

Supplementary data

Unraveling the Synthesis of SbCl(C₃N₆H₃): A Metal-Melamine Obtained through Deprotonation of Melamine with Antimony(III)Chloride

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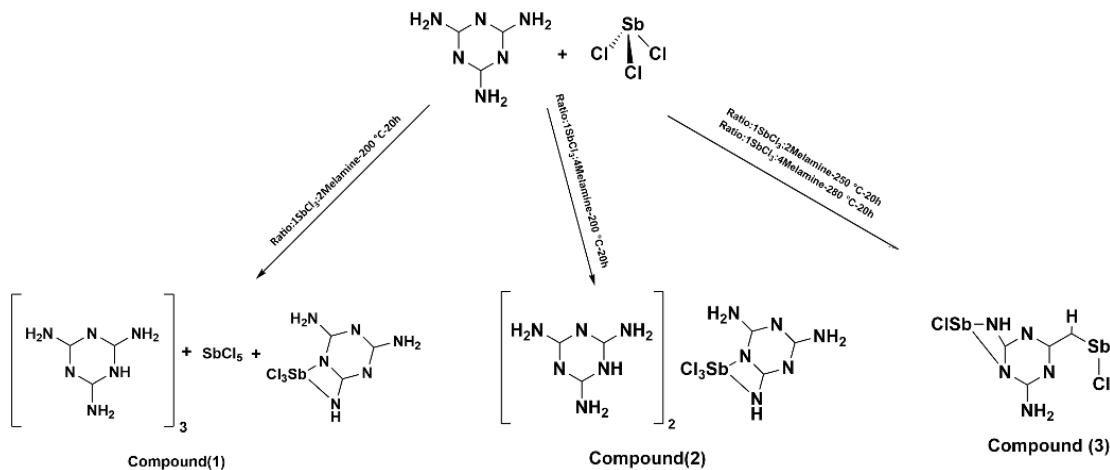


Figure S1: Schematic synthesis of three synthesized compounds ((1),(2),(3)).

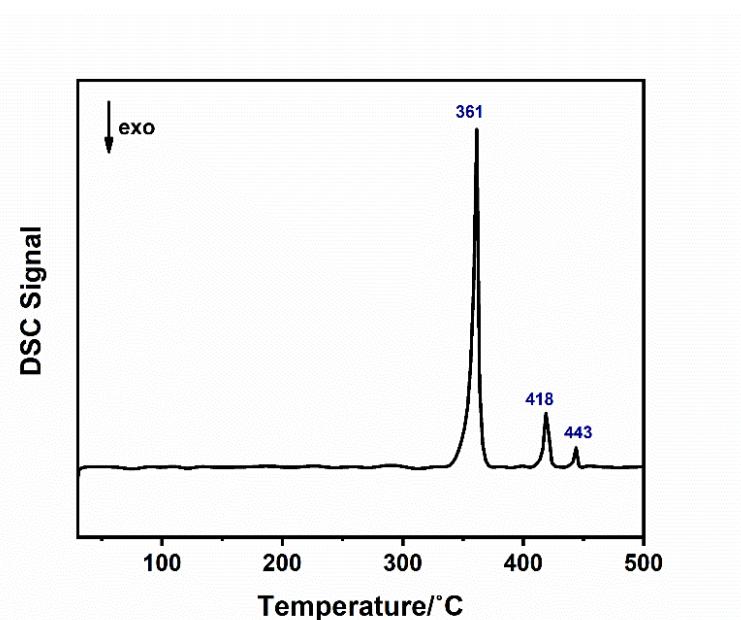


Figure S2: DSC pattern of pure Melamine.

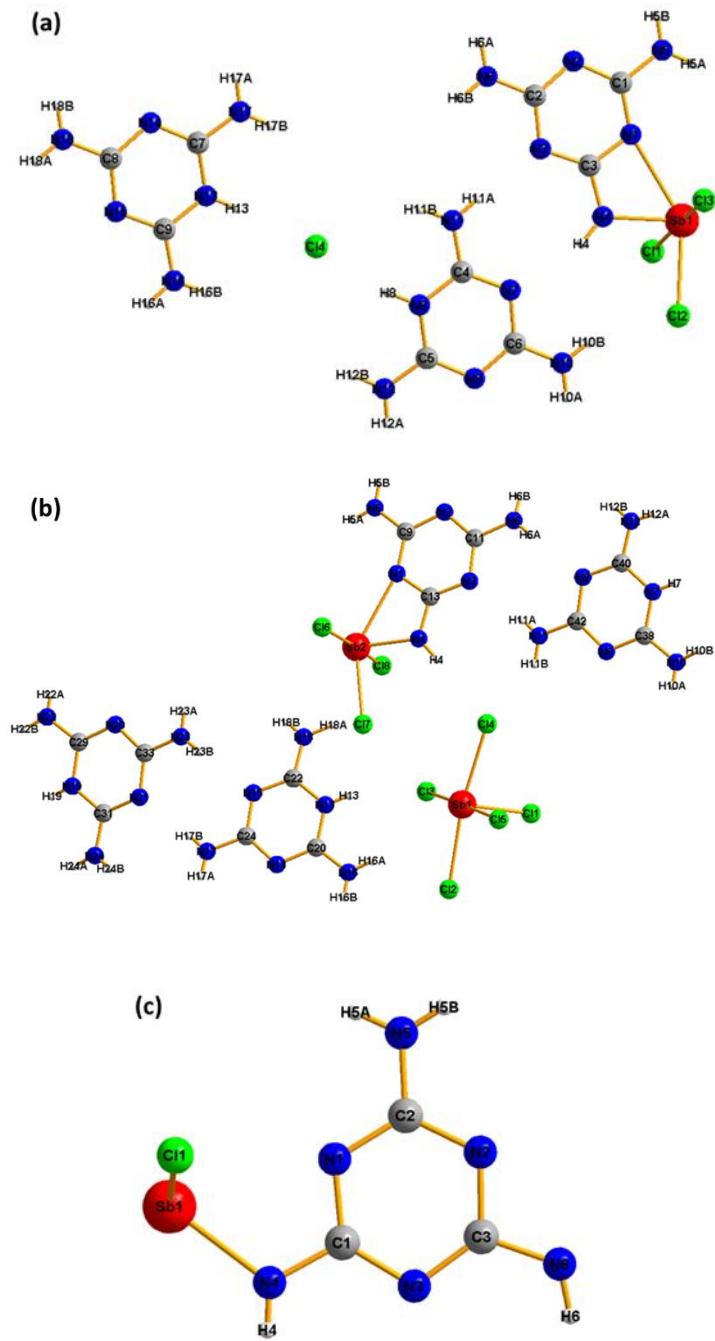


Figure S3: Asymmetric unit of compound a. (1), b. (2), c. (3)

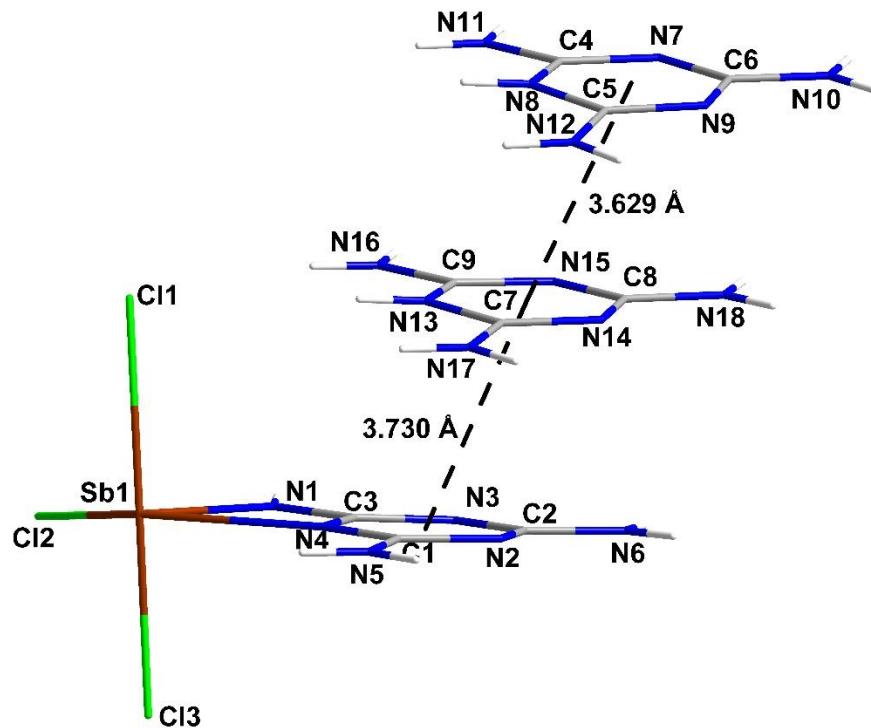


Figure S4: Stacking pattern of the C_3N_3 units in compound (1).

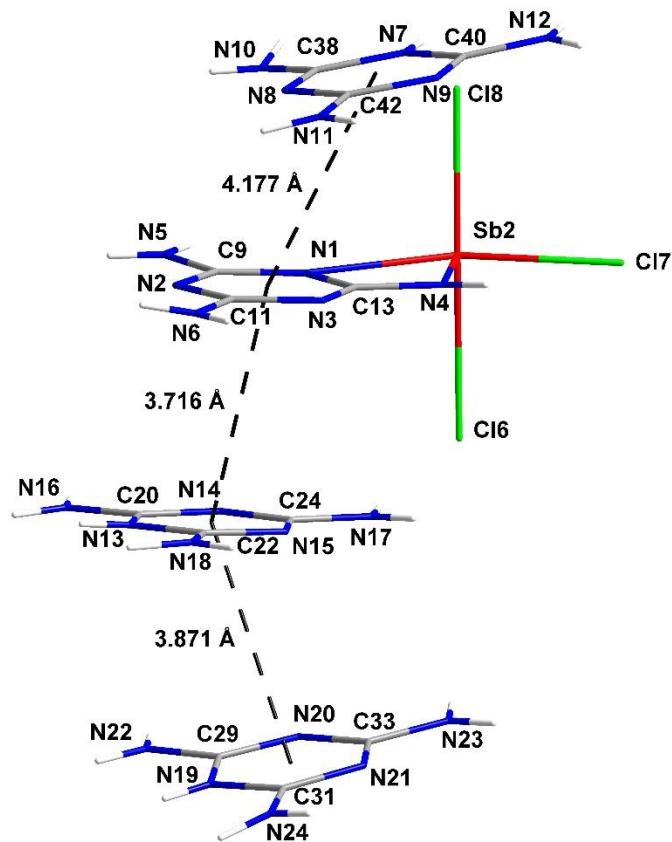


Figure S5: Stacking pattern of the C_3N_3 units in compound (2).

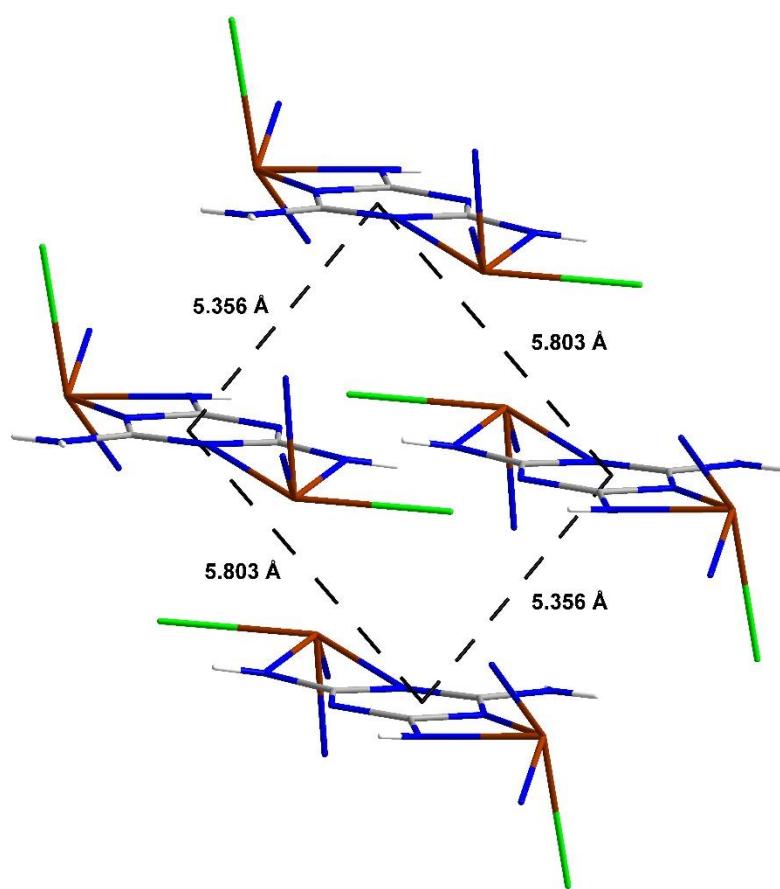


Figure S6: Stacking pattern of the C_3N_3 units in compound (3).

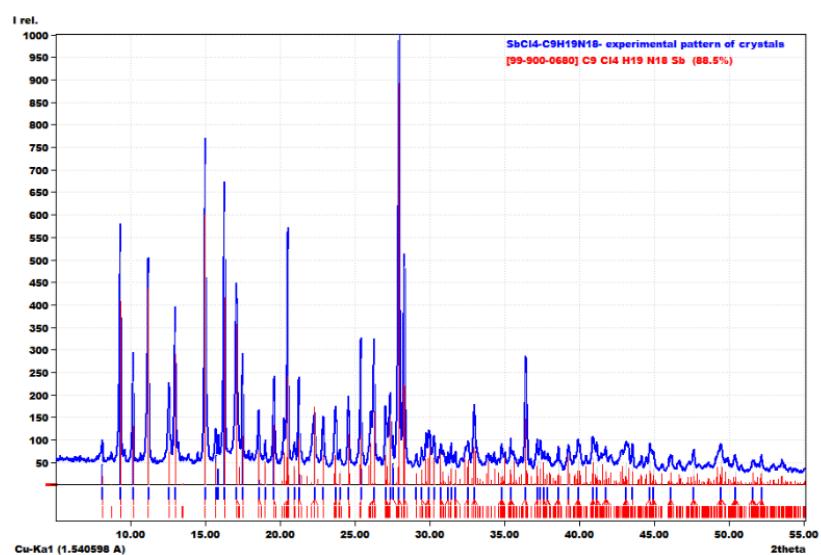


Figure S7: Comparison of the recorded powder pattern of (1) with the calculated pattern. Calculated (red) and recorded (blue)

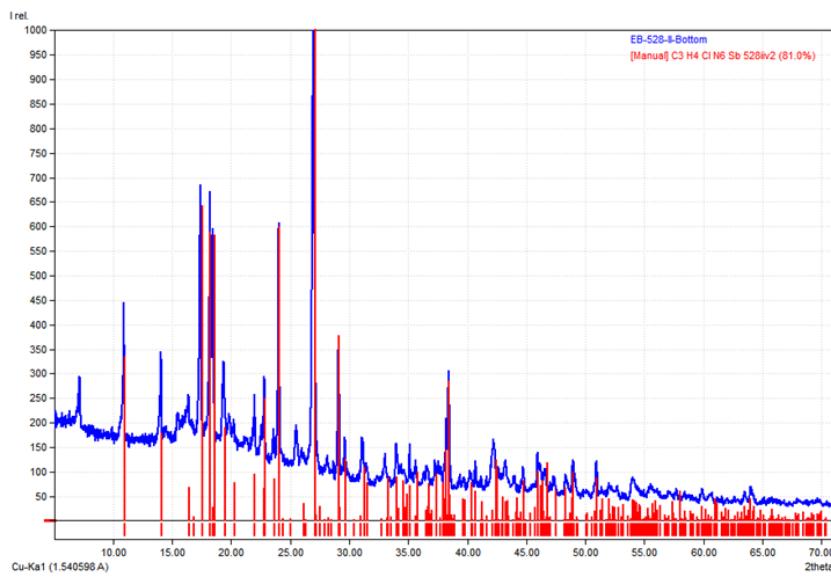


Figure S8: Comparison of the recorded powder pattern of (3) with the calculated pattern. Calculated (red) and recorded (blue)

Table S1. Assignment of recorded infrared wavenumbers (cm^{-1}) of obtained compounds compared to those of melamine [1], and melaminium chloride [2].

Melamine	Melaminium chloride[29]	Compound (1)	Compound (3)	Compound (4)	Tentative assignment
3471	3469	3462			NH ₂ asym stretch
3421	3363	3433	3342	3332	NH ₂ asym stretch
	3363	3370	3334		N-H... Cl stretch
3334		3357			NH ₂ sym stretch
3180				3147	Combination tone: NH ₂ bend+ side chain asym C-N stretch
		3203			N-H... N stretch
3132	3120	3157	3134		N-H... N stretch
		3116	3049		N-H... N stretch
	2945				N-H... N stretch
	2734	2785			Combination tone:
2677	2679	2680			NH ₂ asym stretch side
2368	2356		2364	2370	chain out of plane C-N bend
2198	2175				NH ₂ bend
	1722				NH ₂ bend
	1676	1679			NH ₂ bend
1652	1649	1656	1639	1651	NH ₂ bend
	1620	1612	1600		Side chain asym C-N stretch
1554	1556	1565		1510	
		1521	1515	1508	
1465					Ring semi-circle stretch
	1492	1487	1479		
1438	1452	1448	1375	1390	Side chain C-N breath
	1367	1373	1325	1350	Ring semi-circle stretch
	1336				

1172	1168	1172	1004		Ring semi-circle stretch+NH ₂ rock
		1145			Ring semi-circle stretch
1022	1014				Ring breath
		979			triazine ring, in phase radial
815				802	Ring out of plane bend
769	779	759	792	781	Side chain out of plane bend +Ring-sextant out of plane bend
730					Side chain out of plane bend +Ring-sextant out of plane bend
		692	703		Ring breath and NH ₂ bend (out of plane)
626	655				NH ₂ wag
586	578	568	580		Ring bend
464	495	501		472	Combination tone: NH ₂ bend+NH ₂ rock