Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

First Polar Quaternary Sulphide $CsLiGa_6S_{10}$ with Mixed Ordered Alkali Cations Displaying Excellent Infrared Nonlinear Optical Properties

Zi Wang,[a,b] Bin-Wen Liu,[a,c,*] and Guo-Cong Guo[a,c,*]

[a] State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian, 350002, P. R. China

[c] University of Chinese Academy of Sciences, Beijing 100039, PR China

[b] Fujian Science & Technology Innovation Laboratory for Optoelectronic Information of China, Fuzhou, Fujian 350108, P. R. China

[*] E-mail addresses: bwliu@fjirsm.ac.cn (B.-W. Liu), gcguo@fjirsm.ac.cn (G.-C. Guo)

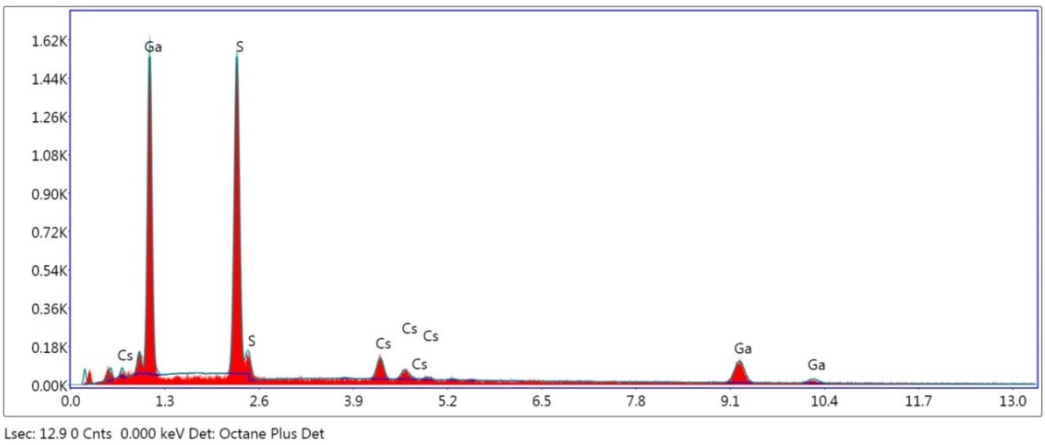

Fig. S1 The EDS result of $CsLiGa_6S_{10}$.

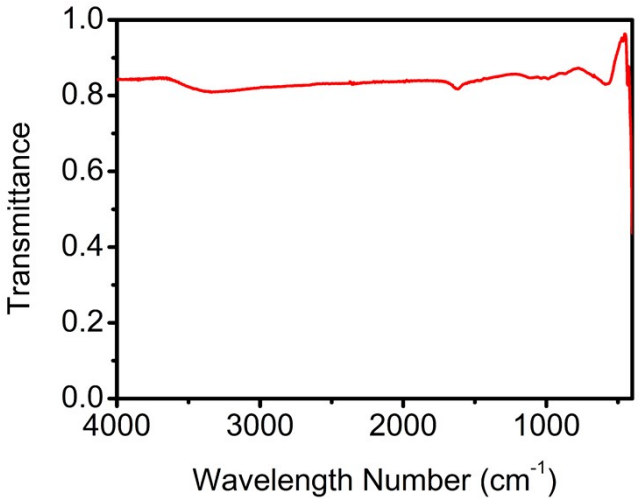

Fig. S2 IR spectrum of $CsLiGa_6S_{10}$.

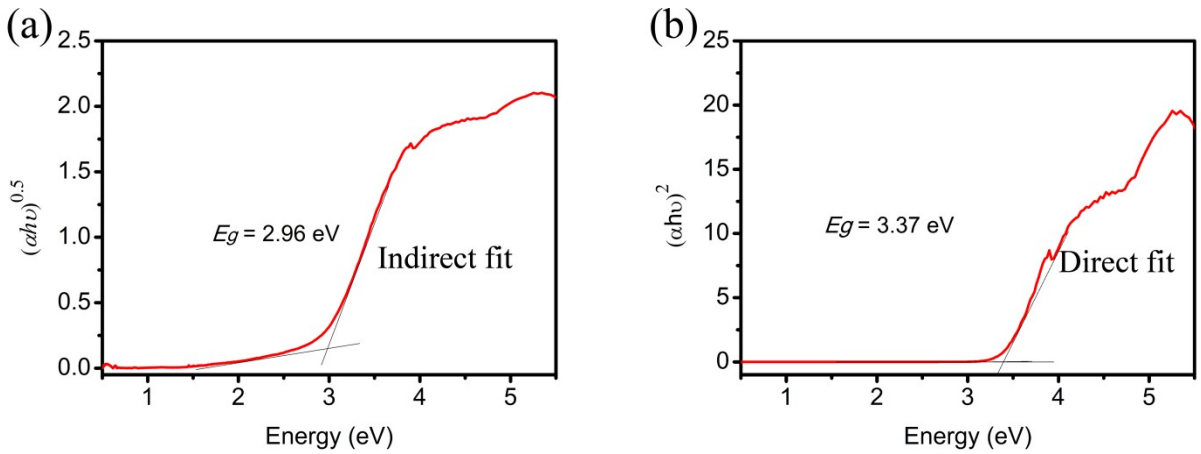

Fig. S3 The indirect and direct models to determine the band gap of $CsLiGa_6S_{10}$.

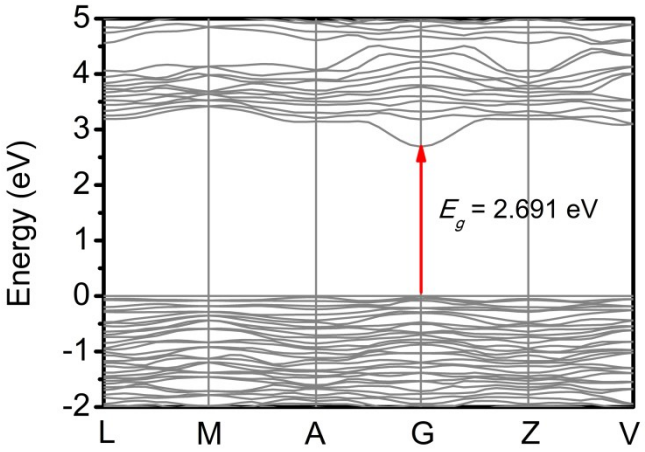

Fig. S4 Band structure of $CsLiGa_6S_{10}$.

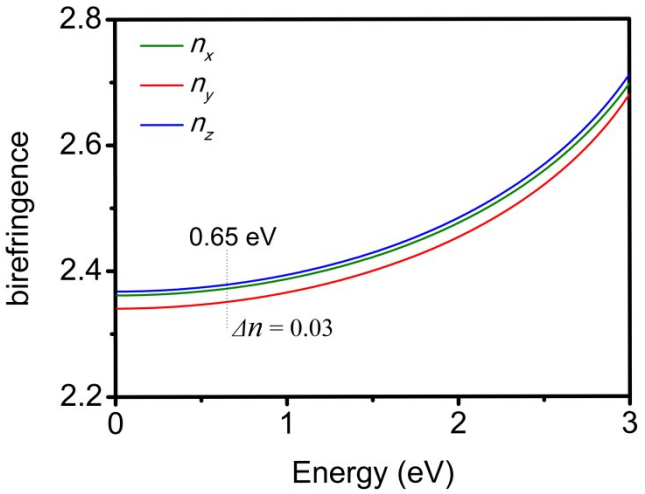

Fig. S5 The energy dependence birefringence of $CsLiGa_6S_{10}$.

Table S1 Crystal data and structure refinements for $CsLiGa_6S_{10}$.

Empirical formula	$CsLiGa_6S_{10}$
CCDC	2154078
Fw	1757.54
Temperature (K)	293(2)
Space group	*Cc*
a (Å)	16.763(1)
b (Å)	6.436(1)
c (Å)	16.192(1)
β (°)	111.03(1)
V (Å^3)	1630.5(1)
Z	2
D_{calcd} (g cm^{-3})	3.580
μ (mm^{-1})	13.224
GOF on F^2	1.031
$R_1{}^a$ ($I > 2\sigma(I)$)	0.0197
$wR_2{}^b$ ($I > 2\sigma(I)$)	0.0402
$R_1{}^a$ (all data)	0.0200
$wR_2{}^b$ (all data)	0.0403
Flack	-0.001(7)
$\Delta\rho_{max}/\Delta\rho_{min,}$ (e Å^{-3})	0.766/−1.018

$^aR = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $^bwR = (\Sigma(w(F_o{}^2-F_c{}^2)^2)/\Sigma(w(F_o{}^2)^2))^{1/2}$.

Table S2. Atomic coordinates and equivalent isotropic displacement parameters (Å^{-2}) of $CsLiGa_6S_{10}$.

atoms	x	y	z	U(eq)
Cs1	0.68507(3)	0.31061(5)	0.64054(3)	0.01925(11)
Li1	0.4181(6)	0.8321(12)	0.8142(7)	0.007(3)
Ga1	0.86362(5)	0.83381(9)	0.89388(6)	0.0090(2)
Ga2	0.63344(4)	0.68567(10)	0.84628(5)	0.0096(2)
Ga3	0.49755(5)	0.82308(11)	0.63012(5)	0.0092(2)
Ga4	0.81262(5)	0.68154(10)	0.48574(5)	0.0093(2)
Ga5	0.94721(6)	0.83936(10)	0.71687(5)	0.00959(19)
Ga6	0.59600(5)	0.83322(9)	0.44352(5)	0.00955(19)
S1	0.55671(9)	0.8299(2)	0.92012(11)	0.0107(4)
S2	0.95240(10)	0.66592(17)	0.59275(10)	0.0084(3)
S3	1.00000(10)	0.8291(2)	1.00000(9)	0.0091(3)
S4	0.40060(10)	0.6631(2)	0.67388(11)	0.0111(3)
S5	0.72420(12)	0.7948(2)	0.55057(12)	0.0127(4)
S6	0.77322(10)	0.6646(2)	0.95028(11)	0.0090(3)
S7	0.63471(12)	0.8186(2)	0.71976(13)	0.0131(4)
S8	0.81480(10)	0.8389(2)	0.36276(10)	0.0101(3)
S9	0.58842(11)	0.3391(2)	0.81538(11)	0.0094(3)
S10	0.85949(9)	0.6694(2)	0.77003(10)	0.0106(4)

Table S3. The selected bonds and distances of $CsLiGa_6S_{10}$.

bond	distances	bond	distances	bond	distances
Cs1−S1	3.5599(16)	Ga1−S10	2.2462(18)	Ga4−S5	2.224(2)
Cs1−S4	3.5840(16)	Ga1−S8	2.2507(15)	Ga4−S8	2.2457(18)
Cs1−S5	3.5984(16)	Ga1−S6	2.3041(18)	Ga4−S6	2.3362(16)
Cs1−S8	3.6035(16)	Ga1−S3	2.315(2)	Ga4−S2	2.3640(18)
Cs1−S7	3.6278(15)	Ga2−S7	2.227(2)	Ga5−S10	2.2378(15)
Cs1−S7	3.7184(15)	Ga2−S1	2.2469(16)	Ga5−S4	2.2465(15)
Cs1−S10	3.7253(15)	Ga2−S6	2.3478(19)	Ga5−S2	2.3277(16)
Cs1−S9	3.7369(15)	Ga2−S9	2.3504(16)	Ga5−S9	2.332(2)
Cs1−S5	3.7763(15)	Ga3−S7	2.236(2)	Ga6−S5	2.2384(19)
Cs1−S2	3.8094(17)	Ga3−S4	2.2427(16)	Ga6−S1	2.2584(16)
Cs1−S6	3.8687(16)	Ga3−S3	2.3370(15)	Ga6−S9	2.3156(18)
Cs1−S3	3.8875(15)	Ga3−S2	2.3407(14)	Ga6−S3	2.3608(17)
		Li1−S1	2.342(10)	Li1−S8	2.409(10)
		Li1−S10	2.384(8)	Li1−S4	2.440(11)

Table S4. Powder LIDTs of $CsLiGa_6S_{10}$ and $AgGaS_2$.

compounds	damage energy (mJ)	spot area (cm^2)	τ_p (ns)	damage threshold [$MW \cdot cm^{-2}$]
$CsLiGa_6S_{10}$	15.3	0.03	10	51.0
$AgGaS_2$	3.4	0.03	10	11.3