Rate and Mechanism of the Reaction of (*E*)-PhCH=CH-CH(Ph)-OAc with Palladium(0) Complexes

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Supporting information

Reaction of (*E*)-1,3-diphenyl-3-acetoxyprop-1-ene (1) with the Pd^0 Complex Generated from $Pd^0(dba)_2$ and $2PPh_3$

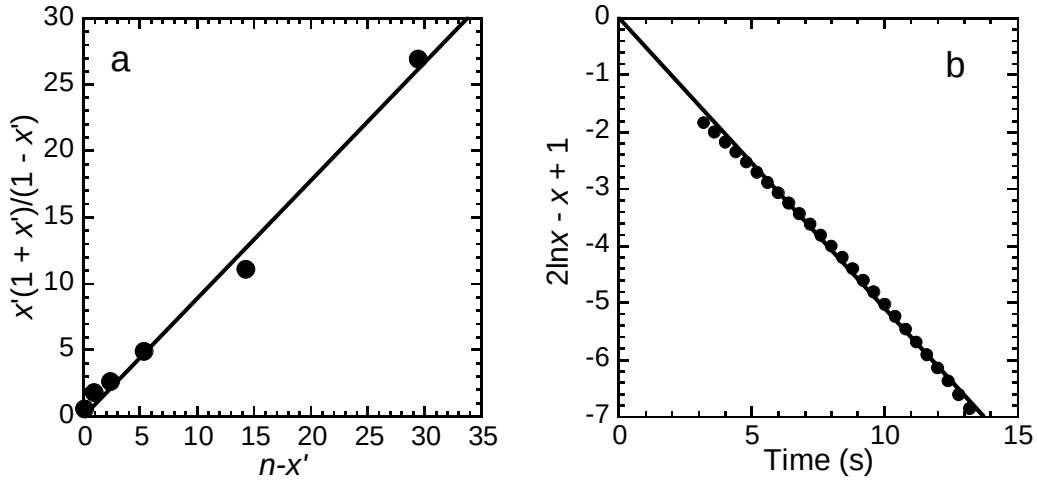

Figure S1. a) Determination of the equilibrium constant K_0K_1 = [**6a**][dba]/[**1**][Pd^0(dba)(PPh_3)$_2$] of the complexation step (see Scheme 4) using the UV data of Fig 3a. $K_0K_1 = x'(1 + x')/(n - x')(1 - x')$ where $x' = (D_0 - D_n)/(D_0 - D_8)$ (D_0: initial absorbance of Pd^0(dba)(PPh_3)$_2$; D_n: absorbance at 425 nm of Pd^0(dba)(PPh_3)$_2$ in the presence of n equiv. of **1** when the equilibrium is fully established; D_8: residual absorbance when the equilibrium is fully displaced toward its right-hand side. The absorbance was measured at 425 nm. K_0K_1 = 0.9 (DMF, 25 °C). b) Kinetics of the overall complexation step (See k_1^{app} in Scheme 3) as monitored by UV spectroscopy in DMF at 25 °C. Reaction between Pd^0(dba)(PPh_3)$_2$ (C_0 = 1 mM) (formed in situ by reacting Pd^0(dba)$_2$ (1 mM) and PPh_3 (2 mM)) with PhCH=CH-CH(Ph)-OAc (94.3 mM). Plot of $2\ln x - x + 1$ *versus* time (x is the molar fraction of Pd^0(dba)(PPh_3)$_2$ that has not reacted: $x = (D_n - D_8)/(D_0 - D_8)$ (D_0: initial absorbance of Pd^0(dba)(PPh_3)$_2$; D_n: absorbance of Pd^0(dba)(PPh_3)$_2$ at t, D_8: residual absorbance at the end of the complexation step). $2\ln x - x + 1 = -k_{exp}t$.

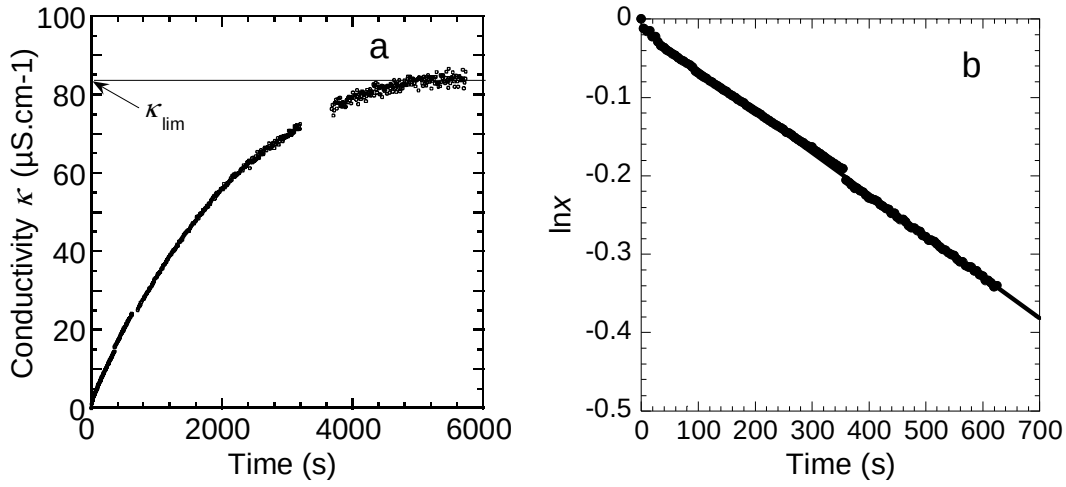

Figure S2. Kinetics of the ionization step in acetonitrile at 25 °C. a) Conductivity measurements *versus* time of [(η^3-PhCH-CH-CHPh)Pd(PPh_3)$_2$]$^+$,AcO$^-$ (**5a**$^+$,AcO$^-$) generated in the reaction of PhCH=CH-CH(Ph)-OAc (46 mM) to Pd^0(dba)(PPh_3)$_2$ (1 mM) formed in situ by reacting Pd^0(dba)$_2$ (1 mM) and PPh_3 (2 mM) at 25 °C. κ_{lim} = 83 µS.cm^{-1} is the theoretical conductivity of **5a**$^+$,AcO$^-$ (1 mM) in acetonitrile at 25 °C (determined as in ref 8b). b) Plot of ln*x* *versus* time ($x = (\kappa_{lim} - \kappa)/\kappa_{lim}$ with κ: conductivity at *t* and κ_{lim} : final conductivity). ln*x* = $-k_2t$. $k_2 = 5.3\times10^{-4}$ s^{-1} (acetonitrile, 25 °C)

Reaction of (*E*)-1,3-diphenyl-3-acetoxyprop-1-ene (1) with $Pd^0(PPh_3)_4$

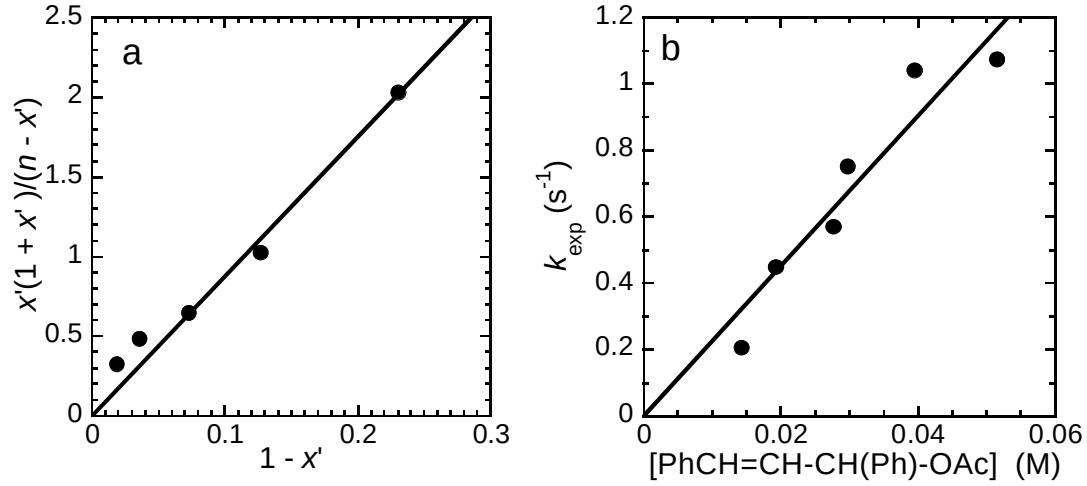

Figure S3. a) Determination of the equilibrium constant K'_0K_1 of the complexation step (see Scheme 7) using the UV data in Fig 4a. $K'_0K_1 = x'(1 + x')/(n - x')(1 - x')$ where $x' = (D_0 - D_n)/(D_0 - D_8)$ (D_0: initial absorbance of $Pd^0(PPh_3)_3$; D_n: absorbance of $Pd^0(PPh_3)_3$ in the presence of *n* equiv. of **1** when the equilibrium is fully established; D_8: residual absorbance when the equilibrium is fully displaced to its right-hand side: *n* = 16) K'_0K_1 = 8.7 (DMF, 25 °C). b) Kinetics of the complexation step (Scheme 6). Determination of the reaction order in

PhCH=CH-CH(Ph)-OAc: plot of k_{exp} versus PhCH=CH-CH(Ph)-OAc concentration. $k_{exp} = K'_0 k_1[\mathbf{1}]/C_0$. $k'^{app}_1 = 23\ M^{-1}s^{-1}$ and $K'_0 k_1 = 23\times10^{-3}\ s^{-1}$ (DMF, 25 °C).

Reaction of (*E*)-1,3-diphenyl-3-acetoxyprop-1-ene (1) with the Pd^0 complex generated from $Pd^0(dba)_2$ and dppb

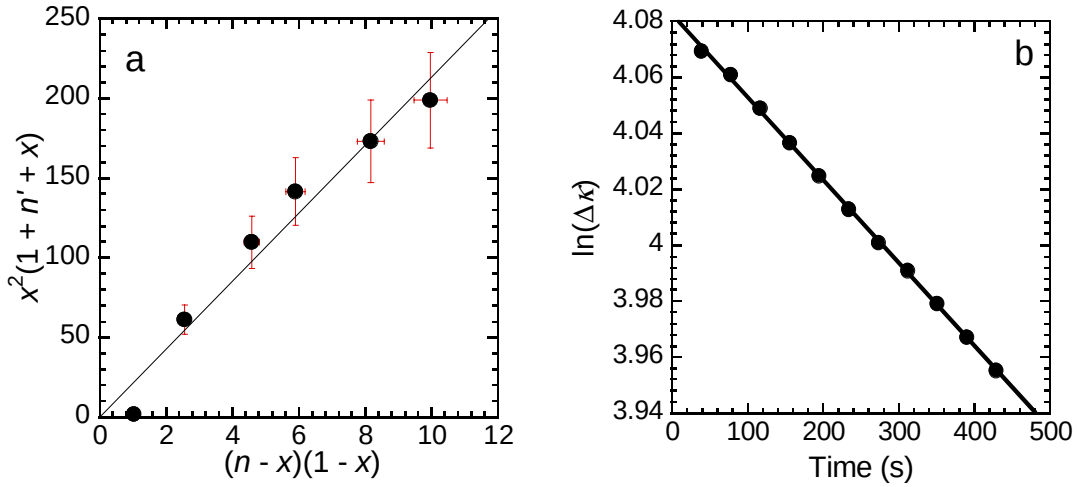

Figure S4. a) Determination of the overall equilibrium constant K (see Scheme 10) using the conductivity data in Fig 5. $K = C_0x^2(1 + n' + x)/(n - x)(1 - x)$ where x is the molar fraction of $\mathbf{5b}^+$ in the equilibrium: $x = (\kappa_{equil} - \kappa_0)/(\kappa_{lim} - \kappa_0)$ as indicated in Fig 5; n' is the total equiv. of added dba and n = 32.1 equiv. of **1** K = 0.021 M (DMF, 30 °C). b) Determination of the rate constant k_2 of the ionization step (Scheme 9) using the conductivity data in Fig 5 and the Guggenheim method. Plot of $\ln(\Delta\kappa)$ *versus* time: $\ln(\Delta\kappa) = -k_2t + A$. $\Delta\kappa$ was measured for Δt = 16500 s and every δt = 40 s. $k_2 = 3\times10^{-4}$ s^{-1} (DMF, 30 °C).

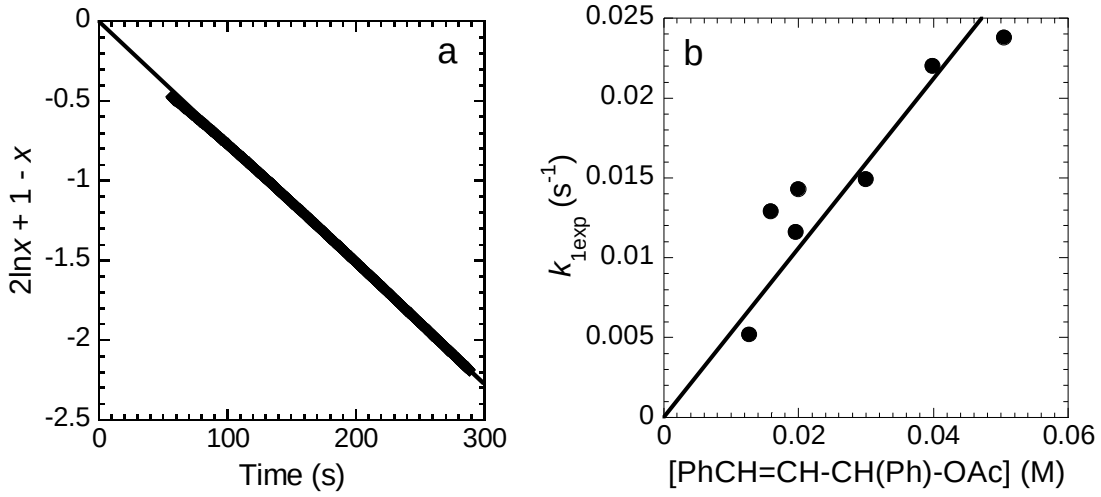

Figure S5. Kinetics of the overall complexation step (k_1^{app} in Scheme 9) as monitored by UV spectroscopy in DMF at 25 °C. a) Reaction between Pd^0(dba)(dppb) (C_0 = 1 mM) (formed in situ by reacting $Pd^0(dba)_2$ (1 mM) and dppb (2 mM)) with PhCH=CH-CH(Ph)-OAc (10 mM). Plot of $2\ln x - x + 1$ *versus* time (x is the molar fraction of Pd^0(dba)(dppb) that has not reacted: $x = (D_n - D_8)/(D_0 - D_8)$ (D_0: initial absorbance of Pd^0(dba)(dppb); D_n: absorbance of Pd^0(dba)(dppb) at t, D_8: residual absorbance at the end of the complexation step). $2\ln x - x + 1 = -k_{exp}t$. b) Determination of the reaction order in PhCH=CH-CH(Ph)-OAc: plot of k_{exp}, determined as in Fig 6, *versus* PhCH=CH-CH(Ph)-OAc concentration. $k_{exp} = K_0k_1[\mathbf{1}]/C_0$.

Table 3. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [(η^3-Ph-CH-CH-CH-Ph)Pd(PPh_3)]$^+BF_4^-$

atom	x	y	z	U(eq)
Pd(1)	6885(1)	-7430(1)	4825(1)	34(1)
Pd(2)	4871(1)	-4466(1)	2671(1)	35(1)
P(1)	5873(1)	-7713(1)	5069(1)	35(1)
P(2)	6451(1)	-7040(1)	4361(1)	37(1)
P(3)	4442(1)	-4079(1)	3139(1)	36(1)
P(4)	5119(1)	-3424(1)	2443(1)	35(1)
C(1)	7600(2)	-7578(2)	5218(1)	38(1)
C(2)	7932(2)	-7214(2)	4988(1)	39(1)
C(3)	8008(2)	-7494(2)	4700(1)	39(1)
C(4)	7460(2)	-7279(2)	5521(1)	41(1)
C(5)	7435(2)	-7703(3)	5774(1)	45(1)
C(6)	7329(3)	-7428(3)	6063(1)	55(2)
C(7)	7236(3)	-6733(3)	6100(1)	56(1)
C(8)	7259(3)	-6319(3)	5851(1)	60(2)
C(9)	7377(3)	-6576(2)	5561(1)	49(1)
C(10)	8373(2)	-7179(2)	4444(1)	42(1)
C(11)	8579(2)	-6493(3)	4438(1)	51(1)
C(12)	8935(3)	-6241(3)	4197(1)	60(2)
C(13)	9088(3)	-6644(3)	3950(2)	67(2)
C(14)	8900(3)	-7316(3)	3952(1)	62(2)
C(15)	8550(3)	-7586(3)	4196(1)	54(1)
C(16)	5911(2)	-8056(2)	5453(1)	36(1)
C(17)	6177(2)	-8709(2)	5491(1)	42(1)
C(18)	6210(2)	-8992(2)	5780(1)	46(1)
C(19)	5996(3)	-8626(2)	6027(1)	48(1)
C(20)	5741(3)	-7981(2)	5990(1)	48(1)
C(21)	5693(2)	-7694(2)	5705(1)	44(1)
C(22)	5324(2)	-6968(2)	5102(1)	33(1)
C(23)	4633(2)	-6947(2)	5042(1)	41(1)
C(24)	4264(2)	-6346(2)	5077(1)	46(1)
C(25)	4583(3)	-5764(2)	5174(1)	49(1)
C(26)	5278(3)	-5769(2)	5233(1)	47(1)
C(27)	5650(3)	-6370(2)	5194(1)	42(1)
C(28)	5437(2)	-8409(2)	4876(1)	37(1)
C(29)	4800(2)	-8645(2)	4965(1)	49(1)
C(30)	4498(3)	-9197(3)	4819(2)	64(2)
C(31)	4854(4)	-9527(3)	4593(2)	74(2)
C(32)	5496(4)	-9316(3)	4509(1)	76(2)
C(33)	5786(3)	-8759(2)	4647(1)	55(1)
C(34)	5542(2)	-6824(2)	4329(1)	39(1)
C(35)	5073(2)	-7345(2)	4285(1)	41(1)
C(36)	4381(2)	-7205(3)	4268(1)	50(1)
C(37)	4149(3)	-6542(3)	4295(1)	55(1)
C(38)	4610(3)	-6020(3)	4333(1)	50(1)
C(39)	5309(2)	-6157(2)	4352(1)	46(1)
C(40)	6587(2)	-7546(2)	4021(1)	39(1)
C(41)	6321(2)	-7340(3)	3742(1)	51(1)
C(42)	6463(3)	-7687(3)	3480(1)	54(1)
C(43)	6853(3)	-8274(3)	3494(1)	55(2)
C(44)	7120(3)	-8498(2)	3766(1)	49(1)
C(45)	6987(2)	-8132(2)	4027(1)	42(1)
C(46)	6896(2)	-6232(2)	4291(1)	42(1)
C(47)	6951(2)	-5788(2)	4537(1)	50(1)
C(48)	7299(3)	-5170(3)	4505(2)	64(2)
C(49)	7594(3)	-5009(3)	4234(2)	68(2)
C(50)	7542(3)	-5437(3)	3992(2)	61(2)
C(51)	7188(3)	-6064(3)	4016(1)	55(1)
C(52)	4985(3)	-5585(2)	2801(1)	41(1)
C(53)	4779(3)	-5506(2)	2500(1)	42(1)

C(54)	5173(3)	-5144(2)	2291(1)	41(1)
C(55)	5009(2)	-4173(2)	3463(1)	37(1)
C(56)	5616(2)	-4537(2)	3434(1)	43(1)
C(57)	6049(3)	-4630(2)	3680(1)	52(1)
C(58)	5868(3)	-4371(2)	3959(1)	52(1)
C(59)	5276(3)	-4003(2)	3989(1)	51(1)
C(60)	4849(2)	-3901(2)	3744(1)	43(1)
C(61)	4606(2)	-5957(2)	3034(1)	37(1)
C(62)	4942(3)	-6125(2)	3304(1)	49(1)
C(63)	4606(3)	-6476(3)	3533(1)	54(1)
C(64)	3947(3)	-6685(2)	3489(1)	53(1)
C(65)	3613(3)	-6542(2)	3223(1)	53(1)
C(66)	3935(3)	-6184(2)	2999(1)	49(1)
C(67)	4927(3)	-5031(2)	1977(1)	48(1)
C(68)	4230(3)	-4976(2)	1916(1)	63(2)
C(69)	3993(5)	-4913(3)	1625(2)	86(2)
C(70)	4433(6)	-4894(3)	1391(2)	94(3)
C(71)	5137(5)	-4952(3)	1437(1)	90(3)
C(72)	5393(3)	-5013(2)	1738(1)	60(2)
C(73)	3668(2)	-4558(2)	3233(1)	38(1)
C(74)	3536(3)	-4815(2)	3522(1)	47(1)
C(75)	2929(3)	-5160(2)	3580(1)	54(1)
C(76)	2455(3)	-5243(3)	3355(2)	58(2)
C(77)	2581(3)	-5006(2)	3064(1)	56(2)
C(78)	3186(2)	-4666(2)	3003(1)	46(1)
C(79)	4183(2)	-3182(2)	3165(1)	38(1)
C(80)	3517(3)	-2982(2)	3100(1)	49(1)
C(81)	3347(3)	-2292(3)	3089(1)	61(2)
C(82)	3837(3)	-1804(3)	3143(1)	56(2)
C(83)	4490(3)	-1995(2)	3217(1)	51(1)
C(84)	4661(3)	-2678(2)	3227(1)	41(1)
C(85)	5734(2)	-2980(2)	2685(1)	36(1)
C(86)	5852(3)	-2285(2)	2687(1)	55(2)
C(87)	6284(3)	-1987(3)	2896(1)	64(2)
C(88)	6615(3)	-2389(3)	3104(1)	55(1)
C(89)	6536(2)	-3083(3)	3094(1)	51(1)
C(90)	6098(2)	-3376(2)	2887(1)	42(1)
C(91)	5528(2)	-3408(2)	2069(1)	37(1)
C(92)	5140(3)	-3307(2)	1812(1)	46(1)
C(93)	5451(3)	-3320(2)	1527(1)	51(1)
C(94)	6142(3)	-3432(3)	1502(1)	54(1)
C(95)	6527(3)	-3543(3)	1762(1)	57(1)
C(96)	6221(3)	-3535(2)	2042(1)	47(1)
C(97)	4341(2)	-2928(2)	2387(1)	36(1)
C(98)	3730(2)	-3284(2)	2372(1)	44(1)
C(99)	3115(3)	-2953(3)	2329(1)	51(1)
C(100)	3105(3)	-2252(3)	2309(1)	55(2)
C(101)	3699(3)	-1892(3)	2321(1)	58(2)
C(102)	4316(3)	-2231(2)	2356(1)	58(2)
B(1)	7308(3)	-4729(3)	5320(2)	63(2)
F(1)	7215(2)	-4517(2)	5610(1)	96(1)
F(2)	6772(2)	-5148(2)	5227(1)	82(1)
F(3)	7347(2)	-4179(2)	5125(1)	86(1)
F(4)	7917(2)	-5099(2)	5294(1)	81(1)
B(2)	7264(5)	-5049(4)	2865(3)	87(3)
F(5)	6633(2)	-5089(2)	2754(1)	121(2)
F(6)	7288(4)	-4779(6)	3153(2)	126(3)
F(7)	7585(4)	-4518(3)	2705(2)	127(3)
F(8)	7644(7)	-5595(5)	2810(4)	166(6)
F(9)	7730(10)	-5430(20)	2714(5)	126(3)
F(10)	7501(8)	-4532(7)	2977(6)	127(3)
F(11)	7071(8)	-5496(7)	3101(5)	166(6)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table 4. Bond lengths (A) and angles (deg) for complex [(η^3-Ph-CH-CH-CH-Ph)Pd(PPh_3)]$^+BF_4^-$

Pd(1)-C(2)	2.212(4)	Pd(1)-C(1)	2.245(4)
Pd(1)-C(3)	2.270(4)	Pd(1)-P(1)	2.319(1)
Pd(1)-P(2)	2.342(1)	Pd(2)-C(53)	2.180(4)
Pd(2)-C(54)	2.218(5)	Pd(2)-C(52)	2.276(4)
Pd(2)-P(4)	2.328(1)	Pd(2)-P(3)	2.349(1)
P(1)-C(22)	1.818(4)	P(1)-C(28)	1.819(4)
P(1)-C(16)	1.820(5)	P(2)-C(40)	1.816(5)
P(2)-C(46)	1.832(5)	P(2)-C(34)	1.833(5)
P(3)-C(55)	1.817(5)	P(3)-C(73)	1.830(5)
P(3)-C(79)	1.831(4)	P(4)-C(97)	1.823(4)
P(4)-C(85)	1.830(5)	P(4)-C(91)	1.831(5)
C(1)-C(2)	1.396(6)	C(1)-C(4)	1.484(6)
C(2)-C(3)	1.392(7)	C(3)-C(10)	1.473(7)
C(4)-C(5)	1.390(6)	C(4)-C(9)	1.398(6)
C(5)-C(6)	1.399(7)	C(6)-C(7)	1.383(7)
C(7)-C(8)	1.366(7)	C(8)-C(9)	1.391(7)
C(10)-C(15)	1.396(7)	C(10)-C(11)	1.402(6)
C(11)-C(12)	1.361(7)	C(12)-C(13)	1.378(8)
C(13)-C(14)	1.366(8)	C(14)-C(15)	1.380(7)
C(16)-C(21)	1.384(6)	C(16)-C(17)	1.391(6)
C(17)-C(18)	1.391(6)	C(18)-C(19)	1.371(6)
C(19)-C(20)	1.367(6)	C(20)-C(21)	1.381(6)
C(22)-C(23)	1.377(6)	C(22)-C(27)	1.397(6)
C(23)-C(24)	1.389(6)	C(24)-C(25)	1.368(7)
C(25)-C(26)	1.384(7)	C(26)-C(27)	1.394(6)
C(28)-C(29)	1.384(6)	C(28)-C(33)	1.401(6)
C(29)-C(30)	1.391(7)	C(30)-C(31)	1.377(8)
C(31)-C(32)	1.375(8)	C(32)-C(33)	1.371(7)
C(34)-C(35)	1.385(6)	C(34)-C(39)	1.387(6)
C(35)-C(36)	1.383(6)	C(36)-C(37)	1.382(7)
C(37)-C(38)	1.373(7)	C(38)-C(39)	1.395(7)
C(40)-C(45)	1.390(6)	C(40)-C(41)	1.392(7)
C(41)-C(42)	1.370(7)	C(42)-C(43)	1.381(7)
C(43)-C(44)	1.379(7)	C(44)-C(45)	1.382(6)
C(46)-C(51)	1.383(7)	C(46)-C(47)	1.393(7)
C(47)-C(48)	1.396(7)	C(48)-C(49)	1.363(8)
C(49)-C(50)	1.360(8)	C(50)-C(51)	1.413(7)
C(52)-C(53)	1.398(7)	C(52)-C(61)	1.459(7)
C(53)-C(54)	1.393(7)	C(54)-C(67)	1.482(7)
C(55)-C(60)	1.384(6)	C(55)-C(56)	1.391(6)
C(56)-C(57)	1.389(7)	C(57)-C(58)	1.378(7)
C(58)-C(59)	1.370(7)	C(59)-C(60)	1.381(7)
C(61)-C(66)	1.394(6)	C(61)-C(62)	1.401(7)
C(62)-C(63)	1.386(7)	C(63)-C(64)	1.367(7)
C(64)-C(65)	1.373(7)	C(65)-C(66)	1.364(7)
C(67)-C(72)	1.391(7)	C(67)-C(68)	1.394(8)
C(68)-C(69)	1.369(8)	C(69)-C(70)	1.35(1)
C(70)-C(71)	1.39(1)	C(71)-C(72)	1.42(1)
C(73)-C(74)	1.394(6)	C(73)-C(78)	1.401(6)
C(74)-C(75)	1.391(7)	C(75)-C(76)	1.367(8)
C(76)-C(77)	1.386(8)	C(77)-C(78)	1.384(7)
C(79)-C(84)	1.387(6)	C(79)-C(80)	1.390(6)
C(80)-C(81)	1.392(7)	C(81)-C(82)	1.375(7)
C(82)-C(83)	1.372(7)	C(83)-C(84)	1.380(6)
C(85)-C(90)	1.379(6)	C(85)-C(86)	1.380(6)
C(86)-C(87)	1.382(7)	C(87)-C(88)	1.368(7)
C(88)-C(89)	1.368(7)	C(89)-C(90)	1.377(7)
C(91)-C(92)	1.380(6)	C(91)-C(96)	1.384(6)
C(92)-C(93)	1.393(7)	C(93)-C(94)	1.373(7)
C(94)-C(95)	1.386(7)	C(95)-C(96)	1.372(7)
C(97)-C(102)	1.373(6)	C(97)-C(98)	1.384(6)

C(98)-C(99)	1.380(7)	C(99)-C(100)	1.375(8)
C(100)-C(101)	1.362(7)	C(101)-C(102)	1.385(7)
B(1)-F(1)	1.356(8)	B(1)-F(3)	1.381(8)
B(1)-F(2)	1.393(7)	B(1)-F(4)	1.399(7)
B(2)-F(10)	1.22(2)	B(2)-F(8)	1.33(1)
B(2)-F(5)	1.33(1)	B(2)-F(9)	1.35(2)
B(2)-F(6)	1.37(1)	B(2)-F(7)	1.41(1)
B(2)-F(11)	1.41(2)		
C(2)-Pd(1)-C(1)	36.5(2)	C(2)-Pd(1)-C(3)	36.2(2)
C(1)-Pd(1)-C(3)	64.9(2)	C(2)-Pd(1)-P(1)	133.2(1)
C(1)-Pd(1)-P(1)	98.2(1)	C(3)-Pd(1)-P(1)	157.7(1)
C(2)-Pd(1)-P(2)	123.8(1)	C(1)-Pd(1)-P(2)	160.2(1)
C(3)-Pd(1)-P(2)		99.0(1)	P(1)-Pd(1)-P(2)
100.04(4)			
C(53)-Pd(2)-C(54)	36.9(2)	C(53)-Pd(2)-C(52)	36.5(2)
C(54)-Pd(2)-C(52)	65.7(2)	C(53)-Pd(2)-P(4)	133.3(1)
C(54)-Pd(2)-P(4)	98.1(1)	C(52)-Pd(2)-P(4)	158.9(1)
C(53)-Pd(2)-P(3)	125.2(1)	C(54)-Pd(2)-P(3)	161.9(1)
C(52)-Pd(2)-P(3)	97.2(1)	P(4)-Pd(2)-P(3)	99.84(4)
C(22)-P(1)-C(28)	111.1(2)	C(22)-P(1)-C(16)	104.3(2)
C(28)-P(1)-C(16)	100.2(2)	C(22)-P(1)-Pd(1)	110.4(2)
C(28)-P(1)-Pd(1)	111.3(2)	C(16)-P(1)-Pd(1)	119.0(2)
C(40)-P(2)-C(46)	105.3(2)	C(40)-P(2)-C(34)	101.8(2)
C(46)-P(2)-C(34)	104.4(2)	C(40)-P(2)-Pd(1)	119.4(2)
C(46)-P(2)-Pd(1)	104.8(2)	C(34)-P(2)-Pd(1)	119.6(2)
C(55)-P(3)-C(73)	106.0(2)	C(55)-P(3)-C(79)	102.5(2)
C(73)-P(3)-C(79)	104.3(2)	C(55)-P(3)-Pd(2)	116.0(2)
C(73)-P(3)-Pd(2)	109.2(2)	C(79)-P(3)-Pd(2)	117.7(2)
C(97)-P(4)-C(85)	111.9(2)	C(97)-P(4)-C(91)	103.7(2)
C(85)-P(4)-C(91)	103.3(2)	C(97)-P(4)-Pd(2)	110.6(2)
C(85)-P(4)-Pd(2)	107.5(2)	C(91)-P(4)-Pd(2)	119.7(1)
C(2)-C(1)-C(4)	122.5(4)	C(2)-C(1)-Pd(1)	70.5(3)
C(4)-C(1)-Pd(1)	121.8(3)	C(3)-C(2)-C(1)	120.6(4)
C(3)-C(2)-Pd(1)	74.2(3)	C(1)-C(2)-Pd(1)	73.0(3)
C(2)-C(3)-C(10)	126.0(4)	C(2)-C(3)-Pd(1)	69.7(2)
C(10)-C(3)-Pd(1)	129.2(3)	C(5)-C(4)-C(9)	118.8(5)
C(5)-C(4)-C(1)	119.5(4)	C(9)-C(4)-C(1)	121.6(4)
C(4)-C(5)-C(6)	120.4(5)	C(7)-C(6)-C(5)	120.4(5)
C(8)-C(7)-C(6)	119.0(5)	C(7)-C(8)-C(9)	121.9(5)
C(8)-C(9)-C(4)	119.5(5)	C(15)-C(10)-C(11)	117.5(5)
C(15)-C(10)-C(3)	118.8(4)	C(11)-C(10)-C(3)	123.7(5)
C(12)-C(11)-C(10)	120.6(5)	C(11)-C(12)-C(13)	121.2(5)
C(14)-C(13)-C(12)	119.4(5)	C(13)-C(14)-C(15)	120.4(6)
C(14)-C(15)-C(10)	120.9(5)	C(21)-C(16)-C(17)	119.2(4)
C(21)-C(16)-P(1)	123.0(4)	C(17)-C(16)-P(1)	117.8(3)
C(18)-C(17)-C(16)	119.7(4)	C(19)-C(18)-C(17)	120.3(4)
C(20)-C(19)-C(18)	120.1(5)	C(19)-C(20)-C(21)	120.5(5)
C(20)-C(21)-C(16)	120.2(5)	C(23)-C(22)-C(27)	118.7(4)
C(23)-C(22)-P(1)	126.1(3)	C(27)-C(22)-P(1)	115.2(3)
C(22)-C(23)-C(24)	120.9(4)	C(25)-C(24)-C(23)	120.3(5)
C(24)-C(25)-C(26)	120.0(4)	C(25)-C(26)-C(27)	119.8(4)
C(26)-C(27)-C(22)	120.3(4)	C(29)-C(28)-C(33)	118.7(4)
C(29)-C(28)-P(1)	122.7(4)	C(33)-C(28)-P(1)	118.4(4)
C(28)-C(29)-C(30)	120.8(5)	C(31)-C(30)-C(29)	119.0(5)
C(32)-C(31)-C(30)	121.1(5)	C(33)-C(32)-C(31)	119.8(6)
C(32)-C(33)-C(28)	120.6(5)	C(35)-C(34)-C(39)	119.0(4)
C(35)-C(34)-P(2)	118.9(3)	C(39)-C(34)-P(2)	122.1(4)
C(36)-C(35)-C(34)	120.7(5)	C(37)-C(36)-C(35)	120.2(5)
C(38)-C(37)-C(36)	119.6(5)	C(37)-C(38)-C(39)	120.5(5)
C(34)-C(39)-C(38)	120.0(5)	C(45)-C(40)-C(41)	117.8(4)
C(45)-C(40)-P(2)	121.1(4)	C(41)-C(40)-P(2)	121.1(4)
C(42)-C(41)-C(40)	121.7(5)	C(41)-C(42)-C(43)	119.1(5)
C(44)-C(43)-C(42)	120.9(5)	C(43)-C(44)-C(45)	119.2(5)
C(44)-C(45)-C(40)	121.2(5)	C(51)-C(46)-C(47)	120.1(5)
C(51)-C(46)-P(2)	123.3(4)	C(47)-C(46)-P(2)	116.6(4)

C(46)-C(47)-C(48)	120.1(5)	C(49)-C(48)-C(47)	119.7(6)
C(50)-C(49)-C(48)	120.9(5)	C(49)-C(50)-C(51)	120.9(6)
C(46)-C(51)-C(50)	118.4(5)	C(53)-C(52)-C(61)	125.3(4)
C(53)-C(52)-Pd(2)	68.0(2)	C(61)-C(52)-Pd(2)	127.4(3)
C(54)-C(53)-C(52)	121.7(5)	C(54)-C(53)-Pd(2)	73.0(3)
C(52)-C(53)-Pd(2)	75.5(3)	C(53)-C(54)-C(67)	120.9(5)
C(53)-C(54)-Pd(2)	70.0(3)	C(67)-C(54)-Pd(2)	122.1(3)
C(60)-C(55)-C(56)	118.2(4)	C(60)-C(55)-P(3)	121.7(4)
C(56)-C(55)-P(3)	120.1(4)	C(57)-C(56)-C(55)	121.1(5)
C(58)-C(57)-C(56)	119.5(5)	C(59)-C(58)-C(57)	119.8(5)
C(58)-C(59)-C(60)	120.8(5)	C(59)-C(60)-C(55)	120.5(5)
C(66)-C(61)-C(62)	117.5(4)	C(66)-C(61)-C(52)	124.1(5)
C(62)-C(61)-C(52)	118.4(4)	C(63)-C(62)-C(61)	120.8(5)
C(64)-C(63)-C(62)	119.6(5)	C(63)-C(64)-C(65)	120.6(5)
C(66)-C(65)-C(64)	120.2(5)	C(65)-C(66)-C(61)	121.3(5)
C(72)-C(67)-C(68)	119.4(5)	C(72)-C(67)-C(54)	119.9(5)
C(68)-C(67)-C(54)	120.6(5)	C(69)-C(68)-C(67)	121.3(7)
C(70)-C(69)-C(68)	120.3(8)	C(69)-C(70)-C(71)	121.2(7)
C(70)-C(71)-C(72)	119.3(6)	C(67)-C(72)-C(71)	118.5(6)
C(74)-C(73)-C(78)	118.9(4)	C(74)-C(73)-P(3)	123.1(4)
C(78)-C(73)-P(3)	118.0(4)	C(75)-C(74)-C(73)	120.0(5)
C(76)-C(75)-C(74)	120.3(5)	C(75)-C(76)-C(77)	120.7(5)
C(78)-C(77)-C(76)	119.6(5)	C(77)-C(78)-C(73)	120.4(5)
C(84)-C(79)-C(80)	118.1(4)	C(84)-C(79)-P(3)	120.5(3)
C(80)-C(79)-P(3)	121.2(4)	C(79)-C(80)-C(81)	120.4(5)
C(82)-C(81)-C(80)	120.1(5)	C(83)-C(82)-C(81)	120.2(5)
C(82)-C(83)-C(84)	119.7(5)	C(83)-C(84)-C(79)	121.5(5)
C(90)-C(85)-C(86)	117.7(4)	C(90)-C(85)-P(4)	116.7(3)
C(86)-C(85)-P(4)	125.6(4)	C(85)-C(86)-C(87)	121.5(5)
C(88)-C(87)-C(86)	119.4(5)	C(89)-C(88)-C(87)	119.9(5)
C(88)-C(89)-C(90)	120.3(5)	C(89)-C(90)-C(85)	120.9(5)
C(92)-C(91)-C(96)	119.5(5)	C(92)-C(91)-P(4)	120.1(4)
C(96)-C(91)-P(4)	120.2(4)	C(91)-C(92)-C(93)	119.8(5)
C(94)-C(93)-C(92)	120.3(5)	C(93)-C(94)-C(95)	119.7(5)
C(96)-C(95)-C(94)	120.2(5)	C(95)-C(96)-C(91)	120.5(5)
C(102)-C(97)-C(98)	117.8(4)	C(102)-C(97)-P(4)	125.0(4)
C(98)-C(97)-P(4)	117.2(3)	C(99)-C(98)-C(97)	121.5(5)
C(100)-C(99)-C(98)	119.3(5)	C(101)-C(100)-C(99)	120.1(5)
C(100)-C(101)-C(102)	120.0(5)	C(97)-C(102)-C(101)	121.2(5)
F(1)-B(1)-F(3)	110.9(5)	F(1)-B(1)-F(2)	110.9(6)
F(3)-B(1)-F(2)	108.4(6)	F(1)-B(1)-F(4)	110.6(5)
F(3)-B(1)-F(4)	107.8(6)	F(2)-B(1)-F(4)	108.2(5)
F(10)-B(2)-F(8)	122(1)	F(10)-B(2)-F(5)	124(1)
F(8)-B(2)-F(5)	114.1(8)	F(10)-B(2)-F(9)	114(2)
F(8)-B(2)-F(9)	24(1)	F(5)-B(2)-F(9)	114(1)
F(10)-B(2)-F(6)	45(1)	F(8)-B(2)-F(6)	117(1)
F(5)-B(2)-F(6)	113.1(8)	F(9)-B(2)-F(6)	130(1)
F(10)-B(2)-F(7)	55(1)	F(8)-B(2)-F(7)	105(1)
F(5)-B(2)-F(7)	105.9(8)	F(9)-B(2)-F(7)	82(1)
F(6)-B(2)-F(7)	99.4(7)	F(10)-B(2)-F(11)	109(2)
F(8)-B(2)-F(11)	78(1)	F(5)-B(2)-F(11)	89.2(8)
F(9)-B(2)-F(11)	101(2)	F(6)-B(2)-F(11)	64(1)
F(7)-B(2)-F(11)	162(1)		

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for $[(\eta^3\text{-Ph-CH-CH-CH-Ph})Pd(PPh_3)]^+BF_4^-$

atom	U11	U22	U33	U23	U13	U12
Pd(1)	31(1)	34(1)	37(1)	1(1)	0(1)	-1(1)
Pd(2)	39(1)	29(1)	36(1)	-1(1)	1(1)	1(1)
P(1)	33(1)	33(1)	39(1)	-2(1)	3(1)	-2(1)
P(2)	33(1)	39(1)	39(1)	3(1)	-1(1)	-1(1)
P(3)	36(1)	35(1)	38(1)	-2(1)	1(1)	2(1)
P(4)	38(1)	32(1)	37(1)	2(1)	0(1)	1(1)
C(1)	36(3)	37(2)	42(3)	-11(2)	-11(2)	3(2)
C(2)	28(3)	44(3)	45(3)	-1(2)	-3(2)	-8(2)
C(3)	29(3)	46(3)	43(3)	4(2)	2(2)	-3(2)
C(4)	34(3)	44(3)	44(3)	-1(2)	-5(2)	-3(2)
C(5)	32(3)	58(3)	45(4)	-2(3)	-5(2)	2(2)
C(6)	43(3)	79(4)	43(4)	-1(3)	-7(3)	0(3)
C(7)	52(3)	82(4)	33(3)	-12(3)	-11(3)	4(3)
C(8)	62(4)	65(3)	52(4)	-27(3)	-14(3)	7(3)
C(9)	53(3)	44(3)	50(4)	-2(2)	-9(3)	-1(2)
C(10)	30(3)	51(3)	44(3)	2(2)	-4(2)	3(2)
C(11)	38(3)	54(3)	62(4)	11(3)	-5(3)	3(2)
C(12)	41(3)	64(4)	75(5)	21(3)	2(3)	-4(3)
C(13)	46(3)	76(4)	79(5)	25(4)	17(3)	8(3)
C(14)	45(3)	82(4)	59(4)	3(3)	9(3)	10(3)
C(15)	48(3)	57(3)	57(4)	2(3)	1(3)	-2(3)
C(16)	31(3)	40(3)	37(3)	1(2)	4(2)	0(2)
C(17)	43(3)	40(3)	43(3)	0(2)	3(2)	-2(2)
C(18)	51(3)	34(2)	52(4)	8(2)	-1(3)	-3(2)
C(19)	55(3)	53(3)	37(3)	5(2)	-1(3)	-8(3)
C(20)	59(4)	54(3)	32(3)	0(2)	2(3)	3(3)
C(21)	42(3)	42(3)	47(4)	-7(2)	-1(3)	0(2)
C(22)	34(3)	31(2)	35(3)	-3(2)	4(2)	1(2)
C(23)	44(3)	43(3)	35(3)	1(2)	12(2)	-3(2)
C(24)	38(3)	51(3)	50(3)	9(2)	2(2)	6(2)
C(25)	56(4)	41(3)	51(4)	4(2)	12(3)	9(3)
C(26)	59(4)	31(3)	50(4)	0(2)	-1(3)	-2(2)
C(27)	43(3)	42(3)	41(3)	5(2)	2(2)	0(2)
C(28)	42(3)	31(2)	38(3)	-2(2)	1(2)	0(2)
C(29)	46(3)	38(3)	62(4)	-8(2)	-4(3)	-7(2)
C(30)	54(4)	47(3)	92(5)	0(3)	-3(3)	-18(3)
C(31)	96(5)	51(4)	74(5)	-13(3)	-8(4)	-24(3)
C(32)	107(6)	57(4)	64(5)	-23(3)	30(4)	-21(4)
C(33)	72(4)	42(3)	51(4)	-5(2)	13(3)	-8(3)
C(34)	34(3)	43(3)	40(3)	-1(2)	2(2)	1(2)
C(35)	36(3)	52(3)	34(3)	1(2)	0(2)	0(2)
C(36)	34(3)	65(3)	51(4)	-1(3)	-1(3)	-8(3)
C(37)	32(3)	75(4)	58(4)	-11(3)	-8(3)	7(3)
C(38)	50(3)	55(3)	46(4)	-13(3)	-1(3)	10(3)
C(39)	40(3)	50(3)	49(4)	-8(2)	-2(2)	3(2)
C(40)	29(3)	52(3)	36(3)	5(2)	-8(2)	-5(2)
C(41)	34(3)	68(3)	50(4)	2(3)	0(3)	7(2)
C(42)	41(3)	78(4)	42(4)	-2(3)	1(3)	-7(3)
C(43)	51(3)	71(4)	44(4)	-15(3)	9(3)	-13(3)
C(44)	57(3)	53(3)	37(3)	-6(2)	9(3)	6(2)
C(45)	41(3)	49(3)	35(3)	6(2)	1(2)	-2(2)
C(46)	31(3)	44(3)	52(4)	12(2)	-5(2)	0(2)
C(47)	50(3)	38(3)	61(4)	6(3)	-9(3)	-5(2)
C(48)	62(4)	45(3)	86(5)	3(3)	-10(3)	-6(3)
C(49)	58(4)	53(3)	92(6)	21(3)	-16(4)	-12(3)
C(50)	46(3)	66(4)	72(5)	32(3)	1(3)	0(3)
C(51)	43(3)	54(3)	67(4)	22(3)	-4(3)	0(3)
C(52)	58(3)	30(2)	35(3)	-4(2)	-1(3)	0(2)
C(53)	58(3)	31(2)	38(3)	-3(2)	-9(3)	3(2)
C(54)	50(3)	38(3)	36(3)	-2(2)	0(2)	3(2)
C(55)	47(3)	34(2)	30(3)	3(2)	1(2)	-5(2)
C(56)	42(3)	38(3)	48(4)	-4(2)	5(3)	2(2)
C(57)	46(3)	47(3)	64(4)	7(3)	-13(3)	2(2)
C(58)	64(4)	51(3)	42(4)	2(2)	-13(3)	2(3)
C(59)	62(4)	52(3)	39(4)	-3(2)	-4(3)	-1(3)
C(60)	42(3)	39(3)	48(4)	0(2)	-4(3)	0(2)

C(61)	45(3)	30(2)	36(3)	1(2)	3(2)	-1(2)
C(62)	52(3)	34(3)	62(4)	2(3)	-2(3)	-4(2)
C(63)	54(4)	54(3)	54(4)	14(3)	1(3)	-3(3)
C(64)	56(4)	42(3)	61(4)	11(3)	7(3)	-4(3)
C(65)	47(3)	44(3)	67(4)	2(3)	2(3)	-9(2)
C(66)	48(3)	41(3)	57(4)	-1(2)	-1(3)	1(2)
C(67)	70(4)	26(3)	49(4)	-3(2)	-5(3)	-1(2)
C(68)	89(5)	48(3)	50(4)	-4(3)	-18(3)	-4(3)
C(69)	128(7)	67(4)	62(5)	-3(4)	-17(5)	-13(4)
C(70)	147(8)	71(5)	65(6)	-10(4)	-44(6)	-7(5)
C(71)	200(10)	40(3)	27(4)	-3(3)	33(5)	2(4)
C(72)	89(4)	37(3)	53(4)	-5(2)	23(3)	6(3)
C(73)	39(3)	37(2)	39(3)	-7(2)	5(2)	0(2)
C(74)	43(3)	47(3)	49(4)	-9(2)	2(3)	-2(2)
C(75)	52(4)	45(3)	66(4)	-6(3)	13(3)	-5(3)
C(76)	42(3)	52(3)	79(5)	-5(3)	12(3)	-11(3)
C(77)	42(3)	54(3)	73(5)	-5(3)	-8(3)	-2(3)
C(78)	42(3)	49(3)	46(4)	2(2)	-3(3)	4(2)
C(79)	42(3)	39(3)	33(3)	5(2)	5(2)	9(2)
C(80)	52(3)	45(3)	51(4)	-2(2)	5(3)	9(2)
C(81)	58(4)	60(4)	66(4)	-7(3)	11(3)	29(3)
C(82)	68(4)	37(3)	65(4)	-5(3)	9(3)	16(3)
C(83)	71(4)	36(3)	47(4)	-3(2)	7(3)	2(3)
C(84)	47(3)	40(3)	36(3)	-4(2)	1(2)	2(2)
C(85)	39(3)	39(3)	31(3)	1(2)	5(2)	-5(2)
C(86)	65(4)	38(3)	62(4)	4(2)	-29(3)	-5(3)
C(87)	59(4)	47(3)	87(5)	-5(3)	-23(3)	-2(3)
C(88)	41(3)	71(4)	53(4)	-14(3)	-3(3)	-6(3)
C(89)	37(3)	72(4)	46(4)	12(3)	-6(3)	-1(3)
C(90)	38(3)	45(3)	44(3)	7(2)	-4(2)	-1(2)
C(91)	40(3)	30(2)	40(3)	1(2)	-2(2)	1(2)
C(92)	46(3)	47(3)	45(4)	0(2)	-6(3)	1(2)
C(93)	60(4)	47(3)	47(4)	1(2)	1(3)	5(3)
C(94)	61(4)	54(3)	46(4)	1(3)	12(3)	0(3)
C(95)	47(3)	61(3)	62(4)	-2(3)	10(3)	1(3)
C(96)	48(3)	48(3)	44(3)	4(2)	2(3)	6(2)
C(97)	34(3)	35(2)	39(3)	-2(2)	-3(2)	0(2)
C(98)	43(3)	43(3)	45(3)	3(2)	-7(2)	-1(2)
C(99)	39(3)	65(4)	47(4)	6(3)	-7(2)	-10(3)
C(100)	48(4)	69(4)	49(4)	-7(3)	-7(3)	18(3)
C(101)	48(3)	41(3)	86(5)	-9(3)	-20(3)	9(3)
C(102)	40(3)	35(3)	100(5)	-3(3)	-8(3)	3(2)
B(1)	46(4)	48(4)	95(6)	-4(4)	-11(4)	-1(3)
F(1)	85(3)	93(3)	110(4)	-34(2)	-4(2)	6(2)
F(2)	56(2)	57(2)	133(3)	-15(2)	-11(2)	-14(2)
F(3)	73(2)	42(2)	145(4)	0(2)	-25(2)	-3(2)
F(4)	50(2)	54(2)	137(3)	0(2)	2(2)	9(2)
B(2)	81(6)	39(4)	140(10)	-18(5)	-2(6)	-14(4)
F(5)	59(3)	89(3)	216(5)	-38(3)	-20(3)	-1(2)
F(6)	91(5)	202(8)	85(5)	-33(5)	15(4)	34(5)
F(7)	110(5)	91(4)	180(10)	-7(5)	67(6)	-35(3)
F(8)	98(6)	74(4)	330(20)	-66(7)	-54(8)	32(4)
F(9)	91(5)	202(8)	85(5)	-33(5)	15(4)	34(5)
F(10)	110(5)	91(4)	180(10)	-7(5)	67(6)	-35(3)
F(11)	98(6)	74(4)	330(20)	-66(7)	-54(8)	32(4)

The anisotropic displacement factor exponent takes the form

2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table 6. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for $[(\eta^3\text{-Ph-CH-CH-CH-Ph})Pd(PPh_3)]^+BF_4^-$

atom	x	y	z	U(eq)
H(1)	7460	-8033	5177	46
H(2)	8106	-6771	5029	46
H(3)	7807	-7929.0005	4666	47
H(5)	7490	-8182	5750	54
H(6)	7322	-7720	6235	66
H(7)	7156	-6547	6296	67
H(8)	7191	-5842.0005	5876	72
H(9)	7402	-6276	5392	59
H(11)	8468	-6202	4603	62
H(12)	9081	-5778	4200	72
H(13)	9321	-6457	3781	80
H(14)	9011	-7598.9995	3784	74
H(15)	8428	-8054.9995	4195	65
H(17)	6334	-8960	5320	50
H(18)	6381	-9442	5806	55
H(19)	6024	-8819	6224	58
H(20)	5596	-7727	6161	58
H(21)	5509	-7248	5681	53
H(23)	4405	-7350	4977	49
H(24)	3789	-6339	5032	56
H(25)	4327	-5356	5201	59
H(26)	5500	-5365	5299	56
H(27)	6129	-6372	5231	50
H(29)	4568	-8427	5128	59
H(30)	4052	-9344	4874	77
H(31)	4652	-9907	4494	88
H(32)	5739	-9555	4355	91
H(33)	6227	-8609	4586	66
H(35)	5228	-7802	4266	49
H(36)	4064	-7567	4238	60
H(37)	3673	-6447	4287	66
H(38)	4453	-5562.0005	4347	60
H(39)	5624	-5795	4381	55
H(41)	6035	-6949	3734	61
H(42)	6294	-7526	3291	65
H(43)	6937	-8526	3314	66
H(44)	7391	-8900	3773	58
H(45)	7174	-8283	4214	50
H(47)	6751	-5905	4726	60
H(48)	7330	-4862	4671	77
H(49)	7839	-4593	4214	81
H(50)	7746	-5313	3804	74
H(51)	7151	-6362	3846	66
H(52)	5405	-5381	2860	50
H(53)	4361	-5704	2435	51
H(54)	5604	-4967	2351	49
H(56)	5736	-4726	3242	52
H(57)	6467	-4871	3656	63
H(58)	6153	-4446	4130	63
H(59)	5158	-3815	4181	61
H(60)	4442	-3641	3768	51
H(62)	5407	-5998	3331	59
H(63)	4832	-6569	3719	65
H(64)	3718	-6932	3644	63
H(65)	3156	-6694	3194	63
H(66)	3698	-6088	2816	58
H(68)	3913	-4983	2079	75
H(69)	3515	-4882	1588	103
H(70)	4263	-4840	1190	113
H(71)	5441	-4950	1269	109
H(72)	5870	-5041.0005	1775	72
H(74)	3862	-4754	3680	56
H(75)	2842	-5339	3776	65
H(76)	2035	-5466	3398	69
H(77)	2255	-5077.0005	2907	68

H(78)	3274	-4504	2803	55
H(80)	3176	-3317	3064	59
H(81)	2891	-2158	3043	74
H(82)	3722	-1333.9999	3130	68
H(83)	4825	-1657	3262	62
H(84)	5115	-2806	3277	49
H(86)	5629	-2006	2541	66
H(87)	6351	-1506	2897	77
H(88)	6899	-2187	3253	66
H(89)	6784	-3362.9998	3231	61
H(90)	6045	-3859	2884	51
H(92)	4663	-3228	1828	55
H(93)	5184	-3251	1350	61
H(94)	6354	-3433.0002	1309	64
H(95)	7004	-3626	1745	68
H(96)	6487	-3617	2218	56
H(98)	3735	-3767.0002	2392	53
H(99)	2703	-3207	2313	61
H(100)	2682	-2019	2286	66
H(101)	3691	-1408	2306	70
H(102)	4729	-1976.0001	2357	70