

# New Metal Chalcogenides $\text{Ba}_4\text{CuGa}_5\text{Q}_{12}$ ( $\text{Q} = \text{S}, \text{Se}$ ) Displaying Strong Infrared Non-Linear Optical Responses

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## Supplementary Data

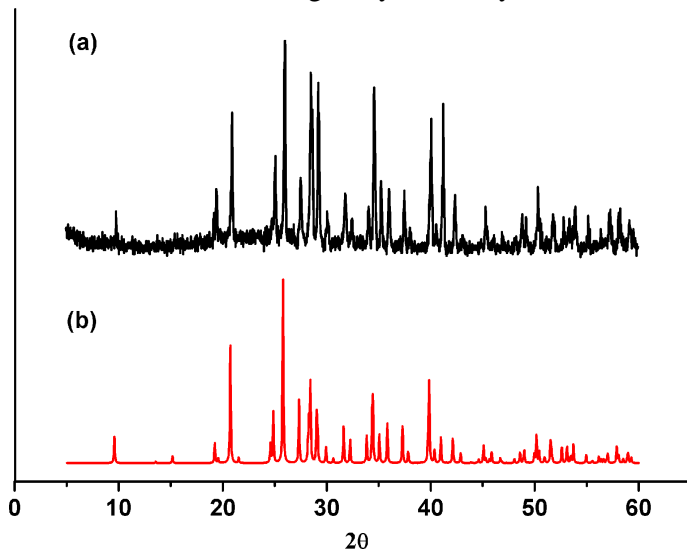
**Figure S1** Powder X-ray diffraction patterns of **1** from (a) the measured data, and (b) the calculated data of single-crystal X-ray structural analyses.

**Figure S2** Powder X-ray diffraction patterns of **2** from (a) the measured data, and (b) the calculated data of single-crystal X-ray structural analyses.

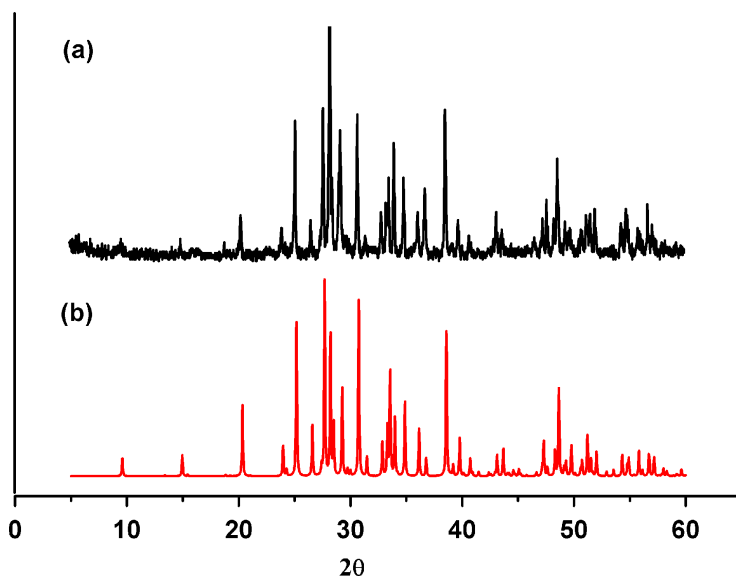
**Figure S3** Powder X-ray diffraction patterns of **3** from (a) the measured data, and (b) the calculated data of single-crystal X-ray structural analyses.

**Figure S4** The SHG response measured as a function of the incident laser intensity of (a) **1**, (b) **2**, (c) **3**, and (d)  $\text{AgGaS}_2$  at 532 nm.

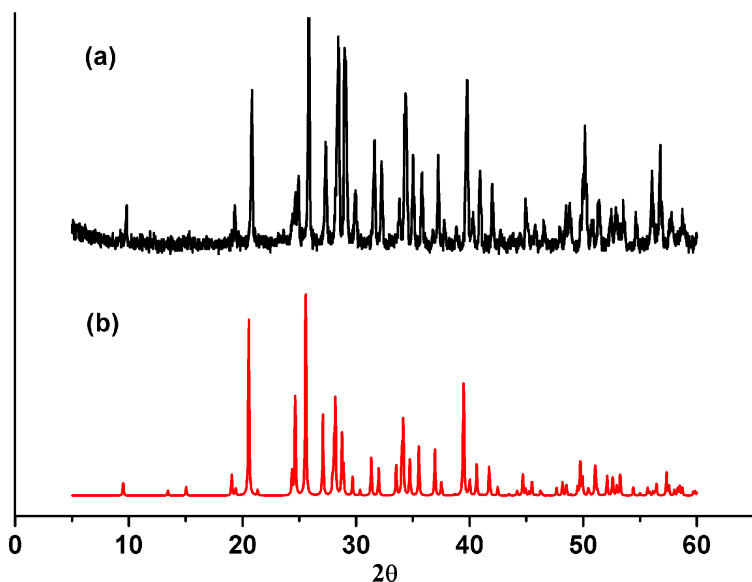
**Figure S1** Powder X-ray diffraction patterns of **1** from (a) the measured data, and (b) the calculated data of single-crystal X-ray structural analyses.



**Figure S2** Powder X-ray diffraction patterns of **2** from (a) the measured data, and (b) the calculated data of single-crystal X-ray structural analyses.



**Figure S3** Powder X-ray diffraction patterns of **3** from (a) the measured data, and (b) the calculated data of single-crystal X-ray structural analyses.



**Figure S4** The SHG response measured as a function of the incident laser (1064 nm) intensity of (a) **1**, (b) **2**, (c) **3**, and (d) AgGaS<sub>2</sub>. The colors represent the data collected at various spots.

