

Table S1 Atomic coordinates and isotropic displacement parameters for 6.

	x	y	z	U(eq)
Pd	13671(1)	7782(1)	9849(1)	26(1)
P(1)	11403(1)	7857(1)	9387(1)	26(1)
O(1)	15833(3)	7564(2)	10436(2)	32(1)
O(2)	13992(4)	7222(2)	8215(2)	48(1)
N(1)	13449(4)	8598(2)	10739(2)	28(1)
C(1)	17483(5)	6689(3)	10664(4)	48(1)
C(2)	16094(5)	6990(2)	10234(3)	32(1)
C(3)	15002(5)	6579(2)	9608(3)	40(1)
C(4)	13815(5)	7007(2)	9020(3)	36(1)
C(5)	15170(6)	7612(3)	8266(4)	54(2)
C(6)	15238(7)	7730(3)	7319(4)	59(2)
C(7)	11104(5)	8201(2)	10387(3)	28(1)
C(8)	9865(5)	8131(2)	10583(3)	35(1)
C(9)	9723(5)	8384(2)	11370(3)	38(1)
C(10)	10842(5)	8700(2)	11976(3)	39(1)
C(11)	12081(5)	8778(2)	11797(3)	33(1)
C(12)	12214(5)	8533(2)	10992(3)	29(1)
C(13)	14291(5)	9088(2)	11056(3)	32(1)
C(14)	15468(4)	9246(2)	10744(3)	30(1)
C(15)	16574(5)	9621(2)	11302(4)	40(1)
C(16)	17647(5)	9819(3)	11006(4)	45(1)
C(17)	17610(5)	9650(2)	10152(4)	42(1)
C(18)	16537(5)	9296(2)	9569(4)	36(1)
C(19)	15460(5)	9099(2)	9870(3)	32(1)
C(20)	10359(5)	7093(2)	9144(3)	30(1)
C(21)	10887(5)	6517(2)	9647(3)	39(1)
C(22)	10121(6)	5922(3)	9495(4)	47(1)
C(23)	8841(6)	5900(3)	8855(4)	49(1)
C(24)	8313(5)	6467(3)	8357(4)	44(1)
C(25)	9078(5)	7064(2)	8496(3)	36(1)
C(26)	10674(4)	8442(2)	8480(3)	29(1)
C(27)	9555(5)	8854(2)	8451(3)	36(1)
C(28)	9052(5)	9307(3)	7743(4)	46(1)
C(29)	9707(6)	9358(3)	7091(4)	51(2)
C(30)	10829(6)	8962(3)	7129(4)	53(2)
C(31)	11311(5)	8499(3)	7815(3)	44(1)
F(1)	18642(3)	9867(2)	9847(3)	62(1)
B(1)	15395(10)	4661(5)	8284(5)	74(3)
F(2)	15457(5)	5351(2)	8162(3)	81(1)
F(3)	16592(5)	4450(3)	8880(4)	119(2)
F(4)	14401(5)	4456(4)	8606(4)	153(3)
F(5)	15582(11)	4288(4)	7516(5)	90(3)
F(5')	14557(13)	4492(6)	7499(7)	87(4)
O(3)	12845(14)	5224(7)	9267(9)	259(6)

Pd-C(4)	2.049(4)	Pd-O(1)	2.156(3)
Pd-N(1)	2.195(4)	Pd-P(1)	2.2059(12)
P(1)-C(26)	1.809(4)	P(1)-C(20)	1.822(4)
P(1)-C(7)	1.824(4)	O(1)-C(2)	1.232(5)
O(2)-C(4)	1.398(6)	O(2)-C(5)	1.410(7)
N(1)-C(13)	1.290(6)	N(1)-C(12)	1.439(5)
C(1)-C(2)	1.493(7)	C(2)-C(3)	1.481(7)
C(3)-C(4)	1.532(7)	C(5)-C(6)	1.529(7)
C(7)-C(8)	1.397(6)	C(7)-C(12)	1.397(6)
C(8)-C(9)	1.383(6)	C(9)-C(10)	1.390(7)
C(10)-C(11)	1.386(7)	C(11)-C(12)	1.400(6)
C(13)-C(14)	1.465(6)	C(14)-C(19)	1.402(6)
C(14)-C(15)	1.407(6)	C(15)-C(16)	1.373(7)
C(16)-C(17)	1.372(8)	C(17)-F(1)	1.355(5)
C(17)-C(18)	1.382(7)	C(18)-C(19)	1.381(6)
C(20)-C(25)	1.388(7)	C(20)-C(21)	1.397(6)
C(21)-C(22)	1.393(7)	C(22)-C(23)	1.380(8)
C(23)-C(24)	1.378(8)	C(24)-C(25)	1.397(6)
C(26)-C(27)	1.394(6)	C(26)-C(31)	1.395(6)
C(27)-C(28)	1.397(7)	C(28)-C(29)	1.390(8)
C(29)-C(30)	1.374(8)	C(30)-C(31)	1.383(7)
B(1)-F(5')	1.308(13)	B(1)-F(4)	1.329(9)
B(1)-F(3)	1.354(10)	B(1)-F(2)	1.384(9)
B(1)-F(5)	1.477(12)		
C(4)-Pd-O(1)	81.8(2)	C(4)-Pd-N(1)	178.0(2)
O(1)-Pd-N(1)	99.71(13)	C(4)-Pd-P(1)	96.6(2)
O(1)-Pd-P(1)	170.12(9)	N(1)-Pd-P(1)	81.69(10)
C(26)-P(1)-C(20)	107.2(2)	C(26)-P(1)-C(7)	107.6(2)
C(20)-P(1)-C(7)	104.4(2)	C(26)-P(1)-Pd	115.85(14)
C(20)-P(1)-Pd	119.9(2)	C(7)-P(1)-Pd	100.3(2)
C(2)-O(1)-Pd	110.4(3)	C(4)-O(2)-C(5)	117.6(4)
C(13)-N(1)-C(12)	119.8(4)	C(13)-N(1)-Pd	127.7(3)
C(12)-N(1)-Pd	112.5(3)	O(1)-C(2)-C(3)	120.0(4)
O(1)-C(2)-C(1)	120.2(5)	C(3)-C(2)-C(1)	119.7(4)
C(2)-C(3)-C(4)	112.9(4)	O(2)-C(4)-C(3)	114.5(4)
O(2)-C(4)-Pd	113.6(3)	C(3)-C(4)-Pd	103.3(3)
O(2)-C(5)-C(6)	108.9(5)	C(8)-C(7)-C(12)	119.7(4)
C(8)-C(7)-P(1)	123.8(4)	C(12)-C(7)-P(1)	116.5(3)
C(9)-C(8)-C(7)	120.9(5)	C(8)-C(9)-C(10)	119.0(4)
C(11)-C(10)-C(9)	121.3(4)	C(10)-C(11)-C(12)	119.6(4)
C(7)-C(12)-C(11)	119.5(4)	C(7)-C(12)-N(1)	116.7(4)
C(11)-C(12)-N(1)	123.8(4)	N(1)-C(13)-C(14)	123.3(4)
C(19)-C(14)-C(15)	118.8(4)	C(19)-C(14)-C(13)	121.8(4)
C(15)-C(14)-C(13)	119.1(4)	C(16)-C(15)-C(14)	120.6(5)
C(17)-C(16)-C(15)	118.6(5)	F(1)-C(17)-C(16)	118.7(5)
F(1)-C(17)-C(18)	118.0(5)	C(16)-C(17)-C(18)	123.3(5)
C(19)-C(18)-C(17)	117.8(5)	C(18)-C(19)-C(14)	120.9(4)
C(25)-C(20)-C(21)	119.5(4)	C(25)-C(20)-P(1)	123.0(4)
C(21)-C(20)-P(1)	117.5(4)	C(22)-C(21)-C(20)	119.7(5)
C(23)-C(22)-C(21)	120.4(5)	C(24)-C(23)-C(22)	120.3(5)
C(23)-C(24)-C(25)	119.9(5)	C(20)-C(25)-C(24)	120.2(5)
C(27)-C(26)-C(31)	119.8(4)	C(27)-C(26)-P(1)	122.2(3)
C(31)-C(26)-P(1)	117.9(4)	C(26)-C(27)-C(28)	119.7(5)
C(29)-C(28)-C(27)	119.5(5)	C(30)-C(29)-C(28)	120.7(5)
C(29)-C(30)-C(31)	120.2(5)	C(30)-C(31)-C(26)	120.1(5)
F(5')-B(1)-F(4)	85.9(8)	F(5')-B(1)-F(3)	139.5(11)
F(4)-B(1)-F(3)	106.0(6)	F(5')-B(1)-F(2)	99.5(8)
F(4)-B(1)-F(2)	115.2(9)	F(3)-B(1)-F(2)	109.3(6)
F(4)-B(1)-F(5)	117.8(8)	F(3)-B(1)-F(5)	95.4(8)
F(2)-B(1)-F(5)	110.8(6)		

Table S3. Anisotropic displacement parameters for 6.

	U11	U22	U33	U23	U13	U12
Pd	26 (1)	24 (1)	27 (1)	-4 (1)	9 (1)	1 (1)
P(1)	27 (1)	24 (1)	28 (1)	-1 (1)	10 (1)	-3 (1)
O(1)	33 (2)	33 (2)	30 (2)	1 (1)	11 (1)	5 (1)
O(2)	58 (2)	47 (2)	43 (2)	-4 (2)	22 (2)	0 (2)
N(1)	27 (2)	28 (2)	28 (2)	2 (2)	7 (2)	5 (2)
C(1)	40 (3)	44 (3)	61 (4)	6 (3)	16 (3)	12 (2)
C(2)	35 (3)	32 (2)	33 (2)	7 (2)	16 (2)	5 (2)
C(3)	50 (3)	28 (2)	47 (3)	-1 (2)	22 (2)	6 (2)
C(4)	43 (3)	35 (2)	33 (2)	-6 (2)	16 (2)	-1 (2)
C(5)	59 (4)	62 (4)	48 (3)	-19 (3)	25 (3)	-7 (3)
C(6)	75 (4)	68 (4)	43 (3)	-6 (3)	30 (3)	-7 (3)
C(7)	35 (2)	22 (2)	30 (2)	2 (2)	15 (2)	3 (2)
C(8)	35 (3)	33 (2)	40 (3)	2 (2)	17 (2)	-1 (2)
C(9)	44 (3)	35 (3)	44 (3)	6 (2)	27 (2)	3 (2)
C(10)	55 (3)	37 (3)	35 (3)	6 (2)	26 (2)	12 (2)
C(11)	38 (3)	32 (2)	28 (2)	-2 (2)	10 (2)	3 (2)
C(12)	37 (2)	22 (2)	32 (2)	6 (2)	16 (2)	6 (2)
C(13)	37 (3)	30 (2)	28 (2)	-6 (2)	7 (2)	1 (2)
C(14)	27 (2)	23 (2)	38 (3)	-2 (2)	6 (2)	1 (2)
C(15)	37 (3)	31 (2)	44 (3)	-7 (2)	4 (2)	-2 (2)
C(16)	31 (3)	35 (3)	61 (4)	-9 (2)	2 (2)	-3 (2)
C(17)	26 (2)	32 (2)	69 (4)	4 (2)	17 (2)	2 (2)
C(18)	31 (2)	29 (2)	50 (3)	-4 (2)	15 (2)	-3 (2)
C(19)	29 (2)	24 (2)	40 (3)	-6 (2)	8 (2)	-4 (2)
C(20)	34 (2)	28 (2)	33 (2)	-8 (2)	19 (2)	-8 (2)
C(21)	45 (3)	32 (2)	39 (3)	-1 (2)	15 (2)	-5 (2)
C(22)	61 (4)	31 (3)	55 (3)	4 (2)	25 (3)	-8 (2)
C(23)	59 (4)	34 (3)	61 (4)	-13 (3)	31 (3)	-18 (3)
C(24)	36 (3)	45 (3)	54 (3)	-17 (3)	17 (2)	-12 (2)
C(25)	32 (2)	33 (3)	44 (3)	-6 (2)	15 (2)	-4 (2)
C(26)	27 (2)	28 (2)	28 (2)	0 (2)	5 (2)	-6 (2)
C(27)	34 (3)	34 (2)	41 (3)	6 (2)	11 (2)	-4 (2)
C(28)	39 (3)	35 (3)	52 (3)	4 (2)	-1 (2)	-1 (2)
C(29)	56 (4)	44 (3)	37 (3)	11 (2)	-9 (3)	-15 (3)
C(30)	60 (4)	61 (4)	35 (3)	13 (3)	11 (3)	-7 (3)
C(31)	44 (3)	55 (3)	34 (3)	2 (2)	16 (2)	-4 (3)
F(1)	35 (2)	55 (2)	102 (3)	-10 (2)	33 (2)	-14 (2)
B(1)	91 (6)	81 (6)	42 (4)	16 (4)	6 (4)	-33 (5)
F(2)	108 (3)	72 (3)	67 (3)	1 (2)	33 (2)	3 (2)
F(3)	92 (3)	115 (4)	134 (5)	21 (4)	13 (3)	14 (3)
F(4)	83 (4)	218 (7)	163 (6)	74 (5)	45 (4)	-34 (4)
F(5)	149 (8)	69 (5)	65 (5)	-3 (4)	53 (6)	-20 (5)
F(5')	99 (9)	87 (8)	59 (7)	-9 (6)	0 (7)	-34 (7)

Table S4 Hydrogen coordinates for 6.

	x	y	z	U (eq)
H(1A)	18081(5)	7024(3)	11056(4)	72
H(1B)	17886(5)	6550(3)	10201(4)	72
H(1C)	17393(5)	6294(3)	11019(4)	72
H(3A)	14632(5)	6255(2)	9956(3)	48
H(3B)	15411(5)	6315(2)	9219(3)	48
H(4A)	12949(5)	6734(2)	8877(3)	43
H(5A)	16009(6)	7372(3)	8628(4)	65
H(5B)	15120(6)	8050(3)	8558(4)	65
H(6A)	16055(7)	8001(3)	7348(4)	89
H(6B)	14409(7)	7971(3)	6967(4)	89
H(6C)	15295(7)	7295(3)	7037(4)	89
H(8A)	9111(5)	7907(2)	10170(3)	42
H(9A)	8873(5)	8342(2)	11494(3)	46
H(10A)	10756(5)	8866(2)	12523(3)	47
H(11A)	12836(5)	8996(2)	12219(3)	39
H(13A)	14141(5)	9360(2)	11515(3)	39
H(15A)	16577(5)	9738(2)	11889(4)	47
H(16A)	18399(5)	10067(3)	11385(4)	55
H(18A)	16539(5)	9191(2)	8979(4)	43
H(19A)	14704(5)	8859(2)	9480(3)	38
H(21A)	11764(5)	6531(2)	10091(3)	46
H(22A)	10481(6)	5529(3)	9833(4)	57
H(23A)	8323(6)	5494(3)	8758(4)	58
H(24A)	7430(5)	6450(3)	7920(4)	53
H(25A)	8719(5)	7452(2)	8146(3)	43
H(27A)	9134(5)	8828(2)	8912(3)	44
H(28A)	8268(5)	9577(3)	7708(4)	55
H(29A)	9375(6)	9670(3)	6613(4)	61
H(30A)	11276(6)	9005(3)	6683(4)	64
H(31A)	12076(5)	8220(3)	7833(3)	52
H(3)	13456	5097	8977	388
H(3')	13144	5102	9860	388