Supplementary Information for:

A new supramolecular semi-conductor palladium (II) complex $[(CH_3)_3N(CH_2)_3Br]_2Pd_2Cl_6$: Structural study, optical and electrical properties

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Table S1. Selected bond distances (Å) and angles (°) for$[(CH_3)_3N(CH_2)_3Br]_2Pd_2Cl_6$.

Distances (Å)		**Angles (°)**	
Pd1−Cl1	2.267(4)	Cl2−Pd1−Cl1	92.14(16)
Pd1− Cl2	2.264(4)	Cl2−Pd1−Cl3$^{(i)}$	176.91(19)
Pd1−Cl3	2.321(5)	Cl1−Pd1−Cl3$^{(i)}$	90.78(17)
Pd1−Cl3$^{(i)}$	2.306(5)	Cl2−Pd1−Cl3	90.84(17)
Pd2−Cl4	2.273(4)	Cl1−Pd1−Cl3	177.02(18)
Pd2− Cl5	2.264(4)	Cl3$^{(i)}$−Pd1−Cl3	86.23(18)
Pd2− Cl6	2.329(4)	Pd1$^{(i)}$−Cl3−Pd1	93.77(18)
Pd2−Cl6$^{(ii)}$	2.335(4)	Cl5−Pd2−Cl4	91.81(16)
N1−C6	1.49(2)	Cl5−Pd2−Cl6	91.74(15)
N1−C3	1.50(2)	Cl4−Pd2−Cl6	176.39(16)
N1−C5	1.503(18)	Cl5−Pd2−Cl6$^{(ii)}$	176.04(17)
N1−C4	1.51(2)	Cl4−Pd2−Cl6$^{(ii)}$	90.97(15)
C1−C2	1.53(2)	Cl6−Pd2−Cl6$^{(ii)}$	85.45(14)
C2−C3	1.49(2)	Pd2−Cl6−Pd2$^{(ii)}$	94.55(14)
Br2A−C7A	1.97(5)	C6−N1−C3	109.5(13)
Br1−C1	1.950(17)	C6−N1−C5	108.1(13)
C7A−C8A	1.49(5)	C3−N1−C5	112.8(13)
C8A−C9A	1.14(4)	C6−N1−C4	107.0(13)
C9A−N2A	1.73(6)	C3−N1−C4	110.1(13)
N2A−C12A	1.37(6)	C5−N1−C4	109.1(12)
N2A−C10A	1.46(8)	C2−C1−Br1	112.1(13)
N2A−C11A	1.55(6)	C3−C2−C1	112.6(16)
Br2B−C7B	1.90(4)	C2−C3−N1	116.1(13)
C7B−C8B	1.55(5)	C8B−C7B−Br2B	110(2)
C8B−C9B	1.37(4)	N2B−C9B−C8B	139(4)
C9B−N2B	1.37(6)	C9B−N2B−C10B	116(5)
N2B - C11B	1.42(7)	C9B −N2B−C12B	107(4)
N2B−C10B	1.52(8)	C10B−N2B−C12B	101(4)
N2B−C12B	1.68(6)	C8A−C7A−Br2A	110(3)
		C9A−C8A−C7A	118(4)
		C8A−C9A−N2A	126(3)
		C12A−N2A−C10A	116(5)
		C12A−N2A−C11A	111(4)
		C10A−N2A−C11A	114(4)
		C12A−N2A−C9A	106(3)
		C10A−N2A−C9A	112(4)
		C11A−N2A−C9A	96(3)
		C9B−C8B−C7B	124(3)
		C9B−N2B−C11B	125(5)
		C11B−N2B−C10B	105(5)

C11B−N2B−C12B	101(4)
Br1−C1−C2−C3	61(2)
C4−N1−C3−C2	64.0(19)
C8A−C9A−N2A−C12A	136(4)
C7B−C8B−C9B−N2B	136(5)
C8B−C9B−N2B−C12B	132(5)
C1−C2−C3−N1	170.9(15)
Br2A−C7A−C8A−C9A	104(4)
Br2B−C7B−C8B−C9B	167(3)
C8B−C9B−N2B−C11B	112(7)

Symmetry codes: **(i)** −x, −y+1, −z+3; **(ii)** −x+1, −y+1, −z+2.

Table S2. Hydrogen-bonding geometry (Å, °) for $[(CH_3)_3N(CH_2)_3Br]_2Pd_2Cl_6$.

D*—H···*A	***D*—H**	**H···*A***	***D*···*A***	***D*—H···*A***
C1—H1*A*···Cl5	0.99	2.84	3.74 (2)	151
C1—H1*B*···Cl5$^{(i)}$	0.99	2.82	3.554 (19)	131
C3—H3*A*···Cl4	0.99	2.95	3.860 (17)	153
C3—H3*B*···Cl1$^{(ii)}$	0.99	2.90	3.814 (17)	153
C4—H4*A*···Cl4 $^{(iii)}$	0.98	2.85	3.737 (19)	152
C4—H4*B*···Cl1 $^{(ii)}$	0.98	2.81	3.759 (18)	163
C4—H4*C*···Cl6$^{(iv)}$	0.98	2.91	3.863 (18)	164
C5—H5*B*···Cl5 $^{(iii)}$	0.98	2.94	3.830 (16)	152
C5—H5*C*···Cl6$^{(iv)}$	0.98	2.98	3.917 (17)	160
C6—H6*B*···Cl2$^{(ii)}$	0.98	2.79	3.669 (19)	150
C7*A*—H7*A*···Cl3$^{(v)}$	0.99	2.74	3.69 (5)	160
C7*A*—H7*B*···Cl1$^{(vi)}$	0.99	2.98	3.95 (5)	168
C7*A*—H7*B*···Cl3$^{(vii)}$	0.99	2.72	3.31 (5)	119
C8*A*—H8*A*···Cl3$^{(vii)}$	0.99	2.26	3.02 (3)	133
C9*A*—H9*B*···Cl3$^{(v)}$	0.99	2.98	3.63 (3)	125
C10*A*—H10*A*···Cl1$^{(ii)}$	0.98	2.79	3.44 (8)	124
C10*A*—H10*A*···Cl2$^{(ii)}$	0.98	2.72	3.67 (7)	163
C10*A*—H10*B*···Cl2$^{(vii)}$	0.98	2.84	3.66 (7)	141
C10*A*—H10*C*···Cl4	0.98	2.96	3.83 (7)	148
C11*A*—H11*A*···Cl4	0.98	2.60	3.52 (5)	157
C11*A*—H11*C*···Br1$^{(viii)}$	0.98	3.09	3.66 (5)	119
C11*A*—H11*C*···Cl1$^{(ix)}$	0.98	2.74	3.65 (5)	156
C12*A*—H12*B*···Cl1$^{(ix)}$	0.98	2.76	3.65 (4)	151
C12*A*—H12*C*···Cl2$^{(ii)}$	0.98	2.78	3.69 (4)	153
C7*B*—H7*C*···Cl3$^{(v)}$	0.99	2.66	3.53 (4)	147
C10*B*—H10*D*···Cl2$^{(vii)}$	0.98	2.69	3.48 (6)	138
C10*B*—H10*E*···Cl4	0.98	2.82	3.73 (6)	155
C10*B*—H10*F*···Cl1$^{(ii)}$	0.98	2.84	3.55 (7)	130

C10*B*—H10*F*···Cl2$^{(ii)}$	0.98	2.96	3.88 (7)	157
C11*B*—H11*D*···Cl1$^{(ix)}$	0.98	2.88	3.71 (6)	142
C11*B*—H11*E*···Cl4	0.98	2.88	3.76 (5)	150
C11*B*—H11*F*···Cl2$^{(vii)}$	0.98	2.96	3.86 (6)	152
C12*B*—H12*D*···Br1$^{(iii)}$	0.98	3.03	3.65 (3)	123
C12*B*—H12*E*···Cl4	0.98	2.77	3.70 (4)	158
C12*B*—H12*F*···Cl1$^{(ix)}$	0.98	2.89	3.77 (4)	150

Symmetry codes: **(i)** −x+1, y+1/2, −z+3/2; **(ii)** −x, y+1/2, −z+5/2; **(iii)** x, −y+3/2, z+1/2; **(iv)** −x+1, −y+2, −z+2; **(v)** x, −y+1/2, z−1/2; **(vi)** x, y, z−1; **(vii)** −x, −y+1, −z+2; **(viii)** x, y−1, z; **(ix)** −x, y−1/2, −z+5/2.

Alert level C

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Author Response: A combination of the weak quality of the data and disordered organic molecule contribute to this alert.