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Supporting information for article:

(H3O)3Sb2Br9: the first member of the *M*3*E*2*X*9 structure family with oxonium cations

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S1. Degree of distortion

The degree of distortion (*dd*) was defined from the dispersion of $d(M\cdots M')$ (*Eq*. S1-S3). $d(M\cdots M')$ are the distances of the *M* atom centering the hexagonal star to the six neighboring *M*′ atoms. (*Chang, et al.* 2016).

$$\bar{d} = \sum d(M\cdots M') / 6 \qquad \text{(S1)}$$

$$\Delta d = [d(M\cdots M')_{max} - d(M\cdots M')_{min}] \qquad \text{(S2)}$$

$$dd \text{ (degree of distortion)} \equiv \Delta d / 2\bar{d} \qquad \text{(S3)}$$

Factor 2 in *Eq*. (S3) is used for normalization.

Figure S1

EDX spectrum of the single crystal recorded after the XRD experiment. The crystal was mounted on a carbon pad of an Al sample holder. Signals of Cs atoms were not detected (expected energies of Cs signals are marked in red).