From AgGaS$_2$ to AgHgPS$_4$: vacancy defects and highly distorted HgS$_4$ tetrahedra double-induced remarkable second-harmonic generation response

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Table S1 Atomic coordinates, equivalent isotropic displacement parameters and bond valence sums (BVS) for $AgHgPS_4$.

Atom	x	y	z	U_{eq} (Å²) [a]	BVS
Hg	0.41570 (4)	0.81444 (8)	0.26543 (4)	0.0238 (2)	2.04
Ag	0.90874 (18)	0.6438 (2)	0.52054 (16)	0.0290 (3)	1.09
P	0.4167(6)	0.3155(4)	0.5180(4	0.0098 (8)	4.81
S1	0.4992 (5)	0.6264 (5)	0.5515 (4)	0.0139 (6)	−2.02
S2	0.5704 (5)	0.1937 (5)	0.3078 (4)	0.0150 (6)	−1.96
S3	0.5069 (5)	0.1464 (5)	0.7370 (4)	0.0143 (6)	−1.94
S4	0.0904 (5)	0.2787 (5)	0.4796 (4)	0.0134 (6)	−2.01

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

Table S2 Selected band distances (Å) and band angles (°) for AgHgPS$_4$.

Hg1—S1	2.536 (3)	Ag1—S3^{iii}	2.624 (3)
Hg1—S2^i	2.613 (3)	Ag1—S4^v	2.601 (4)
Hg1—S3^{ii}	2.559 (3)	P1—S1	2.056 (4)
Hg1—S4^{iii}	2.526 (3)	P1—S2	2.035 (5)
Ag1—S1	2.564 (3)	P1—S3	2.058 (5)
Ag1—S2^{iv}	2.610 (3)	P1—S4	2.058 (5)
S1—Hg1—S2^i	104.98 (10)	S2^{iv}—Ag1—S3^{iii}	113.64 (11)
S1—Hg1—S3^{ii}	107.87 (10)	S4^v—Ag1—S2^{iv}	106.99 (11)
S3^{ii}—Hg1—S2^i	106.49 (10)	S4^v—Ag1—S3^{iii}	104.24 (11)
S4^{iii}—Hg1—S1	123.35 (10)	S1—P1—S3	109.7 (2)
S4^{iii}—Hg1—S2^i	99.22 (10)	S1—P1—S4	111.7 (2)
S4^{iii}—Hg1—S3^{ii}	113.02 (9)	S2—P1—S1	110.1 (2)
S1—Ag1—S2^{iv}	107.93 (11)	S2—P1—S3	108.55 (19)
S1—Ag1—S3^{iii}	110.12 (11)	S2—P1—S4	108.7 (2)
S1—Ag1—S4^v	114.01 (11)	S3—P1—S4	108.1 (2)

Symmetry codes: (i) x, $y+1$, z; (ii) $x-1/2$, $-y+1$, $z-1/2$; (iii) $x+1/2$, $-y+1$, $z-1/2$; (iv) $x+1/2$, $-y+1$, $z+1/2$; (v) $x+1$, y, z; (vi) x, $y-1$, z; (vii) $x-1/2$, $-y+1$, $z+1/2$; (viii) $x-1$, y, z.

Figure S1. The EDX results of AgHgPS$_4$.

Element	Ag L	Hg M	P K	S K
Atomic%	13.3	13.8	14.7	58.2

Sum Spectrum
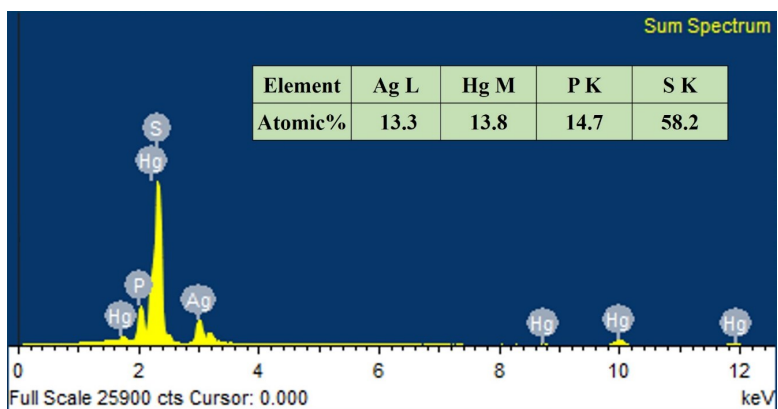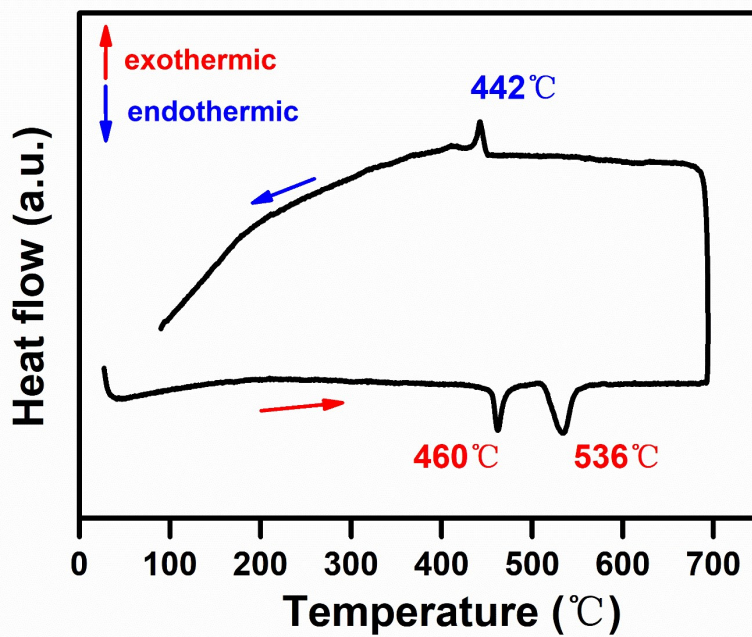
Full Scale 25900 cts Cursor: 0.000 keV

Figure S2. DSC curve of AgHgPS$_4$.

Figure S3. The infrared spectrum of AgHgPS$_4$.