Supplementary Material (ESI) for Chemical Communications

$[H_3N(CH_2)_7NH_3]_8(CH_3NH_3)_2$ Sn(IV)Sn(II)$_{12}I_{46}$ - A Mixed-valent Hybrid Compound with a Uniquely Templated Defect-Perovskite Structure

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(Supplementary Material)

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Table 1S. Crystal data and structure refinement for (1).

Empirical formula	$C_{58}H_{172}I_{46}N_{18}Sn_{13}$
Formula weight	8502.51
Temperature	223(2) K
Wavelength	0.71073 A
Crystal system	Tetragonal
Space group	$P4_2/mnm$
Unit cell dimensions	a = 26.9174(13) Å
	b= 26.9174(13) Å
	c = 12.7329(9) Å
Volume	9225.6(9) $Å^3$
Z	2
Density (calculated)	3.061 g/m^3
Absorption coefficient	9.455 mm^{-1}
F(000)	7468
Crystal size	0.36 x 0.32 x 0.30 mm
Theta range for data collection	1.07 to 25.04º
Index ranges	$-25 \le h \le 32$, $-32 \le k \le 32$, $-15 \le l \le 13$
Reflections collected	47031
Independent reflections	4411 [R(int) = 0.0393]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4399 / 15 / 139
Goodness-of-fit on F^2	1.223
Final R indices [I>2sigma(I)]	R1 = 0.0527, wR2 = 0.1102
R indices (all data)	R1 = 0.0689, wR2 = 0.1320
Extinction coefficient	0.000376(9)
Largest diff. peak and hole	1.192 and -1.345 e. $Å^{-3}$

Table 2S. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (1).

	x	y	z	U(eq)
Sn(1)	3476(1)	3476(1)	5000	51(1)
Sn(2)	3281(1)	3281(1)	0	39(1)
Sn(3)	0	0	-5000	45(1)
Sn(4)	79(1)	3300(1)	-5000	38(1)
Sn(5)	41(1)	3329(1)	0	39(1)
I(1)	3439(1)	3439(1)	2473(1)	85(1)
I(2)	2539(1)	2539(1)	0	77(1)
I(3)	4269(1)	2599(1)	5000	76(1)
I(4)	4102(1)	2443(1)	0	76(1)
I(5)	747(1)	747(1)	-5000	74(1)
I(6)	0	0	-2783(2)	99(1)
I(7)	9(1)	3352(1)	-2504(1)	68(1)
I(8)	952(1)	2740(1)	0	72(1)
I(9)	685(1)	4286(1)	0	67(1)
I(10)	927(1)	4019(1)	-5000	72(1)
I(11)	674(1)	2391(1)	-5000	71(1)
I(12)	4218(1)	4218(1)	5000	88(1)
I(13)	-763(1)	763(1)	-5000	112(1)
N(1)	1413(6)	3634(6)	2097(14)	137(6)
C(1)	1854(8)	3416(8)	2623(18)	139(8)
C(2)	1716(10)	2899(9)	2937(28)	230(16)
C(3)	2118(13)	2675(11)	3511(28)	282(21)
C(4)	2159(14)	2159(14)	3217(51)	309(34)
N(2)	1921(9)	-230(9)	-2824(21)	228(12)
C(5)	1497(11)	-16(11)	-2446(28)	236(17)
C(6)	1586(13)	398(11)	-1731(26)	257(18)
C(7)	1515(13)	861(10)	-2106(26)	232(16)
C(8)	1186(15)	1186(15)	-1473(44)	294(31)
N(3)	0	000	2500	203(21)
C(9)	-333(24)	5336(24)	3033(57)	111(24)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table 3S. Relevant Bond lengths [Å] and angles [°] for (1).

Sn(1)-I(12)	2.823(3)
Sn(1)-I(3)#1	3.1815(12)
Sn(1)-I(3)	3.1815(12)
Sn(1)-I(1)#2	3.2208(14)
Sn(1)-I(1)	3.2208(14)
Sn(2)-I(2)	2.826(2)
Sn(2)-I(4)#3	3.1577(12)
Sn(2)-I(4)	3.1577(12)
Sn(2)-I(1)	3.206(2)
Sn(2)-I(1)#4	3.206(2)
Sn(3)-I(6)#5	2.823(2)
Sn(3)-I(6)	2.823(2)
Sn(3)-I(5)#5	2.905(2)
Sn(4)-I(11)	2.924(2)
Sn(4)-I(10)	2.993(2)
Sn(4)-I(7)	3.108(2)
Sn(5)-I(7)#4	3.1897(8)
Sn(5)-I(7)	3.1897(8)
N(1)-C(1)	1.44(3)
C(4)-C(3)#7	1.44(3)
N(2)-C(5)	1.37(2)
C(5)-C(6)	1.46(2)
C(6)-C(7)	1.35(2)
C(7)-C(8)	1.48(2)
C(8)-C(7)#7	1.48(2)
N(3)-C(9)#8	1.44(3)
N(3)-C(9)	1.44(3)
N(3)-C(9)#9	1.44(3)
N(3)-C(9)#10	1.44(3)
I(12)-Sn(1)-I(3)#1	92.90(5)
I(12)-Sn(1)-I(3)	92.90(5)
I(3)#1-Sn(1)-I(3)	174.21(9)
I(12)-Sn(1)-I(1)#2	92.48(5)
I(3)#1-Sn(1)-I(1)#2	89.875(4)
I(3)-Sn(1)-I(1)#2	89.875(4)
I(12)-Sn(1)-I(1)	92.48(5)
I(3)#1-Sn(1)-I(1)	89.875(4)
I(3)-Sn(1)-I(1)	89.875(4)
I(1)#2-Sn(1)-I(1)	175.04(10)
I(2)-Sn(2)-I(4)#3	89.38(4)
I(2)-Sn(2)-I(4)	89.38(4)
I(4)#3-Sn(2)-I(4)	178.76(8)
I(2)-Sn(2)-I(1)	100.83(4)
I(4)#3-Sn(2)-I(1)	90.117(8)
I(4)-Sn(2)-I(1)	90.117(8)
I(2)-Sn(2)-I(1)#4	100.83(4)
I(4)#3-Sn(2)-I(1)#4	90.117(8)
I(4)-Sn(2)-I(1)#4	90.117(8)
I(1)-Sn(2)-I(1)#4	158.34(8)
I(6)#5-Sn(3)-I(6)	180.0
I(6)#5-Sn(3)-I(5)#5	90.0

I(6)-Sn(3)-I(5)#5	90.0
I(6)#5-Sn(3)-I(5)	90.0
I(6)-Sn(3)-I(5)	90.0
I(5)#5-Sn(3)-I(5)	180.0
I(6)#5-Sn(3)-I(13)	90.0
I(6)-Sn(3)-I(13)	90.0
I(5)#5-Sn(3)-I(13)	90.0
I(5)-Sn(3)-I(13)	90.0
I(6)#5-Sn(3)-I(13)#5	90.0
I(6)-Sn(3)-I(13)#5	90.0
I(5)#5-Sn(3)-I(13)#5	90.0
I(5)-Sn(3)-I(13)#5	90.0
I(13)-Sn(3)-I(13)#5	180.0
I(11)-Sn(4)-I(10)	97.07(5)
I(11)-Sn(4)-I(7)	93.96(3)
I(10)-Sn(4)-I(7)	90.96(3)
I(11)-Sn(4)-I(7)#6	93.96(3)
I(10)-Sn(4)-I(7)#6	90.96(3)
I(7)-Sn(4)-I(7)#6	171.56(5)
I(8)-Sn(5)-I(9)	88.92(5)
I(8)-Sn(5)-I(7)#4	91.90(3)
I(9)-Sn(5)-I(7)#4	89.90(3)
I(8)-Sn(5)-I(7)	91.90(3)
I(9)-Sn(5)-I(7)	89.90(3)
I(7)#4-Sn(5)-I(7)	176.19(5)
Sn(2)-I(1)-Sn(1)	171.65(8)
Sn(4)-I(7)-Sn(5)	173.87(5)
N(1)-C(1)-C(2)	107(2)
C(3)-C(2)-C(1)	110(2)
C(2)-C(3)-C(4)	109(2)
C(3)-C(4)-C(3)#7	94(4)
N(2)-C(5)-C(6)	114(3)
C(7)-C(6)-C(5)	118(3)
C(6)-C(7)-C(8)	116(3)
C(7)#7-C(8)-C(7)	114(5)
C(9)#8-N(3)-C(9)	103(3)
C(9)#8-N(3)-C(9)#9	103(3)
C(9)-N(3)-C(9)#9	124(6)
C(9)#8-N(3)-C(9)#10	124(6)
C(9)-N(3)-C(9)#10	103(3)
C(9)#9-N(3)-C(9)#10	103(3)

Symmetry transformations used to generate equivalent atoms:
#1 y,x,-z+1 #2 x,y,-z+1 #3 y,x,-z #4 x,y,-z
#5 -x,-y,-z-1 #6 x,y,-z-1 #7 y,x,z
#8 -y+1/2,x+1/2,-z+1/2 #9 -x,-y+1,z #10 y-1/2,-x+1/2,-z+1/2

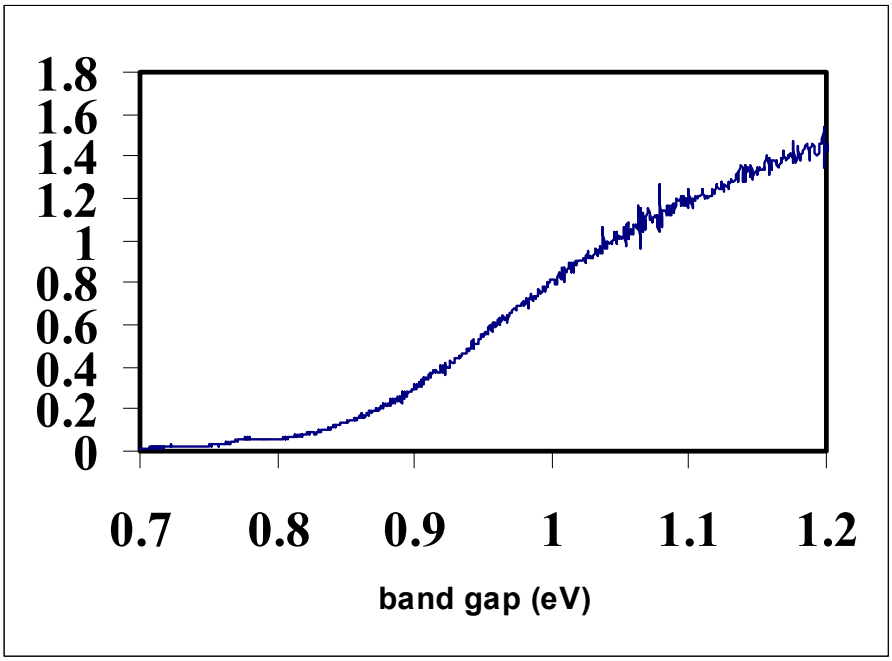

Figure 1S. Reflectance spectrum - $(\alpha/S)^2$ versus band gap ΔE - of compound **(1)**.