Supporting Information for:

Synthesis, Crystal Structure and Properties of a New Candidate for Nonlinear Optical Material in the IR Region: Hg_2BrI_3

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Captions for the figures and table in the ESI:

Figure S1. Experimental and simulated X-ray powder diffraction data of Hg_2BrI_3, $HgBr_2$ and HgI_2. Comparison of an experimental XRD of Hg_2BrI_3 with $HgBr_2$ and HgI_2 as well as the simulated data of Hg_2BrI_3 from single crystal structure.

Figure S2. Packing of Hg_2BrI_3 down the *a*-axis

Table S1. Bond distances (Å) and angles (^{o}) of Hg_2BrI_3

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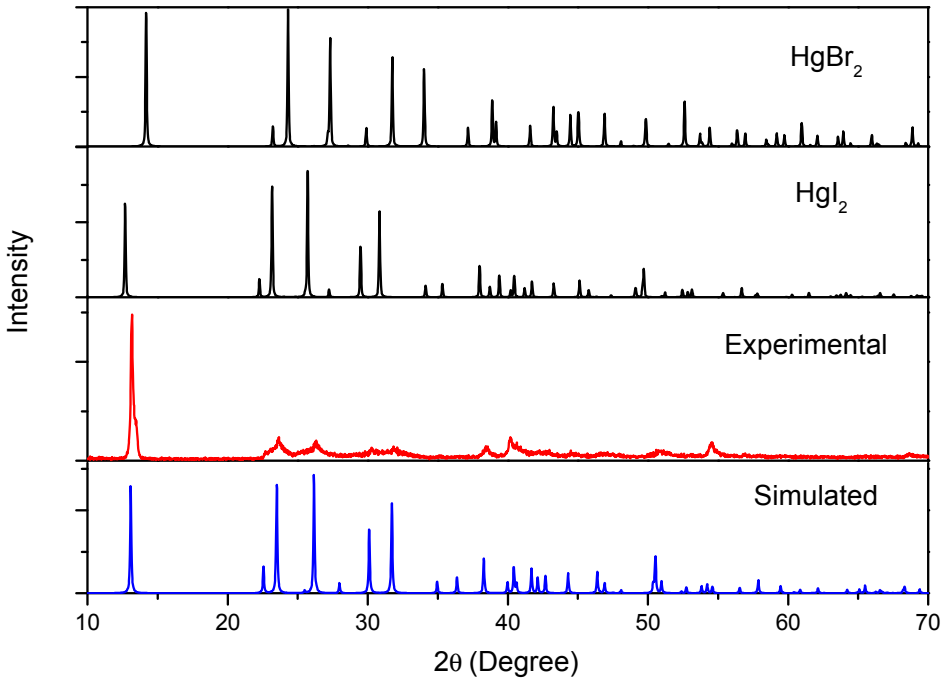

Figure S2. Packing of Hg_2BrI_3 down the *a*-axis

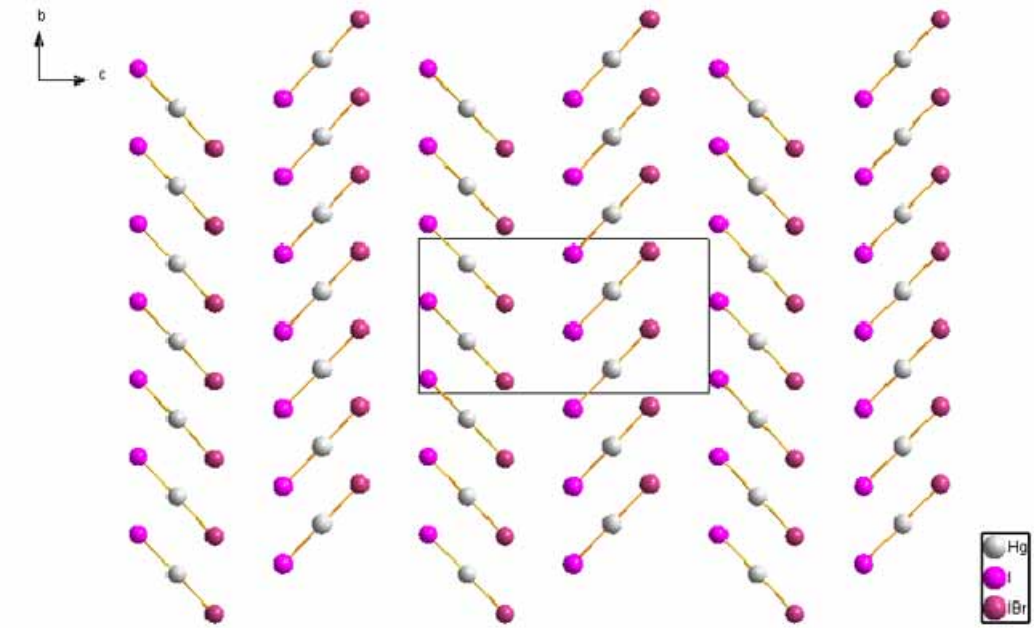

Table S1. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for Hg_2BrI_3

Atom	Site occupancy	*x*	*y*	*z*	Ueq
Hg1	1	0.0000	0.3392(3)	0.1672(2)	0.0516(7)
I1	1	0.0000	0.5964(4)	0.03326(19)	0.0422(9)
I2	0.5	0.0000	0.0826(4)	0.29718(15)	0.0331(9)
Br1	0.5	0.0000	0.0826(4)	0.29718(15)	0.0331(9)