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Supporting information for article:

Formation and distortion of iodidoantimonates(III): the first isolated [SbI₆]³⁻ octahedron

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Table S1 Selected bond lengths and angles (\AA , $^\circ$) for $(\text{C}_4\text{H}_{12}\text{N}_2)_3[\text{SbI}_6]_2 \cdot 5\text{H}_2\text{O}$ (TPBHP), $(\text{C}_4\text{H}_{12}\text{N}_2)[\text{SbI}_4]_2 \cdot 4\text{H}_2\text{O}$ (PBTT) and $(\text{C}_4\text{H}_{12}\text{N}_2)\text{I}_2 \cdot \text{I}_2$ (PDD).

TPBHP	295 K	85 K	PBTT	295 K	85 K	PDD	295 K	85 K
N11–C12	1.494 (7)	1.490 (19)	N11–C12	1.484 (7)	1.506 (6)	N11–C12	1.493 (6)	1.498 (5)
N11–C13	1.489 (7)	1.482 (18)	N11–C13	1.463 (7)	1.481 (6)	N11–C13	1.481 (6)	1.501 (5)
–	–	–	N21–C12	1.57 (2)	–	–	–	–
–	–	–	N21–C13	1.41 (2)	–	–	–	–
C12–C12 ⁱ	1.498 (12)	1.52 (3)	C12–C13 ^{iv}	1.504 (7)	1.506 (6)	C12–C13 ^v	1.494 (7)	1.503 (6)
C13–C13 ⁱ	1.496 (11)	1.51 (3)	–	–	–	–	–	–
N21–C23	1.486 (8)	1.47 (2)	–	–	–	–	–	–
N21–C25	1.502 (7)	1.50 (2)	–	–	–	–	–	–
N22–C24	1.486 (7)	1.465 (19)	–	–	–	–	–	–
N22–C26	1.488 (7)	1.519 (19)	–	–	–	–	–	–
C23–C24	1.492 (8)	1.51 (2)	–	–	–	–	–	–
C25–C26	1.500 (8)	1.48 (2)	–	–	–	–	–	–
N11–C12–C12 ⁱ	110.4 (4)	110.1 (10)	N11–C12–C13 ^{iv}	109.7 (4)	109.1 (4)	N11–C12–C13 ^v	110.7 (4)	110.4 (3)
–	–	–	N21–C13–C12 ^{iv}	112.2 (9)	–	–	–	–
N11–C13–C13 ⁱ	110.2 (4)	110.5 (10)	N11–C13–C12 ^{iv}	110.9 (4)	111.1 (4)	N11–C13–C12 ^v	110.6 (4)	110.5 (3)
–	–	–	N21–C12–C13 ^{iv}	108.9 (7)	–	–	–	–
C12–N11–C13	111.7 (5)	113.2 (11)	C12–N11–C13	112.1 (5)	111.7 (4)	C12–N11–C13	111.8 (3)	111.7 (3)
–	–	–	C12–N21–C13	110.2 (14)	–	–	–	–
N21–C23–C24	110.9 (5)	111.7 (13)	–	–	–	–	–	–
N21–C25–C26	110.3 (5)	112.6 (14)	–	–	–	–	–	–
N22–C24–C23	110.7 (5)	110.8 (13)	–	–	–	–	–	–
N22–C26–C25	110.3 (5)	110.6 (13)	–	–	–	–	–	–
C23–N21–C25	111.9 (5)	112.0 (12)	–	–	–	–	–	–
C24–N22–C26	111.6 (5)	111.4 (12)	–	–	–	–	–	–
–	–	–	–	–	–	I2–I2 ^{vi}	2.7651 (8)	2.7608 (6)

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