Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Metal Halide Structure and Extent of Distortion Controls the Photo-physical Properties of Luminescent Zero Dimensional Organic-Antimony(III) Halide Hybrids

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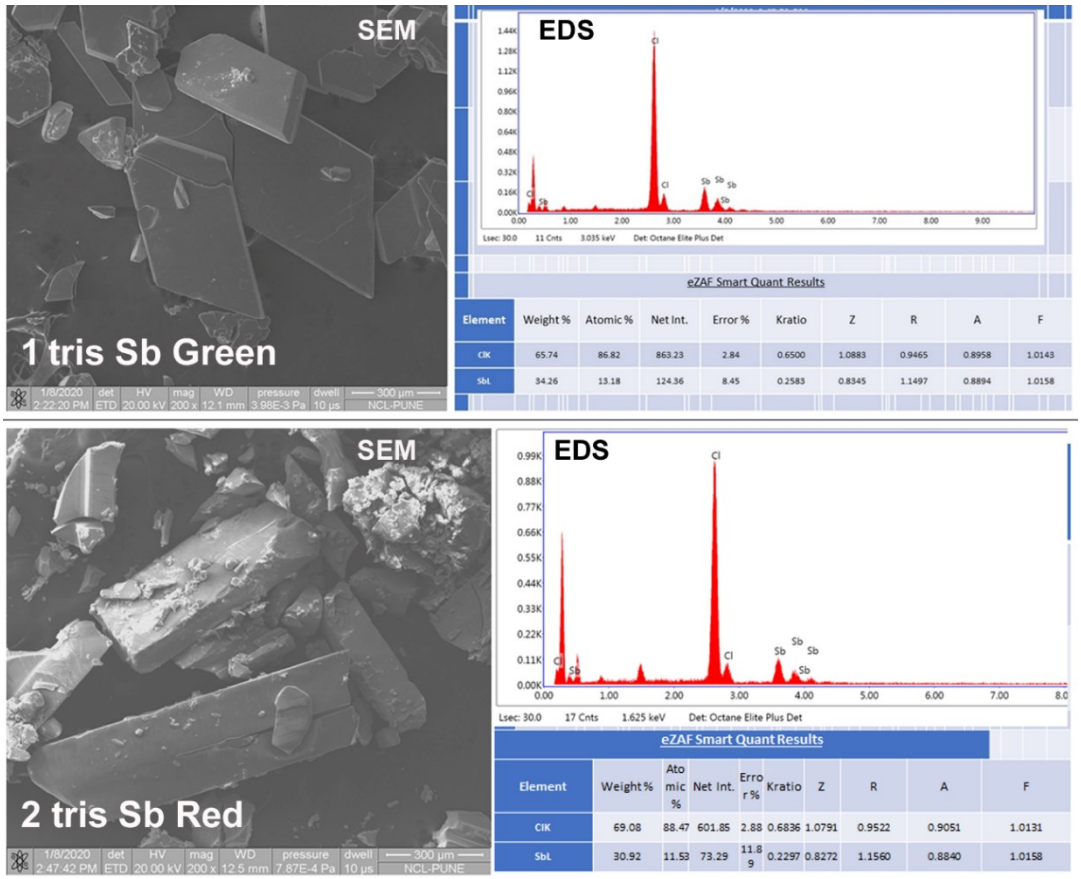


Figure S1: SEM/EDS analysis of **1** tris Sb Green (top) and **2** tris Sb Red (bottom) showing the presence of Antimony and Chlorine.

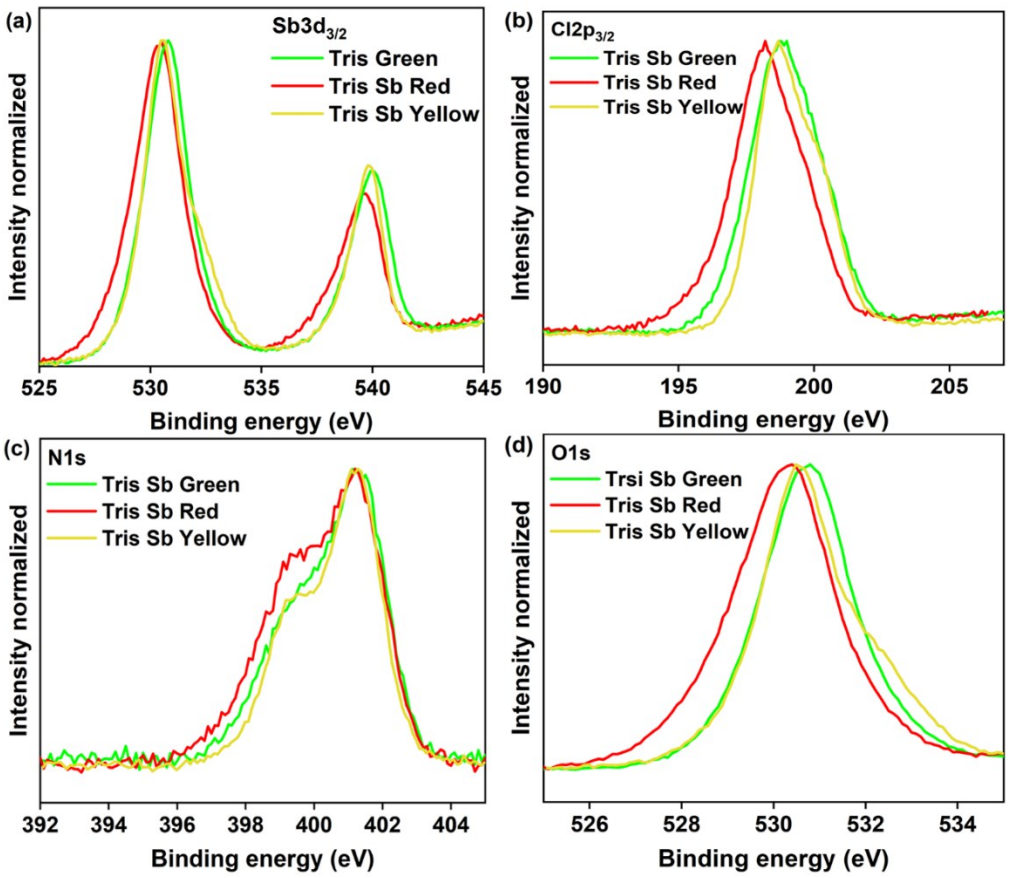


Figure S2: XPS spectra of products **1** tris Sb Green and **2** tris Sb Red showing the presence of Sb(III).

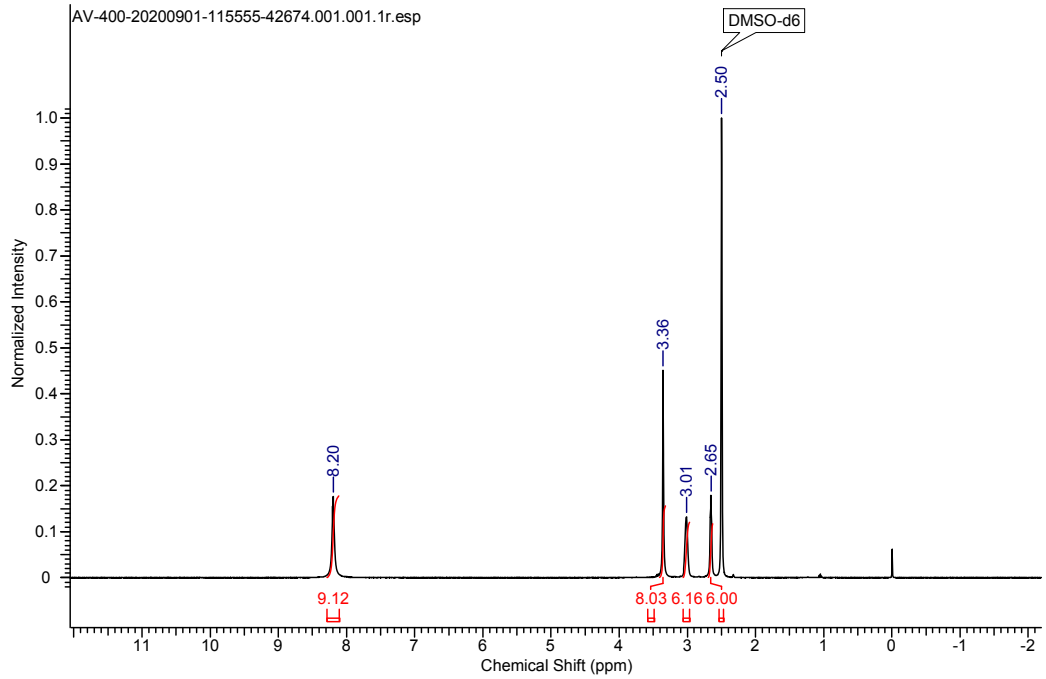


Figure S3 (a). ^{1}H NMR of Tris Cl salt (400 MHz, DMSO-d6, 298 K): δ 8.20 (br, 9H, NH_3), 3.01 (br, 6H, CH_2), 2.65 (br, 6H, CH_2) 3.36(br, 8H, H_2O) ppm.

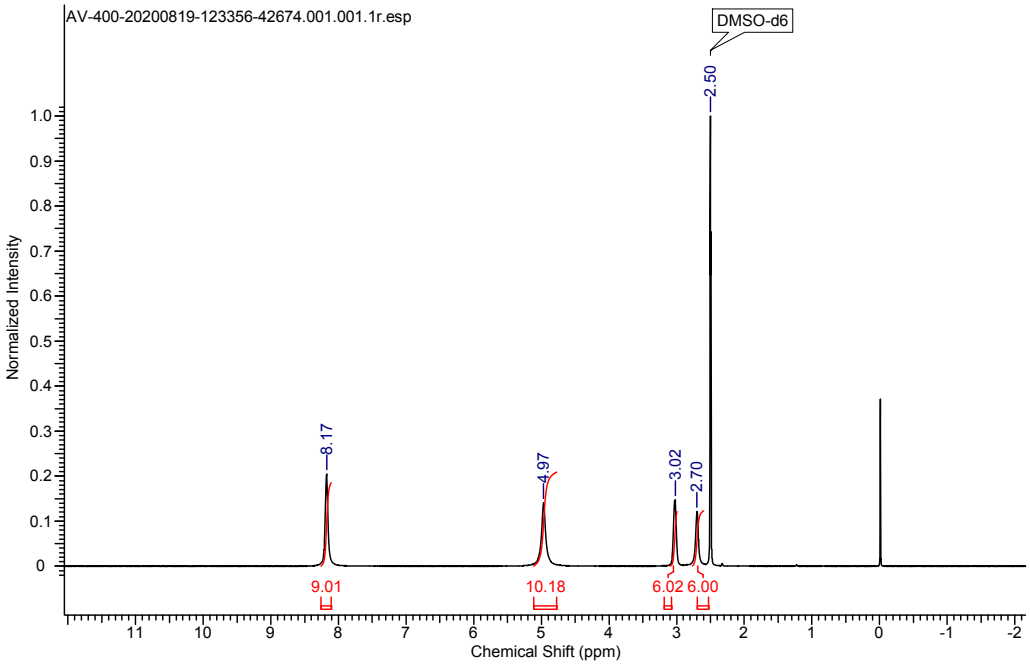


Figure S3 (b). ^{1}H NMR of 1 Tris Sb Green (400 MHz, DMSO-d6, 298 K): δ 8.17 (br, 9H, NH_3), 3.02 (br, 6H, CH_2), 2.70 (br, 6H, CH_2), 4.97 (br, 9H, H_2O & 1H, NH) ppm.

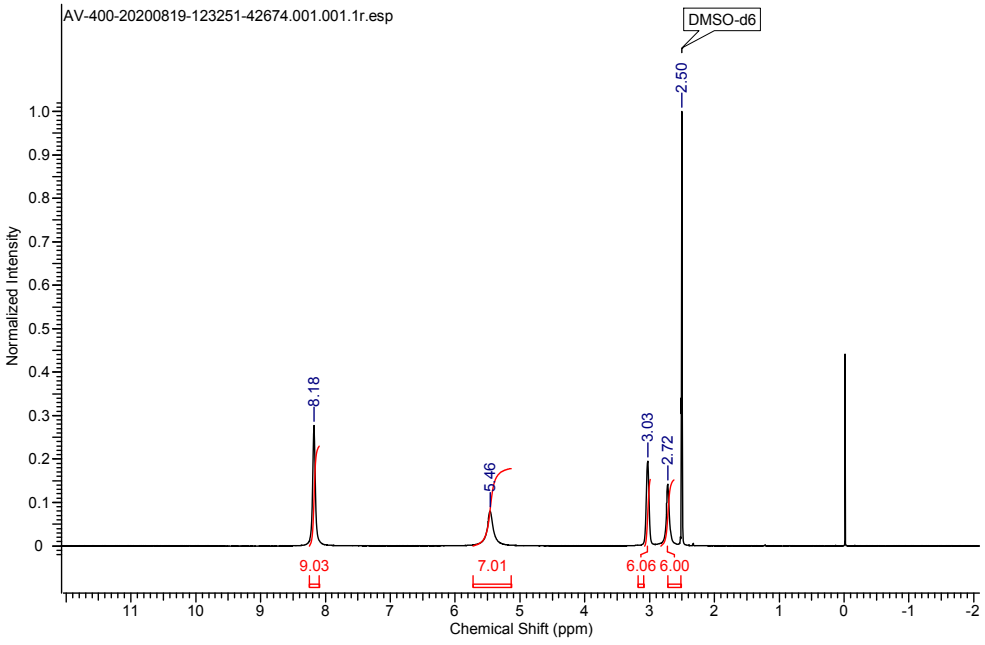


Figure S3 (c). ^{1}H NMR of 1 Tris Sb Red (400 MHz, DMSO-d6, 298 K): δ 8.18 (br, 9H, NH_3), 3.03 (br, 6H, CH_2), 2.72 (br, 6H, CH_2), 5.46 (br, 6H, H_2O & 1H, NH) ppm.

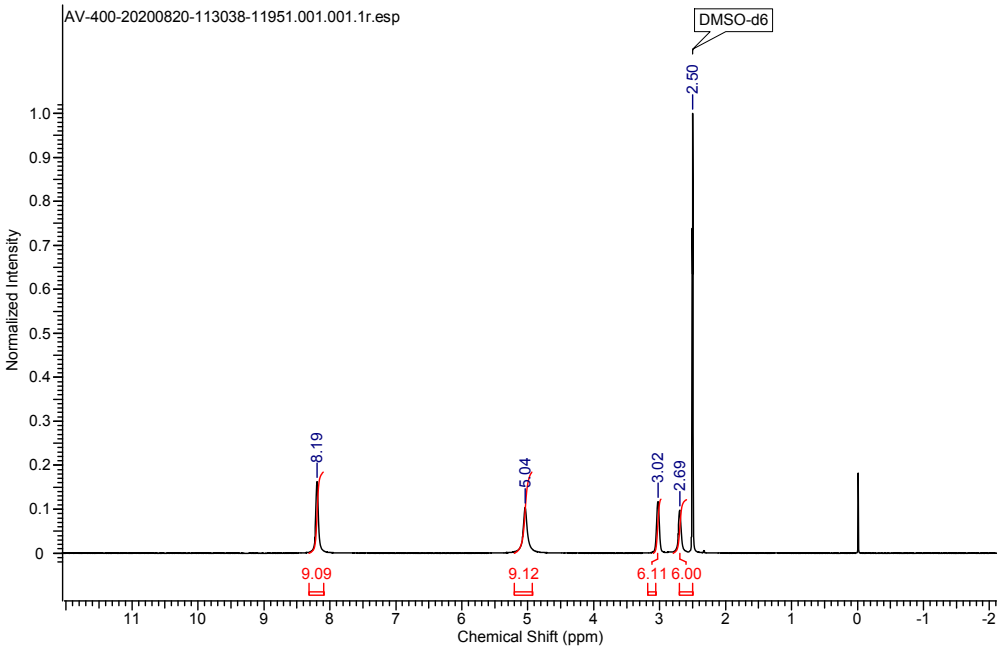
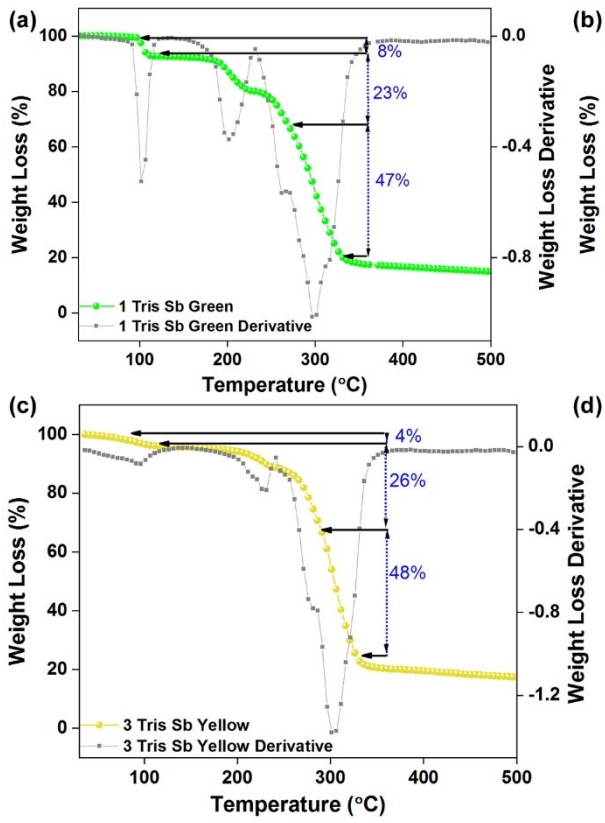


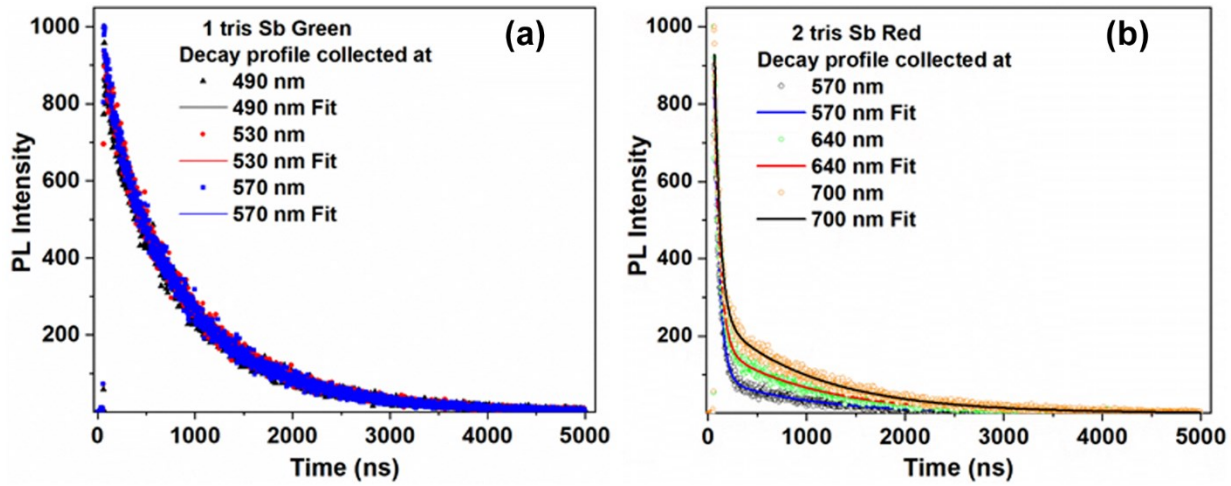
Figure S3 (d). ^{1}H NMR of 1 Tris Sb Yellow (400 MHz, DMSO-d6, 298 K): δ 8.19 (br, 9H, NH_3), 3.02 (br, 6H, CH_2), 2.69 (br, 6H, CH_2), 5.04 (br, 8H, H_2O & 1H, NH) ppm.



(d)

Weight Loss Analysis		Ligand weight (%)	Structural Cl weight (%)	Water weight (%)
1 Tris Sb Green $[(C_6H_{22}N_4)_2(Sb_2Cl_{10})(SbCl_6)(Cl)_2(H_3O)].(3H_2O)$	*Calc.*	21	46	5.3
	Exp.	23	47	8
2 Tris Sb Red $[(C_6H_{22}N_4)_2(SbCl_6)_2(Cl)_2].3(H_2O)$	*Calc.*	21	45	4.9
	Exp.	25	49	4
3 Tris Sb Yellow $[(C_6H_{22}N_4)_4(SbCl_6)_3(Cl)_7].4(H_2O)$	*Calc.*	31	46	3
	Exp.	26	48	4

Figure S4: Thermogravimetric weight loss analysis for a) **1** tris Sb Green, b) **2** tris Sb Red, c) **3** tris Sb Yellow, d) table listing the % weight losses incurred from the plausible structural components.



1 tris Sb Green (c)

Emission (nm)	Lifetime (ns)	Weightage (%)
490	317.6	10
	941.9	90
530	261.6	8
	929.9	92
570	204.6	6
	891.3	94

2 tris Sb Red (d)

Emission (nm)	Lifetime (ns)	Weightage (%)
570	53.3	34
	930.2	66
640	55.8	20
	986.9	80
700	56.4	14
	1015	86

Figure S5: TCSPC Lifetime analysis for products **1** tris Sb Green (a,c) and **2** tris Sb Red (b,d) at room temperature across the broad band emission with estimated lifetimes in nanoseconds.

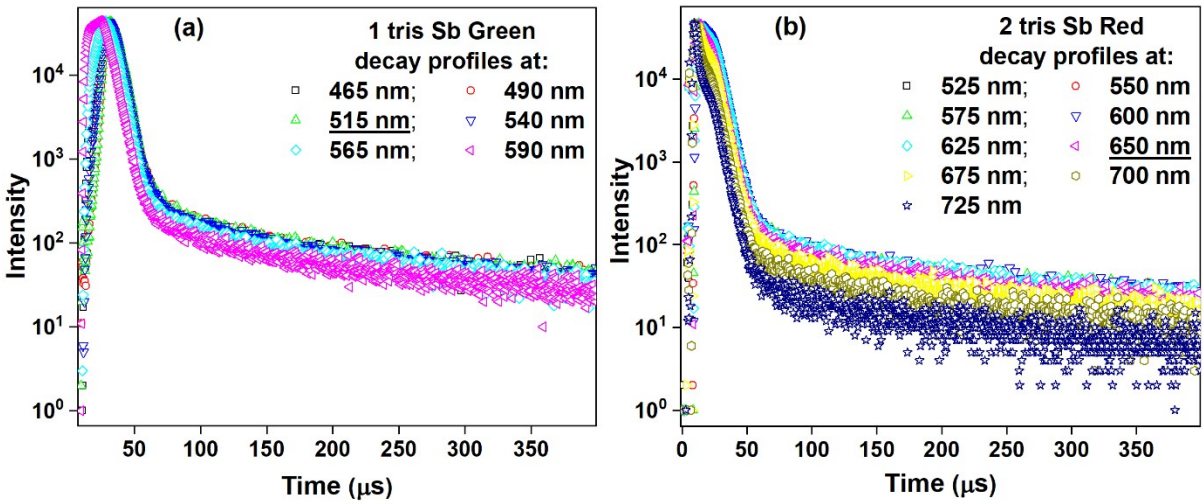


Figure S6: Lifetime decay profiles for products **1** tris Sb Green (a) and **2** tris Sb Red (b) at room temperature collected across emission band using microsecond flash lamp excitation (360 nm).

Table S1: Lifetime (μs) components and their relative weightages (%) for the decay profiles presented above in figure S5.

1 tris Sb Green		
Wavelength (nm)	**Life time (μs) (at room temp.)**	**Relative %**
465	4.88 77.1	69.99 30.01
490	4.91 71.61	76.98 23.02
515	4.77 71.9	72.55 27.45
540	4.89 73.8	73.32 26.68
565	5.01 79.4	80.57 19.43
590	5.25 85.1	86.14 13.86

2 tris Sb Red		
Wavelength (nm)	**Life time (μs) (at room temp.)**	**Relative %**
525	5.6 92.7	90.04 9.96
550	5.61 90.8	90.81 9.29
575	5.62 89.9	90.77 9.23
600	5.65 90.5	90.69 9.31
625	5.57 92.8	89.40 10.60
650	5.66 94.4	90.68 9.32
675	5.63 90.7	90.15 9.85
700	5.68 90.4	90.74 9.26
725	5.68 96.3	89.20 10.80

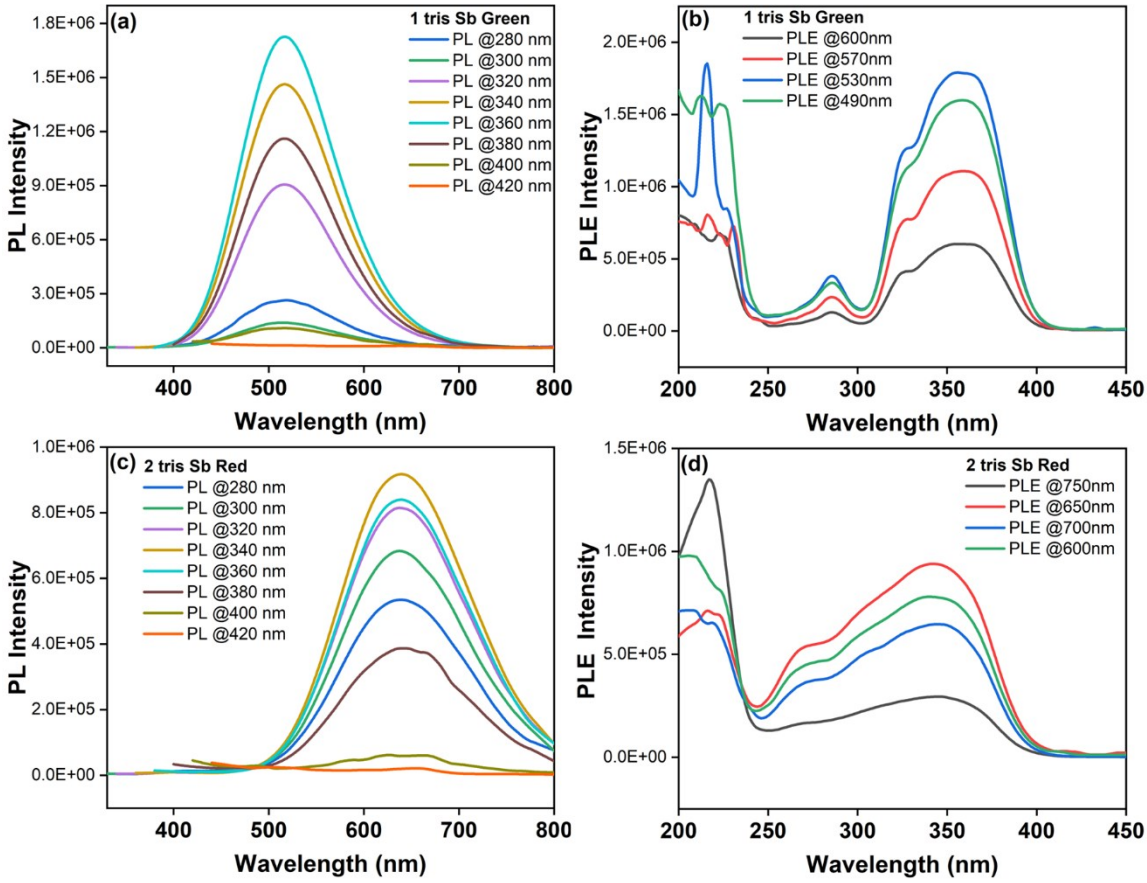


Figure S7: Dependence of photoluminescence (PL) on excitation wavelength and photoluminescence excitation (PLE) spectrum collected across the broad PL peak for a) **1** tris Sb Green, and b) **2** tris Sb Red powder samples.

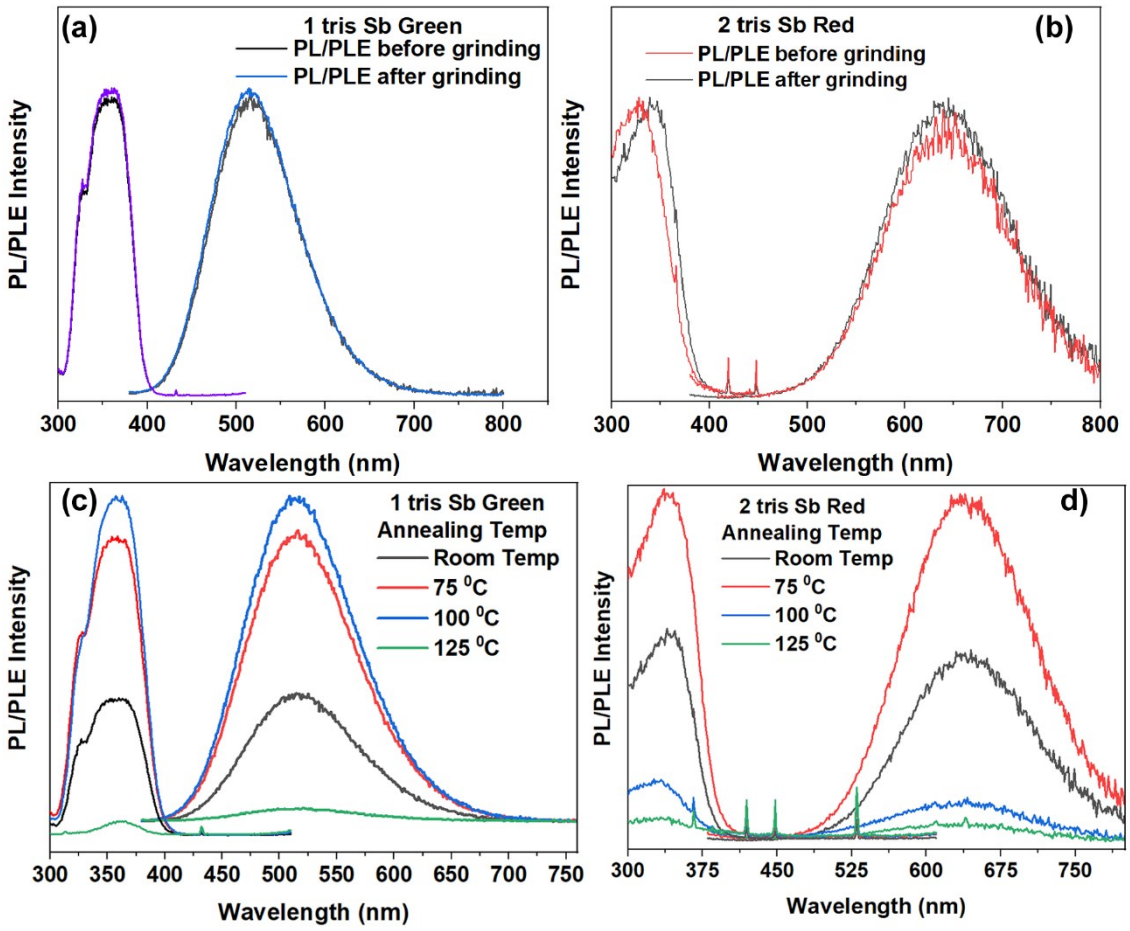


Figure S8: PL/PLE of **1** tris Sb Green and **2** tris Sb Red samples upon a-b) room temperature grinding (10 mins, mortar-pestle) and c-d) annealing of the ground powders at different temperatures. The drastic drop of PL/PLE intensity for **1** and **2** at around 100 °C is related to the loss of solvent (water) molecules that is integral to the stability of the structure of the products through network of hydrogen bonding.

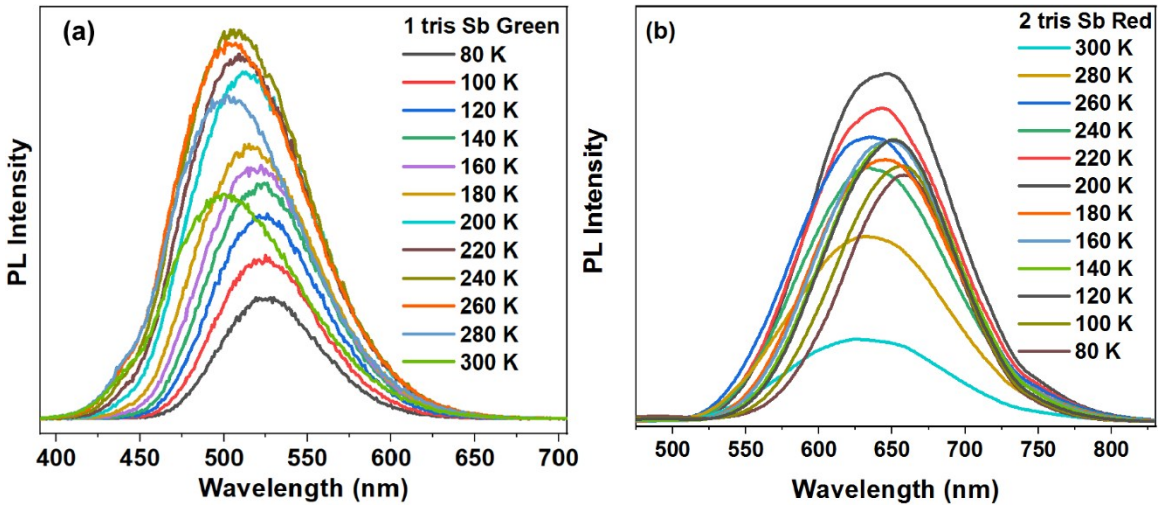


Figure S9: Low temperature photoluminescence spectra of a) **1** tris Sb Green and b) **2** tris Sb Red powder samples excited at 370 nm and 350 nm respectively using a **µs** flash lamp.

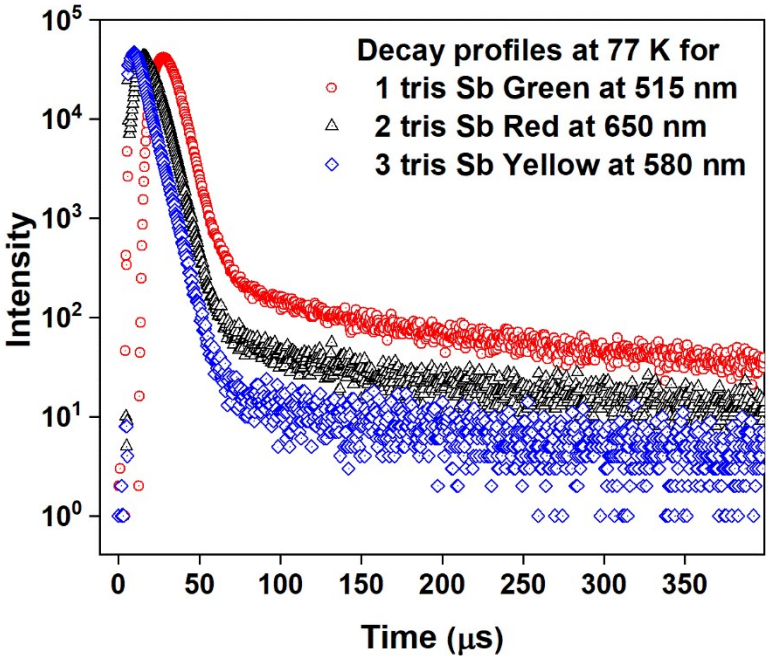


Figure S10: Life time decay profile for powder samples of **1** tris Sb Green, **2** tris Sb Red, and **3** tris Sb Yellow at low temperature (77 K) collected at 515 nm, 650 nm, and 580 nm respectively using microsecond flash lamp excitation (360 nm) with their fitted lifetimes listed below:

Table SX.

Sample	Wavelength (nm)	Life time (μs) (at 77 K)	Relative %
3 tris Sb yellow	580	6.35 131.1	99.16 0.84
2 tris Sb Red	650	6.35 102.8	94.71 5.29
1 tris Sb Green	515	5.98 81.09	88.45 11.55

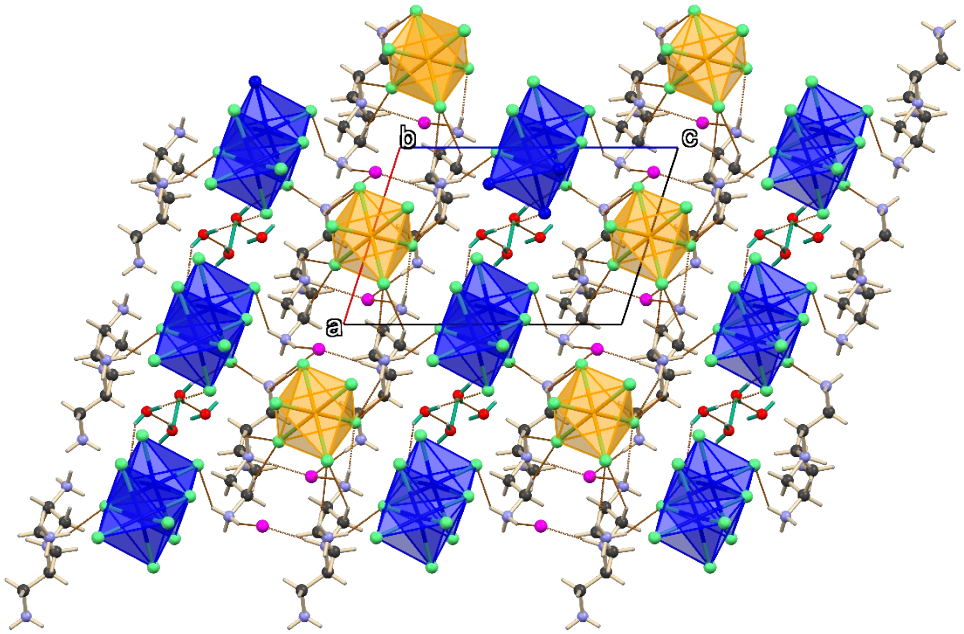


Figure S11 a): A view of the molecular packing down the b-axis in crystals of **1** (*tris Sb Green*) showed the associations of the metal halide, organic ligands, and water molecules through N-H···Cl, O-H···Cl, and O-H···O hydrogen bonds.

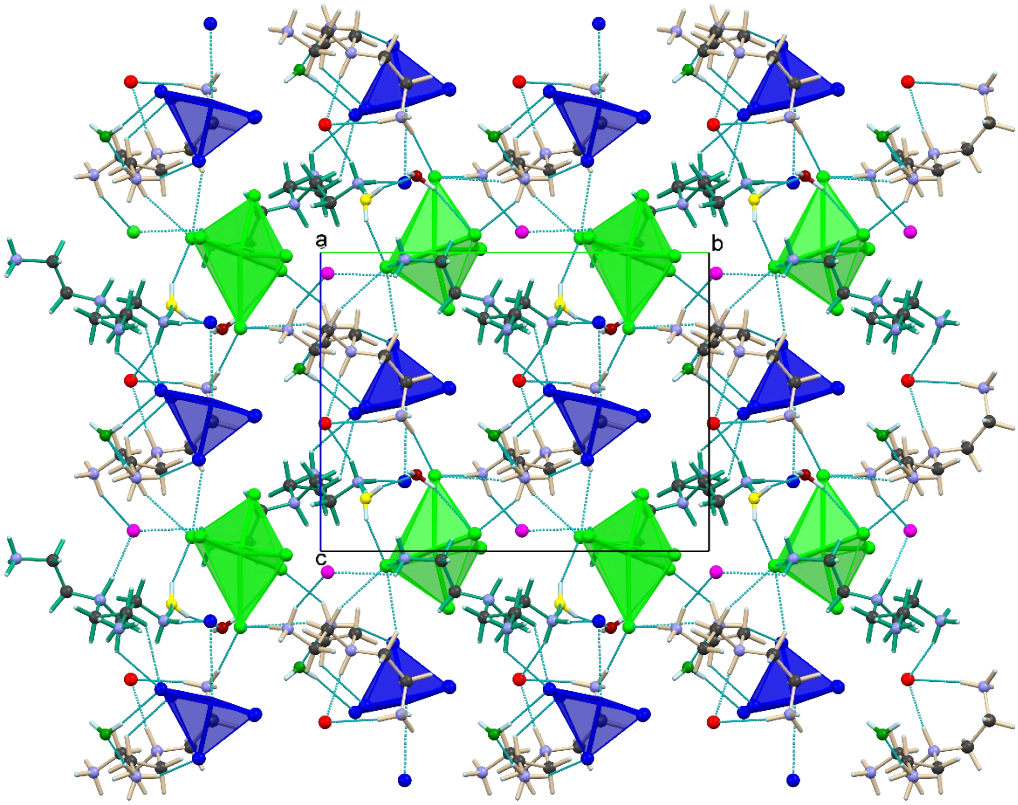


Figure S11 b): A view of the molecular packing down the a-axis in crystals of **2** (*tris Sb Red*) showing the associations of the metal halide, organic ligands, and water molecules through N-H···Cl, O-H···Cl, N-H···O, and O-H···O hydrogen bonds.

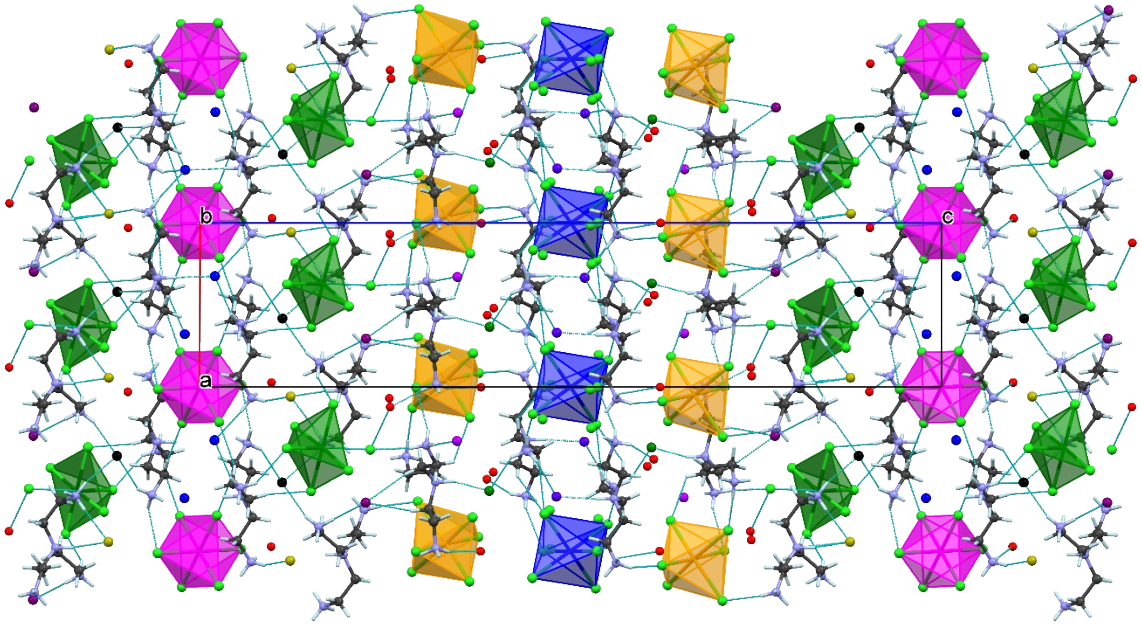


Figure S11 c): A view of the molecular packing down the b-axis in crystals of **3** (*tris Sb Yellow*) showing the associations of the metal halide, organic ligands, and water molecules through N-H···Cl, O-H···Cl, and N-H···O hydrogen bonds.

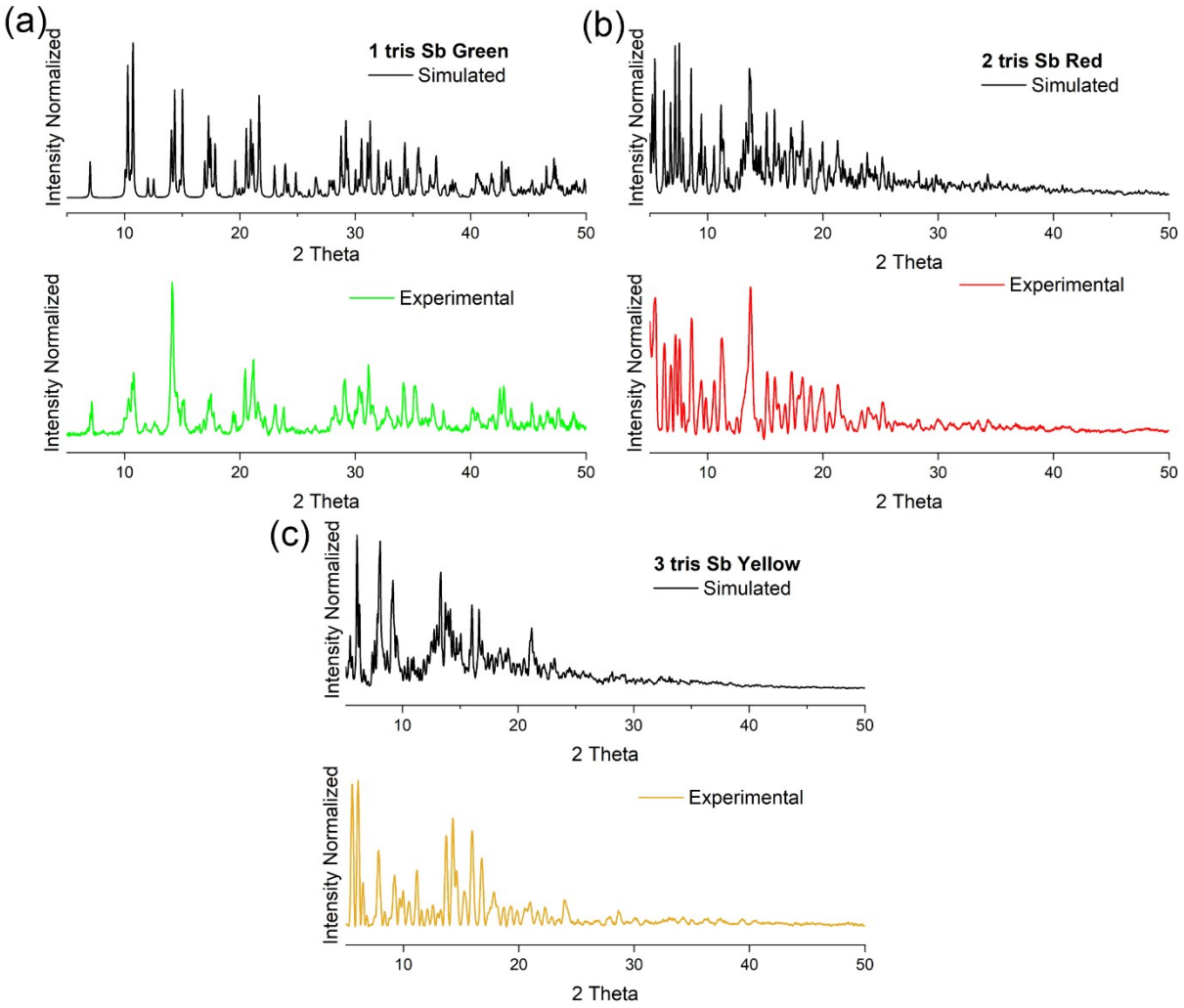


Figure S12: Comparison of the PXRD pattern with the simulated pattern from the single crystal structure data for a) **1** tris Sb Green (collected using Cu source), b) **2** tris Sb Red, and c) **3** tris Sb Yellow (collected using Mo source) samples.

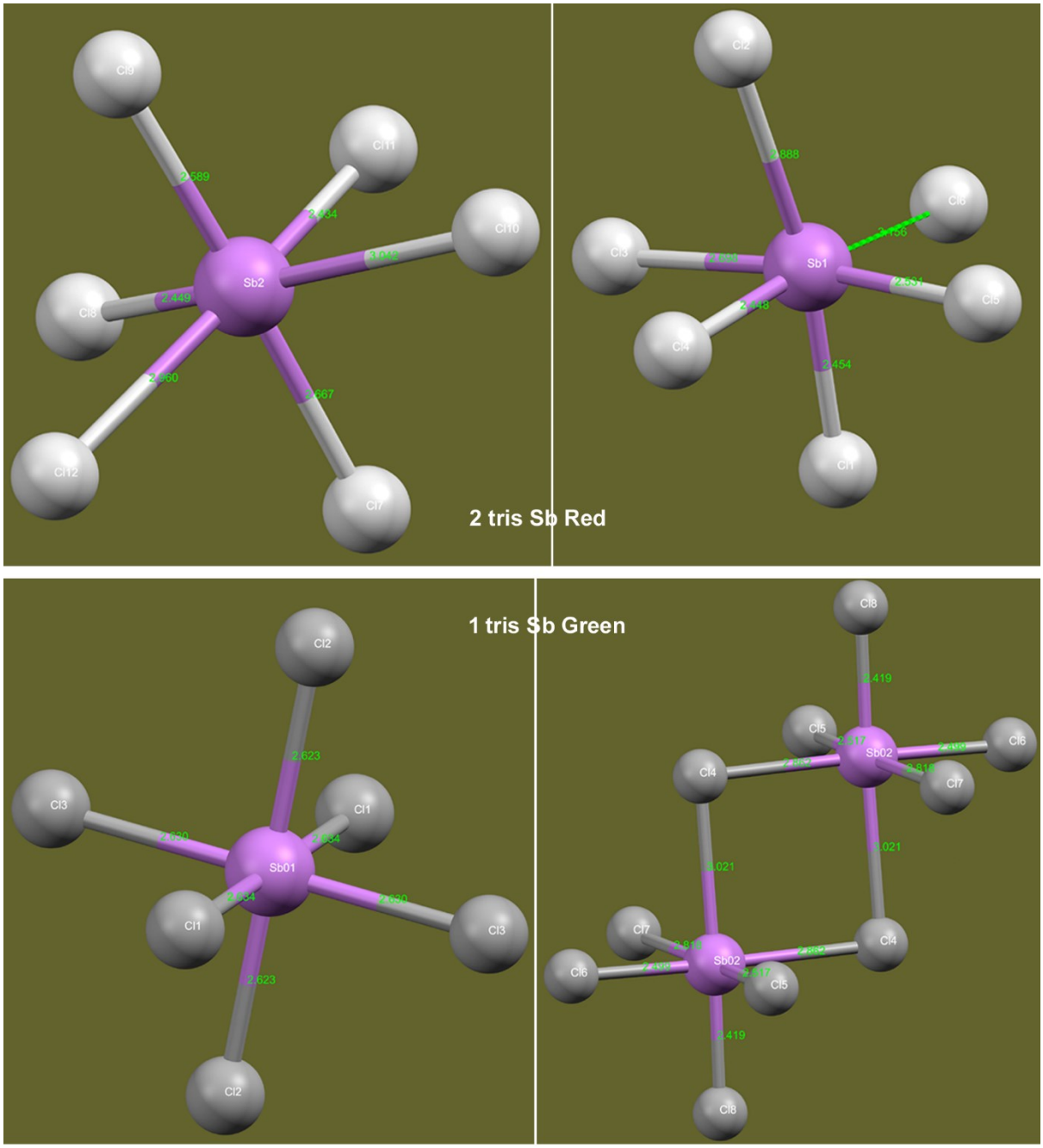


Figure S13: Sb-Cl bond lengths in the metal halide polyhedral framework for **2** tris Sb Red (upper panel) and **1** tris Sb Green (lower panel).

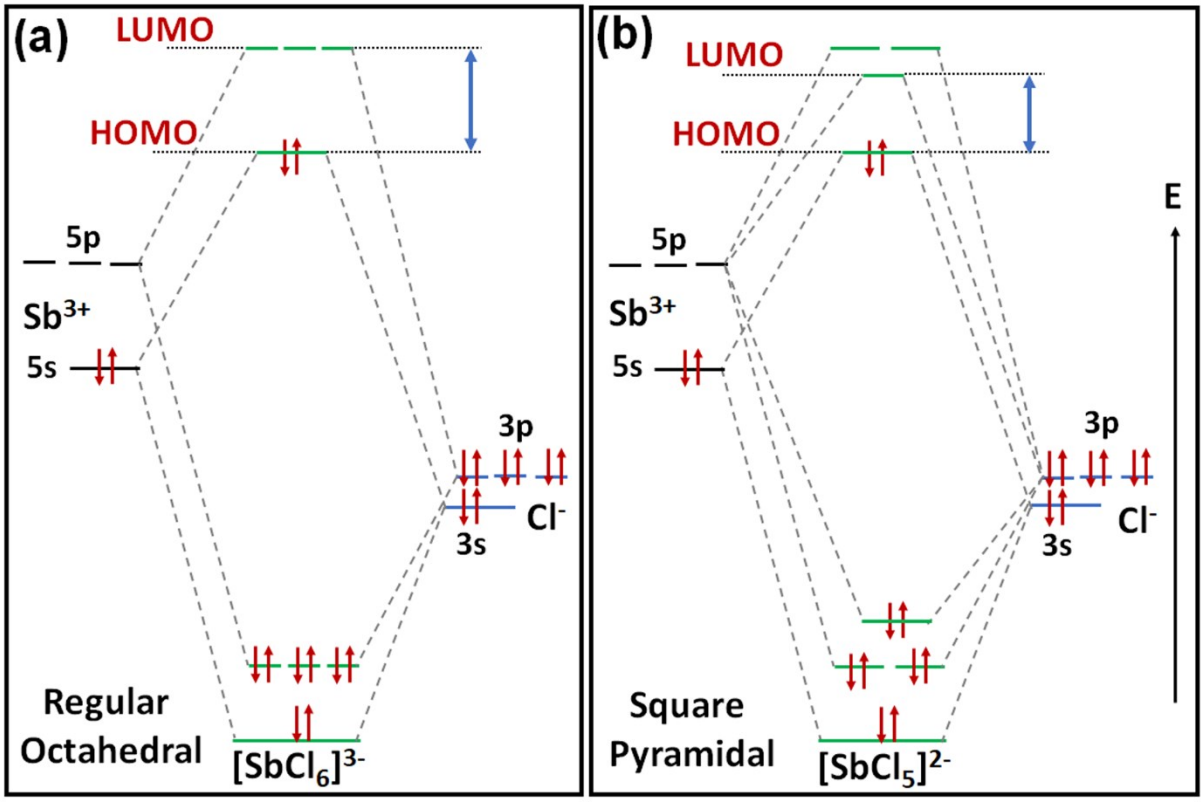


Figure S14: Qualitative molecular orbital diagram of (a) octahedral and (b) square pyramidal metal-halide framework and the associated change in the energy gap between the HOMO and LUMO that manifests as PL emission energy difference between the two structures.

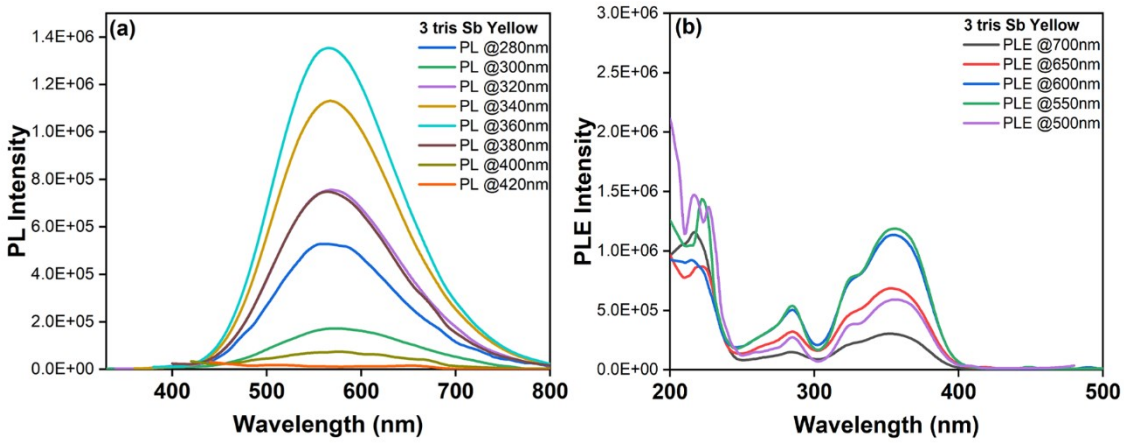


Figure S15: Dependence of photoluminescence (PL) on excitation wavelength and photoluminescence excitation (PLE) spectrum collected across the broad PL peak for **3** *tris Sb Yellow* powder samples.

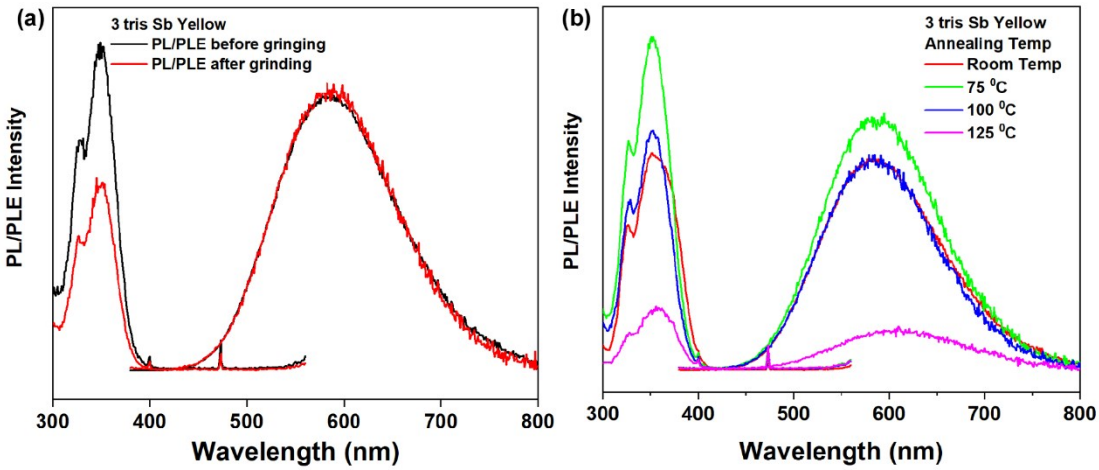


Figure S16: Dependence of PL and PLE on a) grinding and b) annealing for **3** *tris Sb Yellow* powder samples.

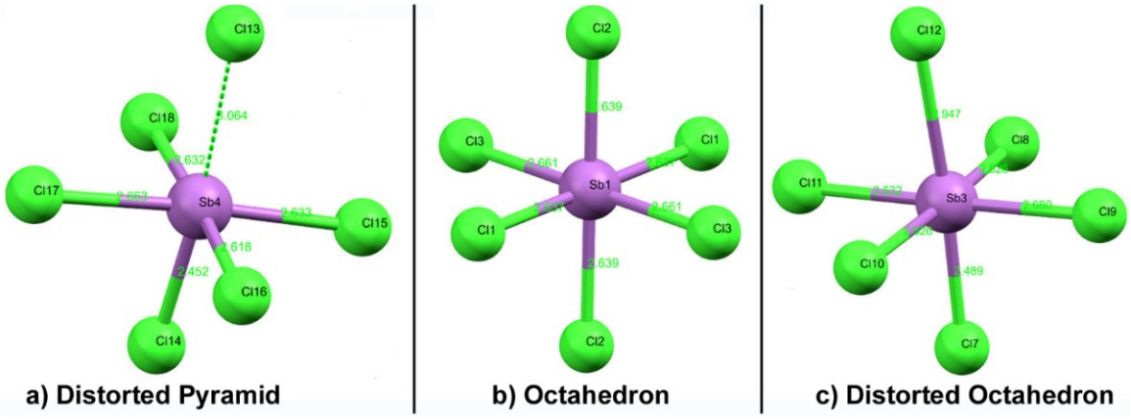


Figure S17: Metal halide frameworks and the associated bond lengths highlighting the bond length distortion for ***3*** *tris Sb Yellow.*

Table S2: List of estimated bond length asymmetry and bond angle variations (from ideal value) in metal halide frameworks of **1**, **2**, **3** as obtained from single crystal structures.

Sb-Cl polyhedra type	λ_{oct}	σ^2
1 tris Sb Green		
Isolated octahedral	3×10^{-6}	3
Dimer octahedral	6.6×10^{-3}	6
2 tris Sb Red		
Distorted octahedral	7.5×10^{-3}	77
Quadrangular pyramid	9×10^{-3}	67
3 tris Sb Yellow		
Octahedra	1.7×10^{-5}	5
Distorted octahedral	3.6×10^{-3}	6.3
Quadrangular pyramidal	4.8×10^{-3}	9.3

$$\lambda_{\text{oct}} = \frac{1}{6}\sum_{n=1}^{6}\left[\left(d_n - d_0\right)/d_0\right]^2; \quad \sigma^2 = \frac{1}{11}\sum_{n=1}^{12}\left(\theta_n - 90^\circ\right)^2$$

For the above calculations the following bond angles and bond lengths were utilized for samples 1, 2, 3

Number	Atom1	Atom2	Atom3	Angle
1	Cl1	Sb1	Cl2	93.22
2	Cl1	Sb1	Cl3	89.79
3	Cl1	Sb1	Cl1	180
4	Cl1	Sb1	Cl2	86.78
5	Cl1	Sb1	Cl3	90.21
6	Cl2	Sb1	Cl3	90.09
7	Cl2	Sb1	Cl1	86.78
8	Cl2	Sb1	Cl2	180
9	Cl2	Sb1	Cl3	89.91
10	Cl3	Sb1	Cl1	90.21
11	Cl3	Sb1	Cl2	89.91
12	Cl3	Sb1	Cl3	180
13	Cl1	Sb1	Cl2	93.22
14	Cl1	Sb1	Cl3	89.79
15	Cl2	Sb1	Cl3	90.09
16	Cl4	Sb2	Cl5	90.58
17	Cl4	Sb2	Cl6	176.70
18	Cl4	Sb2	Cl7	95.27
19	Cl4	Sb2	Cl8	90.38
20	Cl4	Sb2	Cl4	90.01
21	Cl5	Sb2	Cl6	87.12
22	Cl5	Sb2	Cl7	173.84
23	Cl5	Sb2	Cl8	90.38
24	Cl5	Sb2	Cl4	94.25
25	Cl6	Sb2	Cl7	86.96
26	Cl6	Sb2	Cl8	92.00
27	Cl6	Sb2	Cl4	87.8
28	Cl7	Sb2	Cl8	91.54
29	Cl7	Sb2	Cl4	83.82
30	Cl8	Sb2	Cl4	175.36
32	Cl4	Sb2	Cl4	90.01
33	Cl4	Sb2	Cl5	94.25
34	Cl4	Sb2	Cl6	87.81
35	Cl4	Sb2	Cl7	83.82
36	Cl4	Sb2	Cl8	175.36
37	Cl4	Sb2	Cl5	90.58
38	Cl4	Sb2	Cl6	176.70
39	Cl4	Sb2	Cl7	95.27

40	Cl4	Sb2	Cl8	90.38
41	Cl5	Sb2	Cl6	87.12
42	Cl5	Sb2	Cl7	173.84
43	Cl5	Sb2	Cl8	90.38
44	Cl6	Sb2	Cl7	86.96
45	Cl6	Sb2	Cl8	92.00
46	Cl7	Sb2	Cl8	91.54

1 Tris Sb Green Bond Angle

Number	Atom1	Atom2	Length
1	Sb1	Cl1	2.634
2	Sb1	Cl2	2.623
3	Sb1	Cl3	2.63
4	Sb1	Cl1	2.634
5	Sb1	Cl2	2.623
6	Sb1	Cl3	2.63
7	Sb2	Cl4	2.862
8	Sb2	Cl5	2.517
9	Sb2	Cl6	2.499
10	Sb2	Cl7	2.818
11	Sb2	Cl8	2.419
12	Sb2	Cl4	3.021
13	Cl4	Sb2	3.021
14	Sb2	Cl4	2.862
15	Sb2	Cl5	2.517
16	Sb2	Cl6	2.499
17	Sb2	Cl7	2.818
18	Sb2	Cl8	2.419

1 Tris Sb Green Bond Length

Number	Atom1	Atom2	Atom3	Angle
1	Cl12	Sb2	Cl10	113.15
2	Cl12	Sb2	Cl7	84.41
3	Cl12	Sb2	Cl8	79.88
4	Cl12	Sb2	Cl9	94.01
5	Cl12	Sb2	Cl11	166.37
6	Cl10	Sb2	Cl7	86.94
7	Cl10	Sb2	Cl8	165.46
8	Cl10	Sb2	Cl9	94.69
9	Cl10	Sb2	Cl11	79.36

10	Cl7	Sb2	Cl8	88.03
11	Cl7	Sb2	Cl9	178.08
12	Cl7	Sb2	Cl11	91.12
13	Cl8	Sb2	Cl9	90.62
14	Cl8	Sb2	Cl11	87.11
15	Cl9	Sb2	Cl11	90.17
16	Cl1	Sb1	Cl2	169.04
17	Cl1	Sb1	Cl3	86.81
18	Cl1	Sb1	Cl4	88.97
19	Cl1	Sb1	Cl5	88.11
20	Cl2	Sb1	Cl3	89.28
21	Cl2	Sb1	Cl4	80.49
22	Cl2	Sb1	Cl5	94.74
23	Cl3	Sb1	Cl4	85.15
24	Cl3	Sb1	Cl5	172.58
25	Cl4	Sb1	Cl5	89.36

2 Tris Sb Red Bond Angle

Number	Atom1	Atom2	Length
1	Sb2	Cl12	2.960
2	Sb2	Cl10	3.042
3	Sb2	Cl7	2.667
4	Sb2	Cl8	2.449
5	Sb2	Cl9	2.589
6	Sb2	Cl11	2.434
7	Sb1	Cl1	2.454
8	Sb1	Cl2	2.888
9	Sb1	Cl3	2.698
10	Sb1	Cl4	2.448
11	Sb1	Cl5	2.531

2 Tris Sb Red Bond Length

Number	Atom1	Atom2	Atom3	Angle
1	Cl1	Sb1	Cl2	93.31
2	Cl1	Sb1	Cl3	90.72
3	Cl1	Sb1	Cl1	180
4	Cl1	Sb1	Cl2	86.69
5	Cl1	Sb1	Cl3	89.28
6	Cl2	Sb1	Cl3	92.25
7	Cl2	Sb1	Cl1	86.69
8	Cl2	Sb1	Cl2	180
9	Cl2	Sb1	Cl3	87.75

10	Cl3	Sb1	Cl1	89.28
11	Cl3	Sb1	Cl2	87.75
12	Cl3	Sb1	Cl3	180
13	Cl1	Sb1	Cl2	93.31
14	Cl1	Sb1	Cl3	90.72
15	Cl2	Sb1	Cl3	92.25
16	Cl4	Sb2	Cl5	90.9
17	Cl4	Sb2	Cl6	96.9
18	Cl4	Sb2	Cl4	180
19	Cl4	Sb2	Cl5	89.1
20	Cl4	Sb2	Cl6	83.1
21	Cl5	Sb2	Cl6	96.7
22	Cl5	Sb2	Cl4	89.1
23	Cl5	Sb2	Cl5	180
24	Cl5	Sb2	Cl6	83.3
25	Cl6	Sb2	Cl4	83.1
26	Cl6	Sb2	Cl5	83.3
27	Cl6	Sb2	Cl6	180
28	Cl4	Sb2	Cl5	90.9
29	Cl4	Sb2	Cl6	96.9
30	Cl5	Sb2	Cl6	96.7
32	Cl7	Sb3	Cl8	90.6
33	Cl7	Sb3	Cl9	89.0
34	Cl7	Sb3	Cl10	88.93
35	Cl7	Sb3	Cl11	90.8
36	Cl7	Sb3	Cl12	175.7
37	Cl8	Sb3	Cl9	90.1
38	Cl8	Sb3	Cl10	175.3
39	Cl8	Sb3	Cl11	87.5
40	Cl8	Sb3	Cl12	93.3
41	Cl9	Sb3	Cl10	94.5
42	Cl9	Sb3	Cl11	177.6
43	Cl9	Sb3	Cl12	93.0
44	Cl10	Sb3	Cl11	87.89
45	Cl10	Sb3	Cl12	87.06
46	Cl11	Sb3	Cl12	87.34
47	Cl14	Sb4	Cl15	88.73
48	Cl14	Sb4	Cl16	90.4
49	Cl14	Sb4	Cl17	88.97
50	Cl14	Sb4	Cl18	87.2
51	Cl15	Sb4	Cl16	90.4
52	Cl15	Sb4	Cl17	176.75
53	Cl15	Sb4	Cl18	91.4
54	Cl16	Sb4	Cl17	87.4

55	Cl16	Sb4	Cl18	177.0
56	Cl17	Sb4	Cl18	90.8

3 Tris Sb Yellow Bond Angle

Number	Atom1	Atom2	Length
1	Sb1	Cl1	2.637
2	Sb1	Cl2	2.639
3	Sb1	Cl3	2.662
4	Sb1	Cl1	2.637
5	Sb1	Cl2	2.639
6	Sb1	Cl3	2.662
7	Sb2	Cl4	2.65
8	Sb2	Cl5	2.64
9	Sb2	Cl6	2.7
10	Sb2	Cl4	2.65
11	Sb2	Cl5	2.64
12	Sb2	Cl6	2.7
13	Sb3	Cl7	2.488
14	Sb3	Cl8	2.526
15	Sb3	Cl9	2.679
16	Sb3	Cl10	2.826
17	Sb3	Cl11	2.632
18	Sb3	Cl12	2.948
19	Sb4	Cl14	2.451
20	Sb4	Cl15	2.634
21	Sb4	Cl16	2.619
22	Sb4	Cl17	2.663
23	Sb4	Cl18	2.632

3 Tris Sb Yellow Bond Length

Details on Single Crystal Structures:

Single crystals X-ray intensity data measurements of compounds TrisSbCl Green and TrisSbCl Red were carried out on a Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer equipped with Incoatech multilayer mirrors optics. The intensity measurements were carried out at 100(2) K temperature with Mo micro-focus sealed tube diffraction source (MoKα= 0.71073 Å). The X-ray generator was operated at 50 kV and 1.4. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 36 frames. Data were collected with ω scan width of 0.5° at different settings of ϕ and 2θ with a frame time of 10 secs keeping the sample-to-detector distance fixed at 5.00 cm. The X-ray data collection was monitored by APEX3 program (Bruker, 2016).[1] All the data were corrected for Lorentzian, polarization and absorption effects using SAINT and SADABS programs (Bruker, 2016).1 Using APEX3 (Bruker) program suite, the structure was solved with the ShelXS-97 (Sheldrick, 2008)[2] structure solution program, using direct methods. The model was refined with version of ShelXL-2013 (Sheldrick, 2015)[3] using Least Squares minimisation. All the hydrogen atoms were placed in a geometrically idealized position and constrained to ride on its parent atoms. An ORTEP III[4] view of compounds was drawn with 50% probability displacement ellipsoids and H atoms are shown as small spheres of arbitrary radii.

Table S3. Crystal data and structure refinement for **1** tris Sb Green.

Identification code	ANUP	
Empirical formula	C6 H26 Cl9 N4 O2 Sb1.50	
Formula weight	687.98	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.116(4) Å	α= 97.69(2)°.
	b = 10.249(6) Å	β= 101.372(16)°.
	c = 13.343(5) Å	γ = 119.379(13)°.
Volume	1138.0(9) $Å^3$	
Z	2	
Density (calculated)	2.008 Mg/m^3	
Absorption coefficient	2.858 mm^{-1}	
F(000)	671	
Crystal size	0.350 x 0.280 x 0.130 mm^3	
Theta range for data collection	2.426 to 27.998°.	
Index ranges	-13<=h<=13, -13<=k<=13, -17<=l<=17	
Reflections collected	24249	
Independent reflections	5453 [R(int) = 0.0617]	
Completeness to theta = 25.242°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.708 and 0.435	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5453 / 4 / 220	
Goodness-of-fit on F^2	1.091	
Final R indices [I>2sigma(I)]	R1 = 0.0356, wR2 = 0.0920	
R indices (all data)	R1 = 0.0376, wR2 = 0.0930	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.694 and -0.967 $e.Å^{-3}$	

Table S4. Bond lengths [Å] and angles [°] for **1** tris Sb Green.

Sb(01)-Cl(2)	2.6233(14)
Sb(01)-Cl(2)#1	2.6233(14)
Sb(01)-Cl(3)	2.6296(16)
Sb(01)-Cl(3)#1	2.6296(16)
Sb(01)-Cl(1)	2.6337(13)
Sb(01)-Cl(1)#1	2.6337(13)
Sb(02)-Cl(8)	2.4189(14)
Sb(02)-Cl(6)	2.4987(11)
Sb(02)-Cl(5)	2.5173(15)
Sb(02)-Cl(7)	2.8180(16)
Sb(02)-Cl(4)	2.8615(13)
N(1)-C(3)	1.511(4)
N(1)-C(1)	1.513(4)
N(1)-C(5)	1.515(4)
N(1)-H(1)	1.0000
N(2)-C(2)	1.487(4)
N(2)-H(2NA)	0.9100
N(2)-H(2NB)	0.9100
N(2)-H(2NC)	0.9100
N(3)-C(4)	1.480(4)
N(3)-H(3NA)	0.9100
N(3)-H(3NB)	0.9100
N(3)-H(3NC)	0.9100
N(4)-C(6)	1.480(4)
N(4)-H(4NA)	0.9100
N(4)-H(4NB)	0.9100
N(4)-H(4NC)	0.9100
C(1)-C(2)	1.523(5)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.524(5)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-H(4A)	0.9900

C(4)-H(4B)	0.9900
C(5)-C(6)	1.523(5)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
O(1)-H(1OA)	0.827(19)
O(1)-H(1OB)	0.8290
O(2)-H(2OA)	0.829(19)
O(2)-H(2OB)	0.8299

Cl(2)-Sb(01)-Cl(2)#1	180.0
Cl(2)-Sb(01)-Cl(3)	90.09(4)
Cl(2)#1-Sb(01)-Cl(3)	89.91(4)
Cl(2)-Sb(01)-Cl(3)#1	89.91(4)
Cl(2)#1-Sb(01)-Cl(3)#1	90.09(4)
Cl(3)-Sb(01)-Cl(3)#1	180.00(5)
Cl(2)-Sb(01)-Cl(1)	93.22(4)
Cl(2)#1-Sb(01)-Cl(1)	86.78(4)
Cl(3)-Sb(01)-Cl(1)	89.79(5)
Cl(3)#1-Sb(01)-Cl(1)	90.21(6)
Cl(2)-Sb(01)-Cl(1)#1	86.78(4)
Cl(2)#1-Sb(01)-Cl(1)#1	93.22(4)
Cl(3)-Sb(01)-Cl(1)#1	90.21(6)
Cl(3)#1-Sb(01)-Cl(1)#1	89.79(5)
Cl(1)-Sb(01)-Cl(1)#1	180.0
Cl(8)-Sb(02)-Cl(6)	92.00(4)
Cl(8)-Sb(02)-Cl(5)	90.38(5)
Cl(6)-Sb(02)-Cl(5)	87.12(5)
Cl(8)-Sb(02)-Cl(7)	91.54(5)
Cl(6)-Sb(02)-Cl(7)	86.96(5)
Cl(5)-Sb(02)-Cl(7)	173.84(3)
Cl(8)-Sb(02)-Cl(4)	90.38(4)
Cl(6)-Sb(02)-Cl(4)	176.70(3)
Cl(5)-Sb(02)-Cl(4)	90.58(5)
Cl(7)-Sb(02)-Cl(4)	95.26(5)
C(3)-N(1)-C(1)	110.7(3)
C(3)-N(1)-C(5)	110.7(3)

C(1)-N(1)-C(5)	111.3(3)
C(3)-N(1)-H(1)	108.0
C(1)-N(1)-H(1)	108.0
C(5)-N(1)-H(1)	108.0
C(2)-N(2)-H(2NA)	109.5
C(2)-N(2)-H(2NB)	109.5
H(2NA)-N(2)-H(2NB)	109.5
C(2)-N(2)-H(2NC)	109.5
H(2NA)-N(2)-H(2NC)	109.5
H(2NB)-N(2)-H(2NC)	109.5
C(4)-N(3)-H(3NA)	109.5
C(4)-N(3)-H(3NB)	109.5
H(3NA)-N(3)-H(3NB)	109.5
C(4)-N(3)-H(3NC)	109.5
H(3NA)-N(3)-H(3NC)	109.5
H(3NB)-N(3)-H(3NC)	109.5
C(6)-N(4)-H(4NA)	109.5
C(6)-N(4)-H(4NB)	109.5
H(4NA)-N(4)-H(4NB)	109.5
C(6)-N(4)-H(4NC)	109.5
H(4NA)-N(4)-H(4NC)	109.5
H(4NB)-N(4)-H(4NC)	109.5
N(1)-C(1)-C(2)	110.5(3)
N(1)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1A)	109.5
N(1)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	108.1
N(2)-C(2)-C(1)	109.6(3)
N(2)-C(2)-H(2A)	109.7
C(1)-C(2)-H(2A)	109.7
N(2)-C(2)-H(2B)	109.7
C(1)-C(2)-H(2B)	109.7
H(2A)-C(2)-H(2B)	108.2
N(1)-C(3)-C(4)	109.8(3)
N(1)-C(3)-H(3A)	109.7
C(4)-C(3)-H(3A)	109.7
N(1)-C(3)-H(3B)	109.7

C(4)-C(3)-H(3B)	109.7
H(3A)-C(3)-H(3B)	108.2
N(3)-C(4)-C(3)	108.8(3)
N(3)-C(4)-H(4A)	109.9
C(3)-C(4)-H(4A)	109.9
N(3)-C(4)-H(4B)	109.9
C(3)-C(4)-H(4B)	109.9
H(4A)-C(4)-H(4B)	108.3
N(1)-C(5)-C(6)	109.5(3)
N(1)-C(5)-H(5A)	109.8
C(6)-C(5)-H(5A)	109.8
N(1)-C(5)-H(5B)	109.8
C(6)-C(5)-H(5B)	109.8
H(5A)-C(5)-H(5B)	108.2
N(4)-C(6)-C(5)	109.9(3)
N(4)-C(6)-H(6A)	109.7
C(5)-C(6)-H(6A)	109.7
N(4)-C(6)-H(6B)	109.7
C(5)-C(6)-H(6B)	109.7
H(6A)-C(6)-H(6B)	108.2
H(1OA)-O(1)-H(1OB)	118.2
H(2OA)-O(2)-H(2OB)	117.8

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z+2

Table S5. Torsion angles [°] for **1** tris Sb Green.

C(3)-N(1)-C(1)-C(2)	-82.1(3)
C(5)-N(1)-C(1)-C(2)	154.4(3)
N(1)-C(1)-C(2)-N(2)	178.8(3)
C(1)-N(1)-C(3)-C(4)	150.3(3)
C(5)-N(1)-C(3)-C(4)	-85.7(3)
N(1)-C(3)-C(4)-N(3)	176.6(3)
C(3)-N(1)-C(5)-C(6)	153.6(3)
C(1)-N(1)-C(5)-C(6)	-82.8(3)
N(1)-C(5)-C(6)-N(4)	174.2(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z+2

Table S6. Crystal data and structure refinement for **2** tris Sb Red.

Identification code	TrisSbClRed_0m	
Empirical formula	C6 H25 Cl7 N4 O1.50 Sb	
Formula weight	547.20	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 10.3972(5) Å	α= 90°.
	b = 15.6011(8) Å	β= 95.622(2)°.
	c = 12.0441(6) Å	γ = 90°.
Volume	1944.25(17) Å^3	
Z	4	
Density (calculated)	1.869 Mg/m^3	
Absorption coefficient	2.382 mm^{-1}	
F(000)	1084	
Crystal size	0.400 x 0.210 x 0.090 mm^3	
Theta range for data collection	2.362 to 29.995°.	
Index ranges	-14<=h<=14, -21<=k<=21, -16<=l<=16	
Reflections collected	39790	
Independent reflections	11149 [R(int) = 0.0636]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.814 and 0.449	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11149 / 7 / 377	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0309, wR2 = 0.0791	
R indices (all data)	R1 = 0.0322, wR2 = 0.0803	
Absolute structure parameter	0.490(15)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.561 and -0.804 e.Å^{-3}	

Table S7. Bond lengths [Å] and angles [°] for **2** tris Sb Red.

Sb(1)-Cl(4)	2.4481(11)
Sb(1)-Cl(1)	2.4535(10)
Sb(1)-Cl(5)	2.5314(10)
Sb(1)-Cl(3)	2.6982(10)
Sb(1)-Cl(2)	2.8878(10)
N(1)-C(1)	1.504(5)
N(1)-C(3)	1.508(5)
N(1)-C(5)	1.515(5)
N(1)-H(1)	1.0000
N(2)-C(2)	1.494(5)
N(2)-H(2NA)	0.9100
N(2)-H(2NB)	0.9100
N(2)-H(2NC)	0.9100
N(3)-C(4)	1.490(5)
N(3)-H(3NA)	0.9100
N(3)-H(3NB)	0.9100
N(3)-H(3NC)	0.9100
N(4)-C(6)	1.490(5)
N(4)-H(4NA)	0.9100
N(4)-H(4NB)	0.9100
N(4)-H(4NC)	0.9100
C(1)-C(2)	1.533(6)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.523(6)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.504(5)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900

Sb(2)-Cl(11)	2.4339(10)
Sb(2)-Cl(8)	2.4495(11)
Sb(2)-Cl(9)	2.5890(10)
Sb(2)-Cl(7)	2.6674(10)
N(5)-C(11)	1.509(5)
N(5)-C(9)	1.512(5)
N(5)-C(7)	1.512(5)
N(5)-H(5)	1.0000
N(6)-C(8)	1.485(5)
N(6)-H(6NA)	0.9100
N(6)-H(6NB)	0.9100
N(6)-H(6NC)	0.9100
N(7)-C(10)	1.486(5)
N(7)-H(7NA)	0.9100
N(7)-H(7NB)	0.9100
N(7)-H(7NC)	0.9100
N(8)-C(12)	1.486(5)
N(8)-H(8NA)	0.9100
N(8)-H(8NB)	0.9100
N(8)-H(8NC)	0.9100
C(7)-C(8)	1.522(5)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.523(6)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.525(6)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
O(1)-H(1OA)	0.83(2)
O(1)-H(1OB)	0.8398
O(2)-H(2OA)	0.82(2)

O(2)-H(2OB)	0.8433
O(3)-H(3OA)	0.86(2)
O(3)-H(3OB)	0.8273

Cl(4)-Sb(1)-Cl(1)	88.97(4)
Cl(4)-Sb(1)-Cl(5)	89.37(4)
Cl(1)-Sb(1)-Cl(5)	88.11(4)
Cl(4)-Sb(1)-Cl(3)	85.14(3)
Cl(1)-Sb(1)-Cl(3)	86.81(3)
Cl(5)-Sb(1)-Cl(3)	172.58(4)
Cl(4)-Sb(1)-Cl(2)	80.49(3)
Cl(1)-Sb(1)-Cl(2)	169.04(3)
Cl(5)-Sb(1)-Cl(2)	94.74(3)
Cl(3)-Sb(1)-Cl(2)	89.28(3)
C(1)-N(1)-C(3)	110.3(3)
C(1)-N(1)-C(5)	108.3(3)
C(3)-N(1)-C(5)	112.2(3)
C(1)-N(1)-H(1)	108.7
C(3)-N(1)-H(1)	108.7
C(5)-N(1)-H(1)	108.7
C(2)-N(2)-H(2NA)	109.5
C(2)-N(2)-H(2NB)	109.5
H(2NA)-N(2)-H(2NB)	109.5
C(2)-N(2)-H(2NC)	109.5
H(2NA)-N(2)-H(2NC)	109.5
H(2NB)-N(2)-H(2NC)	109.5
C(4)-N(3)-H(3NA)	109.5
C(4)-N(3)-H(3NB)	109.5
H(3NA)-N(3)-H(3NB)	109.5
C(4)-N(3)-H(3NC)	109.5
H(3NA)-N(3)-H(3NC)	109.5
H(3NB)-N(3)-H(3NC)	109.5
C(6)-N(4)-H(4NA)	109.5
C(6)-N(4)-H(4NB)	109.5
H(4NA)-N(4)-H(4NB)	109.5
C(6)-N(4)-H(4NC)	109.5
H(4NA)-N(4)-H(4NC)	109.5
H(4NB)-N(4)-H(4NC)	109.5

N(1)-C(1)-C(2)	110.2(3)
N(1)-C(1)-H(1A)	109.6
C(2)-C(1)-H(1A)	109.6
N(1)-C(1)-H(1B)	109.6
C(2)-C(1)-H(1B)	109.6
H(1A)-C(1)-H(1B)	108.1
N(2)-C(2)-C(1)	108.4(3)
N(2)-C(2)-H(2A)	110.0
C(1)-C(2)-H(2A)	110.0
N(2)-C(2)-H(2B)	110.0
C(1)-C(2)-H(2B)	110.0
H(2A)-C(2)-H(2B)	108.4
N(1)-C(3)-C(4)	114.0(3)
N(1)-C(3)-H(3A)	108.8
C(4)-C(3)-H(3A)	108.8
N(1)-C(3)-H(3B)	108.8
C(4)-C(3)-H(3B)	108.8
H(3A)-C(3)-H(3B)	107.6
N(3)-C(4)-C(3)	111.9(3)
N(3)-C(4)-H(4A)	109.2
C(3)-C(4)-H(4A)	109.2
N(3)-C(4)-H(4B)	109.2
C(3)-C(4)-H(4B)	109.2
H(4A)-C(4)-H(4B)	107.9
C(6)-C(5)-N(1)	111.6(3)
C(6)-C(5)-H(5A)	109.3
N(1)-C(5)-H(5A)	109.3
C(6)-C(5)-H(5B)	109.3
N(1)-C(5)-H(5B)	109.3
H(5A)-C(5)-H(5B)	108.0
N(4)-C(6)-C(5)	109.0(3)
N(4)-C(6)-H(6A)	109.9
C(5)-C(6)-H(6A)	109.9
N(4)-C(6)-H(6B)	109.9
C(5)-C(6)-H(6B)	109.9
H(6A)-C(6)-H(6B)	108.3
Cl(11)-Sb(2)-Cl(8)	87.11(4)
Cl(11)-Sb(2)-Cl(9)	90.17(4)

Cl(8)-Sb(2)-Cl(9)	90.62(4)
Cl(11)-Sb(2)-Cl(7)	91.11(4)
Cl(8)-Sb(2)-Cl(7)	88.03(4)
Cl(9)-Sb(2)-Cl(7)	178.09(3)
C(11)-N(5)-C(9)	113.4(3)
C(11)-N(5)-C(7)	109.6(3)
C(9)-N(5)-C(7)	109.5(3)
C(11)-N(5)-H(5)	108.1
C(9)-N(5)-H(5)	108.1
C(7)-N(5)-H(5)	108.1
C(8)-N(6)-H(6NA)	109.5
C(8)-N(6)-H(6NB)	109.5
H(6NA)-N(6)-H(6NB)	109.5
C(8)-N(6)-H(6NC)	109.5
H(6NA)-N(6)-H(6NC)	109.5
H(6NB)-N(6)-H(6NC)	109.5
C(10)-N(7)-H(7NA)	109.5
C(10)-N(7)-H(7NB)	109.5
H(7NA)-N(7)-H(7NB)	109.5
C(10)-N(7)-H(7NC)	109.5
H(7NA)-N(7)-H(7NC)	109.5
H(7NB)-N(7)-H(7NC)	109.5
C(12)-N(8)-H(8NA)	109.5
C(12)-N(8)-H(8NB)	109.5
H(8NA)-N(8)-H(8NB)	109.5
C(12)-N(8)-H(8NC)	109.5
H(8NA)-N(8)-H(8NC)	109.5
H(8NB)-N(8)-H(8NC)	109.5
N(5)-C(7)-C(8)	110.5(3)
N(5)-C(7)-H(7A)	109.6
C(8)-C(7)-H(7A)	109.6
N(5)-C(7)-H(7B)	109.6
C(8)-C(7)-H(7B)	109.6
H(7A)-C(7)-H(7B)	108.1
N(6)-C(8)-C(7)	107.8(3)
N(6)-C(8)-H(8A)	110.2
C(7)-C(8)-H(8A)	110.2
N(6)-C(8)-H(8B)	110.2

C(7)-C(8)-H(8B)	110.2
H(8A)-C(8)-H(8B)	108.5
N(5)-C(9)-C(10)	111.8(3)
N(5)-C(9)-H(9A)	109.3
C(10)-C(9)-H(9A)	109.3
N(5)-C(9)-H(9B)	109.3
C(10)-C(9)-H(9B)	109.3
H(9A)-C(9)-H(9B)	107.9
N(7)-C(10)-C(9)	108.0(3)
N(7)-C(10)-H(10A)	110.1
C(9)-C(10)-H(10A)	110.1
N(7)-C(10)-H(10B)	110.1
C(9)-C(10)-H(10B)	110.1
H(10A)-C(10)-H(10B)	108.4
N(5)-C(11)-C(12)	108.9(3)
N(5)-C(11)-H(11A)	109.9
C(12)-C(11)-H(11A)	109.9
N(5)-C(11)-H(11B)	109.9
C(12)-C(11)-H(11B)	109.9
H(11A)-C(11)-H(11B)	108.3
N(8)-C(12)-C(11)	111.6(3)
N(8)-C(12)-H(12A)	109.3
C(11)-C(12)-H(12A)	109.3
N(8)-C(12)-H(12B)	109.3
C(11)-C(12)-H(12B)	109.3
H(12A)-C(12)-H(12B)	108.0
H(1OA)-O(1)-H(1OB)	117.0
H(2OA)-O(2)-H(2OB)	117.4
H(3OA)-O(3)-H(3OB)	115.2

Symmetry transformations used to generate equivalent atoms:

Table S8. Torsion angles [°] for **2** tris Sb Red.

C(3)-N(1)-C(1)-C(2)	159.9(3)
C(5)-N(1)-C(1)-C(2)	-77.0(4)
N(1)-C(1)-C(2)-N(2)	-177.0(3)

C(1)-N(1)-C(3)-C(4)	-71.2(4)
C(5)-N(1)-C(3)-C(4)	168.1(3)
N(1)-C(3)-C(4)-N(3)	-90.3(4)
C(1)-N(1)-C(5)-C(6)	165.4(4)
C(3)-N(1)-C(5)-C(6)	-72.7(4)
N(1)-C(5)-C(6)-N(4)	-169.8(3)
C(11)-N(5)-C(7)-C(8)	-156.8(3)
C(9)-N(5)-C(7)-C(8)	78.3(4)
N(5)-C(7)-C(8)-N(6)	175.7(3)
C(11)-N(5)-C(9)-C(10)	74.3(4)
C(7)-N(5)-C(9)-C(10)	-163.0(3)
N(5)-C(9)-C(10)-N(7)	162.6(3)
C(9)-N(5)-C(11)-C(12)	-157.8(3)
C(7)-N(5)-C(11)-C(12)	79.6(4)
N(5)-C(11)-C(12)-N(8)	-156.7(3)

Symmetry transformations used to generate equivalent atoms:

Table S9: List of strong intermolecular interactions for the products **1,2,3** evaluated in detail using PLATON.

Sr No.	**Entry**	**D-H⋯A**	**D-H (Å)**	**H⋯A (Å)**	**D⋯A/ Cg⋯Cg (Å)**	**D-H⋯A /α (º)**
1	N1-H1⋯Cl9	1	2.15	3.1463	177	x,y,1+z
2	N2-H2NA⋯Cl7	0.91	2.44	3.1794	138	-1+x,y,z
3	N2-H2NB⋯Cl9	0.91	2.36	3.2215	158	1-x,1-y,1-z
5	N3-H3NA⋯Cl4	0.91	2.4	3.1735	143	2-x,1-y,1-z
6	N3-H3NB⋯Cl9	0.91	2.48	3.2864	147	2-x,2-y,1-z
7	N3-H3NC⋯Cl3	0.91	2.55	3.3115	142	x,y,z
8	N4-H4NA⋯Cl6	0.91	2.5	3.2374	138	x,y,z
9	N4-H4NA⋯Cl7	0.91	2.77	3.3155	120	x,y,z
10	N4-H4NB⋯Cl9	0.91	2.35	3.2284	161	2-x,1-y,1-z
11	N4-H4NC⋯Cl3	0.91	2.38	3.1305	139	1+x,y,z
12	O1-H1OA⋯Cl5	0.83	2.52	3.2765	152	x,1+y,z
13	O1-H1OB⋯Cl8	0.83	2.74	3.4295	142	1-x,1-y,1-z
14	O2-H2OA⋯Cl7	0.83	2.21	3.0135	163	-1+x,y,z

15	O2-H2OB···O1	0.83	1.86	2.6396	156	x,y,z
16	C1-H1A···Cl1	0.99	2.61	3.3815	134	x,-1+y,z
17	C3-H3A···Cl3	0.99	2.52	3.3345	139	x,y,z
18	C3-H3B···Cl4	0.99	2.8	3.5155	130	2-x,1-y,1-z
19	C4-H4B···Cl2	0.99	2.62	3.6035	173	1+x,y,z
20	C5-H5A···Cl2	0.99	2.69	3.4995	139	1+x,y,z
21	C6-H6B···Cl1	0.99	2.67	3.6455	169	x,-1+y,z

Table for **1 Tris Sb Green**: D-H = Donor- Hydrogen bond length in Angstrom (Å), H···A = Hydrogen···Acceptor bond length in Angstrom (Å), D···A = Donor···Acceptor bond length in Angstrom (Å), D-H···A = bond angle in degrees (°), Cg···Cg = Distance between ring Centroids in Angstrom (Å), α= Dihedral angle between planes of two aromatic rings in degrees (°)

Sr No.	**Entry**	**D-H···A**	**D-H (Å)**	**H···A (Å)**	**D···A/ Cg···Cg (Å)**	**D-H···A /α (º)**
1	N1-H1···Cl14	1	2.08	3.0754	172	x,y,z
2	N2-H2NA···Cl7	0.91	2.38	3.1474	141	1-x,-1/2+y,1-z
3	N2-H2NB···O1	0.91	1.85	2.7545	170	x,y,z
4	N2-H2NC···Cl4	0.91	2.45	3.2233	143	1-x,1/2+y,1-z
6	N3-H3NA···Cl2	0.91	2.45	3.2143	142	2-x,1/2+y,1-z
7	N5-H5···Cl13	1	2.11	3.1024	173	-1+x,y,-1+z
8	N3-H3NB···Cl10	0.91	2.25	3.1574	171	x,y,z
9	N3-H3NC···Cl14	0.91	2.34	3.1933	156	x,y,z
10	N4-H4NA···Cl13	0.91	2.37	3.2074	153	x,y,z
11	N4-H4NB···O1	0.91	2.12	2.8755	140	1+x,y,z
12	N4-H4NC···Cl10	0.91	2.32	3.1953	161	1-x,-1/2+y,1-z
13	N6-H6NA···Cl8	0.91	2.43	3.2733	154	-x,-1/2+y,-z
14	N6-H6NB···O2	0.91	1.86	2.7465	164	-1+x,y,z
15	N6-H6NC···Cl5	0.91	2.69	3.3394	129	-1+x,y,z
17	N7-H7NA···Cl6	0.91	2.51	3.3843	160	1-x,1/2+y,1-z
18	N7-H7NB···O2	0.91	2.03	2.8614	151	x,y,z
19	N7-H7NC···Cl14	0.91	2.39	3.2114	150	x,y,z
21	N8-H8NA···Cl12	0.91	2.2	3.1033	174	1-x,-1/2+y,-z
22	N8-H8NB···Cl6	0.91	2.31	3.1554	154	-1+x,y,-1+z
24	O1-H1OA···Cl3	0.83	2.45	3.2733	171	1-x,1/2+y,1-z
25	O1-H1OB···Cl2	0.84	2.24	3.0773	171	-1+x,y,z
26	O2-H2OA···Cl12	0.82	2.28	3.0414	154	x,y,z
27	O2-H2OB···O3	0.84	1.97	2.7615	157	x,y,z
28	O3-H3OA···Cl6	0.86	2.46	3.2623	156	2-x,1/2+y,1-z
29	O3-H3OB···Cl7	0.83	2.57	3.3734	165	x,y,z
32	C3-H3B···Cl12	0.99	2.74	3.5714	142	x,y,1+z
33	C5-H5A···Cl12	0.99	2.59	3.4774	149	x,y,1+z
34	C5-H5B···Cl10	0.99	2.74	3.5745	143	1-x,-1/2+y,1-z
38	C9-H9A···Cl2	0.99	2.71	3.5904	149	-1+x,y,z
39	C11-H11A···Cl4	0.99	2.79	3.6805	149	-1+x,y,z

40	C11-H11B···Cl7	0.99	2.79	3.5515	135	1-x,-1/2+y,-z

Table For **2 Tris Sb Red**: D-H = Donor- Hydrogen bond length in Angstrom (Å), H···A = Hydrogen···Acceptor bond length in Angstrom (Å), D···A = Donor···Acceptor bond length in Angstrom (Å), D-H···A = bond angle in degrees (°), Cg···Cg = Distance between ring Centroids in Angstrom (Å), α= Dihedral angle between planes of two aromatic rings in degrees (°)

Sr No.	**Entry**	**D-H···A**	**D-H (Å)**	**H···A (Å)**	**D···A/ Cg···Cg (Å)**	**D-H···A /α (º)**
1	N1-H···Cl24	0.98	2.17	3.1488	179	1-x,1-y,-z
2	N2-H2A···O3	0.89	1.94	2.81713	169	x,y,z
3	N2-H2B···Cl24	0.89	2.51	3.2949	148	1+x,-1+y,z
4	N2-H2C···Cl22	0.89	2.31	3.1479	156	1+x,-1+y,z
5	N3-H3A···Cl3	0.89	2.52	3.35410	156	1+x,-1+y,z
6	N3-H3B···Cl24	0.89	2.37	3.18810	153	x,-1+y,z
7	N3-H3C···Cl14	0.89	2.71	3.4179	137	x,y,z
8	N3-H3C···Cl23	0.89	2.7	3.3179	127	x,-1+y,z
9	N4-H4A···Cl3	0.89	2.57	3.30211	141	x,y,z
10	N4-H4B···Cl24	0.89	2.42	3.2539	156	x,y,z
11	N4-H4C···Cl23	0.89	2.47	3.26510	149	x,y,z
12	N5-H5···Cl22	0.98	2.11	3.0818	171	x,y,z
13	N6-H6A···Cl22	0.89	2.25	3.08512	155	x,y,z
14	N6-H6B···Cl23	0.89	2.29	3.17011	168	x,y,z
15	N6-H6C···Cl17	0.89	2.41	3.23712	155	x,1+y,z
16	N7-H7A···Cl18	0.89	2.54	3.32110	147	x,y,z
17	N7-H7B···Cl23	0.89	2.36	3.22511	163	-1+x,y,z
18	N7-H7C···Cl21	0.89	2.25	3.13510	170	-1+x,y,z
20	N8-H8A···Cl16	0.89	2.44	3.2069	144	-1+x,1+y,z
21	N8-H8B···Cl21	0.89	2.26	3.12610	165	-1+x,1+y,z
22	N8-H8C···Cl10	0.89	2.31	3.1999	174	-1+x,y,z
23	N9-H9···Cl19	0.98	2.05	2.9928	161	x,y,z
24	N10-H10A···O4	0.89	1.88	2.769	167	1+x,y,z
25	N10-H10A···O4	0.89	1.96	2.8110	159	1+x,y,z
26	N10-H10B···Cl12	0.89	2.68	3.38611	137	x,-1+y,z
27	N10-H10C···O2	0.89	2.01	2.87417	164	1+x,y,z
28	N11-H11A···Cl11	0.89	2.46	3.26211	151	-1+x,y,z
29	N11-H11B···Cl20	0.89	2.24	3.12210	175	x,y,z
30	N11-H11C···Cl13	0.89	2.31	3.1899	168	x,y,z
31	N12-H12A···Cl12	0.89	2.38	3.22512	159	-1+x,y,z
32	N12-H12B···Cl17	0.89	2.57	3.2639	135	x,1+y,z
34	N12-H12C···Cl20	0.89	2.46	3.1809	139	x,1+y,z
35	N13-H13···Cl25	0.98	2.16	3.1417	176	1-x,1-y,1-z
36	N14-H14A···Cl4	0.89	2.61	3.153	120	1-x,1-y,1-z
38	N14-H14B···Cl25	0.89	2.41	3.23710	155	x,1+y,z
40	N14-H14C···O1	0.89	1.87	2.713	154	x,y,z
41	N14-H14C···O1	0.89	2.12	2.843	137	x,y,z
42	N15-H15A···Cl6	0.89	2.37	3.132	143	x,y,z

43	N15-H15A···Cl6	0.89	2.55	3.213	132	x,y,z
44	N15-H15B···Cl25	0.89	2.43	3.29510	164	x,y,z
45	N15-H15C···Cl19	0.89	2.35	3.09311	140	x,y,z
46	N16-H16A···Cl6	0.89	2.65	3.442	148	x,1+y,z
49	N16-H16B···Cl25	0.89	2.47	3.25910	149	-1+x,1+y,z
50	N16-H16C···Cl9	0.89	2.64	3.40510	145	-1+x,y,z
51	C1-H1E···Cl2	0.97	2.82	3.5249	131	1-x,1-y,-z
52	C3-H3D···Cl3	0.97	2.65	3.5079	148	1+x,-1+y,z
53	C3-H3E···Cl16	0.97	2.68	3.5339	147	x,y,z
54	C4-H4D···Cl1	0.97	2.69	3.60112	156	-x,1-y,-z
55	C4-H4E···Cl1	0.97	2.78	3.57510	139	1+x,-1+y,z
56	C6-H6D···Cl2	0.97	2.64	3.60312	172	1-x,1-y,-z
57	C6-H6E···Cl2	0.97	2.79	3.61410	144	x,y,z
58	C8-H8E···Cl15	0.97	2.76	3.72512	176	x,y,z
59	C9-H9E···Cl15	0.97	2.79	3.5279	134	x,y,z
60	C13-H13E···Cl21	0.97	2.71	3.5299	142	x,y,z
62	C15-H15D···Cl21	0.97	2.72	3.63510	157	x,y,z
63	C16-H16D···Cl10	0.97	2.68	3.50011	143	x,-1+y,z
65	C17-H17D···Cl7	0.97	2.8	3.72212	160	x,y,z
66	C19-H19D···Cl5	0.97	2.69	3.492	140	1-x,1-y,1-z
67	C19-H19D···Cl5	0.97	2.64	3.383	133	1-x,1-y,1-z
68	C20-H20D···Cl6	0.97	2.75	3.703	168	x,1+y,z
69	C21-H21E···Cl4	0.97	2.58	3.373	139	-x,1-y,1-z
70	C22-H22D···Cl5	0.97	2.74	3.713	176	1-x,1-y,1-z
71	C22-H22D···Cl5	0.97	2.67	3.634	174	1-x,1-y,1-z
72	C23-H23E···Cl6	0.97	2.6	3.452	146	x,1+y,z
73	C23-H23E···Cl6	0.97	2.61	3.423	141	x,1+y,z
74	C24-H24D···Cl4	0.97	2.71	3.653	165	-x,1-y,1-z
75	C24-H24D···Cl4	0.97	2.68	3.602	159	-x,1-y,1-z

Table for **3 Tris Sb Yellow:** D-H = Donor- Hydrogen bond length in Angstrom (Å), H···A = Hydrogen···Acceptor bond length in Angstrom (Å), D···A = Donor···Acceptor bond length in Angstrom (Å), D-H···A = bond angle in degrees (°), Cg···Cg = Distance between ring Centroids in Angstrom (Å), α= Dihedral angle between planes of two aromatic rings in degrees (°)

Table S10: Lifetime (μs) components and their relative weightages (%) for 3 tris Sb Yellow

3 tris Sb Yellow		
Wavelength (nm)	**Life time (μs) (at room temp.)**	**Relative %**
480	5.18 92.05	82.59 17.41
530	5.25 87.20	84.97 15.03
580	5.20 84.6	83.90 16.10
630	5.28 89.39	84.68 15.32
680	5.52 93.51	89.46 10.54
730	5.67 97.91	91.37 8.63

Table S11. Crystal data and structure refinement for **3** tris Sb Yellow.

Identification code	**3** tris Sb Yellow	
Empirical formula	C24 H88 Cl25 N16 O4 Sb3	
Formula weight	1916.60	
Temperature	301(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.229(4) Å	α= 86.054(17)°.
	b = 10.266(4) Å	β= 88.191(17)°.
	c = 40.365(16) Å	γ = 60.550(15)°.
Volume	3682(3) $Å^3$	
Z	2	
Density (calculated)	1.729 Mg/m^3	
Absorption coefficient	2.041 mm^{-1}	
F(000)	1908	
Crystal size	0.485 x 0.345 x 0.100 mm^3	
Theta range for data collection	2.283 to 25.999°.	
Index ranges	-12<=h<=12, -12<=k<=12, -49<=l<=49	

Reflections collected	68358
Independent reflections	13650 [R(int) = 0.0706]
Completeness to theta = 25.242°	93.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.822 and 0.438
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13650 / 0 / 665
Goodness-of-fit on F^2	1.332
Final R indices [I>2sigma(I)]	R1 = 0.0765, wR2 = 0.2054
R indices (all data)	R1 = 0.0781, wR2 = 0.2063
Extinction coefficient	0.0090(8)
Largest diff. peak and hole	1.440 and -1.531 e.$Å^{-3}$

Table S12. Bond lengths [Å] and angles [°] for **3** tris Sb Yellow.

N(1)-C(1)	1.505(10)
N(1)-C(3)	1.516(11)
N(1)-C(5)	1.519(11)
N(1)-H(1)	0.9800
N(2)-C(2)	1.485(12)
N(2)-H(2A)	0.8900
N(2)-H(2B)	0.8900
N(2)-H(2C)	0.8900
N(3)-C(4)	1.486(12)
N(3)-H(3A)	0.8900
N(3)-H(3B)	0.8900
N(3)-H(3C)	0.8900
N(4)-C(6)	1.494(12)
N(4)-H(4A)	0.8900
N(4)-H(4B)	0.8900
N(4)-H(4C)	0.8900
C(1)-C(2)	1.513(13)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-H(2D)	0.9700
C(2)-H(2E)	0.9700

C(3)-C(4)	1.513(12)
C(3)-H(3D)	0.9700
C(3)-H(3E)	0.9700
C(4)-H(4D)	0.9700
C(4)-H(4E)	0.9700
C(5)-C(6)	1.506(12)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
N(5)-C(7)	1.512(11)
N(5)-C(11)	1.519(11)
N(5)-C(9)	1.521(12)
N(5)-H(5)	0.9800
N(6)-C(8)	1.485(14)
N(6)-H(6C)	0.8900
N(6)-H(6D)	0.8900
N(6)-H(6E)	0.8900
N(7)-C(10)	1.480(13)
N(7)-H(7A)	0.8900
N(7)-H(7B)	0.8900
N(7)-H(7C)	0.8900
N(8)-C(12)	1.483(14)
N(8)-H(8A)	0.8900
N(8)-H(8B)	0.8900
N(8)-H(8C)	0.8900
C(7)-C(8)	1.522(13)
C(7)-H(7D)	0.9700
C(7)-H(7E)	0.9700
C(8)-H(8D)	0.9700
C(8)-H(8E)	0.9700
C(9)-C(10)	1.530(13)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-C(12)	1.503(13)
C(11)-H(11A)	0.9700

C(11)-H(11B)	0.9700
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
N(9)-C(17)	1.490(13)
N(9)-C(15)	1.513(11)
N(9)-C(13)	1.515(12)
N(9)-H(9)	0.9800
N(10)-C(14)	1.474(12)
N(10)-H(10C)	0.8900
N(10)-H(10D)	0.8900
N(10)-H(10E)	0.8900
N(11)-C(16)	1.475(12)
N(11)-H(11C)	0.8900
N(11)-H(11D)	0.8900
N(11)-H(11E)	0.8900
N(12)-C(18)	1.470(13)
N(12)-H(12C)	0.8900
N(12)-H(12D)	0.8900
N(12)-H(12E)	0.8900
C(13)-C(14)	1.518(14)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-C(16)	1.531(13)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.504(13)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
N(13)-C(23)	1.505(11)
N(13)-C(21)	1.511(11)
N(13)-C(19)	1.519(11)
N(13)-H(13)	0.9800

N(14)-C(20)	1.479(12)
N(14)-H(14C)	0.8900
N(14)-H(14D)	0.8900
N(14)-H(14E)	0.8900
N(15)-C(22)	1.480(13)
N(15)-H(15C)	0.8900
N(15)-H(15D)	0.8900
N(15)-H(15E)	0.8900
N(16)-C(24)	1.468(13)
N(16)-H(16C)	0.8900
N(16)-H(16D)	0.8900
N(16)-H(16E)	0.8900
C(19)-C(20)	1.517(13)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(21)-C(22)	1.523(13)
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-C(24)	1.520(13)
C(23)-H(23A)	0.9700
C(23)-H(23B)	0.9700
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
Sb(1)-Cl(1)	2.637(3)
Sb(1)-Cl(1)#1	2.637(3)
Sb(1)-Cl(2)	2.638(2)
Sb(1)-Cl(2)#1	2.638(2)
Sb(1)-Cl(3)#1	2.661(3)
Sb(1)-Cl(3)	2.661(3)
Sb(2)-Cl(4)	2.622(3)
Sb(2)-Cl(4)#2	2.622(3)
Sb(2)-Cl(5)#2	2.624(3)
Sb(2)-Cl(5)	2.625(3)
Sb(2)-Cl(6)	2.650(4)

Sb(2)-Cl(6)#2	2.650(4)
Sb(3)-Cl(7)	2.489(3)
Sb(3)-Cl(8)	2.526(3)
Sb(3)-Cl(11)	2.632(3)
Sb(3)-Cl(9)	2.680(3)
Sb(3)-Cl(10)	2.826(3)
Sb(4)-Cl(14)	2.452(3)
Sb(4)-Cl(16)	2.619(3)
Sb(4)-Cl(18)	2.632(3)
Sb(4)-Cl(15)	2.634(3)
Sb(4)-Cl(17)	2.663(3)

C(1)-N(1)-C(3)	109.0(6)
C(1)-N(1)-C(5)	110.7(7)
C(3)-N(1)-C(5)	111.8(6)
C(1)-N(1)-H(1)	108.4
C(3)-N(1)-H(1)	108.4
C(5)-N(1)-H(1)	108.4
C(2)-N(2)-H(2A)	109.5
C(2)-N(2)-H(2B)	109.5
H(2A)-N(2)-H(2B)	109.5
C(2)-N(2)-H(2C)	109.5
H(2A)-N(2)-H(2C)	109.5
H(2B)-N(2)-H(2C)	109.5
C(4)-N(3)-H(3A)	109.5
C(4)-N(3)-H(3B)	109.5
H(3A)-N(3)-H(3B)	109.5
C(4)-N(3)-H(3C)	109.5
H(3A)-N(3)-H(3C)	109.5
H(3B)-N(3)-H(3C)	109.5
C(6)-N(4)-H(4A)	109.5
C(6)-N(4)-H(4B)	109.5
H(4A)-N(4)-H(4B)	109.5
C(6)-N(4)-H(4C)	109.5
H(4A)-N(4)-H(4C)	109.5
H(4B)-N(4)-H(4C)	109.5
N(1)-C(1)-C(2)	112.9(7)
N(1)-C(1)-H(1A)	109.0

C(2)-C(1)-H(1A)	109.0
N(1)-C(1)-H(1B)	109.0
C(2)-C(1)-H(1B)	109.0
H(1A)-C(1)-H(1B)	107.8
N(2)-C(2)-C(1)	109.6(8)
N(2)-C(2)-H(2D)	109.8
C(1)-C(2)-H(2D)	109.8
N(2)-C(2)-H(2E)	109.8
C(1)-C(2)-H(2E)	109.8
H(2D)-C(2)-H(2E)	108.2
C(4)-C(3)-N(1)	111.5(7)
C(4)-C(3)-H(3D)	109.3
N(1)-C(3)-H(3D)	109.3
C(4)-C(3)-H(3E)	109.3
N(1)-C(3)-H(3E)	109.3
H(3D)-C(3)-H(3E)	108.0
N(3)-C(4)-C(3)	109.9(7)
N(3)-C(4)-H(4D)	109.7
C(3)-C(4)-H(4D)	109.7
N(3)-C(4)-H(4E)	109.7
C(3)-C(4)-H(4E)	109.7
H(4D)-C(4)-H(4E)	108.2
C(6)-C(5)-N(1)	110.6(7)
C(6)-C(5)-H(5A)	109.5
N(1)-C(5)-H(5A)	109.5
C(6)-C(5)-H(5B)	109.5
N(1)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	108.1
N(4)-C(6)-C(5)	110.5(7)
N(4)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6A)	109.5
N(4)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	108.1
C(7)-N(5)-C(11)	111.1(7)
C(7)-N(5)-C(9)	111.9(7)
C(11)-N(5)-C(9)	109.6(7)
C(7)-N(5)-H(5)	108.0

C(11)-N(5)-H(5)	108.0
C(9)-N(5)-H(5)	108.0
C(8)-N(6)-H(6C)	109.5
C(8)-N(6)-H(6D)	109.5
H(6C)-N(6)-H(6D)	109.5
C(8)-N(6)-H(6E)	109.5
H(6C)-N(6)-H(6E)	109.5
H(6D)-N(6)-H(6E)	109.5
C(10)-N(7)-H(7A)	109.5
C(10)-N(7)-H(7B)	109.5
H(7A)-N(7)-H(7B)	109.5
C(10)-N(7)-H(7C)	109.5
H(7A)-N(7)-H(7C)	109.5
H(7B)-N(7)-H(7C)	109.5
C(12)-N(8)-H(8A)	109.5
C(12)-N(8)-H(8B)	109.5
H(8A)-N(8)-H(8B)	109.5
C(12)-N(8)-H(8C)	109.5
H(8A)-N(8)-H(8C)	109.5
H(8B)-N(8)-H(8C)	109.5
N(5)-C(7)-C(8)	115.5(8)
N(5)-C(7)-H(7D)	108.4
C(8)-C(7)-H(7D)	108.4
N(5)-C(7)-H(7E)	108.4
C(8)-C(7)-H(7E)	108.4
H(7D)-C(7)-H(7E)	107.5
N(6)-C(8)-C(7)	113.7(9)
N(6)-C(8)-H(8D)	108.8
C(7)-C(8)-H(8D)	108.8
N(6)-C(8)-H(8E)	108.8
C(7)-C(8)-H(8E)	108.8
H(8D)-C(8)-H(8E)	107.7
N(5)-C(9)-C(10)	111.1(7)
N(5)-C(9)-H(9A)	109.4
C(10)-C(9)-H(9A)	109.4
N(5)-C(9)-H(9B)	109.4
C(10)-C(9)-H(9B)	109.4
H(9A)-C(9)-H(9B)	108.0

N(7)-C(10)-C(9)	109.2(8)
N(7)-C(10)-H(10A)	109.8
C(9)-C(10)-H(10A)	109.8
N(7)-C(10)-H(10B)	109.8
C(9)-C(10)-H(10B)	109.8
H(10A)-C(10)-H(10B)	108.3
C(12)-C(11)-N(5)	111.8(7)
C(12)-C(11)-H(11A)	109.2
N(5)-C(11)-H(11A)	109.2
C(12)-C(11)-H(11B)	109.2
N(5)-C(11)-H(11B)	109.2
H(11A)-C(11)-H(11B)	107.9
N(8)-C(12)-C(11)	108.7(8)
N(8)-C(12)-H(12A)	110.0
C(11)-C(12)-H(12A)	110.0
N(8)-C(12)-H(12B)	110.0
C(11)-C(12)-H(12B)	110.0
H(12A)-C(12)-H(12B)	108.3
C(17)-N(9)-C(15)	112.0(7)
C(17)-N(9)-C(13)	110.8(7)
C(15)-N(9)-C(13)	115.3(8)
C(17)-N(9)-H(9)	106.0
C(15)-N(9)-H(9)	106.0
C(13)-N(9)-H(9)	106.0
C(14)-N(10)-H(10C)	109.5
C(14)-N(10)-H(10D)	109.5
H(10C)-N(10)-H(10D)	109.5
C(14)-N(10)-H(10E)	109.5
H(10C)-N(10)-H(10E)	109.5
H(10D)-N(10)-H(10E)	109.5
C(16)-N(11)-H(11C)	109.5
C(16)-N(11)-H(11D)	109.5
H(11C)-N(11)-H(11D)	109.5
C(16)-N(11)-H(11E)	109.5
H(11C)-N(11)-H(11E)	109.5
H(11D)-N(11)-H(11E)	109.5
C(18)-N(12)-H(12C)	109.5
C(18)-N(12)-H(12D)	109.5

H(12C)-N(12)-H(12D)	109.5
C(18)-N(12)-H(12E)	109.5
H(12C)-N(12)-H(12E)	109.5
H(12D)-N(12)-H(12E)	109.5
N(9)-C(13)-C(14)	112.3(8)
N(9)-C(13)-H(13A)	109.1
C(14)-C(13)-H(13A)	109.1
N(9)-C(13)-H(13B)	109.1
C(14)-C(13)-H(13B)	109.1
H(13A)-C(13)-H(13B)	107.9
N(10)-C(14)-C(13)	109.6(8)
N(10)-C(14)-H(14A)	109.7
C(13)-C(14)-H(14A)	109.7
N(10)-C(14)-H(14B)	109.7
C(13)-C(14)-H(14B)	109.7
H(14A)-C(14)-H(14B)	108.2
N(9)-C(15)-C(16)	111.0(8)
N(9)-C(15)-H(15A)	109.4
C(16)-C(15)-H(15A)	109.4
N(9)-C(15)-H(15B)	109.4
C(16)-C(15)-H(15B)	109.4
H(15A)-C(15)-H(15B)	108.0
N(11)-C(16)-C(15)	109.9(8)
N(11)-C(16)-H(16A)	109.7
C(15)-C(16)-H(16A)	109.7
N(11)-C(16)-H(16B)	109.7
C(15)-C(16)-H(16B)	109.7
H(16A)-C(16)-H(16B)	108.2
N(9)-C(17)-C(18)	113.1(8)
N(9)-C(17)-H(17A)	109.0
C(18)-C(17)-H(17A)	109.0
N(9)-C(17)-H(17B)	109.0
C(18)-C(17)-H(17B)	109.0
H(17A)-C(17)-H(17B)	107.8
N(12)-C(18)-C(17)	109.7(9)
N(12)-C(18)-H(18A)	109.7
C(17)-C(18)-H(18A)	109.7
N(12)-C(18)-H(18B)	109.7

C(17)-C(18)-H(18B)	109.7
H(18A)-C(18)-H(18B)	108.2
C(23)-N(13)-C(21)	111.6(7)
C(23)-N(13)-C(19)	110.9(7)
C(21)-N(13)-C(19)	110.5(7)
C(23)-N(13)-H(13)	107.9
C(21)-N(13)-H(13)	107.9
C(19)-N(13)-H(13)	107.9
C(20)-N(14)-H(14C)	109.5
C(20)-N(14)-H(14D)	109.5
H(14C)-N(14)-H(14D)	109.5
C(20)-N(14)-H(14E)	109.5
H(14C)-N(14)-H(14E)	109.5
H(14D)-N(14)-H(14E)	109.5
C(22)-N(15)-H(15C)	109.5
C(22)-N(15)-H(15D)	109.5
H(15C)-N(15)-H(15D)	109.5
C(22)-N(15)-H(15E)	109.5
H(15C)-N(15)-H(15E)	109.5
H(15D)-N(15)-H(15E)	109.5
C(24)-N(16)-H(16C)	109.5
C(24)-N(16)-H(16D)	109.5
H(16C)-N(16)-H(16D)	109.5
C(24)-N(16)-H(16E)	109.5
H(16C)-N(16)-H(16E)	109.5
H(16D)-N(16)-H(16E)	109.5
C(20)-C(19)-N(13)	110.9(7)
C(20)-C(19)-H(19A)	109.5
N(13)-C(19)-H(19A)	109.5
C(20)-C(19)-H(19B)	109.5
N(13)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	108.1
N(14)-C(20)-C(19)	110.2(8)
N(14)-C(20)-H(20A)	109.6
C(19)-C(20)-H(20A)	109.6
N(14)-C(20)-H(20B)	109.6
C(19)-C(20)-H(20B)	109.6
H(20A)-C(20)-H(20B)	108.1

N(13)-C(21)-C(22)	109.8(7)
N(13)-C(21)-H(21A)	109.7
C(22)-C(21)-H(21A)	109.7
N(13)-C(21)-H(21B)	109.7
C(22)-C(21)-H(21B)	109.7
H(21A)-C(21)-H(21B)	108.2
N(15)-C(22)-C(21)	109.5(8)
N(15)-C(22)-H(22A)	109.8
C(21)-C(22)-H(22A)	109.8
N(15)-C(22)-H(22B)	109.8
C(21)-C(22)-H(22B)	109.8
H(22A)-C(22)-H(22B)	108.2
N(13)-C(23)-C(24)	111.4(7)
N(13)-C(23)-H(23A)	109.4
C(24)-C(23)-H(23A)	109.3
N(13)-C(23)-H(23B)	109.4
C(24)-C(23)-H(23B)	109.4
H(23A)-C(23)-H(23B)	108.0
N(16)-C(24)-C(23)	110.7(8)
N(16)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24A)	109.5
N(16)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	108.1
Cl(1)-Sb(1)-Cl(1)#1	180.0
Cl(1)-Sb(1)-Cl(2)	93.32(9)
Cl(1)#1-Sb(1)-Cl(2)	86.68(9)
Cl(1)-Sb(1)-Cl(2)#1	86.68(9)
Cl(1)#1-Sb(1)-Cl(2)#1	93.32(9)
Cl(2)-Sb(1)-Cl(2)#1	180.0
Cl(1)-Sb(1)-Cl(3)#1	89.28(9)
Cl(1)#1-Sb(1)-Cl(3)#1	90.72(9)
Cl(2)-Sb(1)-Cl(3)#1	87.73(9)
Cl(2)#1-Sb(1)-Cl(3)#1	92.27(9)
Cl(1)-Sb(1)-Cl(3)	90.72(9)
Cl(1)#1-Sb(1)-Cl(3)	89.28(9)
Cl(2)-Sb(1)-Cl(3)	92.27(9)
Cl(2)#1-Sb(1)-Cl(3)	87.73(9)

Cl(3)#1-Sb(1)-Cl(3)	180.00(6)
Cl(4)-Sb(2)-Cl(4)#2	180.0
Cl(4)-Sb(2)-Cl(5)#2	86.71(12)
Cl(4)#2-Sb(2)-Cl(5)#2	93.29(12)
Cl(4)-Sb(2)-Cl(5)	93.29(12)
Cl(4)#2-Sb(2)-Cl(5)	86.71(12)
Cl(5)#2-Sb(2)-Cl(5)	180.00(15)
Cl(4)-Sb(2)-Cl(6)	88.36(17)
Cl(4)#2-Sb(2)-Cl(6)	91.64(17)
Cl(5)#2-Sb(2)-Cl(6)	90.23(15)
Cl(5)-Sb(2)-Cl(6)	89.77(15)
Cl(4)-Sb(2)-Cl(6)#2	91.64(17)
Cl(4)#2-Sb(2)-Cl(6)#2	88.37(17)
Cl(5)#2-Sb(2)-Cl(6)#2	89.77(15)
Cl(5)-Sb(2)-Cl(6)#2	90.23(15)
Cl(6)-Sb(2)-Cl(6)#2	180.0(2)
Cl(7)-Sb(3)-Cl(8)	90.54(12)
Cl(7)-Sb(3)-Cl(11)	90.84(10)
Cl(8)-Sb(3)-Cl(11)	87.45(10)
Cl(7)-Sb(3)-Cl(9)	89.00(11)
Cl(8)-Sb(3)-Cl(9)	90.16(11)
Cl(11)-Sb(3)-Cl(9)	177.60(10)
Cl(7)-Sb(3)-Cl(10)	88.93(10)
Cl(8)-Sb(3)-Cl(10)	175.29(10)
Cl(11)-Sb(3)-Cl(10)	87.88(9)
Cl(9)-Sb(3)-Cl(10)	94.51(10)
Cl(14)-Sb(4)-Cl(16)	90.39(9)
Cl(14)-Sb(4)-Cl(18)	87.19(11)
Cl(16)-Sb(4)-Cl(18)	176.96(11)
Cl(14)-Sb(4)-Cl(15)	88.75(10)
Cl(16)-Sb(4)-Cl(15)	90.38(9)
Cl(18)-Sb(4)-Cl(15)	91.41(10)
Cl(14)-Sb(4)-Cl(17)	88.98(10)
Cl(16)-Sb(4)-Cl(17)	87.36(10)
Cl(18)-Sb(4)-Cl(17)	90.76(11)
Cl(15)-Sb(4)-Cl(17)	176.78(9)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z #2 -x,-y+1,-z+1

Table S13. Torsion angles [°] for **3** tris Sb Yellow.

C(3)-N(1)-C(1)-C(2)	78.7(9)
C(5)-N(1)-C(1)-C(2)	-157.8(7)
N(1)-C(1)-C(2)-N(2)	-168.9(7)
C(1)-N(1)-C(3)-C(4)	-161.3(7)
C(5)-N(1)-C(3)-C(4)	75.9(9)
N(1)-C(3)-C(4)-N(3)	179.3(7)
C(1)-N(1)-C(5)-C(6)	85.2(9)
C(3)-N(1)-C(5)-C(6)	-153.0(7)
N(1)-C(5)-C(6)-N(4)	-165.6(7)
C(11)-N(5)-C(7)-C(8)	-158.4(8)
C(9)-N(5)-C(7)-C(8)	78.7(10)
N(5)-C(7)-C(8)-N(6)	82.9(11)
C(7)-N(5)-C(9)-C(10)	-155.5(8)
C(11)-N(5)-C(9)-C(10)	80.8(9)
N(5)-C(9)-C(10)-N(7)	-176.8(8)
C(7)-N(5)-C(11)-C(12)	69.5(10)
C(9)-N(5)-C(11)-C(12)	-166.3(7)
N(5)-C(11)-C(12)-N(8)	165.3(8)
C(17)-N(9)-C(13)-C(14)	172.4(8)
C(15)-N(9)-C(13)-C(14)	-59.1(10)
N(9)-C(13)-C(14)-N(10)	-159.5(8)
C(17)-N(9)-C(15)-C(16)	-139.4(8)
C(13)-N(9)-C(15)-C(16)	92.6(10)
N(9)-C(15)-C(16)-N(11)	165.3(8)
C(15)-N(9)-C(17)-C(18)	-71.4(10)
C(13)-N(9)-C(17)-C(18)	58.9(11)
N(9)-C(17)-C(18)-N(12)	162.3(8)
C(23)-N(13)-C(19)-C(20)	82.9(9)
C(21)-N(13)-C(19)-C(20)	-152.8(8)
N(13)-C(19)-C(20)-N(14)	-178.9(8)
C(23)-N(13)-C(21)-C(22)	-152.7(7)
C(19)-N(13)-C(21)-C(22)	83.5(9)
N(13)-C(21)-C(22)-N(15)	-171.2(7)
C(21)-N(13)-C(23)-C(24)	80.8(9)
C(19)-N(13)-C(23)-C(24)	-155.6(8)

N(13)-C(23)-C(24)-N(16) -179.8(8)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z #2 -x,-y+1,-z+1

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