Supporting Information

Bromination of organic spacer impacts on the structural arrangement, phase transitions, optical and electrical properties of hybrid halide compound:$[(CH_3)_3N(CH_2)_3Br]_2PdBr_4$

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Table S1. Selected bond distances (Å) and angles (°) for $[(CH_3)_3N(CH_2)_3Br]_2PdBr_4$.

Table S2. Hydrogen-bonding geometry (Å, °) for $[(CH_3)_3N(CH_2)_3Br]_2PdBr_4$.

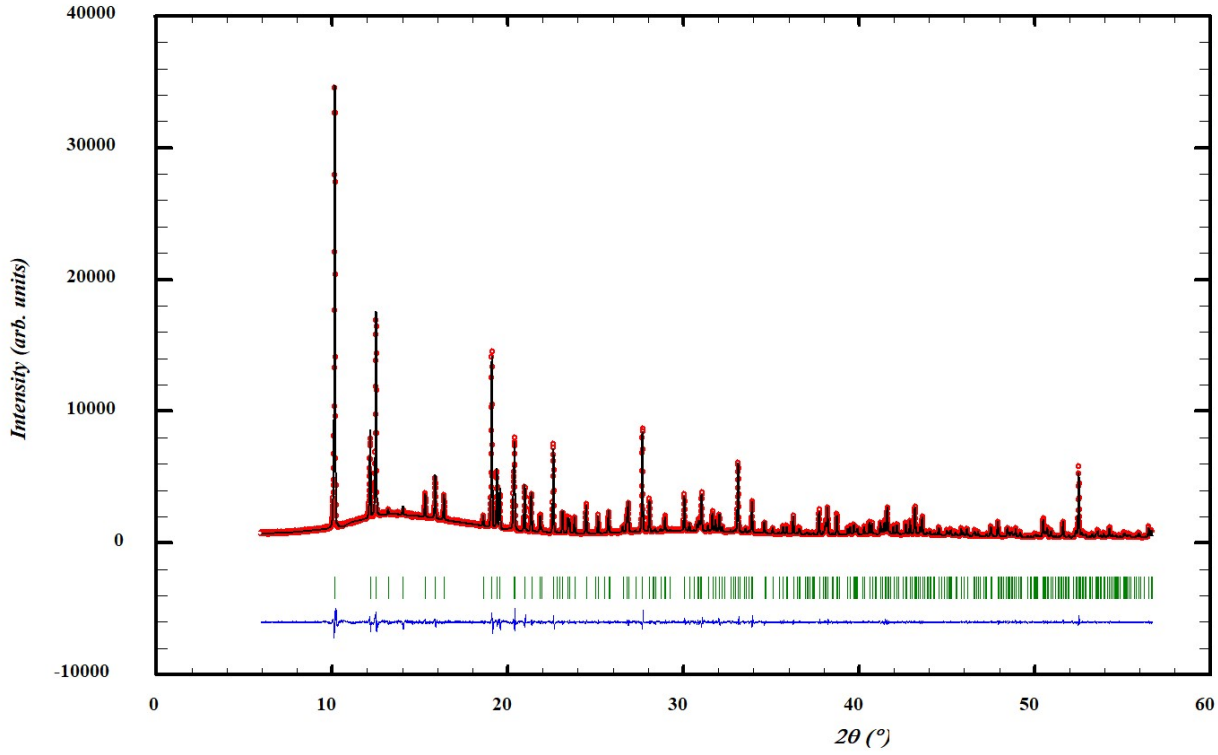

Figure S1. Plot of the Le Bail fit of powder X-ray diffraction pattern recorded at 293 K for $[(CH_3)_3N(CH_2)_3Br]_2PdBr_4$: orthorhombic space group *Pbca*, lattice parameters of a = 9.1496(1)Å, b = 14.5376(2) Å, c = 17.4081(2) Å; Rp = 3.99, Rwp = 5.33, Rexp = 2.89.

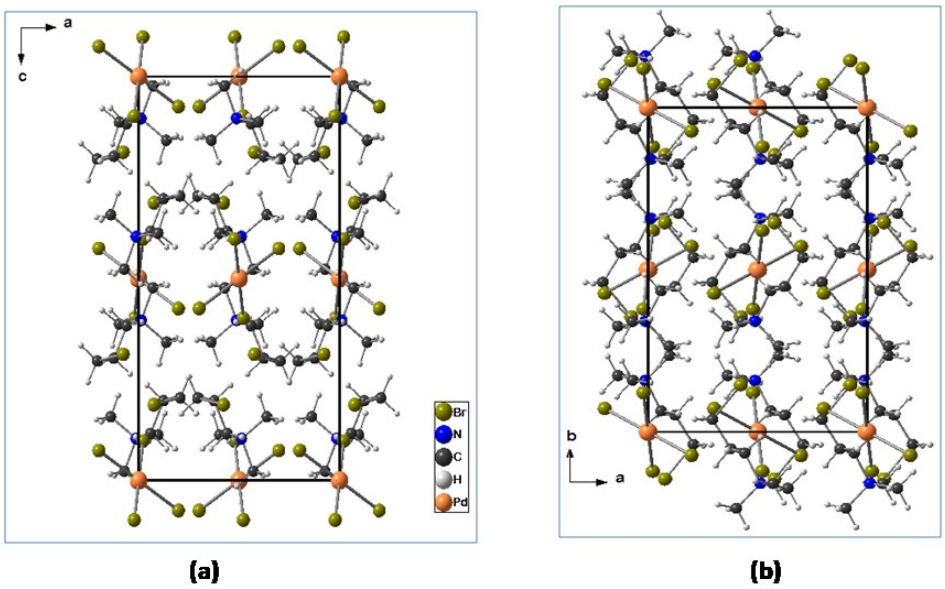

Figure S2. Packing structure of the $[(CH_3)_3N(CH_2)_3Br]_2PdBr_4$ compound along the *b* and *c*-axes.

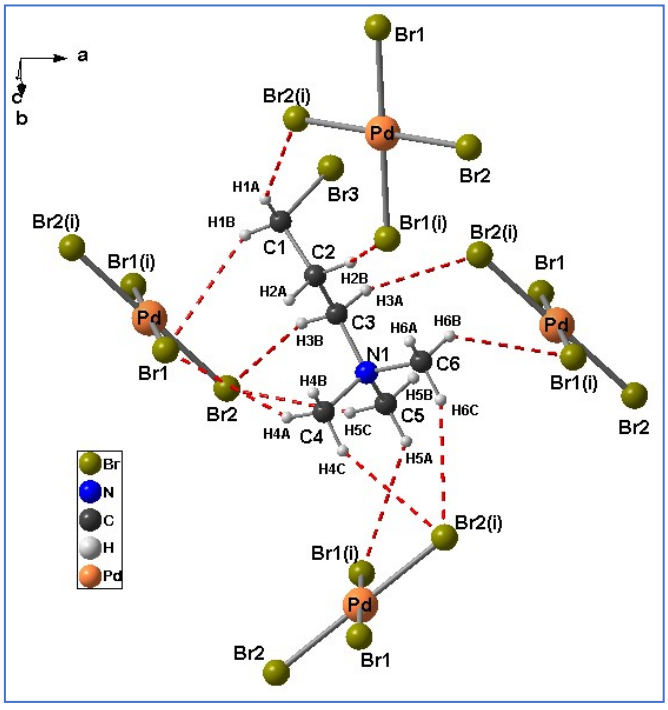

Figure S3. Hydrogen-bonding interactions for $[(CH_3)_3N(CH_2)_3Br]_2PdBr_4$.

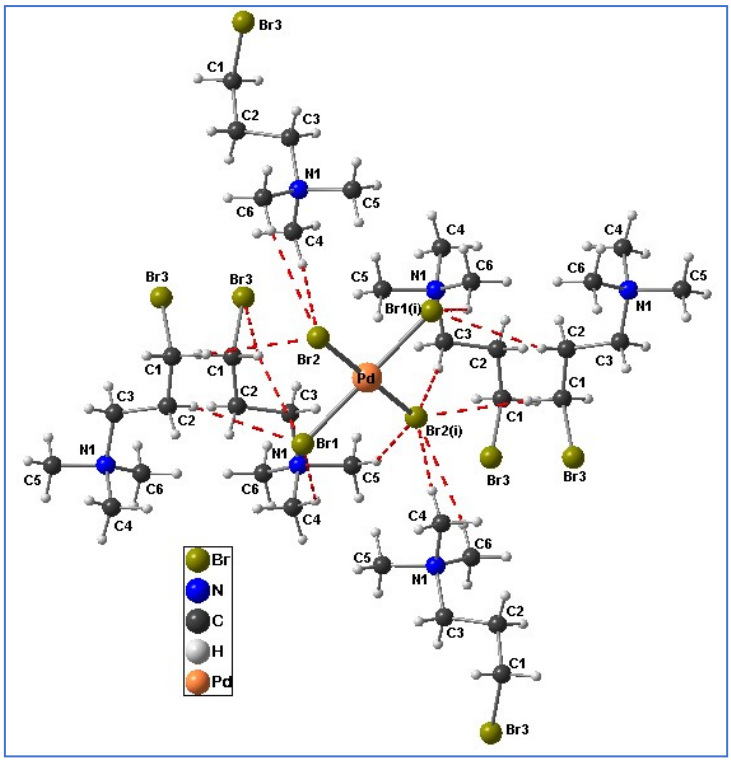

Figure S4. Molecular structure of $[(CH_3)_3N(CH_2)_3Br]_2PdBr_4$ highlighting the hydrogen-bonding interactions between the $[(CH_3)_3N(CH_2)_3Br]^+$ cations and the bromine atoms.

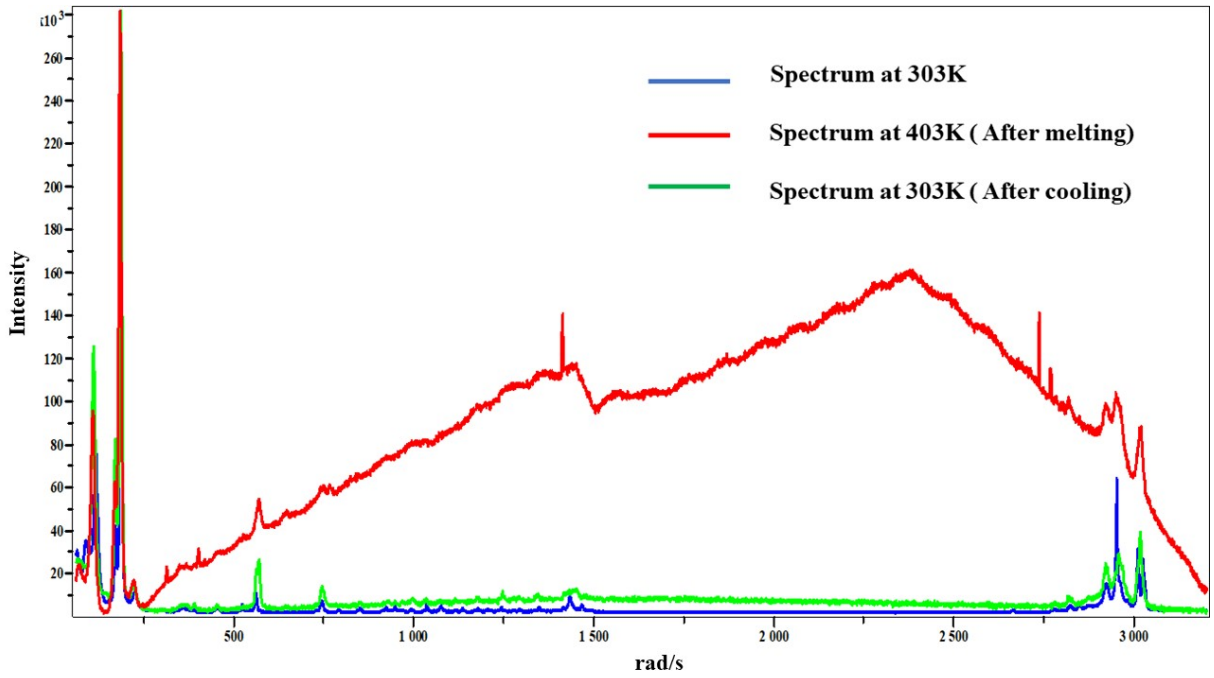

Figure S5. Raman spectra of $[(CH_3)_3N(CH_2)_3Br]_2PdBr_4$ at room temperature before heating, after cooling and at 403K.

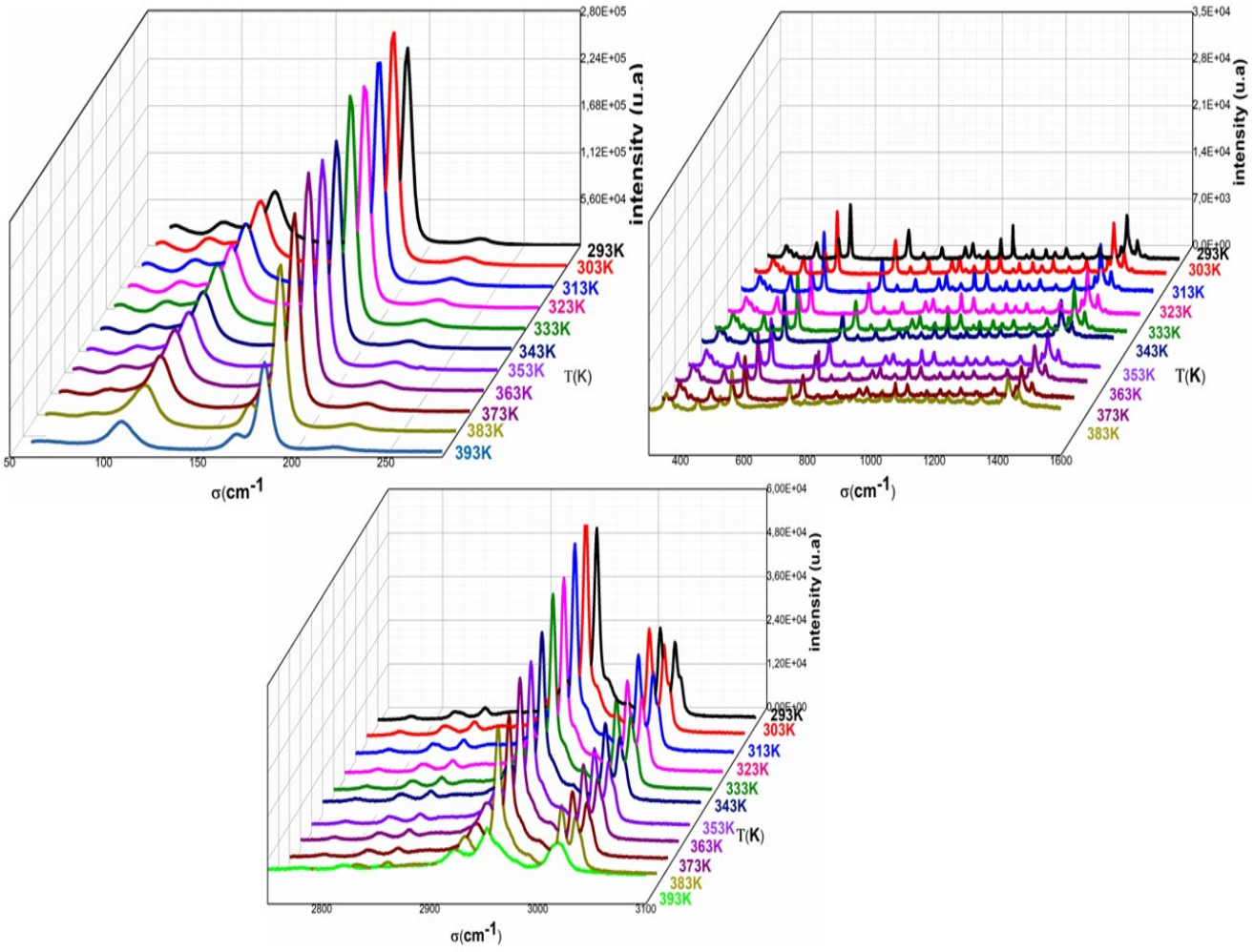

Figure S6. Evolution of Raman spectra *vs* temperature for $[(CH_3)_3N(CH_2)_3Br]_2PdBr_4$.

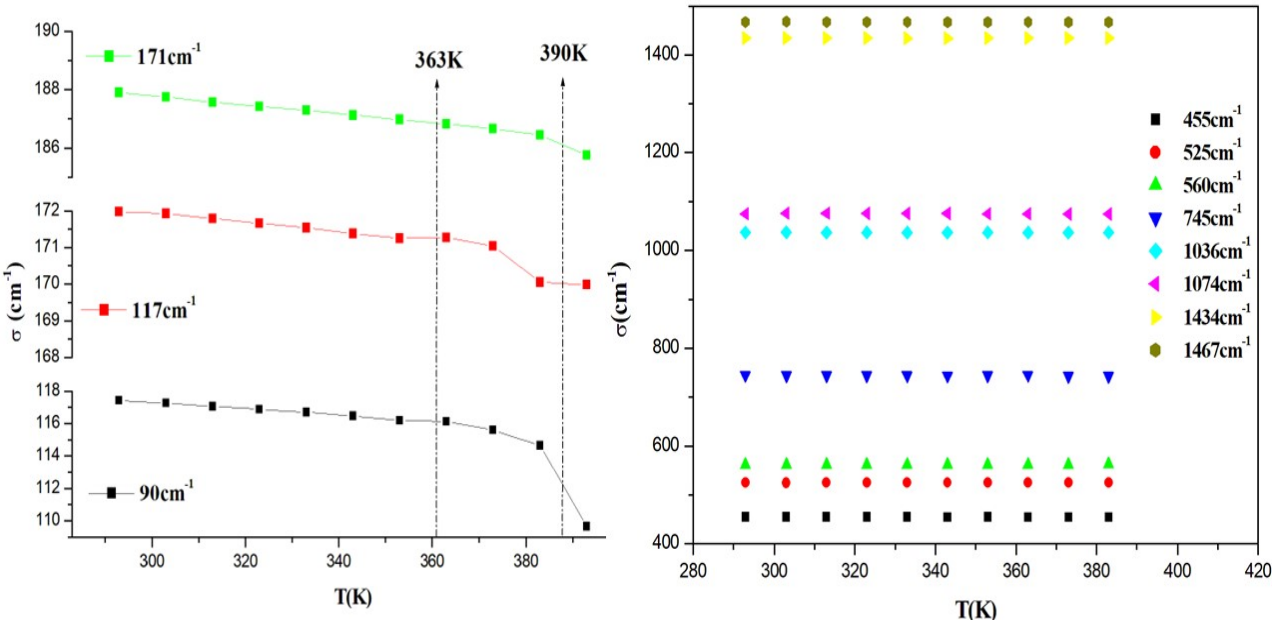

Figure S7. Variation of the position of the vibration modes as function temperature of $[(CH_3)_3N(CH_2)_3Br]_2PdBr_4$.

Table S1. Selected bond distances (Å) and angles (°) for $[(CH_3)_3N(CH_2)_3Br]_2PdBr_4$.

Pd1—Br1	2.4358 (4)	C6—N1—C5	108.1 (3)
Pd1—Br1$^{(i)}$	2.4358 (4)	C6—N1—C4	109.5 (3)
Pd1—Br2	2.4415 (4)	C5—N1—C4	109.0 (3)
Pd1—Br2$^{(i)}$	2.4415 (4)	C6—N1—C3	111.4 (3)
Br1$^{(i)}$—Pd1—Br1	180.0	C5—N1—C3	107.4 (3)
Br1$^{(i)}$—Pd1—Br2$^{(i)}$	89.806 (15)	C4—N1—C3	111.2 (3)
Br1—Pd1—Br2$^{(i)}$	90.194 (15)	C2—C1—Br3	111.7 (3)
Br1$^{(i)}$—Pd1—Br2	90.195 (15)	C1—C2—C3	111.7 (3)
Br1—Pd1—Br2	89.805 (15)	C2—C3—N1	114.3 (3)
Br2$^{(i)}$—Pd1—Br2	180.0	Br3—C1—C2—C3	62.4 (4)
Br3—C1	1.963 (4)	C1—C2—C3—N1	174.1 (3)
N1—C6	1.489 (5)	C6—N1—C3—C2	60.9 (4)
N1—C5	1.491 (5)	C5—N1—C3—C2	179.1 (3)
N1—C4	1.494 (5)	C4—N1—C3—C2	61.6 (4)
N1—C3	1.520 (4)		
C1—C2	1.508 (5)		
C2—C3	1.517 (5)		

Symmetry codes: (i) −x+2, −y, −z.

Table S2. Hydrogen-bonding geometry (Å, °) for $[(CH_3)_3N(CH_2)_3Br]_2PdBr_4$.

D*—H···*A	***D*—H**	**H···*A***	***D*···*A***	***D*—H···*A***
C1—H1*A*···Br2$^{(ii)}$	0.99	2.99	3.849 (4)	146
C1—H1*B*···Br1	0.99	3.12	3.841 (4)	131
C2—H2*B*···Br1$^{(iii)}$	0.99	3.08	3.897 (4)	140
C3—H3*A*···Br2$^{(iv)}$	0.99	2.95	3.899 (4)	160
C3—H3*B*···Br2	0.99	3.02	3.962 (4)	159
C4—H4*A*···Br1	0.98	3.10	3.844 (4)	134
C4—H4*C*···Br2$^{(v)}$	0.98	3.00	3.914 (4)	157
C5—H5*A*···Br1$^{(v)}$	0.98	3.13	3.819 (4)	129
C5—H5*C*···Br2	0.98	3.06	3.976 (4)	156
C6—H6*B*···Br1$^{(vi)}$	0.98	2.97	3.705 (4)	133
C6—H6*C*···Br2$^{(v)}$	0.98	3.07	3.979 (4)	154

Symmetry codes:(ii) −x+3/2, −y, z+1/2; (iii) x−1/2, y, −z+1/2; (iv) −x+1, −y, −z; (v) x−1/2, −y+1/2, −z; (vi) x−1, y, z