Supporting Information

Balanced Second-Order Nonlinear Optical Properties of Adducts $CHI_3 \cdot (S_8)_3$ and $AsI_3 \cdot (S_8)_3$: A Systematic Survey

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Table 1. Crystal data and structure refinement parameters for **1** and **2**.

Chemical formula	**1**	**2**
Fw	1163.16	1225.06
T (K)	293	
crystal system, space group	trigonal, $R3m$	
Z	3	
a (Å)	24.4393(6)	24.7274(7)
c (Å)	4.4548(2)	4.4094(3)
V (Å^3)	2304.29(15)	2334.9(2)
D_{calcd} (g cm^{-3})	2.515	2.614
μ (mm^{-1})	4.683	5.676
F(000)	1650	1728
2θ range (°)	5.774 to 54.988	3.294 to 52.988
measd. reflns	8007	7440
indep. reflns/R_{int}	1253/0.0282	1147/0.0303
obs. reflns	1189	1126
R1, wR2 ($I > 2\sigma(I)$)[a]	0.0178, 0.0315	0.0166, 0.0418
R1, wR2 (all data)[a]	0.0205, 0.0320	0.0189, 0.0685
GOF on F^2	1.086	0.962
$\Delta\rho_{max}/\Delta\rho_{min,}$ e/Å^3	0.43/–0.43	0.56/–0.72

[a]R1 = $||F_o| - |F_c||/|F_o|$; wR2 = $[w(F_o^2 - F_c^2)^2]/[w(F_o^2)^2]^{1/2}$.

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (U_{eq}[a], $Å^2 \times 10^3$) for **1** and **2**.

atom	*x*	*y*	*z*	U_{eq}/Å^2
		1		
C(1)	3333	6667	6840(20)	28.8(19)
I(1)	2848.8(2)	5697.7(2)	5472.0(8)	41.05(13)
S(1)	2030.8(3)	4061.6(6)	3607(3)	33.4(3)
S(2)	1176.6(5)	3694.3(5)	5744(2)	37.0(2)
S(3)	523.1(4)	2963.0(5)	3203(2)	36.4(2)
S(4)	392.8(5)	2135.2(5)	5036(2)	36.7(2)
S(5)	930.7(3)	1861.4(7)	2656(3)	40.2(3)
		2		
As(1)	6667	3333	7873(3)	28.7(3)
I(1)	6136.4(2)	3863.6(2)	5130.0(13)	38.2(2)
S(1)	5343.1(5)	4656.9(5)	2675(5)	34.2(5)
S(2)	5835.9(8)	5492.4(8)	4899(4)	36.7(4)
S(3)	5753.5(8)	6150.2(8)	2461(4)	36.8(4)
S(4)	5071.0(8)	6271.3(7)	4450(4)	37.0(4)
S(5)	4256.8(6)	5743.2(6)	2111(65)	40.3(6)

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

Table S3. Important bond lengths (Å) for **1** and **2**.

Bond	Dist./Å	Bond	Dist./Å
		1	
C(1)–I(1)	2.139(3)	S(3)–S(4)	2.054(1)
S(1)–S(2)	2.048 (1)	S(4)–S(5)	2.044(1)
S(2)–S(3)	2.043(1)		
		2	
As(1)–I(1)	2.573(1)	S(3)–S(4)	2.052(2)
S(1)–S(2)#3	2.049(2)	S(4)–S(5)	2.048(2)
S(2)–S(3)	2.043(2)		

Symmetry transformations used to generate equivalent atoms: #1 +*y*-*x*, +*y*, +*z*; #2 1-*y*, 1+*x*-*y*, +*z*; #3 +*y*-*x*, 1-*x*, +*z* for **1**. #1 1+*y*-*x*, 1-*x*, +*z*; #2 1-*y*, +*x*-*y*, +*z*; #3 1-*y*, 1-*x*, +*z* for **2**.

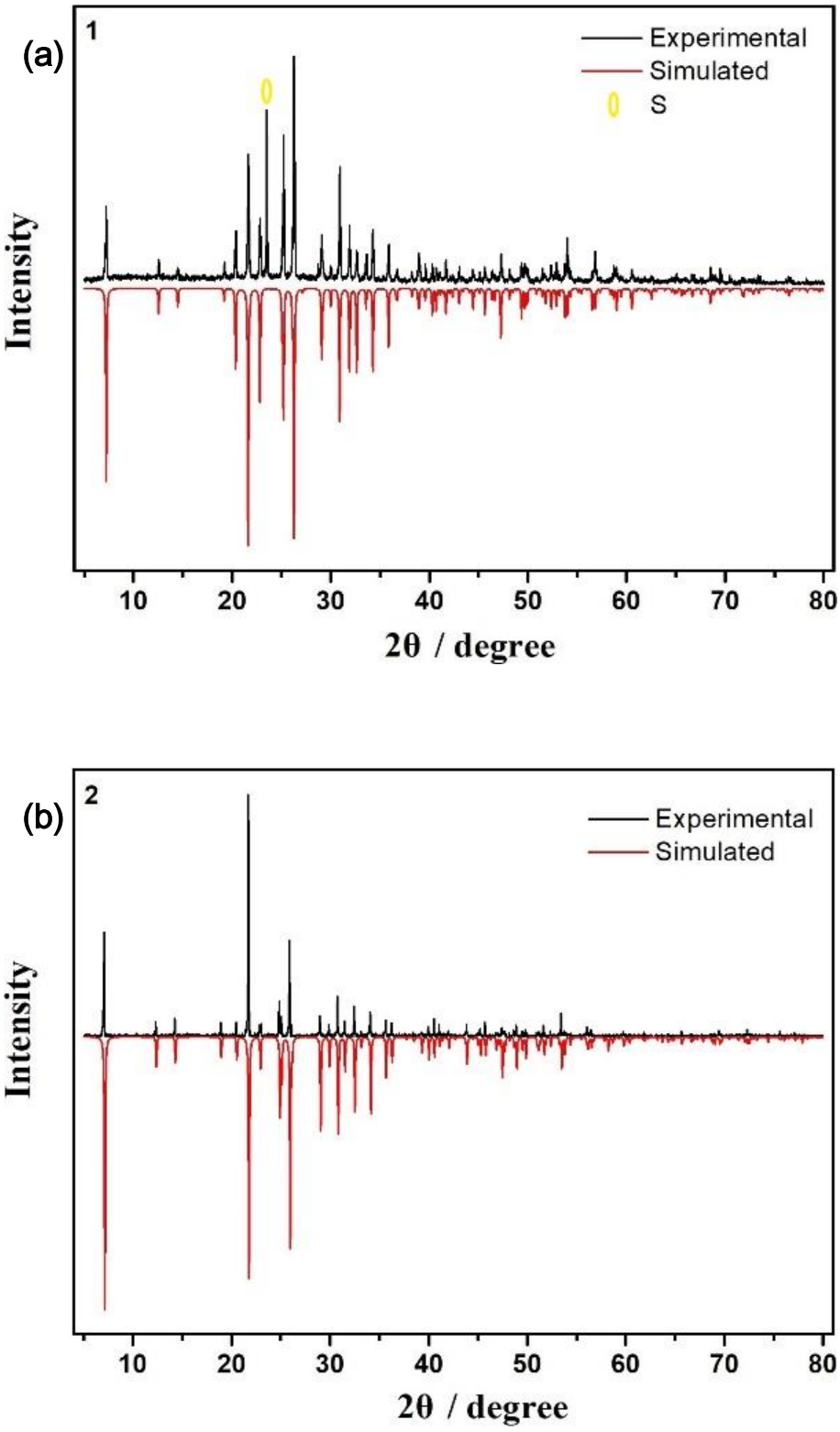


Fig. S1 The PXRD patterns of **1** (a) and **2** (b).

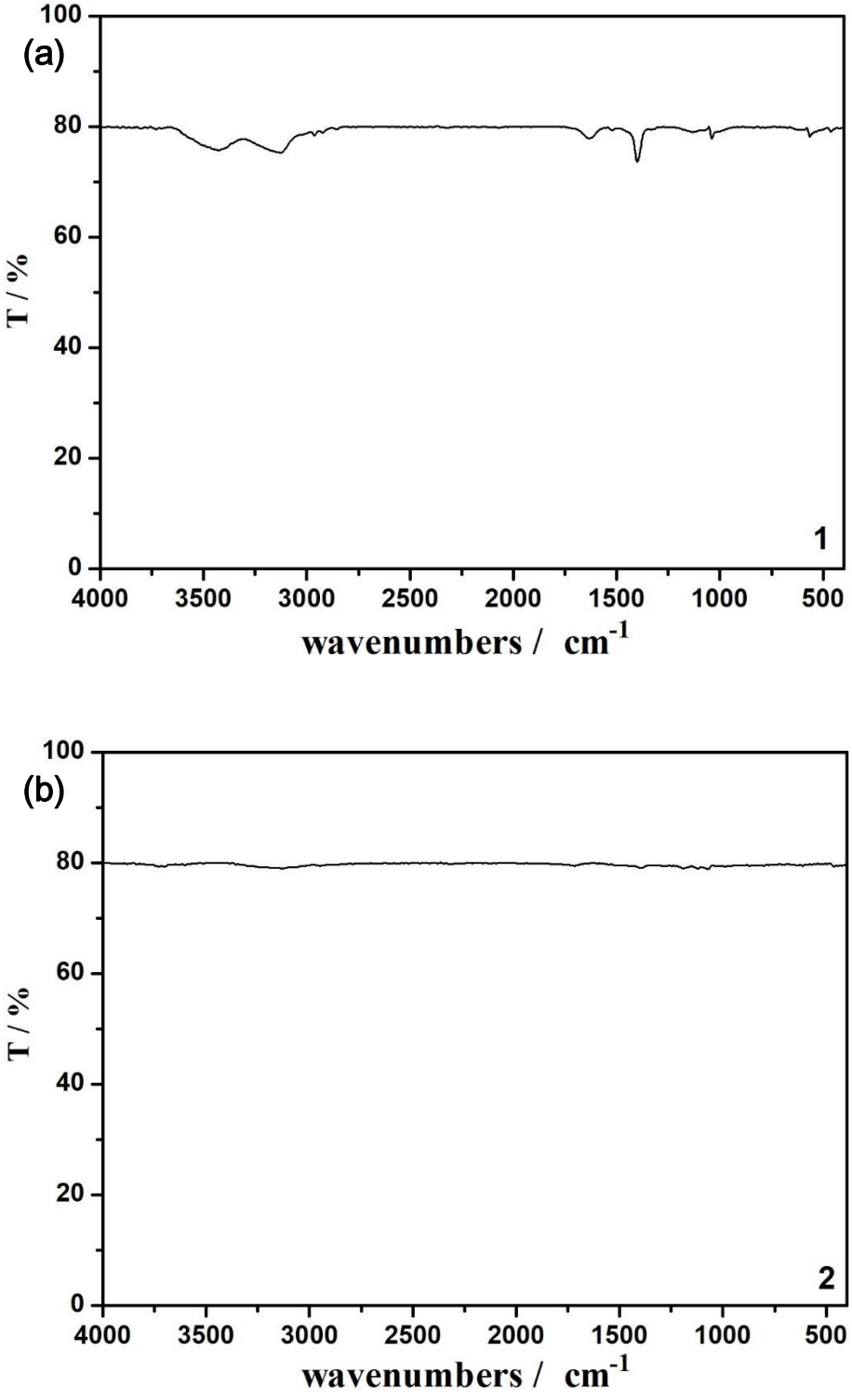
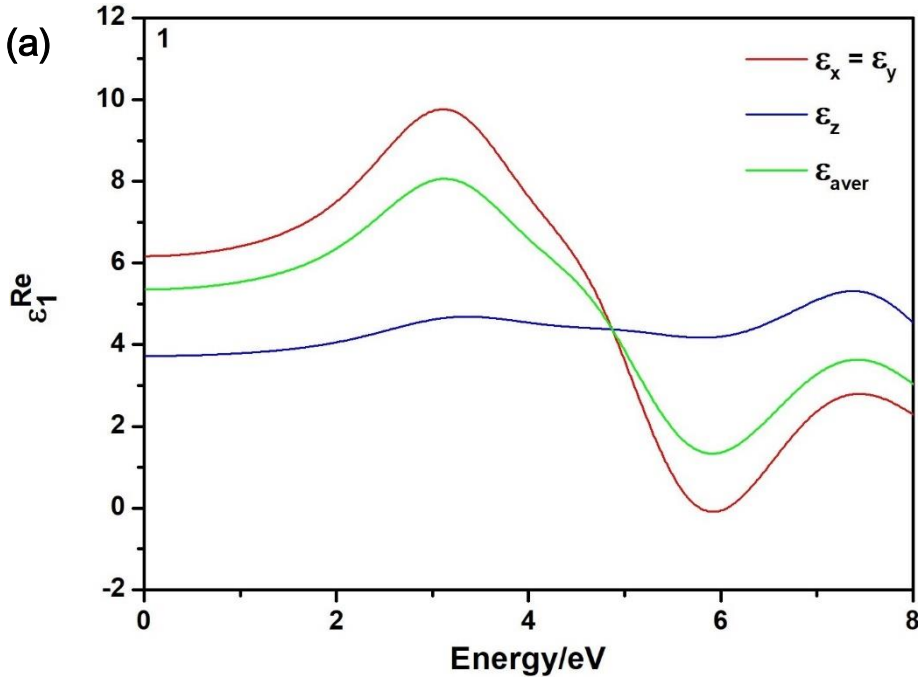
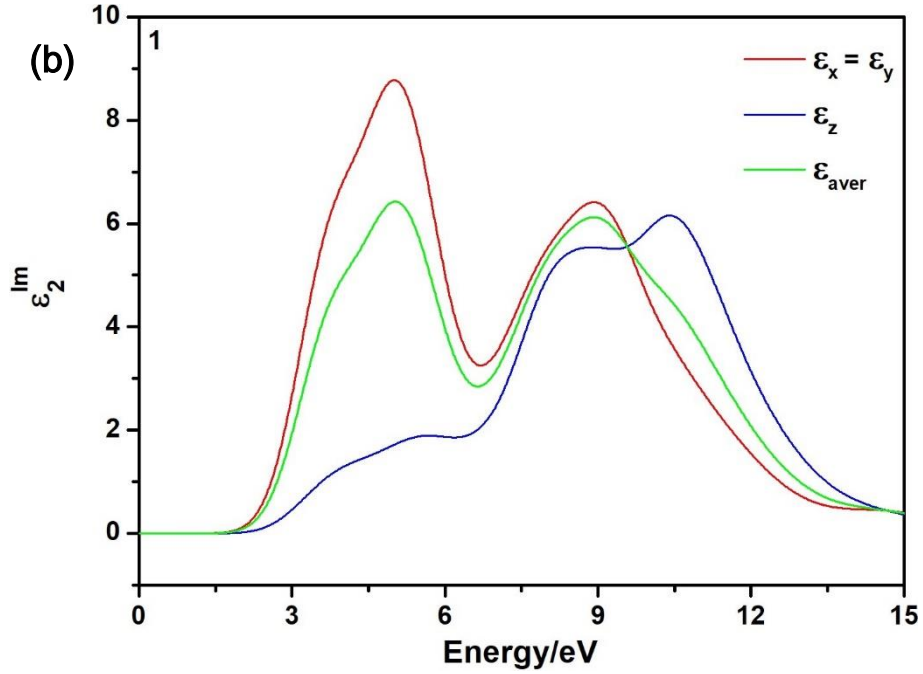


Fig. S2. The IR spectra of **1** (a) and **2** (b).


(a)
1
$\varepsilon_x = \varepsilon_y$
ε_z
ε_{aver}
ε_1^{Re}
Energy/eV


(b)
1
$\varepsilon_x = \varepsilon_y$
ε_z
ε_{aver}
ε_2^{Im}
Energy/eV

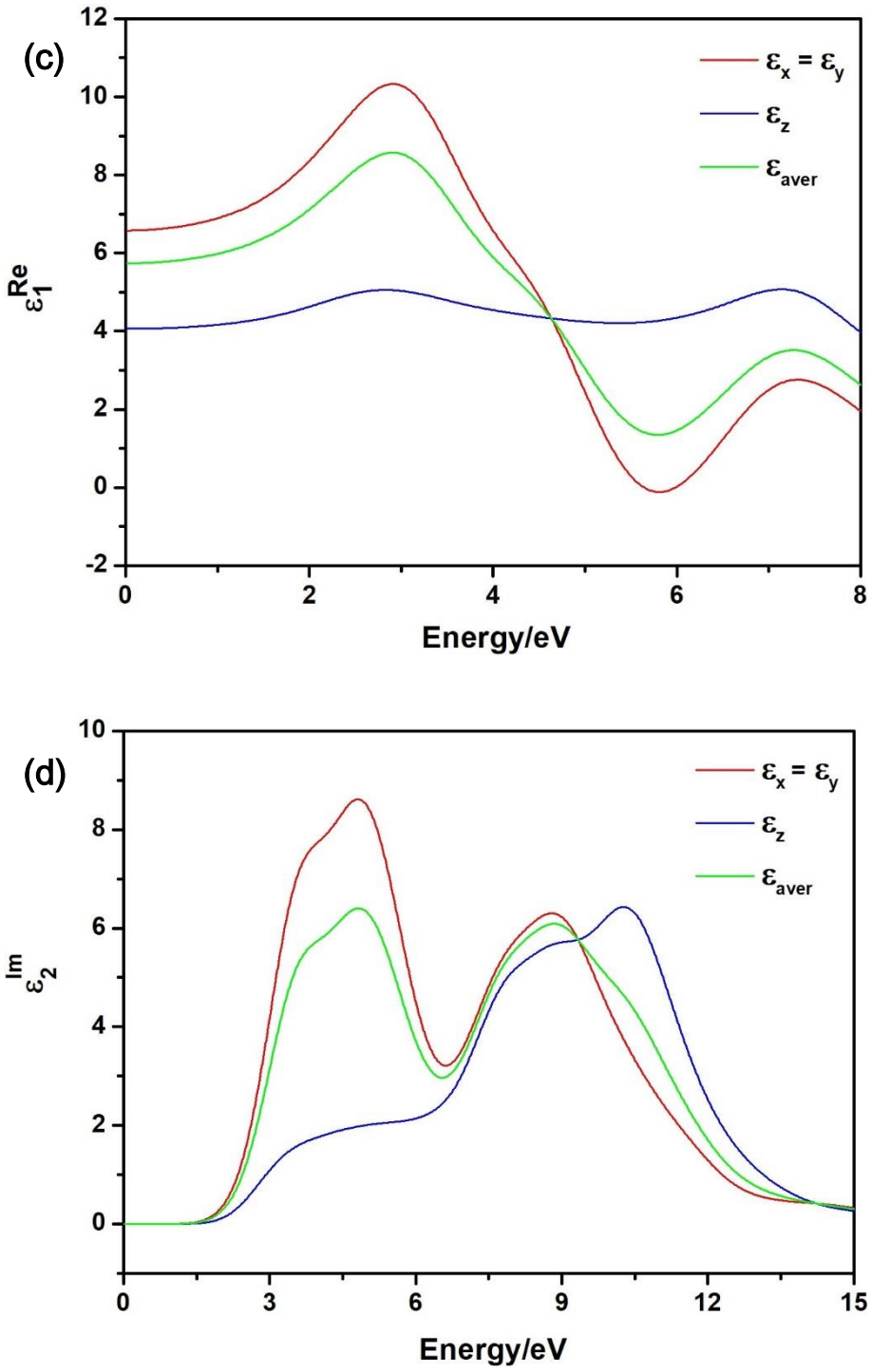


Fig. S3 The calculated real parts (a and c) and imaginary parts (b and d) of optical dielectric functions for **1** and **2**.

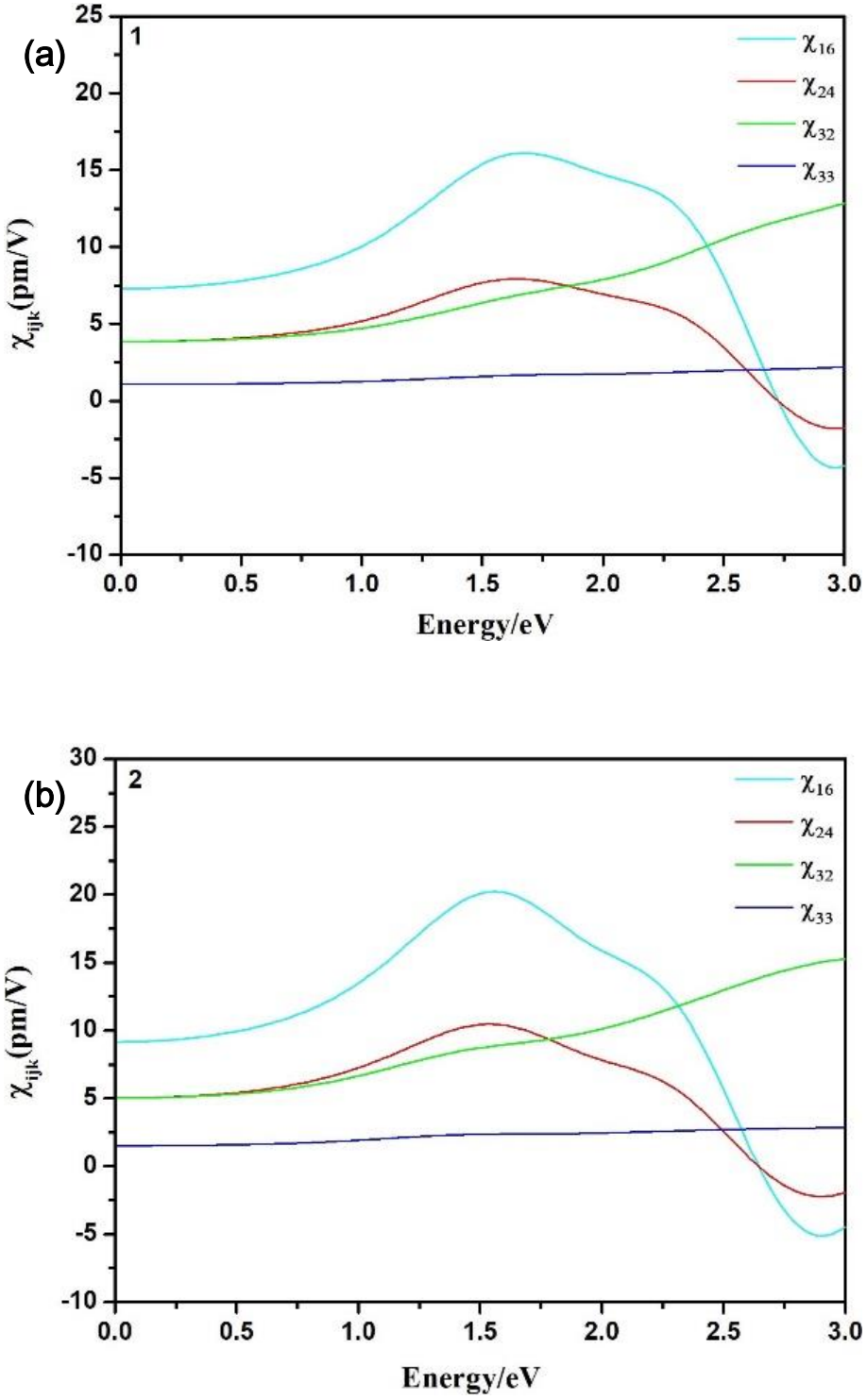


Fig. S4 The calculated frequency-dependent SHG coefficients of **1** (a) and **2** (b).