

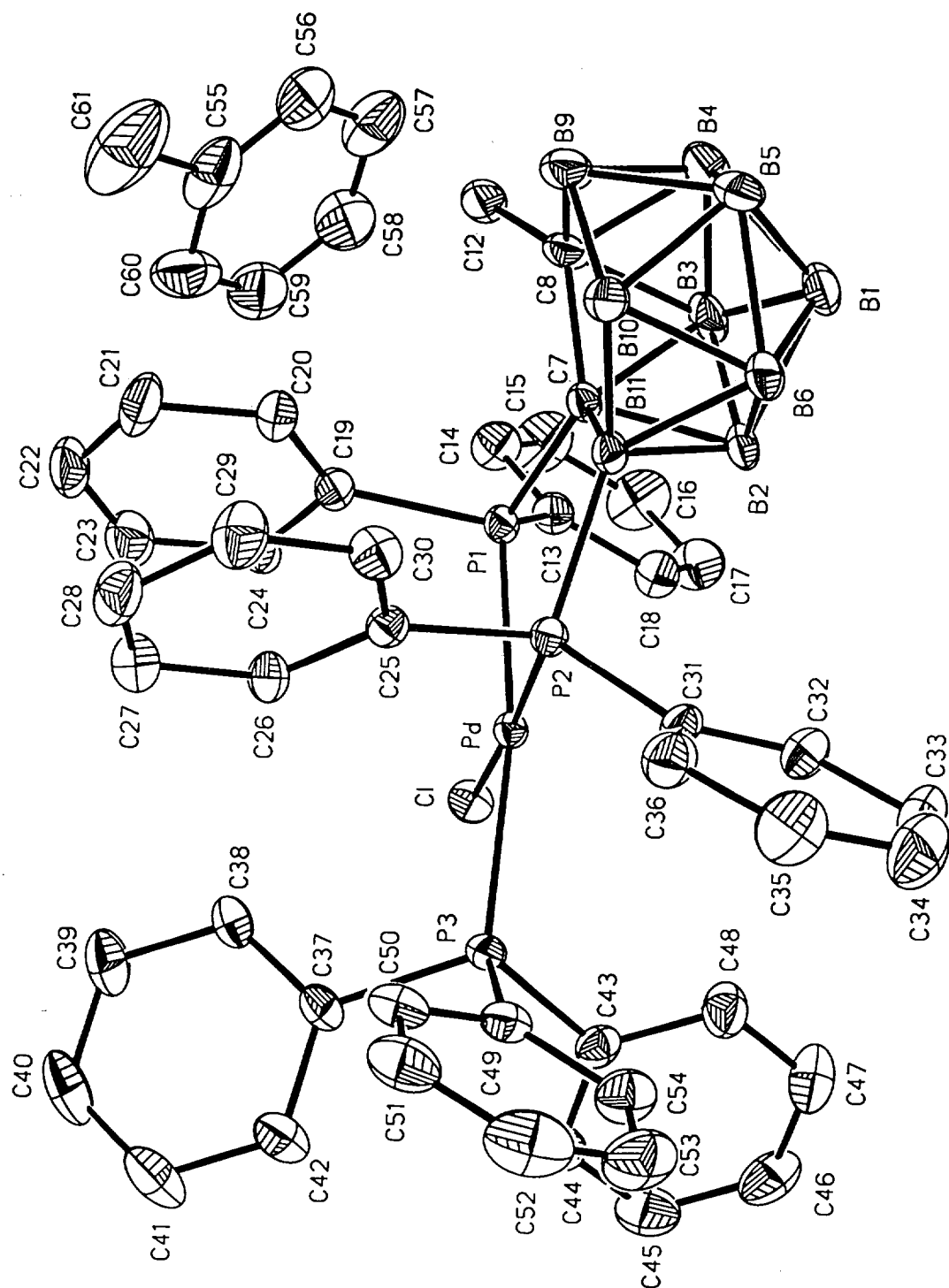


Table 1. Crystal data and structure refinement for C52 H55 B9 Cl P3 Pd.

Identification code	L2FNPd.toluene
Chemical formula	C52 H55 B9 Cl P3 Pd
Formula weight	1012.01
Temperature	193(2) K
Wavelength	0.71069 Å
Crystal system, space group	monoclinic, P2(1)/n (no. 14)
Unit cell dimensions	a = 19.007(6) Å alpha = 90 deg. b = 10.863(5) Å beta = 96.15(2) deg. c = 25.454(7) Å gamma = 90 deg.
Volume	5225(3) Å ³
Z, Calculated density	4, 1.286 Mg/m ³
Absorption coefficient	0.533 mm ⁻¹
F(000)	2080
Crystal size	0.45 x 0.45 x 0.08 mm
Theta range for data collection	2.54 to 26.00 deg.
Index ranges	0 ≤ h ≤ 23, 0 ≤ k ≤ 13, -31 ≤ l ≤ 31
Reflections collected / unique	9249 / 9249 [R(int) = 0.0000]
Reflections observed [I > 2σI]	7296
Completeness to theta = 26.00	90.0%
Max. and min. transmission	0.9586 and 0.7955
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9249 / 28 / 606
Goodness-of-fit on F ²	1.050
Final R indices [I > 2σ(I)]	R1 = 0.0688, wR2 = 0.1309
R indices (all data)	R1 = 0.0896, wR2 = 0.1418
Largest diff. peak and hole	0.511 and -0.819 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for C52 H55 B9 Cl P3 Pd. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd	4932 (1)	3540 (1)	7297 (1)	24 (1)
Cl	4217 (1)	5310 (1)	7230 (1)	38 (1)
P1	4741 (1)	3359 (1)	8178 (1)	27 (1)
P2	5590 (1)	1796 (1)	7423 (1)	25 (1)
P3	4918 (1)	3736 (1)	6379 (1)	30 (1)
B1	6756 (4)	2345 (8)	9068 (3)	46 (2)
B2	6274 (3)	2891 (7)	8476 (3)	36 (2)
B3	5928 (4)	3070 (8)	9094 (3)	43 (2)
B4	6156 (4)	1757 (8)	9471 (3)	47 (2)
B5	6631 (4)	714 (8)	9112 (3)	46 (2)
B6	6715 (3)	1450 (7)	8485 (3)	36 (2)
C7	5422 (3)	2429 (5)	8556 (2)	27 (1)
C8	5345 (3)	1863 (6)	9119 (2)	37 (2)
B9	5694 (3)	478 (8)	9150 (3)	46 (2)
B10	6109 (2)	212 (4)	8528 (3)	38 (2)
B11	5855 (3)	1589 (6)	8171 (3)	28 (1)
C12	4704 (3)	2128 (7)	9414 (2)	45 (2)
C13	4633 (3)	4809 (6)	8513 (2)	35 (1)
C14	4130 (4)	5003 (7)	8863 (3)	49 (2)
C15	4100 (5)	6137 (7)	9115 (3)	71 (3)
C16	4560 (5)	7052 (8)	9025 (3)	74 (3)
C17	5062 (4)	6864 (7)	8683 (3)	62 (2)
C18	5098 (3)	5759 (6)	8424 (3)	42 (2)
C19	3921 (3)	2500 (6)	8141 (2)	35 (1)
C20	3926 (3)	1221 (6)	8206 (2)	39 (2)
C21	3307 (4)	546 (8)	8099 (3)	63 (2)
C22	2687 (4)	1137 (8)	7923 (3)	63 (2)
C23	2677 (4)	2390 (8)	7849 (3)	61 (2)
C24	3289 (3)	3082 (8)	7960 (3)	51 (2)
C25	5062 (3)	469 (5)	7199 (2)	28 (1)
C26	4369 (3)	609 (6)	6985 (2)	35 (1)
C27	3943 (4)	-391 (6)	6841 (3)	48 (2)
C28	4225 (4)	-1576 (7)	6912 (3)	52 (2)
C29	4908 (4)	-1743 (6)	7135 (3)	51 (2)
C30	5323 (3)	-732 (6)	7277 (2)	40 (2)
C31	6404 (3)	1782 (6)	7102 (2)	32 (1)
C32	6844 (3)	2814 (7)	7187 (3)	47 (2)
C33	7490 (4)	2849 (8)	6975 (3)	64 (2)
C34	7698 (4)	1849 (9)	6700 (4)	76 (3)
C35	7272 (4)	847 (9)	6603 (3)	72 (3)
C36	6619 (3)	793 (7)	6810 (3)	46 (2)
C37	4028 (3)	3544 (6)	6050 (2)	38 (1)
C38	3460 (3)	3314 (6)	6332 (3)	42 (2)
C39	2798 (4)	3066 (8)	6074 (3)	64 (2)
C40	2703 (4)	3039 (9)	5531 (4)	82 (3)
C41	3256 (5)	3301 (9)	5246 (3)	75 (3)
C42	3916 (4)	3524 (7)	5498 (3)	52 (2)
C43	5245 (3)	5257 (6)	6219 (2)	37 (1)
C44	4888 (4)	6033 (7)	5851 (3)	51 (2)
C45	5185 (5)	7147 (8)	5738 (3)	68 (2)
C46	5828 (5)	7498 (7)	5990 (3)	66 (2)

C47	6182 (4)	6761 (7)	6359 (3)	63 (2)
C48	5885 (4)	5634 (7)	6478 (3)	54 (2)
C49	5396 (3)	2686 (6)	5988 (2)	36 (1)
C50	5126 (4)	1525 (6)	5869 (2)	44 (2)
C51	5458 (4)	697 (7)	5571 (3)	56 (2)
C52	6083 (5)	1020 (8)	5380 (3)	74 (3)
C53	6368 (4)	2172 (8)	5487 (3)	69 (2)
C54	6035 (4)	3007 (7)	5798 (3)	51 (2)
C55	2774 (5)	2369 (8)	9616 (3)	87 (3)
C56	3213 (4)	2676 (9)	10065 (3)	80 (3)
C57	3295 (6)	3870 (9)	10239 (4)	96 (3)
C58	2897 (5)	4750 (11)	9952 (4)	98 (3)
C59	2454 (6)	4464 (11)	9507 (4)	89 (3)
C60	2370 (5)	3270 (10)	9322 (4)	93 (3)
C61	2664 (7)	1086 (10)	9426 (5)	157 (6)

Table 3. Bond lengths [Å] and angles [deg] for C52 H55 B9 Cl P3 Pd.

Pd-P2	2.2742(16)
Pd-P1	2.3178(16)
Pd-P3	2.3459(16)
Pd-Cl	2.3504(17)
P1-C19	1.811(6)
P1-C13	1.813(6)
P1-C7	1.831(5)
P2-C25	1.814(6)
P2-C31	1.825(5)
P2-B11	1.928(7)
P3-C37	1.818(6)
P3-C49	1.821(6)
P3-C43	1.827(6)
B1-B4	1.735(11)
B1-B3	1.766(11)
B1-B6	1.768(11)
B1-B2	1.779(10)
B1-B5	1.792(12)
B1-H1	1.1200
B2-C7	1.729(8)
B2-B11	1.763(10)
B2-B6	1.774(11)
B2-B3	1.779(10)
B2-H2	1.1200
B3-C8	1.723(10)
B3-C7	1.732(8)
B3-B4	1.747(12)
B3-H3	1.1200
B4-C8	1.701(9)
B4-B5	1.764(11)
B4-B9	1.792(12)
B4-H4	1.1200
B5-B10	1.782(10)
B5-B6	1.806(10)
B5-B9	1.813(10)
B5-H5	1.1200
B6-B11	1.747(8)
B6-B10	1.780(8)
B6-H6	1.1200
C7-C8	1.579(8)
C7-B11	1.627(8)
C8-C12	1.526(8)
C8-B9	1.642(11)
B9-B10	1.866(10)
B9-H9	1.1200
B9-H10B	1.35(6)
B10-B11	1.790(8)
B10-H10A	1.1200
B10-H10B	1.1200
C12-H12A	0.9800
C12-H12B	0.9800
C12-H12C	0.9800
C13-C14	1.391(8)
C13-C18	1.392(8)
C14-C15	1.393(9)
C14-H14	0.9500
C15-C16	1.361(11)

C15-H15	0.9500
C16-C17	1.373 (10)
C16-H16	0.9500
C17-C18	1.375 (9)
C17-H17	0.9500
C18-H18	0.9500
C19-C24	1.393 (8)
C19-C20	1.398 (9)
C20-C21	1.389 (8)
C20-H20	0.9500
C21-C22	1.373 (11)
C21-H21	0.9500
C22-C23	1.374 (11)
C22-H22	0.9500
C23-C24	1.388 (10)
C23-H23	0.9500
C24-H24	0.9500
C25-C26	1.378 (7)
C25-C30	1.403 (8)
C26-C27	1.381 (8)
C26-H26	0.9500
C27-C28	1.399 (10)
C27-H27	0.9500
C28-C29	1.373 (9)
C28-H28	0.9500
C29-C30	1.378 (9)
C29-H29	0.9500
C30-H30	0.9500
C31-C36	1.393 (9)
C31-C32	1.401 (9)
C32-C33	1.395 (9)
C32-H32	0.9500
C33-C34	1.374 (11)
C33-H33	0.9500
C34-C35	1.363 (12)
C34-H34	0.9500
C35-C36	1.400 (9)
C35-H35	0.9500
C36-H36	0.9500
C37-C38	1.380 (8)
C37-C42	1.398 (8)
C38-C39	1.383 (8)
C38-H38	0.9500
C39-C40	1.375 (12)
C39-H39	0.9500
C40-C41	1.369 (12)
C40-H40	0.9500
C41-C42	1.368 (10)
C41-H41	0.9500
C42-H42	0.9500
C43-C48	1.382 (9)
C43-C44	1.383 (9)
C44-C45	1.378 (10)
C44-H44	0.9500
C45-C46	1.371 (11)
C45-H45	0.9500
C46-C47	1.357 (10)
C46-H46	0.9500
C47-C48	1.395 (10)
C47-H47	0.9500
C48-H48	0.9500
C49-C50	1.382 (9)

C49-C54	1.397(9)
C50-C51	1.374(9)
C50-H50	0.9500
C51-C52	1.377(11)
C51-H51	0.9500
C52-C53	1.379(7)
C52-H52	0.9500
C53-C54	1.399(10)
C53-H53	0.9500
C54-H54	0.9500
C55-C56	1.381(7)
C55-C60	1.409(7)
C55-C61	1.483(7)
C56-C57	1.374(7)
C56-H56	0.9500
C57-C58	1.379(7)
C57-H57	0.9500
C58-C59	1.372(13)
C58-H58	0.9500
C59-C60	1.383(7)
C59-H59	0.9500
C60-H60	0.9500
C61-H61A	0.9800
C61-H61B	0.9800
C61-H61C	0.9800

P2-Pd-P1	86.22(5)
P2-Pd-P3	99.40(5)
P1-Pd-P3	170.39(5)
P2-Pd-Cl	175.59(6)
P1-Pd-Cl	89.50(6)
P3-Pd-Cl	84.70(6)
C19-P1-C13	109.4(3)
C19-P1-C7	107.4(3)
C13-P1-C7	110.0(3)
C19-P1-Pd	102.48(19)
C13-P1-Pd	114.7(2)
C7-P1-Pd	112.34(18)
C25-P2-C31	108.7(3)
C25-P2-B11	107.2(3)
C31-P2-B11	107.3(3)
C25-P2-Pd	109.86(18)
C31-P2-Pd	115.05(19)
B11-P2-Pd	108.5(2)
C37-P3-C49	99.9(3)
C37-P3-C43	108.9(3)
C49-P3-C43	104.1(3)
C37-P3-Pd	111.0(2)
C49-P3-Pd	122.3(2)
C43-P3-Pd	109.6(2)
B4-B1-B3	59.9(4)
B4-B1-B6	108.7(6)
B3-B1-B6	108.5(5)
B4-B1-B2	108.2(5)
B3-B1-B2	60.2(4)
B6-B1-B2	60.0(4)
B4-B1-B5	60.0(5)
B3-B1-B5	108.3(5)
B6-B1-B5	61.0(4)
B2-B1-B5	108.8(5)
B4-B1-H1	121.7
B3-B1-H1	121.6

B6-B1-H1	121.1
B2-B1-H1	121.5
B5-B1-H1	121.1
C7-B2-B11	55.5 (3)
C7-B2-B6	100.9 (5)
B11-B2-B6	59.2 (4)
C7-B2-B3	59.2 (4)
B11-B2-B3	106.6 (5)
B6-B2-B3	107.6 (5)
C7-B2-B1	101.9 (5)
B11-B2-B1	105.9 (5)
B6-B2-B1	59.7 (4)
B3-B2-B1	59.5 (4)
C7-B2-H2	127.4
B11-B2-H2	123.2
B6-B2-H2	123.4
B3-B2-H2	121.1
B1-B2-H2	123.5
C8-B3-C7	54.4 (3)
C8-B3-B4	58.7 (4)
C7-B3-B4	100.9 (5)
C8-B3-B1	103.9 (6)
C7-B3-B1	102.3 (5)
B4-B3-B1	59.2 (5)
C8-B3-B2	104.4 (5)
C7-B3-B2	59.0 (3)
B4-B3-B2	107.7 (6)
B1-B3-B2	60.2 (4)
C8-B3-H3	125.1
C7-B3-H3	127.2
B4-B3-H3	123.3
B1-B3-H3	123.7
B2-B3-H3	121.4
C8-B4-B1	106.2 (5)
C8-B4-B3	59.9 (4)
B1-B4-B3	61.0 (5)
C8-B4-B5	104.8 (5)
B1-B4-B5	61.6 (5)
B3-B4-B5	110.5 (6)
C8-B4-B9	56.0 (4)
B1-B4-B9	109.7 (6)
B3-B4-B9	107.6 (5)
B5-B4-B9	61.3 (4)
C8-B4-H4	125.3
B1-B4-H4	120.7
B3-B4-H4	120.4
B5-B4-H4	120.8
B9-B4-H4	122.1
B4-B5-B10	111.0 (5)
B4-B5-B1	58.4 (5)
B10-B5-B1	108.4 (5)
B4-B5-B6	105.8 (6)
B10-B5-B6	59.5 (4)
B1-B5-B6	58.9 (4)
B4-B5-B9	60.1 (5)
B10-B5-B9	62.5 (4)
B1-B5-B9	106.3 (6)
B6-B5-B9	106.8 (5)
B4-B5-H5	121.8
B10-B5-H5	119.3
B1-B5-H5	123.1
B6-B5-H5	123.6

B9-B5-H5	121.7
B11-B6-B1	107.0(5)
B11-B6-B2	60.1(4)
B1-B6-B2	60.3(4)
B11-B6-B10	61.0(3)
B1-B6-B10	109.6(5)
B2-B6-B10	111.1(4)
B11-B6-B5	106.1(5)
B1-B6-B5	60.2(4)
B2-B6-B5	108.4(5)
B10-B6-B5	59.6(4)
B11-B6-H6	122.8
B1-B6-H6	121.6
B2-B6-H6	120.4
B10-B6-H6	119.8
B5-B6-H6	122.7
C8-C7-B11	115.5(5)
C8-C7-B2	113.5(4)
B11-C7-B2	63.3(4)
C8-C7-B3	62.5(4)
B11-C7-B3	115.3(4)
B2-C7-B3	61.8(4)
C8-C7-P1	124.2(4)
B11-C7-P1	111.5(4)
B2-C7-P1	113.3(4)
B3-C7-P1	119.6(4)
C12-C8-C7	122.0(5)
C12-C8-B9	119.2(5)
C7-C8-B9	109.0(5)
C12-C8-B4	118.6(5)
C7-C8-B4	109.7(5)
B9-C8-B4	64.8(4)
C12-C8-B3	115.2(6)
C7-C8-B3	63.1(4)
B9-C8-B3	116.2(5)
B4-C8-B3	61.4(4)
C8-B9-B4	59.2(4)
C8-B9-B5	105.2(6)
B4-B9-B5	58.6(4)
C8-B9-B10	107.8(5)
B4-B9-B10	106.0(5)
B5-B9-B10	57.9(3)
C8-B9-H9	126(3)
B4-B9-H9	120(3)
B5-B9-H9	119(3)
B10-B9-H9	121(3)
C8-B9-H10B	99(2)
B4-B9-H10B	132(2)
B5-B9-H10B	94.4(6)
B10-B9-H10B	36.5(5)
H9-B9-H10B	107(4)
B6-B10-B5	60.9(4)
B6-B10-B11	58.6(3)
B5-B10-B11	105.3(4)
B6-B10-B9	105.7(5)
B5-B10-B9	59.5(4)
B11-B10-B9	100.8(4)
B6-B10-H10A	121(3)
B5-B10-H10A	120(3)
B11-B10-H10A	127(3)
B9-B10-H10A	125(3)
B6-B10-H10B	133(3)

B5-B10-H10B	105 (3)
B11-B10-H10B	88 (3)
B9-B10-H10B	46 (3)
H10A-B10-H10B	104 (4)
C7-B11-B6	106.3 (5)
C7-B11-B2	61.2 (4)
B6-B11-B2	60.7 (4)
C7-B11-B10	106.7 (4)
B6-B11-B10	60.4 (3)
B2-B11-B10	111.2 (4)
C7-B11-P2	115.8 (4)
B6-B11-P2	126.5 (4)
B2-B11-P2	113.5 (4)
B10-B11-P2	128.8 (4)
C8-C12-H12A	109.5
C8-C12-H12B	109.5
H12A-C12-H12B	109.5
C8-C12-H12C	109.5
H12A-C12-H12C	109.5
H12B-C12-H12C	109.5
C14-C13-C18	118.9 (6)
C14-C13-P1	123.6 (5)
C18-C13-P1	117.5 (4)
C13-C14-C15	119.6 (7)
C13-C14-H14	120.2
C15-C14-H14	120.2
C16-C15-C14	120.6 (7)
C16-C15-H15	119.7
C14-C15-H15	119.7
C15-C16-C17	120.1 (7)
C15-C16-H16	119.9
C17-C16-H16	119.9
C16-C17-C18	120.4 (7)
C16-C17-H17	119.8
C18-C17-H17	119.8
C17-C18-C13	120.3 (6)
C17-C18-H18	119.8
C13-C18-H18	119.8
C24-C19-C20	119.0 (6)
C24-C19-P1	119.4 (5)
C20-C19-P1	120.8 (5)
C21-C20-C19	120.5 (7)
C21-C20-H20	119.8
C19-C20-H20	119.8
C22-C21-C20	119.7 (8)
C22-C21-H21	120.1
C20-C21-H21	120.1
C21-C22-C23	120.5 (7)
C21-C22-H22	119.8
C23-C22-H22	119.8
C22-C23-C24	120.6 (7)
C22-C23-H23	119.7
C24-C23-H23	119.7
C23-C24-C19	119.7 (7)
C23-C24-H24	120.1
C19-C24-H24	120.1
C26-C25-C30	117.9 (5)
C26-C25-P2	120.7 (4)
C30-C25-P2	121.2 (4)
C25-C26-C27	121.7 (6)
C25-C26-H26	119.1
C27-C26-H26	119.1

C26-C27-C28	119.0 (6)
C26-C27-H27	120.5
C28-C27-H27	120.5
C29-C28-C27	120.4 (6)
C29-C28-H28	119.8
C27-C28-H28	119.8
C28-C29-C30	119.6 (6)
C28-C29-H29	120.2
C30-C29-H29	120.2
C29-C30-C25	121.3 (6)
C29-C30-H30	119.3
C25-C30-H30	119.3
C36-C31-C32	119.7 (5)
C36-C31-P2	123.8 (5)
C32-C31-P2	116.4 (5)
C33-C32-C31	119.9 (7)
C33-C32-H32	120.1
C31-C32-H32	120.1
C34-C33-C32	119.3 (8)
C34-C33-H33	120.4
C32-C33-H33	120.4
C35-C34-C33	121.7 (7)
C35-C34-H34	119.1
C33-C34-H34	119.1
C34-C35-C36	119.9 (8)
C34-C35-H35	120.0
C36-C35-H35	120.0
C31-C36-C35	119.4 (7)
C31-C36-H36	120.3
C35-C36-H36	120.3
C38-C37-C42	118.5 (6)
C38-C37-P3	121.5 (5)
C42-C37-P3	119.8 (5)
C37-C38-C39	120.7 (7)
C37-C38-H38	119.6
C39-C38-H38	119.6
C40-C39-C38	119.8 (8)
C40-C39-H39	120.1
C38-C39-H39	120.1
C41-C40-C39	120.1 (7)
C41-C40-H40	119.9
C39-C40-H40	119.9
C42-C41-C40	120.5 (8)
C42-C41-H41	119.8
C40-C41-H41	119.8
C41-C42-C37	120.4 (7)
C41-C42-H42	119.8
C37-C42-H42	119.8
C48-C43-C44	119.1 (6)
C48-C43-P3	117.7 (5)
C44-C43-P3	123.2 (5)
C45-C44-C43	119.6 (7)
C45-C44-H44	120.2
C43-C44-H44	120.2
C46-C45-C44	120.7 (7)
C46-C45-H45	119.6
C44-C45-H45	119.6
C47-C46-C45	120.7 (8)
C47-C46-H46	119.6
C45-C46-H46	119.6
C46-C47-C48	119.1 (7)
C46-C47-H47	120.5

C48-C47-H47	120.5
C43-C48-C47	120.8 (7)
C43-C48-H48	119.6
C47-C48-H48	119.6
C50-C49-C54	118.0 (6)
C50-C49-P3	119.7 (5)
C54-C49-P3	122.4 (5)
C51-C50-C49	122.4 (7)
C51-C50-H50	118.8
C49-C50-H50	118.8
C50-C51-C52	119.6 (8)
C50-C51-H51	120.2
C52-C51-H51	120.2
C51-C52-C53	119.7 (8)
C51-C52-H52	120.1
C53-C52-H52	120.1
C52-C53-C54	120.6 (8)
C52-C53-H53	119.7
C54-C53-H53	119.7
C49-C54-C53	119.7 (7)
C49-C54-H54	120.1
C53-C54-H54	120.1
C56-C55-C60	121.2 (9)
C56-C55-C61	123.2 (10)
C60-C55-C61	115.5 (10)
C57-C56-C55	122.2 (10)
C57-C56-H56	118.9
C55-C56-H56	118.9
C56-C57-C58	116.4 (11)
C56-C57-H57	121.8
C58-C57-H57	121.8
C59-C58-C57	122.3 (12)
C59-C58-H58	118.9
C57-C58-H58	118.9
C58-C59-C60	122.1 (11)
C58-C59-H59	118.9
C60-C59-H59	118.9
C59-C60-C55	115.7 (10)
C59-C60-H60	122.1
C55-C60-H60	122.1
C55-C61-H61A	109.5
C55-C61-H61B	109.5
H61A-C61-H61B	109.5
C55-C61-H61C	109.5
H61A-C61-H61C	109.5
H61B-C61-H61C	109.5

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for C52 H55 B9 Cl P3 Pd.

The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Pd	21(1)	27(1)	25(1)	0(1)	2(1)	0(1)
Cl	37(1)	34(1)	41(1)	2(1)	2(1)	9(1)
P1	21(1)	35(1)	25(1)	-2(1)	4(1)	1(1)
P2	21(1)	29(1)	25(1)	1(1)	4(1)	2(1)
P3	29(1)	35(1)	24(1)	3(1)	1(1)	1(1)
B1	27(4)	72(6)	36(4)	-5(4)	-4(3)	-9(4)
B2	19(3)	54(5)	34(4)	0(3)	-3(3)	-5(3)
B3	37(4)	59(5)	31(4)	-15(4)	-6(3)	-9(4)
B4	36(4)	66(6)	39(4)	-3(4)	-3(3)	7(4)
B5	38(4)	61(5)	36(4)	19(4)	-3(3)	5(4)
B6	20(3)	50(4)	39(4)	3(4)	1(3)	2(3)
C7	20(3)	33(3)	28(3)	-1(2)	1(2)	0(2)
C8	34(3)	58(4)	19(3)	5(3)	2(2)	4(3)
B9	40(4)	69(6)	29(4)	12(4)	6(3)	4(4)
B10	28(4)	50(5)	37(4)	9(3)	4(3)	1(3)
B11	20(3)	31(3)	33(3)	2(3)	2(2)	1(3)
C12	37(3)	70(5)	29(3)	2(3)	7(3)	-3(3)
C13	37(3)	40(4)	30(3)	-6(3)	6(3)	0(3)
C14	57(4)	48(4)	42(4)	-10(3)	14(3)	-1(3)
C15	87(6)	58(5)	76(6)	-23(4)	41(5)	4(5)
C16	108(7)	50(5)	70(6)	-27(4)	31(5)	-3(5)
C17	86(6)	46(5)	53(5)	-11(4)	9(4)	-12(4)
C18	46(4)	42(4)	39(4)	-13(3)	10(3)	-4(3)
C19	28(3)	52(4)	28(3)	-3(3)	8(2)	-3(3)
C20	33(3)	41(4)	44(4)	-3(3)	5(3)	-6(3)
C21	62(5)	69(5)	60(5)	-17(4)	22(4)	-38(4)
C22	34(4)	99(6)	56(4)	-9(4)	7(3)	-25(4)
C23	38(3)	82(4)	61(4)	0(3)	3(3)	-3(3)
C24	29(3)	76(5)	47(4)	3(4)	0(3)	1(3)
C25	28(3)	29(3)	28(3)	0(2)	5(2)	0(2)
C26	34(3)	30(3)	41(4)	-6(3)	2(3)	-5(3)
C27	41(4)	50(4)	52(4)	-3(3)	1(3)	-6(3)
C28	53(4)	38(4)	65(5)	-2(4)	3(4)	-17(3)
C29	50(4)	32(4)	71(5)	-1(3)	5(4)	-2(3)
C30	41(4)	36(4)	44(4)	-1(3)	1(3)	4(3)
C31	23(3)	41(4)	31(3)	8(3)	8(2)	2(2)
C32	35(3)	62(5)	45(4)	2(3)	15(3)	-5(3)
C33	42(4)	88(6)	64(5)	-1(5)	17(4)	-19(4)
C34	46(4)	103(6)	83(5)	-2(5)	28(4)	-2(4)
C35	49(5)	103(7)	68(6)	-10(5)	30(4)	21(5)
C36	39(4)	53(4)	46(4)	2(3)	11(3)	4(3)
C37	32(3)	45(4)	35(3)	-2(3)	-6(3)	5(3)
C38	29(3)	47(4)	46(4)	-3(3)	-7(3)	1(3)
C39	33(4)	80(6)	77(6)	-8(5)	-9(4)	-6(4)
C40	45(5)	107(8)	86(7)	-11(6)	-30(5)	-6(5)
C41	69(6)	99(7)	52(5)	-13(5)	-24(4)	1(5)
C42	55(4)	64(5)	36(4)	-7(4)	-4(3)	4(4)
C43	33(3)	41(4)	38(4)	4(3)	11(3)	5(3)
C44	52(4)	55(5)	46(4)	11(3)	0(3)	0(4)
C45	85(6)	60(5)	57(5)	19(4)	0(4)	10(5)
C46	73(6)	50(5)	79(6)	23(4)	28(5)	4(4)

C47	41 (4)	50 (5)	97 (7)	-1 (4)	6 (4)	-6 (3)
C48	43 (4)	47 (4)	70 (5)	16 (4)	-5 (4)	-8 (3)
C49	38 (3)	44 (4)	26 (3)	0 (3)	3 (3)	8 (3)
C50	57 (4)	46 (4)	27 (3)	-1 (3)	-1 (3)	7 (3)
C51	80 (6)	50 (5)	37 (4)	-10 (3)	-1 (4)	11 (4)
C52	94 (7)	75 (6)	56 (5)	-9 (5)	16 (5)	35 (5)
C53	65 (5)	88 (7)	58 (5)	2 (5)	27 (4)	17 (5)
C54	53 (4)	55 (4)	48 (4)	-1 (3)	14 (3)	10 (4)
C55	98 (8)	94 (8)	78 (7)	-35 (6)	59 (6)	-40 (6)
C56	60 (6)	108 (8)	79 (7)	2 (6)	36 (5)	-5 (5)
C57	104 (9)	95 (9)	96 (8)	-3 (7)	43 (7)	-22 (7)
C58	94 (8)	120 (10)	82 (8)	6 (7)	15 (6)	-13 (7)
C59	95 (8)	111 (9)	63 (6)	-7 (6)	24 (6)	-17 (7)
C60	88 (7)	125 (10)	69 (7)	32 (7)	21 (5)	13 (7)
C61	203 (15)	143 (13)	144 (12)	-44 (10)	108 (11)	-74 (11)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for C52 H55 B9 Cl P3 Pd.

	x	y	z	U(eq)
H1	7262	2791	9236	55
H2	6438	3709	8250	43
H3	5864	4002	9270	52
H4	6261	1822	9911	57
H5	7040	80	9313	55
H6	7188	1323	8264	44
H9	5520(3)	-310(4)	9390(2)	55
H10A	6210(3)	-710(2)	8350(2)	46
H10B	5554(11)	160(5)	8640(2)	46
H12A	4629	3019	9429	67
H12B	4788	1799	9774	67
H12C	4284	1735	9229	67
H14	3808	4366	8929	58
H15	3754	6272	9352	86
H16	4535	7822	9199	89
H17	5386	7503	8625	74
H18	5441	5643	8184	51
H20	4355	812	8325	47
H21	3312	-322	8146	75
H22	2263	676	7853	75
H23	2247	2786	7720	73
H24	3276	3950	7913	61
H26	4180	1415	6935	42
H27	3466	-276	6696	57
H28	3941	-2271	6805	63
H29	5094	-2550	7191	61
H30	5796	-851	7432	48
H32	6702	3488	7389	56
H33	7784	3557	7021	77
H34	8150	1856	6573	91
H35	7418	186	6396	86
H36	6325	88	6751	55
H38	3526	3326	6707	50
H39	2410	2915	6271	77
H40	2253	2838	5353	98
H41	3181	3327	4871	90
H42	4302	3667	5297	63
H44	4441	5799	5676	62
H45	4942	7677	5483	81
H46	6027	8265	5904	79
H47	6625	7010	6534	75
H48	6126	5120	6741	65
H50	4694	1293	5998	52
H51	5258	-94	5498	67
H52	6317	452	5174	89
H53	6794	2400	5349	83
H54	6241	3789	5880	61
H56	3467	2041	10259	96
H57	3609	4078	10542	115
H58	2931	5583	10065	118
H59	2196	5106	9321	106
H60	2059	3071	9017	111
H61A	3011	888	9180	235

H61B	2185	1001	9245	235
H61C	2724	520	9727	235

Table 6. Torsion angles [deg] for C52 H55 B9 Cl P3 Pd.

P2-Pd-P1-C19	-92.9(2)
P3-Pd-P1-C19	33.3(4)
Cl-Pd-P1-C19	86.0(2)
P2-Pd-P1-C13	148.7(2)
P3-Pd-P1-C13	-85.2(4)
Cl-Pd-P1-C13	-32.4(2)
P2-Pd-P1-C7	22.0(2)
P3-Pd-P1-C7	148.2(4)
Cl-Pd-P1-C7	-159.0(2)
P1-Pd-P2-C25	97.37(19)
P3-Pd-P2-C25	-74.77(19)
Cl-Pd-P2-C25	83.5(8)
P1-Pd-P2-C31	-139.6(2)
P3-Pd-P2-C31	48.3(2)
Cl-Pd-P2-C31	-153.5(7)
P1-Pd-P2-B11	-19.5(2)
P3-Pd-P2-B11	168.4(2)
Cl-Pd-P2-B11	-33.3(8)
P2-Pd-P3-C37	114.5(2)
P1-Pd-P3-C37	-10.8(5)
Cl-Pd-P3-C37	-63.9(2)
P2-Pd-P3-C49	-3.0(3)
P1-Pd-P3-C49	-128.3(4)
Cl-Pd-P3-C49	178.6(3)
P2-Pd-P3-C43	-125.1(2)
P1-Pd-P3-C43	109.6(4)
Cl-Pd-P3-C43	56.5(2)
B4-B1-B2-C7	-5.8(7)
B3-B1-B2-C7	-43.0(5)
B6-B1-B2-C7	95.7(5)
B5-B1-B2-C7	57.9(6)
B4-B1-B2-B11	-63.0(7)
B3-B1-B2-B11	-100.2(5)
B6-B1-B2-B11	38.5(4)
B5-B1-B2-B11	0.6(7)
B4-B1-B2-B6	-101.5(6)
B3-B1-B2-B6	-138.7(5)
B5-B1-B2-B6	-37.9(5)
B4-B1-B2-B3	37.2(5)
B6-B1-B2-B3	138.7(5)
B5-B1-B2-B3	100.8(6)
B4-B1-B3-C8	-39.6(5)
B6-B1-B3-C8	61.8(6)
B2-B1-B3-C8	98.9(5)
B5-B1-B3-C8	-2.8(6)
B4-B1-B3-C7	-95.5(6)
B6-B1-B3-C7	5.9(7)
B2-B1-B3-C7	42.9(5)
B5-B1-B3-C7	-58.8(6)
B6-B1-B3-B4	101.4(6)
B2-B1-B3-B4	138.4(6)
B5-B1-B3-B4	36.7(5)
B4-B1-B3-B2	-138.4(6)
B6-B1-B3-B2	-37.1(5)
B5-B1-B3-B2	-101.7(6)
C7-B2-B3-C8	31.1(4)
B11-B2-B3-C8	1.0(6)

B6-B2-B3-C8	-61.3 (6)
B1-B2-B3-C8	-98.0 (6)
B11-B2-B3-C7	-30.1 (4)
B6-B2-B3-C7	-92.4 (5)
B1-B2-B3-C7	-129.1 (6)
C7-B2-B3-B4	92.3 (5)
B11-B2-B3-B4	62.2 (6)
B6-B2-B3-B4	0.0 (6)
B1-B2-B3-B4	-36.7 (5)
C7-B2-B3-B1	129.1 (6)
B11-B2-B3-B1	99.0 (6)
B6-B2-B3-B1	36.7 (5)
B3-B1-B4-C8	40.7 (5)
B6-B1-B4-C8	-60.3 (7)
B2-B1-B4-C8	3.4 (8)
B5-B1-B4-C8	-98.4 (6)
B6-B1-B4-B3	-101.0 (6)
B2-B1-B4-B3	-37.3 (5)
B5-B1-B4-B3	-139.0 (5)
B3-B1-B4-B5	139.0 (5)
B6-B1-B4-B5	38.1 (5)
B2-B1-B4-B5	101.7 (6)
B3-B1-B4-B9	99.7 (6)
B6-B1-B4-B9	-1.2 (7)
B2-B1-B4-B9	62.4 (7)
B5-B1-B4-B9	-39.3 (5)
C7-B3-B4-C8	-35.8 (4)
B1-B3-B4-C8	-133.7 (5)
B2-B3-B4-C8	-96.5 (5)
C8-B3-B4-B1	133.7 (5)
C7-B3-B4-B1	97.9 (5)
B2-B3-B4-B1	37.2 (5)
C8-B3-B4-B5	95.7 (6)
C7-B3-B4-B5	59.9 (6)
B1-B3-B4-B5	-38.0 (5)
B2-B3-B4-B5	-0.8 (7)
C8-B3-B4-B9	30.5 (4)
C7-B3-B4-B9	-5.3 (6)
B1-B3-B4-B9	-103.2 (6)
B2-B3-B4-B9	-66.0 (6)
C8-B4-B5-B10	1.4 (7)
B1-B4-B5-B10	-99.3 (5)
B3-B4-B5-B10	-61.6 (7)
B9-B4-B5-B10	37.8 (5)
C8-B4-B5-B1	100.7 (6)
B3-B4-B5-B1	37.7 (5)
B9-B4-B5-B1	137.1 (5)
C8-B4-B5-B6	64.2 (6)
B1-B4-B5-B6	-36.5 (5)
B3-B4-B5-B6	1.3 (7)
B9-B4-B5-B6	100.7 (5)
C8-B4-B5-B9	-36.5 (5)
B1-B4-B5-B9	-137.1 (5)
B3-B4-B5-B9	-99.4 (6)
B3-B1-B5-B4	-36.7 (5)
B6-B1-B5-B4	-138.1 (5)
B2-B1-B5-B4	-100.6 (6)
B4-B1-B5-B10	103.8 (5)
B3-B1-B5-B10	67.1 (6)
B6-B1-B5-B10	-34.3 (4)
B2-B1-B5-B10	3.2 (7)
B4-B1-B5-B6	138.1 (5)

B3-B1-B5-B6	101.4(5)
B2-B1-B5-B6	37.5(5)
B4-B1-B5-B9	37.9(5)
B3-B1-B5-B9	1.2(7)
B6-B1-B5-B9	-100.2(5)
B2-B1-B5-B9	-62.7(6)
B4-B1-B6-B11	61.5(7)
B3-B1-B6-B11	-2.0(7)
B2-B1-B6-B11	-39.2(5)
B5-B1-B6-B11	99.1(5)
B4-B1-B6-B2	100.7(6)
B3-B1-B6-B2	37.2(5)
B5-B1-B6-B2	138.3(5)
B4-B1-B6-B10	-3.0(7)
B3-B1-B6-B10	-66.6(7)
B2-B1-B6-B10	-103.7(5)
B5-B1-B6-B10	34.6(5)
B4-B1-B6-B5	-37.7(5)
B3-B1-B6-B5	-101.2(6)
B2-B1-B6-B5	-138.3(5)
C7-B2-B6-B11	38.2(4)
B3-B2-B6-B11	99.1(5)
B1-B2-B6-B11	135.8(5)
C7-B2-B6-B1	-97.6(5)
B11-B2-B6-B1	-135.8(5)
B3-B2-B6-B1	-36.7(5)
C7-B2-B6-B10	3.6(6)
B11-B2-B6-B10	-34.7(5)
B3-B2-B6-B10	64.5(6)
B1-B2-B6-B10	101.1(6)
C7-B2-B6-B5	-60.1(5)
B11-B2-B6-B5	-98.4(5)
B3-B2-B6-B5	0.8(6)
B1-B2-B6-B5	37.4(5)
B4-B5-B6-B11	-64.4(6)
B10-B5-B6-B11	41.0(4)
B1-B5-B6-B11	-100.7(6)
B9-B5-B6-B11	-1.5(7)
B4-B5-B6-B1	36.3(5)
B10-B5-B6-B1	141.6(5)
B9-B5-B6-B1	99.2(6)
B4-B5-B6-B2	-1.2(6)
B10-B5-B6-B2	104.1(5)
B1-B5-B6-B2	-37.5(5)
B9-B5-B6-B2	61.7(7)
B4-B5-B6-B10	-105.4(5)
B1-B5-B6-B10	-141.6(5)
B9-B5-B6-B10	-42.5(5)
B11-B2-C7-C8	107.8(5)
B6-B2-C7-C8	67.7(6)
B3-B2-C7-C8	-36.5(5)
B1-B2-C7-C8	6.7(7)
B6-B2-C7-B11	-40.2(4)
B3-B2-C7-B11	-144.3(5)
B1-B2-C7-B11	-101.2(5)
B11-B2-C7-B3	144.3(5)
B6-B2-C7-B3	104.2(5)
B1-B2-C7-B3	43.2(5)
B11-B2-C7-P1	-103.3(4)
B6-B2-C7-P1	-143.5(4)
B3-B2-C7-P1	112.3(5)
B1-B2-C7-P1	155.5(4)

B4-B3-C7-C8	37.9(4)
B1-B3-C7-C8	98.4(6)
B2-B3-C7-C8	142.1(5)
C8-B3-C7-B11	-106.9(5)
B4-B3-C7-B11	-69.0(6)
B1-B3-C7-B11	-8.4(7)
B2-B3-C7-B11	35.2(5)
C8-B3-C7-B2	-142.1(5)
B4-B3-C7-B2	-104.2(6)
B1-B3-C7-B2	-43.6(5)
C8-B3-C7-P1	115.7(5)
B4-B3-C7-P1	153.6(4)
B1-B3-C7-P1	-145.9(5)
B2-B3-C7-P1	-102.2(5)
C19-P1-C7-C8	-52.2(5)
C13-P1-C7-C8	66.8(5)
Pd-P1-C7-C8	-164.1(4)
C19-P1-C7-B11	93.7(4)
C13-P1-C7-B11	-147.3(4)
Pd-P1-C7-B11	-18.2(4)
C19-P1-C7-B2	162.9(4)
C13-P1-C7-B2	-78.2(4)
Pd-P1-C7-B2	50.9(4)
C19-P1-C7-B3	-127.4(4)
C13-P1-C7-B3	-8.4(5)
Pd-P1-C7-B3	120.7(4)
B11-C7-C8-C12	-149.2(6)
B2-C7-C8-C12	140.5(6)
B3-C7-C8-C12	104.2(7)
P1-C7-C8-C12	-4.5(8)
B11-C7-C8-B9	-3.8(6)
B2-C7-C8-B9	-74.2(6)
B3-C7-C8-B9	-110.4(5)
P1-C7-C8-B9	140.9(4)
B11-C7-C8-B4	65.5(6)
B2-C7-C8-B4	-4.9(7)
B3-C7-C8-B4	-41.2(5)
P1-C7-C8-B4	-149.9(5)
B11-C7-C8-B3	106.6(5)
B2-C7-C8-B3	36.2(5)
P1-C7-C8-B3	-108.7(5)
B1-B4-C8-C12	-145.9(6)
B3-B4-C8-C12	-104.7(7)
B5-B4-C8-C12	149.9(6)
B9-B4-C8-C12	110.9(7)
B1-B4-C8-C7	0.8(7)
B3-B4-C8-C7	42.0(5)
B5-B4-C8-C7	-63.4(7)
B9-B4-C8-C7	-102.3(5)
B1-B4-C8-B9	103.1(6)
B3-B4-C8-B9	144.3(5)
B5-B4-C8-B9	38.9(5)
B1-B4-C8-B3	-41.2(5)
B5-B4-C8-B3	-105.4(6)
B9-B4-C8-B3	-144.3(5)
C7-B3-C8-C12	-114.7(5)
B4-B3-C8-C12	110.2(6)
B1-B3-C8-C12	150.0(5)
B2-B3-C8-C12	-147.6(5)
B4-B3-C8-C7	-135.1(5)
B1-B3-C8-C7	-95.3(5)
B2-B3-C8-C7	-33.0(4)

C7-B3-C8-B9	99.1(5)
B4-B3-C8-B9	-36.0(5)
B1-B3-C8-B9	3.8(7)
B2-B3-C8-B9	66.1(6)
C7-B3-C8-B4	135.1(5)
B1-B3-C8-B4	39.8(5)
B2-B3-C8-B4	102.1(6)
C12-C8-B9-B4	-110.0(6)
C7-C8-B9-B4	103.5(5)
B3-C8-B9-B4	34.8(5)
C12-C8-B9-B5	-147.8(5)
C7-C8-B9-B5	65.7(6)
B4-C8-B9-B5	-37.8(5)
B3-C8-B9-B5	-3.0(7)
C12-C8-B9-B10	151.6(5)
C7-C8-B9-B10	5.1(6)
B4-C8-B9-B10	-98.4(5)
B3-C8-B9-B10	-63.6(6)
B1-B4-B9-C8	-96.7(6)
B3-B4-B9-C8	-32.0(5)
B5-B4-B9-C8	-136.1(5)
C8-B4-B9-B5	136.1(5)
B1-B4-B9-B5	39.5(5)
B3-B4-B9-B5	104.2(6)
C8-B4-B9-B10	101.4(5)
B1-B4-B9-B10	4.8(7)
B3-B4-B9-B10	69.5(6)
B5-B4-B9-B10	-34.7(4)
B4-B5-B9-C8	38.1(5)
B10-B5-B9-C8	-101.7(5)
B1-B5-B9-C8	0.9(7)
B6-B5-B9-C8	-60.7(7)
B10-B5-B9-B4	-139.8(5)
B1-B5-B9-B4	-37.1(5)
B6-B5-B9-B4	-98.8(6)
B4-B5-B9-B10	139.8(5)
B1-B5-B9-B10	102.7(5)
B6-B5-B9-B10	41.0(5)
B11-B6-B10-B5	-133.9(5)
B1-B6-B10-B5	-34.9(5)
B2-B6-B10-B5	-99.6(5)
B1-B6-B10-B11	99.1(5)
B2-B6-B10-B11	34.3(4)
B5-B6-B10-B11	133.9(5)
B11-B6-B10-B9	-93.2(4)
B1-B6-B10-B9	5.8(6)
B2-B6-B10-B9	-58.9(5)
B5-B6-B10-B9	40.7(5)
B4-B5-B10-B6	96.4(6)
B1-B5-B10-B6	34.1(5)
B9-B5-B10-B6	133.3(5)
B4-B5-B10-B11	56.8(6)
B1-B5-B10-B11	-5.6(6)
B6-B5-B10-B11	-39.6(4)
B9-B5-B10-B11	93.6(5)
B4-B5-B10-B9	-36.8(5)
B1-B5-B10-B9	-99.2(6)
B6-B5-B10-B9	-133.3(5)
C8-B9-B10-B6	55.7(5)
B4-B9-B10-B6	-6.4(6)
B5-B9-B10-B6	-41.4(5)
C8-B9-B10-B5	97.1(6)

B4-B9-B10-B5	35.0(5)
C8-B9-B10-B11	-4.5(5)
B4-B9-B10-B11	-66.6(5)
B5-B9-B10-B11	-101.5(4)
C8-C7-B11-B6	-62.7(6)
B2-C7-B11-B6	42.1(5)
B3-C7-B11-B6	7.4(7)
P1-C7-B11-B6	148.2(4)
C8-C7-B11-B2	-104.8(5)
B3-C7-B11-B2	-34.7(5)
P1-C7-B11-B2	106.1(4)
C8-C7-B11-B10	0.6(6)
B2-C7-B11-B10	105.4(4)
B3-C7-B11-B10	70.7(6)
P1-C7-B11-B10	-148.5(3)
C8-C7-B11-P2	151.3(4)
B2-C7-B11-P2	-103.9(5)
B3-C7-B11-P2	-138.6(5)
P1-C7-B11-P2	2.2(5)
B1-B6-B11-C7	-3.0(7)
B2-B6-B11-C7	-42.3(4)
B10-B6-B11-C7	100.3(5)
B5-B6-B11-C7	60.0(6)
B1-B6-B11-B2	39.3(5)
B10-B6-B11-B2	142.6(5)
B5-B6-B11-B2	102.3(6)
B1-B6-B11-B10	-103.3(6)
B2-B6-B11-B10	-142.6(5)
B5-B6-B11-B10	-40.3(5)
B1-B6-B11-P2	138.2(5)
B2-B6-B11-P2	98.9(6)
B10-B6-B11-P2	-118.5(6)
B5-B6-B11-P2	-158.7(5)
B6-B2-B11-C7	132.5(5)
B3-B2-B11-C7	31.5(4)
B1-B2-B11-C7	93.8(5)
C7-B2-B11-B6	-132.5(5)
B3-B2-B11-B6	-101.0(5)
B1-B2-B11-B6	-38.7(5)
C7-B2-B11-B10	-98.0(5)
B6-B2-B11-B10	34.5(4)
B3-B2-B11-B10	-66.5(6)
B1-B2-B11-B10	-4.2(6)
C7-B2-B11-P2	107.5(4)
B6-B2-B11-P2	-120.0(5)
B3-B2-B11-P2	139.0(4)
B1-B2-B11-P2	-158.7(4)
B6-B10-B11-C7	-99.6(5)
B5-B10-B11-C7	-58.8(5)
B9-B10-B11-C7	2.3(5)
B5-B10-B11-B6	40.7(4)
B9-B10-B11-B6	101.9(5)
B6-B10-B11-B2	-34.6(4)
B5-B10-B11-B2	6.1(6)
B9-B10-B11-B2	67.3(5)
B6-B10-B11-P2	114.9(5)
B5-B10-B11-P2	155.6(4)
B9-B10-B11-P2	-143.2(4)
C25-P2-B11-C7	-104.0(4)
C31-P2-B11-C7	139.4(4)
Pd-P2-B11-C7	14.6(5)
C25-P2-B11-B6	117.9(5)

C31-P2-B11-B6	1.3 (6)
Pd-P2-B11-B6	-123.5 (5)
C25-P2-B11-B2	-172.1 (4)
C31-P2-B11-B2	71.4 (4)
Pd-P2-B11-B2	-53.5 (4)
C25-P2-B11-B10	39.0 (5)
C31-P2-B11-B10	-77.6 (5)
Pd-P2-B11-B10	157.6 (4)
C19-P1-C13-C14	23.8 (6)
C7-P1-C13-C14	-93.9 (6)
Pd-P1-C13-C14	138.3 (5)
C19-P1-C13-C18	-158.4 (5)
C7-P1-C13-C18	83.9 (5)
Pd-P1-C13-C18	-44.0 (6)
C18-C13-C14-C15	0.2 (11)
P1-C13-C14-C15	177.9 (6)
C13-C14-C15-C16	-0.4 (13)
C14-C15-C16-C17	-0.1 (15)
C15-C16-C17-C18	0.8 (14)
C16-C17-C18-C13	-1.1 (12)
C14-C13-C18-C17	0.6 (10)
P1-C13-C18-C17	-177.3 (5)
C13-P1-C19-C24	48.9 (6)
C7-P1-C19-C24	168.3 (5)
Pd-P1-C19-C24	-73.2 (5)
C13-P1-C19-C20	-141.8 (5)
C7-P1-C19-C20	-22.4 (6)
Pd-P1-C19-C20	96.1 (5)
C24-C19-C20-C21	-0.8 (10)
P1-C19-C20-C21	-170.2 (5)
C19-C20-C21-C22	0.5 (10)
C20-C21-C22-C23	0.6 (12)
C21-C22-C23-C24	-1.3 (12)
C22-C23-C24-C19	1.0 (11)
C20-C19-C24-C23	0.1 (10)
P1-C19-C24-C23	169.6 (5)
C31-P2-C25-C26	-126.1 (5)
B11-P2-C25-C26	118.3 (5)
Pd-P2-C25-C26	0.6 (5)
C31-P2-C25-C30	59.3 (5)
B11-P2-C25-C30	-56.4 (5)
Pd-P2-C25-C30	-174.1 (4)
C30-C25-C26-C27	-1.2 (9)
P2-C25-C26-C27	-176.0 (5)
C25-C26-C27-C28	-0.4 (10)
C26-C27-C28-C29	1.8 (11)
C27-C28-C29-C30	-1.6 (11)
C28-C29-C30-C25	0.0 (11)
C26-C25-C30-C29	1.4 (9)
P2-C25-C30-C29	176.2 (5)
C25-P2-C31-C36	-10.1 (6)
B11-P2-C31-C36	105.5 (5)
Pd-P2-C31-C36	-133.7 (5)
C25-P2-C31-C32	173.5 (5)
B11-P2-C31-C32	-70.9 (5)
Pd-P2-C31-C32	49.9 (5)
C36-C31-C32-C33	0.6 (10)
P2-C31-C32-C33	177.1 (5)
C31-C32-C33-C34	-2.2 (11)
C32-C33-C34-C35	3.6 (14)
C33-C34-C35-C36	-3.3 (14)
C32-C31-C36-C35	-0.2 (10)

P2-C31-C36-C35	-176.5 (5)
C34-C35-C36-C31	1.6 (12)
C49-P3-C37-C38	130.4 (6)
C43-P3-C37-C38	-120.8 (6)
Pd-P3-C37-C38	0.0 (6)
C49-P3-C37-C42	-44.2 (6)
C43-P3-C37-C42	64.6 (6)
Pd-P3-C37-C42	-174.6 (5)
C42-C37-C38-C39	0.2 (10)
P3-C37-C38-C39	-174.5 (6)
C37-C38-C39-C40	0.5 (12)
C38-C39-C40-C41	-2.4 (14)
C39-C40-C41-C42	3.6 (15)
C40-C41-C42-C37	-2.9 (14)
C38-C37-C42-C41	1.0 (11)
P3-C37-C42-C41	175.8 (6)
C37-P3-C43-C48	173.0 (5)
C49-P3-C43-C48	-81.2 (6)
Pd-P3-C43-C48	51.3 (6)
C37-P3-C43-C44	-7.7 (6)
C49-P3-C43-C44	98.2 (6)
Pd-P3-C43-C44	-129.4 (5)
C48-C43-C44-C45	1.9 (11)
P3-C43-C44-C45	-177.5 (6)
C43-C44-C45-C46	-0.4 (12)
C44-C45-C46-C47	-0.7 (13)
C45-C46-C47-C48	0.4 (13)
C44-C43-C48-C47	-2.2 (11)
P3-C43-C48-C47	177.2 (6)
C46-C47-C48-C43	1.1 (12)
C37-P3-C49-C50	-45.8 (5)
C43-P3-C49-C50	-158.3 (5)
Pd-P3-C49-C50	77.0 (5)
C37-P3-C49-C54	134.0 (6)
C43-P3-C49-C54	21.5 (6)
Pd-P3-C49-C54	-103.2 (5)
C54-C49-C50-C51	-0.5 (9)
P3-C49-C50-C51	179.3 (5)
C49-C50-C51-C52	-0.2 (10)
C50-C51-C52-C53	-0.2 (12)
C51-C52-C53-C54	1.3 (13)
C50-C49-C54-C53	1.6 (10)
P3-C49-C54-C53	-178.2 (6)
C52-C53-C54-C49	-2.0 (12)
C60-C55-C56-C57	-2.0 (14)
C61-C55-C56-C57	-178.5 (9)
C55-C56-C57-C58	2.0 (14)
C56-C57-C58-C59	-1.4 (15)
C57-C58-C59-C60	0.8 (16)
C58-C59-C60-C55	-0.7 (15)
C56-C55-C60-C59	1.2 (13)
C61-C55-C60-C59	178.1 (9)
P1-C7-B11-P2	2.2 (5)
P1-C7-C8-C12	-4.5 (8)

Table 7. Least-squares planes (x,y,z in crystal coordinates) and deviations [A] from them for C52 H55 B9 Cl P3 Pd. (* indicates atom used to define plane)

$$15.2555 (0.0087) x + 6.1230 (0.0049) y + 2.7504 (0.0113) z = 11.6068 (0.0091)$$

* 0.0669 (0.0007) Cl
 * -0.0674 (0.0008) P1
 * 0.0629 (0.0007) P2
 * -0.0624 (0.0007) P3
 0.0920 (0.0008) Pd

Rms deviation of fitted atoms = 0.0649

$$12.7346 (0.0286) x + 8.0583 (0.0144) y - 2.5513 (0.0473) z = 6.6654 (0.0448)$$

Angle to previous plane (with approximate esd) = 18.14 (0.17)

* -0.0071 (0.0018) P1
 * 0.0136 (0.0033) C7
 * -0.0135 (0.0033) B11
 * 0.0070 (0.0017) P2
 0.6062 (0.0043) Pd

Rms deviation of fitted atoms = 0.0108