## **Supporting Information for**

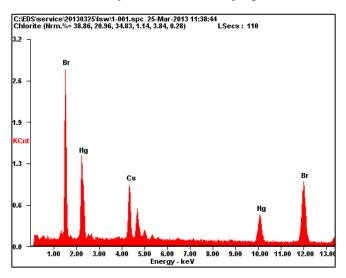
## A Promising New Nonlinear Optical Crystal with high laser damage threshold for application in the IR Region:

## Synthesis, Crystal Structure and Properties of the

## Noncentrosymmetric CsHgBr<sub>3</sub>

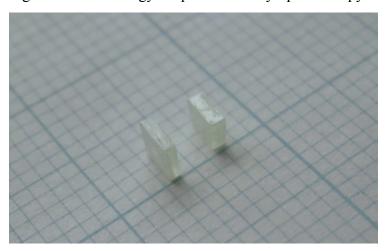
Songwei Lv,<sup>†</sup> Qi Wu,<sup>†</sup> Xianggao Meng,<sup>‡</sup> Lei Kang,<sup>ξ</sup> Cheng Zhong,<sup>†</sup> Zheshuai Lin,<sup>ξ</sup>
Zhanggui Hu,<sup>ξ</sup> Xingguo Chen,<sup>†</sup> Jingui Qin<sup>\*†</sup>

<sup>&</sup>lt;sup>§</sup> Beijing Center for Crystal R & D, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, China



Element	Wt %	At %
CsL	22.31	19.06
HgL	34.43	19.49
BrK	43.26	61.45

Figure S1. The Energy Dispersive X-Ray Spectroscopy of CsHgBr<sub>3</sub>



<sup>†</sup> Department of Chemistry, Wuhan University, Wuhan 430072, China,

<sup>&</sup>lt;sup>‡</sup> College of Chemistry, Central China Normal University, Wuhan, 430079, China

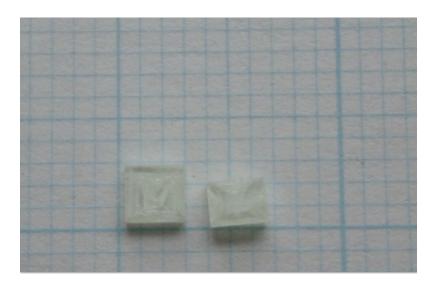


Figure S2. The photograph of CsHgBr<sub>3</sub> crystal

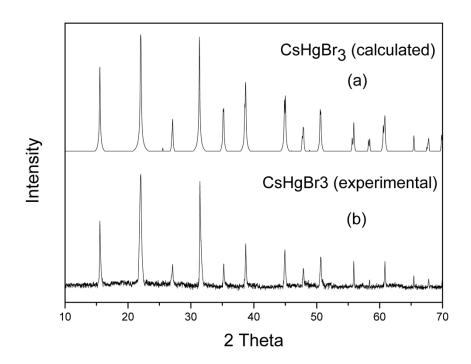


Figure S3. Comparison of experimental and calculated powder X-ray diffraction patterns (a) The calculated powder X-ray diffraction data of CsHgBr<sub>3</sub> from single crystal structure data (b) The experimental powder X-ray diffraction data of CsHgBr<sub>3</sub> of powders obtained from the solution reaction.