944	2.339154
18	6	0	3.009851	2.681484	3.425910
19	6	0	4.363219	2.350607	3.331413
20	6	0	4.867192	1.819052	2.143075
21	6	0	4.020645	1.615755	1.051059
22	6	0	-2.987040	0.777365	0.015644
23	6	0	-3.528977	0.839691	-1.279761
24	6	0	-4.860360	0.498574	-1.526307
25	6	0	-5.685294	0.103564	-0.469689
26	6	0	-5.170629	0.067127	0.829191
27	6	0	-3.837045	0.405803	1.066135
28	6	0	-7.130410	-0.210875	-0.717402

29	9	0	-7.924074	0.882136	-0.593954
30	6	0	-1.665238	3.116719	0.495040
31	9	0	-0.624081	3.945387	0.869595
32	9	0	-2.563752	3.232815	1.509894
33	9	0	-2.239339	3.731284	-0.583611
34	6	0	1.977509	0.436384	-1.504917
35	6	0	2.238109	-0.893881	-1.172849
36	6	0	2.375571	-1.873527	-2.224740
37	6	0	2.266459	-1.471209	-3.595176
38	6	0	2.020232	-0.108067	-3.885057
39	6	0	1.875181	0.808742	-2.875524
40	6	0	1.760036	3.374937	-1.236256
41	6	0	0.698939	3.986928	-1.915356
42	6	0	0.916902	5.148161	-2.660170
43	6	0	2.191243	5.712406	-2.727083
44	6	0	3.250133	5.111161	-2.044067
45	6	0	3.036526	3.948261	-1.302396
46	6	0	1.431083	-1.597468	1.138188
47	6	0	2.467188	-1.365391	0.237042
48	6	0	3.823968	-1.658287	0.629478
49	6	0	4.091208	-2.168975	1.940628
50	6	0	3.005239	-2.389878	2.821825
51	6	0	1.718726	-2.113615	2.431979
52	9	0	-7.340147	-0.697104	-1.965162
53	9	0	-7.609182	-1.130573	0.155039
54	1	0	3.201801	-2.787506	3.814649
55	6	0	5.429191	-2.449427	2.329104
56	1	0	-2.911012	1.158843	-2.115716
57	1	0	-5.257780	0.541054	-2.536219
58	1	0	-5.810579	-0.231649	1.654405
59	1	0	-3.464272	0.371170	2.084485
60	1	0	0.905260	-2.296208	3.123119
61	1	0	1.676674	1.842356	-3.129863
62	1	0	1.945484	0.207981	-4.922820
63	6	0	2.410453	-2.434813	-4.629123
64	1	0	0.381565	-4.130606	0.641402
65	1	0	-0.364680	-6.044269	-0.736526
66	1	0	-2.051743	-5.705779	-2.532369
67	1	0	-2.991734	-3.438268	-2.934248
68	1	0	-2.255238	-1.524368	-1.549297
69	1	0	-2.255064	-3.352568	1.768844
70	1	0	-3.467024	-3.571647	3.907746
71	1	0	-3.182935	-1.861752	5.691147
72	1	0	-1.673765	0.081531	5.306488
73	1	0	-0.476790	0.314860	3.158233
74	1	0	1.111232	2.750098	2.403216
75	1	0	2.613067	3.104132	4.345018
76	1	0	5.023354	2.508756	4.180083
77	1	0	5.918365	1.556129	2.062691
78	1	0	4.423046	1.200426	0.133411
79	1	0	3.867187	3.499785	-0.767723
80	1	0	4.244724	5.547609	-2.083871
81	1	0	2.357626	6.619573	-3.301913
82	1	0	0.082988	5.616029	-3.176191
83	1	0	-0.301364	3.576489	-1.849929
84	6	0	2.650308	-3.756281	-4.333961
85	1	0	2.325236	-2.103660	-5.661286
86	1	0	2.758757	-4.486558	-5.131080
87	6	0	2.750976	-4.164799	-2.983172
88	6	0	2.619382	-3.252193	-1.960302
89	1	0	2.932135	-5.210442	-2.749821
90	6	0	6.476013	-2.238455	1.462449
91	1	0	5.607985	-2.835480	3.329778
92	1	0	7.495233	-2.457789	1.768395
93	6	0	6.221066	-1.736225	0.163694
94	6	0	4.934509	-1.456285	-0.241057
95	1	0	7.048094	-1.573181	-0.522027
96	1	0	4.760945	-1.075048	-1.240618
97	1	0	2.695235	-3.589425	-0.933835

TSrd (BINAP)

SCF Done: E(RB3LYP) = -2741.93469554 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.609948	-1.828115	-0.736127
2	6	0	3.597365	-1.975987	0.254773
3	6	0	3.972051	-2.550132	1.512485
4	6	0	5.318612	-2.947845	1.730403
5	6	0	6.269618	-2.790672	0.749015
6	6	0	5.907122	-2.224018	-0.496320
7	6	0	2.981734	-2.706088	2.512553
8	6	0	1.687793	-2.306539	2.286822
9	6	0	1.293677	-1.729524	1.048421
10	6	0	2.236223	-1.561664	0.033128
11	15	0	-0.495335	-1.110741	0.852902
12	46	0	-0.804820	1.375440	0.322798
13	6	0	-1.973826	3.382549	0.453704
14	9	0	-1.631661	3.979817	-0.717930
15	6	0	1.881015	-1.013354	-1.322382
16	6	0	1.743097	0.350590	-1.573306
17	6	0	1.383769	0.795560	-2.878669
18	6	0	1.215178	-0.085675	-3.915402
19	6	0	1.388742	-1.478094	-3.717367
20	6	0	1.721908	-1.952057	-2.406927
21	6	0	1.238464	-2.402455	-4.784963
22	6	0	1.414068	-3.751823	-4.582079
23	6	0	1.745311	-4.228225	-3.292330
24	6	0	1.892622	-3.355533	-2.236603
25	15	0	1.664064	1.673423	-0.222489
26	6	0	2.260602	3.246685	-1.079880
27	6	0	1.667828	4.453071	-0.686778
28	6	0	2.111162	5.664830	-1.222992
29	6	0	3.142910	5.682115	-2.161576
30	6	0	3.734007	4.481773	-2.563579
31	6	0	3.298807	3.271137	-2.023282
32	6	0	-1.370074	-2.489130	-0.081964
33	6	0	-2.595445	-2.181907	-0.687611
34	6	0	-3.333046	-3.175136	-1.333799
35	6	0	-2.842556	-4.480930	-1.395641
36	6	0	-1.616191	-4.790917	-0.804021
37	6	0	-0.883728	-3.801298	-0.144252
38	6	0	-1.202265	-1.324362	2.595694
39	6	0	-1.810021	-2.506000	3.038454
40	6	0	-2.336206	-2.588614	4.330410
41	6	0	-2.259269	-1.494277	5.193586
42	6	0	-1.659465	-0.310399	4.757934
43	6	0	-1.141074	-0.225450	3.464757
44	6	0	-2.832176	1.644824	0.133473
45	6	0	-3.272568	1.600298	-1.205927
46	6	0	-4.499367	1.025826	-1.531378
47	6	0	-5.331603	0.528454	-0.523706
48	6	0	-4.935607	0.633800	0.817538
49	6	0	-3.712692	1.207224	1.145667
50	6	0	-6.608375	-0.165151	-0.888771
51	9	0	-7.515734	-0.137396	0.112230
52	6	0	3.061408	1.414558	1.019836
53	6	0	2.717768	1.373869	2.375884
54	6	0	3.708129	1.287686	3.357354
55	6	0	5.052671	1.243041	2.989796
56	6	0	5.403433	1.283746	1.638069
57	6	0	4.414439	1.373465	0.658860
58	9	0	-7.191712	0.377139	-1.982266
59	9	0	-6.404008	-1.481010	-1.183489
60	9	0	-1.078496	3.830120	1.410538
61	9	0	-3.133129	3.977720	0.838804

62	1	0	3.259062	-3.147656	3.466966
63	1	0	-2.649254	2.011892	-1.992948
64	1	0	-4.815133	0.973609	-2.569014
65	1	0	-5.588910	0.264597	1.601844
66	1	0	-3.423176	1.286743	2.188689
67	1	0	0.950066	-2.432803	3.070318
68	1	0	1.237359	1.855529	-3.054524
69	1	0	0.946318	0.278605	-4.904124
70	1	0	0.062996	-4.054331	0.323477
71	1	0	-1.228927	-5.805589	-0.850299
72	1	0	-3.413691	-5.254757	-1.901813
73	1	0	-4.291984	-2.920364	-1.775156
74	1	0	-2.978336	-1.168023	-0.652847
75	1	0	-1.881635	-3.362531	2.375580
76	1	0	-2.809602	-3.510083	4.659328
77	1	0	-2.671577	-1.560280	6.196918
78	1	0	-1.604765	0.550702	5.418852
79	1	0	-0.702792	0.706637	3.114394
80	1	0	1.671220	1.411594	2.663832
81	1	0	3.425593	1.258360	4.406355
82	1	0	5.825367	1.178717	3.751336
83	1	0	6.448936	1.245993	1.344307
84	1	0	4.705330	1.412580	-0.385604
85	1	0	3.759310	2.345130	-2.354952
86	1	0	4.535198	4.486696	-3.298179
87	1	0	3.482816	6.624471	-2.582915
88	1	0	1.641201	6.593231	-0.909915
89	1	0	0.855280	4.444363	0.031223
90	1	0	0.982114	-2.019243	-5.769794
91	1	0	1.298427	-4.450934	-5.405705
92	1	0	1.884042	-5.294000	-3.131843
93	1	0	5.582347	-3.380232	2.692697
94	1	0	7.296302	-3.099898	0.925194
95	1	0	6.659695	-2.101524	-1.270715
96	1	0	4.349486	-1.395387	-1.695171
97	1	0	2.149184	-3.742170	-1.257625

(BINAP)Pd(CF_3)$_2$

SCF Done: E(RB3LYP) = -2510.93326547 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.562398	-3.322957	1.355749
2	6	0	-0.349744	-2.622142	1.346390
3	6	0	0.428350	-2.574075	2.510515
4	6	0	-0.007412	-3.216105	3.670899
5	6	0	-1.218662	-3.909871	3.677326
6	6	0	-1.994495	-3.964318	2.517884
7	15	0	0.327430	-1.794598	-0.192188
8	6	0	0.967851	-3.230704	-1.233476
9	6	0	1.899136	-2.949500	-2.242792
10	6	0	2.394699	-3.973760	-3.050462
11	6	0	1.976109	-5.290143	-2.848718
12	6	0	1.059022	-5.577030	-1.836615
13	6	0	0.554241	-4.552608	-1.032834
14	46	0	2.124371	-0.000117	0.000126
15	15	0	0.327601	1.794592	0.192077
16	6	0	0.968133	3.230906	1.232967
17	6	0	0.554718	4.552828	1.031980
18	6	0	1.059536	5.577343	1.835609
19	6	0	1.976467	5.290554	2.847879
20	6	0	2.394929	3.974174	3.049917
21	6	0	1.899330	2.949815	2.242407
22	6	0	-1.159357	1.167691	1.202192
23	6	0	-1.247087	1.599059	2.554882
24	6	0	-2.219620	1.125584	3.398780
25	6	0	-3.180817	0.191839	2.944153

26	6	0	-3.116484	-0.256525	1.585639
27	6	0	-2.078005	0.237527	0.713658
28	6	0	-4.204284	-0.294327	3.801944
29	6	0	-5.144358	-1.187600	3.344716
30	6	0	-5.090839	-1.634561	2.003199
31	6	0	-4.106069	-1.185822	1.151414
32	6	0	-2.078113	-0.237307	-0.713349
33	6	0	-1.159613	-1.167475	-1.202097
34	6	0	-1.247541	-1.598704	-2.554821
35	6	0	-2.220109	-1.125039	-3.398558
36	6	0	-3.181212	-0.191266	-2.943717
37	6	0	-3.116744	0.256872	-1.585136
38	6	0	-4.106246	1.186138	-1.150686
39	6	0	-5.091075	1.635058	-2.002317
40	6	0	-5.144716	1.188335	-3.343897
41	6	0	-4.204700	0.295102	-3.801348
42	6	0	-0.349502	2.621771	-1.346731
43	6	0	0.428519	2.573245	-2.510879
44	6	0	-0.007266	3.214879	-3.671472
45	6	0	-1.218486	3.908694	-3.678117
46	6	0	-1.994248	3.963608	-2.518654
47	6	0	-1.562111	3.322670	-1.356306
48	1	0	-2.265107	1.474109	4.427787
49	1	0	-0.531345	2.319606	2.929617
50	1	0	-0.531929	-2.319312	-2.929696
51	1	0	-2.265729	-1.473422	-4.427607
52	1	0	-2.174610	3.363230	-0.460820
53	1	0	-2.940453	4.497486	-2.518259
54	1	0	-1.557262	4.405793	-4.583155
55	1	0	0.603640	3.172324	-4.569023
56	1	0	1.383056	2.058986	-2.498042
57	1	0	-0.149611	4.792972	0.242865
58	1	0	0.736423	6.600957	1.665207
59	1	0	2.370094	6.089821	3.470129
60	1	0	3.120900	3.742428	3.824250
61	1	0	2.254454	1.934157	2.385616
62	1	0	1.382933	-2.059892	2.497730
63	1	0	0.603528	-3.173906	4.568443
64	1	0	-1.557414	-4.407310	4.582188
65	1	0	-2.940717	-4.498170	2.517362
66	1	0	-2.174871	-3.363197	0.460226
67	1	0	-0.150285	-4.792859	-0.243931
68	1	0	0.735739	-6.600635	-1.666478
69	1	0	2.369720	-6.089332	-3.471082
70	1	0	3.120739	-3.741925	-3.824704
71	1	0	2.254318	-1.933851	-2.385822
72	1	0	-4.230497	-0.058902	-4.829116
73	1	0	-5.926491	1.550782	-4.005723
74	1	0	-5.834720	2.339773	-1.639781
75	1	0	-4.229994	0.059867	4.829649
76	1	0	-5.926107	-1.549901	4.006654
77	1	0	-5.834541	-2.339319	1.640866
78	1	0	-4.084847	-1.543058	0.128926
79	1	0	-4.084922	1.543241	-0.128156
80	6	0	3.627669	-1.364018	0.312464
81	6	0	3.627716	1.363799	-0.312033
82	9	0	4.584579	-0.915103	1.168426
83	9	0	3.139761	-2.509368	0.911203
84	9	0	4.285562	-1.791605	-0.797099
85	9	0	4.285575	1.791275	0.797612
86	9	0	4.584584	0.914993	-1.167990
87	9	0	3.139791	2.509266	-0.910547

(BINAP)Pd(Ar)$_2$

SCF Done: E(RB3LYP) = -2973.01668151 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-5.441406	1.209223	-0.003847
2	6	0	-4.624450	0.301252	-0.738821
3	6	0	-5.115456	-0.159428	-2.002892
4	6	0	-6.376743	0.291784	-2.477223
5	6	0	-7.136348	1.170298	-1.740436
6	6	0	-6.658384	1.632789	-0.491100
7	6	0	-4.325859	-1.063960	-2.752855
8	6	0	-3.103845	-1.480027	-2.287348
9	6	0	-2.589766	-1.024596	-1.042422
10	6	0	-3.338773	-0.147981	-0.261266
11	15	0	-0.875753	-1.626151	-0.474628
12	46	0	0.996553	0.071706	-0.060818
13	6	0	2.409114	-1.408317	0.038253
14	6	0	2.810683	-1.931516	1.278793
15	6	0	3.727768	-2.980700	1.371351
16	6	0	4.278870	-3.527799	0.210853
17	6	0	3.910315	-3.009042	-1.034341
18	6	0	2.990578	-1.963153	-1.113867
19	6	0	5.302723	-4.619735	0.289164
20	9	0	5.150347	-5.530048	-0.704776
21	6	0	-2.921529	0.313609	1.109240
22	6	0	-1.990361	1.328902	1.334182
23	6	0	-1.773328	1.803092	2.658270
24	6	0	-2.443326	1.274709	3.731970
25	6	0	-3.367783	0.216680	3.558431
26	6	0	-3.612484	-0.272005	2.234335
27	6	0	-4.054494	-0.356150	4.662287
28	6	0	-4.950882	-1.383041	4.480023
29	6	0	-5.190923	-1.879538	3.177247
30	6	0	-4.545056	-1.339082	2.087567
31	15	0	-0.739303	1.941108	0.039114
32	6	0	-0.193990	3.632244	0.689627
33	6	0	0.875675	3.686006	1.594385
34	6	0	1.319822	4.910254	2.096664
35	6	0	0.706533	6.097210	1.694218
36	6	0	-0.352529	6.052457	0.786612
37	6	0	-0.801271	4.828508	0.286145
38	6	0	-1.318638	-2.902627	0.830644
39	6	0	-0.615493	-2.911421	2.039330
40	6	0	-0.921918	-3.853212	3.024757
41	6	0	-1.932088	-4.790290	2.808093
42	6	0	-2.641961	-4.782592	1.604423
43	6	0	-2.340406	-3.840550	0.620904
44	6	0	-0.283238	-2.647544	-1.943691
45	6	0	-0.071372	-4.027637	-1.872956
46	6	0	0.447007	-4.718538	-2.972540
47	6	0	0.751513	-4.040143	-4.151846
48	6	0	0.546221	-2.659624	-4.227721
49	6	0	0.043297	-1.966881	-3.127304
50	6	0	-1.641353	2.393797	-1.543270
51	6	0	-0.958487	2.189519	-2.749631
52	6	0	-1.531874	2.576163	-3.962719
53	6	0	-2.796923	3.165682	-3.980900
54	6	0	-3.485348	3.368328	-2.782999
55	6	0	-2.909284	2.988414	-1.569350
56	9	0	6.569340	-4.146784	0.177641
57	9	0	5.245360	-5.296151	1.461083
58	1	0	-4.700697	-1.429469	-3.705974
59	1	0	2.412424	-1.516268	2.202227
60	1	0	4.011709	-3.375089	2.342427
61	1	0	4.338150	-3.427231	-1.941272
62	1	0	2.723417	-1.584116	-2.095468
63	1	0	-2.521516	-2.173816	-2.880544
64	1	0	-1.066504	2.607135	2.823549
65	1	0	-2.266656	1.665786	4.731162
66	1	0	-2.901051	-3.836951	-0.309861
67	1	0	-3.432324	-5.508398	1.431848
68	1	0	-2.168633	-5.523690	3.574272

69	1	0	-0.368864	-3.852288	3.959958
70	1	0	0.172830	-2.185817	2.205161
71	1	0	-0.297070	-4.569330	-0.961008
72	1	0	0.614415	-5.789729	-2.900328
73	1	0	1.153192	-4.579848	-5.005055
74	1	0	0.787597	-2.120376	-5.139919
75	1	0	-0.098235	-0.890950	-3.188761
76	1	0	0.027064	1.731753	-2.736201
77	1	0	-0.989691	2.416063	-4.890775
78	1	0	-3.245911	3.464394	-4.924281
79	1	0	-4.474990	3.816537	-2.789500
80	1	0	-3.455858	3.148975	-0.645732
81	1	0	-1.616709	4.817896	-0.427778
82	1	0	-0.831869	6.971833	0.460661
83	1	0	1.058670	7.051362	2.076807
84	1	0	2.158802	4.932638	2.786330
85	1	0	1.381766	2.774226	1.888238
86	1	0	-3.853666	0.034978	5.656810
87	1	0	-5.470750	-1.816144	5.330120
88	1	0	-5.891433	-2.697748	3.034347
89	1	0	-6.729318	-0.072734	-3.439131
90	1	0	-8.099902	1.508621	-2.111463
91	1	0	-7.258941	2.325924	0.091748
92	1	0	-5.096769	1.574523	0.956386
93	1	0	-4.740176	-1.740712	1.100780
94	6	0	2.647187	1.280018	0.023700
95	6	0	2.951132	2.096885	-1.078999
96	6	0	4.022813	2.991652	-1.055536
97	6	0	4.827016	3.089212	0.082330
98	6	0	4.554896	2.275178	1.185868
99	6	0	3.487246	1.377715	1.146275
100	1	0	2.343689	2.048767	-1.979449
101	1	0	4.236106	3.610911	-1.921891
102	6	0	5.932630	4.099120	0.146873
103	1	0	5.189135	2.330119	2.066241
104	1	0	3.320695	0.737180	2.007877
105	9	0	6.967454	3.676841	0.911096
106	9	0	6.430130	4.395656	-1.076733
107	9	0	5.517177	5.275691	0.686818

TS$^{Ar\text{-}Ar}$(BINAP)

SCF Done: E(RB3LYP) = -2973.00542542 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.329437	1.543056	-1.210562
2	6	0	-2.912872	0.953198	0.002657
3	6	0	-3.444107	1.495005	1.195052
4	6	0	-4.300997	2.591766	1.179546
5	6	0	-4.679444	3.173071	-0.036776
6	6	0	-4.192481	2.633862	-1.233047
7	46	0	-1.022799	0.084889	0.148107
8	15	0	0.743019	1.901794	-0.115471
9	6	0	1.838304	2.487807	1.304640
10	6	0	1.465274	2.124069	2.603106
11	6	0	2.170420	2.609532	3.707036
12	6	0	3.255537	3.465402	3.519182
13	6	0	3.631252	3.836095	2.225538
14	6	0	2.923613	3.355023	1.124334
15	6	0	-5.533340	4.402394	-0.051049
16	9	0	-4.787377	5.542809	0.049439
17	15	0	0.842034	-1.650249	0.625388
18	6	0	0.328131	-2.528290	2.218720
19	6	0	0.494581	-3.902267	2.428760
20	6	0	0.065214	-4.491899	3.621111
21	6	0	-0.528076	-3.715751	4.617357
22	6	0	-0.699881	-2.344260	4.414660

23	6	0	-0.282814	-1.758184	3.219338
24	6	0	2.583347	-1.009317	1.053373
25	6	0	3.139690	-1.334034	2.320761
26	6	0	4.358334	-0.840691	2.716461
27	6	0	5.099836	0.019560	1.870893
28	6	0	4.562652	0.355049	0.586086
29	6	0	3.286663	-0.176280	0.182423
30	6	0	6.356194	0.551015	2.268450
31	6	0	7.065751	1.385480	1.436495
32	6	0	6.539886	1.724644	0.166902
33	6	0	5.324745	1.224678	-0.245976
34	6	0	2.793580	0.142932	-1.202702
35	6	0	1.802462	1.089659	-1.454007
36	6	0	1.361088	1.312492	-2.791030
37	6	0	1.928221	0.655314	-3.852121
38	6	0	2.972115	-0.281510	-3.649054
39	6	0	3.407400	-0.550071	-2.310775
40	6	0	4.451393	-1.502415	-2.135591
41	6	0	5.030638	-2.136589	-3.212751
42	6	0	4.597418	-1.862337	-4.530693
43	6	0	3.585306	-0.954055	-4.739202
44	6	0	1.169084	-3.088929	-0.542002
45	6	0	0.145876	-3.468685	-1.419704
46	6	0	0.320069	-4.560262	-2.272897
47	6	0	1.517745	-5.277020	-2.260182
48	6	0	2.542282	-4.900429	-1.389418
49	6	0	2.369706	-3.811832	-0.532377
50	6	0	-2.791815	-1.020066	-0.043653
51	6	0	-3.069224	-1.580938	-1.310555
52	6	0	-3.804522	-2.755001	-1.443351
53	6	0	-4.298573	-3.408260	-0.308547
54	6	0	-4.049474	-2.864762	0.956208
55	6	0	-3.314147	-1.689714	1.082799
56	6	0	-5.143830	-4.636735	-0.456966
57	9	0	-4.774311	-5.378679	-1.529301
58	9	0	-5.073902	-5.439396	0.630908
59	9	0	-6.456012	-4.339604	-0.632410
60	6	0	0.254630	3.568179	-0.853702
61	6	0	-0.988548	4.089601	-0.476640
62	6	0	-1.395599	5.349626	-0.923211
63	6	0	-0.560567	6.098960	-1.752030
64	6	0	0.682349	5.586352	-2.133256
65	6	0	1.089794	4.328810	-1.685944
66	9	0	-6.248510	4.520322	-1.191803
67	9	0	-6.404974	4.436351	0.982226
68	1	0	4.766662	-1.107479	3.688523
69	1	0	-2.707511	-1.089430	-2.209476
70	1	0	-3.992814	-3.169906	-2.429348
71	1	0	-4.423067	-3.368407	1.842615
72	1	0	-3.139881	-1.292539	2.078217
73	1	0	2.590628	-1.986602	2.989181
74	1	0	0.560009	2.020550	-2.972099
75	1	0	1.580918	0.849196	-4.864239
76	1	0	3.171286	-3.527107	0.142845
77	1	0	3.478045	-5.453164	-1.376053
78	1	0	1.653307	-6.125084	-2.926119
79	1	0	-0.482356	-4.848196	-2.946728
80	1	0	-0.788392	-2.916213	-1.430899
81	1	0	0.953621	-4.518475	1.662741
82	1	0	0.194888	-5.560951	3.767710
83	1	0	-0.861108	-4.176768	5.543330
84	1	0	-1.167771	-1.732939	5.182012
85	1	0	-0.439814	-0.695366	3.053528
86	1	0	0.615884	1.462638	2.747202
87	1	0	1.868642	2.319914	4.710111
88	1	0	3.805347	3.846104	4.375824
89	1	0	4.476009	4.502212	2.072722
90	1	0	3.219830	3.662438	0.126759
91	1	0	2.052192	3.936748	-2.001913

92	1	0	1.336432	6.164819	-2.780755
93	1	0	-0.877302	7.076764	-2.105225
94	1	0	-2.372040	5.725390	-0.633060
95	1	0	-1.646082	3.509002	0.161223
96	1	0	3.237057	-0.734181	-5.745622
97	1	0	5.061918	-2.369971	-5.371554
98	1	0	5.828094	-2.856029	-3.047382
99	1	0	6.745915	0.283631	3.247787
100	1	0	8.026524	1.785215	1.749215
101	1	0	7.101140	2.385276	-0.488520
102	1	0	4.936700	1.496222	-1.220989
103	1	0	4.799446	-1.726949	-1.134646
104	1	0	-3.184959	1.051086	2.152171
105	1	0	-4.684033	2.994699	2.112595
106	1	0	-4.486595	3.072470	-2.181742
107	1	0	-2.973044	1.144779	-2.155871
