

## Electronic Supplementary Information for:

# A Promising Nonlinear Optical Material in the Mid-IR Region: New Results on Synthesis, Crystal Structure and Properties of Noncentrosymmetric $\beta$ -HgBrCl

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### Captions for tables and figures in the ESI

**Table S1** Selected bond lengths (Å) and angles (deg) for HgCl<sub>2</sub>.<sup>1</sup>

**Table S2** Selected bond lengths (Å) and angles (deg) for HgBr<sub>2</sub>.<sup>2</sup>

**Table S3** The proportion of element in  $\alpha$ -HgBrCl by EDX

**Table S4** The proportion of element in  $\beta$ -HgBrCl by EDX

**Fig. S1** The EDX spectrum of  $\alpha$ -HgBrCl.

**Fig. S2** The EDX spectrum of  $\beta$ -HgBrCl.

**Fig. S3** Calculated and experimental powder X-ray diffraction patterns for  $\alpha$ -HgBrCl and  $\beta$ -HgBrCl.

**Fig. S4** The photograph of  $\alpha$ -HgBrCl crystals.

**Fig. S5** The photograph of  $\beta$ -HgBrCl crystals.

**Table S1** Selected bond lengths (Å) and angles (deg) for HgCl<sub>2</sub>.<sup>1</sup>

bond	bond length (Å)	bond	Bond angle (deg)
Hg-Cl(1)	2.2913	Cl(1)-Hg-Cl(2)	178.604
Hg-Cl(2)	2.2734		

**Table S2** Selected bond lengths (Å) and angles (deg) for HgBr<sub>2</sub>.<sup>2</sup>

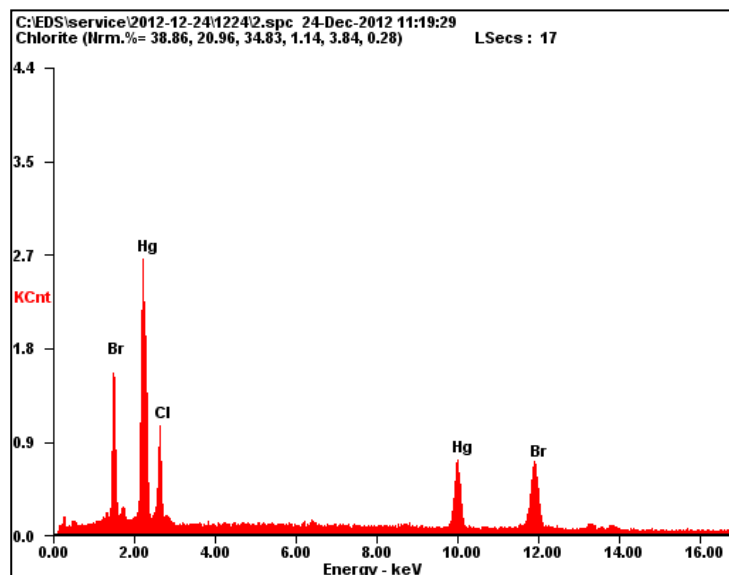
bond	bond length (Å)	bond	Bond angle (deg)
Hg-Br(1)	2.4446	Br(1)-Hg-Br(2)	179.881
Hg-Br(2)	2.4447		

**Table S3** The proportion of element in  $\alpha$ -HgBrCl by EDX

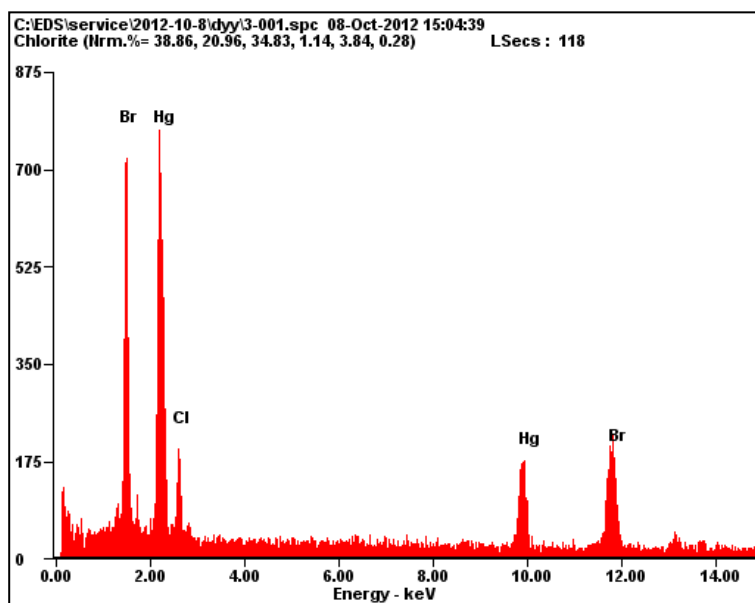
Element	Experimental values	
	Weight/%	Atomic weight/%
Hg <i>L</i>	63.14	31.27
Br <i>K</i>	22.17	27.56
Cl <i>K</i>	14.69	41.17

**Table S4** The proportion of element in  $\beta$ -HgBrCl by EDX

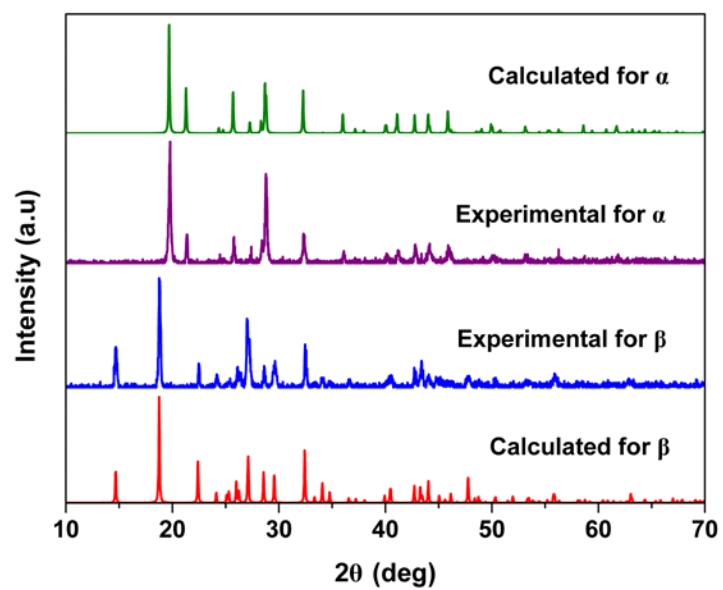
Element	Experimental values	
	Weight/%	Atomic weight/%
Hg <i>L</i>	59.84	30.93
Br <i>K</i>	29.73	38.57
Cl <i>K</i>	10.43	30.51



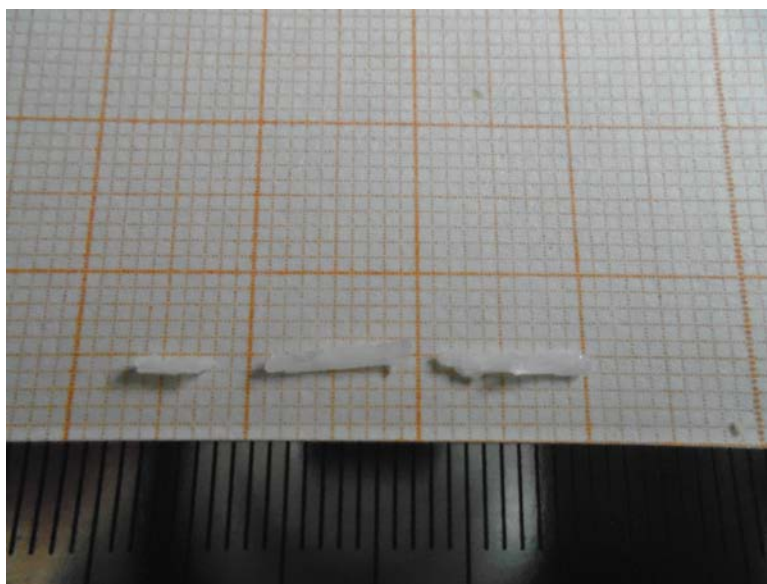
**Fig. S1** The EDX spectrum of  $\alpha$ -HgBrCl



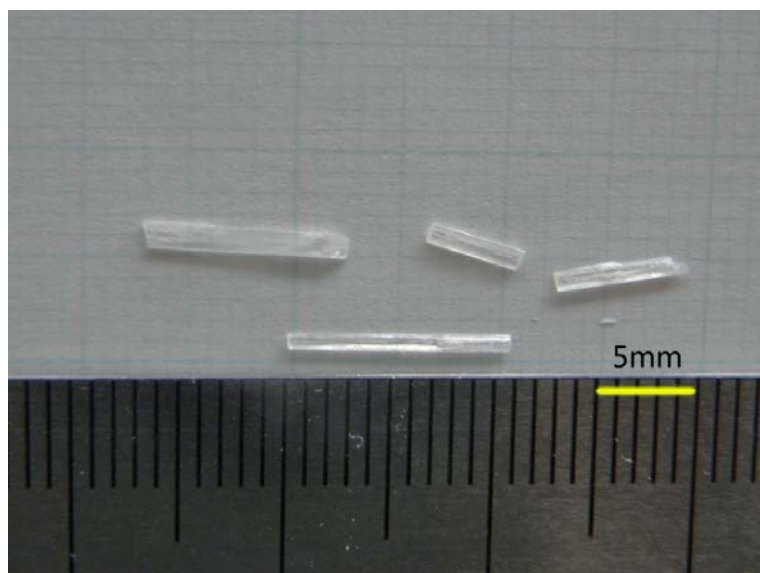
**Fig. S2** The EDX spectrum of  $\beta$ -HgBrCl



**Fig. S3** Calculated and experimental powder X-ray diffraction patterns for  $\alpha$ -HgBrCl and  $\beta$ -HgBrCl.



**Fig. S4** The photograph of  $\alpha$ -HgBrCl crystals.



**Fig. S5** The photograph of  $\beta$ -HgBrCl crystals.

## References

1. V. Subramanian, K. Seff, *Acta Crystallographica B*, 1980, **36**, 2132.
2. V. I. Pakhomov, A. V. Goryunov, I. N. Ivanova-Korfini, A. A. Boguslavskii, R. Sh. Lotfullin, *Zhurnal Neorganicheskoi Khimii*, 1990, **35**,2476.