

Supporting Information

Highly distorted HgS₄ tetrahedra induced moderate second-harmonic generation response of EuHgGeS₄

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Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (U_{eq}^a , $\text{\AA}^2 \times 10^3$) for **1**.

atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{eq}}/\text{\AA}^2$
Eu(1)	5000	5000	3218.4(13)	11.5(3)
Hg(1)	7500	3290.2(6)	8716.9(18)	45.5(4)
Ge(1)	7500	2158.1(15)	3365(3)	9.4(3)
S(1)	5791(3)	2276(3)	1271(5)	10.7(5)
S(2)	7500	4043(3)	5163(5)	8.7(7)
S(3)	7500	629(4)	5734(6)	13.2(8)

^a U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Eu-based quaternary chalcogenides.

Compounds	Space group	Band gap (eV)	SHG intensity	Phase matchability	Reference
Cu ₂ EuSiS ₄	<i>P</i> 3 ₁ 21	2.36	-	no	1
Cu ₂ EuGeS ₄	<i>P</i> 3 ₂ 21	2.32	-	no	1
Cu ₂ EuGeSe ₄	<i>Ama</i> 2	1.74	-	no	1
EuCdGeS ₄	<i>Ama</i> 2	2.50	2.6 × AGS	yes	2
EuCdGeSe ₄	<i>Ama</i> 2	2.25	3.8 × AGS	yes	2
EuZnGeS ₄	<i>Fdd</i> 2	2.26	-	-	3
Eu ₂ Ga ₂ GeS ₇	<i>P</i> $\bar{4}$ ₂ <i>m</i>	1.70	1.6 × AGS	yes	4
EuCu ₂ GeS ₄	<i>P</i> 3 ₁ 21	1.57	-	-	5
EuCu ₂ SnS ₄	<i>P</i> 3 ₁ 21	2.22	-	-	5

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