Electronic Supplementary Information:

$Li_5Cs(SO_4)_3$: A Potential Zero-order Wave Plate Material with Short Deep-ultraviolet Cutoff Edge

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Table S1 Atomic coordinates (× 10^4), equivalent isotropic displacement parameters ($Å^2$ × 10^3) for $Li_5Cs(SO_4)_3$. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor. Bond valence sums (BVS) are calculated by using bond-valence theory (Si = exp[(*R*o−*R*i)/B], where *R*o is an empirical constant, *R*i is the length of bond *I* (in angstroms), and B= 0.37).

Atoms	**x**	**y**	**z**	**$U_{(eq)}$**	**S.O.F.**	**BVS**
Cs(1)	2526(1)	5662(1)	2342(1)	42(1)		0.72
Li(1)	3044(18)	7392(6)	4340(6)	34(2)		0.92
Li(2)	-2201(17)	4323(5)	631(6)	27(2)		1.18
Li(3)	1893(16)	2863(5)	1569(5)	25(2)		1.15
Li(4)	-2900(15)	4165(5)	4412(5)	20(2)		1.13
Li(5)	-1998(16)	8067(5)	1333(5)	27(2)		1.05
S(1)	-2152(2)	6164(1)	4442(1)	14(1)		6.15
S(2)	-2687(3)	6354(1)	275(1)	26(1)		6.4
S(3)	6991(2)	3452(1)	2474(1)	16(1)		6.09
O(1)	-3433(6)	6801(2)	3835(2)	29(1)		2.09
O(2)	-2498(7)	5320(2)	4038(2)	31(1)		2.03
O(3)	-3440(6)	6203(2)	5343(2)	30(1)		2.05
O(4)	765(6)	6364(2)	4563(2)	20(1)		2.02
O(5)	8141(6)	2720(2)	1963(2)	19(1)		2.02
O(6)	4047(6)	3323(2)	2562(2)	22(1)		2.09
O(7)	8274(6)	3480(2)	3392(2)	21(1)		2.07
O(8)	7482(7)	4248(2)	1983(2)	29(1)		1.99
O(9A)	-1820(30)	5459(8)	373(9)	68(4)	0.5	/
O(9B)	-2990(30)	5519(8)	683(10)	62(4)	0.5	/
O(10)	-5437(8)	6559(2)	-56(3)	47(1)		2.04
O(11)	-1971(8)	6873(3)	1052(3)	52(1)		2.07
O(12)	-892(9)	6504(3)	-481(3)	67(1)		2.18

Table S2 Selected bond lengths (Å) and angles (°) for $Li_5Cs(SO_4)_3$.

Cs(1)-O(9B)#1	3.320(10)	S(1)-O(2)	1.447(3)
Cs(1)-O(8)	3.339(4)	S(1)-O(1)	1.461(3)
Cs(1)-O(8)#2	3.352(3)	S(1)-O(3)	1.474(3)
Cs(1)-O(5)#3	3.376(3)	S(1)-O(4)	1.478(3)
Cs(1)-O(1)#1	3.411(3)	S(2)-O(11)	1.428(4)
Cs(1)-O(11)	3.435(4)	S(2)-O(9B)	1.438(13)
Cs(1)-O(2)#1	3.481(3)	S(2)-O(12)	1.449(4)
Cs(1)-O(4)	3.542(3)	S(2)-O(10)	1.463(4)
Cs(1)-O(9A)	3.554(14)	S(2)-O(9A)	1.464(11)
Cs(1)-O(2)	3.579(4)	S(3)-O(8)	1.453(3)
Cs(1)-O(9B)	3.604(18)	S(3)-O(7)	1.466(3)
Cs(1)-O(6)	3.728(4)	S(3)-O(6)	1.474(3)
		S(3)-O(5)	1.481(3)
Li(1)-O(4)	1.985(9)		
Li(1)-O(10)#4	1.991(10)	O(2)-S(1)-O(1)	109.0(2)
Li(1)-O(5)#3	2.038(9)	O(2)-S(1)-O(3)	110.5(2)
Li(1)-O(1)#1	2.113(10)	O(1)-S(1)-O(3)	108.8(2)
Li(1)-O(12)#5	2.608(11)	O(2)-S(1)-O(4)	110.2(2)
Li(2)-O(9A)	1.817(15)	O(1)-S(1)-O(4)	109.57(18)
Li(2)-O(9B)	1.903(15)	O(3)-S(1)-O(4)	108.83(17)
Li(2)-O(10)#8	1.973(9)	O(8)-S(3)-O(7)	110.50(19)
Li(2)-O(8)#2	1.983(9)	O(8)-S(3)-O(6)	109.5(2)
Li(2)-O(12)#9	2.011(9)	O(7)-S(3)-O(6)	109.21(18)
Li(2)-O(9A)#9	2.514(17)	O(8)-S(3)-O(5)	109.72(19)
Li(3)-O(6)	1.913(8)	O(7)-S(3)-O(5)	108.65(17)
Li(3)-O(1)#10	1.916(8)	O(6)-S(3)-O(5)	109.19(18)
Li(3)-O(12)#9	1.920(9)	O(11)-S(2)-O(9B)	102.1(7)
Li(3)-O(5)#2	1.962(9)	O(11)-S(2)-O(12)	111.6(3)
Li(4)-O(2)	1.889(8)	O(9B)-S(2)-O(12)	122.1(4)
		O(11)-S(2)-O(10)	110.4(2)
Li(5)-O(11)	1.902(9)	O(9B)-S(2)-O(10)	103.1(7)
Li(5)-O(3)#13	1.956(9)	O(12)-S(2)-O(10)	107.0(2)
Li(5)-O(6)#6	1.960(8)		
Li(5)-O(7)#3	1.977(9)		

Symmetry transformations used to generate equivalent atoms:

#1 x+1, y, z #2 x-1, y, z #3 -x+1, y+1/2,-z+1/2

#4 x+1, -y+3/2, z+1/2 #5 x, -y+3/2, z+1/2

#6 -x, y+1/2, -z+1/2 #8 -x-1, -y+1, -z

#9 -x, -y+1, -z #10 -x, y-1/2, -z+1/2

#13 x,-y+3/2, z-1/2

Table S3 Birefringence and cutoff edge comparison for wave plate.

	Birefringence	**Cutoff Edge**(nm)
$CaCO_3$	0.172	200
MgF_2	0.0118	110
Al_2O_3	0.01	170
quartz crystals (SiO_2)	0.0059	200
$Li_5Cs(SO_4)_3$	0.0047	180

Table S4 Comparison of basic information on alkali metal sulfates.

Collection Code	Space group	Formula	Type of S-O units	A:S
2512	*P*2$_1$/*c*	$Li_2(SO_4)$	Isolated $[SO_4]$	2
153806	*Cmcm*		Isolated $[SO_4]$	2
37435	*F*-43*m*		Isolated $[SO_4]$	2
201117	*Fm*-3*m*		Isolated $[SO_4]$	2
2895	*Fddd*	$Na_2(SO_4)$	Isolated $[SO_4]$	2
62516	*P*63/*mmc*		Isolated $[SO_4]$	2
66554	*Cmcm*		Isolated $[SO_4]$	2
81504	*Pbnm*		Isolated $[SO_4]$	2
27955	*P*-3*m*		Isolated $[SO_4]$	2
31687	*Pbnn*		Isolated $[SO_4]$	2
31816	*P*-3	$Na_2(SO_3)$	Isolated $[SO_3]$	2
44800	*P*6/*m*		Isolated $[SO_3]$	2
60762	*P*-3*m*	$K_2(SO_3)$	Isolated $[SO_3]$	2
2827	*Pnam*	$K_2(SO_4)$	Isolated $[SO_4]$	2
14084	*P*63/*mmc*		Isolated $[SO_4]$	2
31533	*Pmcn*		Isolated $[SO_4]$	2
27956	*P*-3*m*		Isolated $[SO_4]$	2
2105	*Pnam*	$Rb_2(SO_4)$	Isolated $[SO_4]$	2
27462	*P*63/*mmc*		Isolated $[SO_4]$	2
56103	*Pmcn*		Isolated $[SO_4]$	2
27463	*P*63/*mmc*	$Cs_2(SO_4)$	Isolated $[SO_4]$	2
52382	*Pnam*		Isolated $[SO_4]$	2
14364	*P*3$_1$*c*	$LiNa(SO_4)$	Isolated $[SO_4]$	2
20851	*P*63	$LiK(SO_4)$	Isolated $[SO_4]$	2
71365	*P*3$_1$*c*		Isolated $[SO_4]$	2
71366	*Cc*		Isolated $[SO_4]$	2
151622	*Pmcn*		Isolated $[SO_4]$	2
151625	*P*63*mc*		Isolated $[SO_4]$	2
151626	*P*63/*mmc*		Isolated $[SO_4]$	2
280392	*Pmcn*		Isolated $[SO_4]$	2
88831	*Cmc*2$_1$		Isolated $[SO_4]$	2
88832	*P*2$_1$*cn*		Isolated $[SO_4]$	2
174056	*Pmcn*	$LiRb(SO_4)$	Isolated $[SO_4]$	2
174057	*P*2$_1$/*c*		Isolated $[SO_4]$	2
174058	*Pn*		Isolated $[SO_4]$	2
63179	*Pmcn*	$LiCs(SO_4)$	Isolated $[SO_4]$	2
63181	*P*2$_1$/*n*		Isolated $[SO_4]$	2
26014	*P*-3*m*	$K_3Na(SO_4)_2$	Isolated $[SO_4]$	2
77343	*P*-3*m*	$KNa(SO_4)$	Isolated $[SO_4]$	2
2102195	*P*2$_1$/*n*	$Li_5Cs(SO_4)_3$	Isolated $[SO_4]$	2

16646	*P*2/*c*	$Na_2(S_2O_4)$	Isolated [SO_2]	1
59949	*P*2$_1$/*n*	$Na_2S_2O_5$	Isolated [SO_3] and Isolated [SO_2]	1
59950	*P*2$_1$		Isolated [SO_3] and Isolated [SO_2]	1
31817	*P*2$_1$/*m*	$K_2S_2O_5$	Isolated [SO_3] and Isolated [SO_2]	1
188009	*Pnma*	$Li_2(S_2O_7)$	Isolated [SO_3] and Isolated [SO_2]	1
413049	*P*-1	$Na_2(S_2O_7)$	Isolated [SO_3] and Isolated [SO_2]	1
249741	*C*2/*c*	$K_2(S_2O_7)$	Isolated [SO_3] and Isolated [SO_2]	1
418071	*P*-1	$Cs_2(S_2O_7)$	Isolated [SO_3] and Isolated [SO_2]	1
413050	*P*-1	$KNa(S_2O_7)$	Isolated [SO_3] and Isolated [SO_2]	1
431359	*C*2/*c*	$Li_2(S_5O_{16})$	Isolated [S_5O_{16}]	0.4
431363	*Pbcn*	$Na_2(S_5O_{16})$	Isolated [S_5O_{16}]	0.4
26180	*Pbcn*	$K_2(S_5O_{16})$	Isolated [S_5O_{16}]	0.4
428769	*P*2$_1$	$Cs_2(S_5O_{16})$	Isolated [S_5O_{16}]	0.4
428770	*P*2$_1$/*c*	$Rb_2(S_6O_{19})$	Isolated [S_4O_{13}] and Isolated [SO_2]	0.33

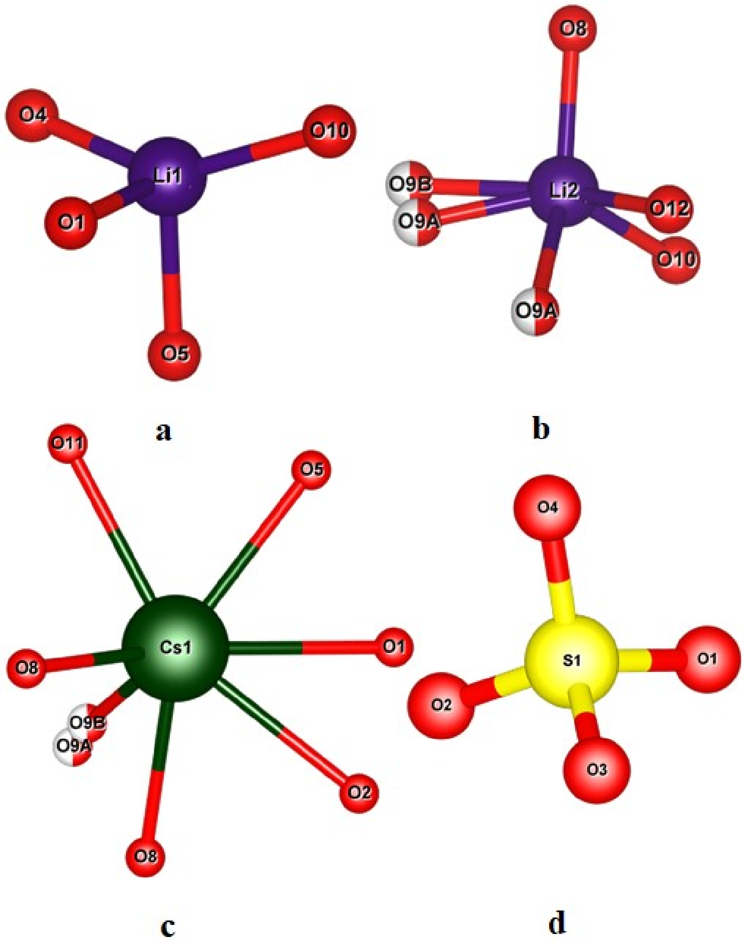

Figure S1 The coordination environments of cations in the crystal structure of $Li_5Cs(SO_4)_3$.

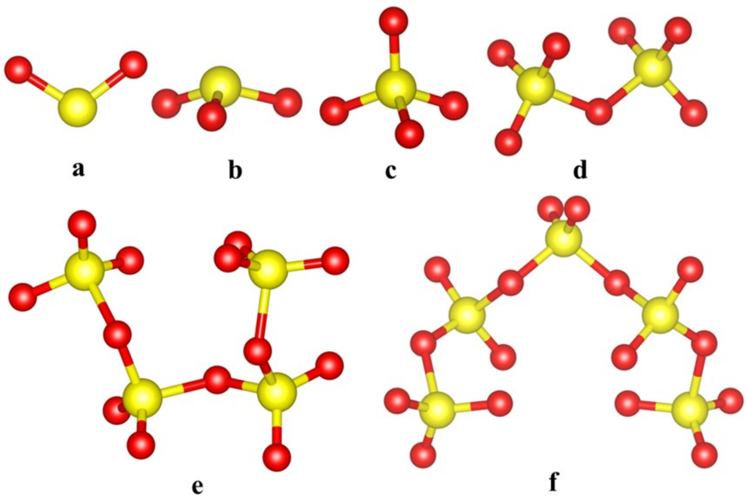

Figure S2 Basic type of S-O group in alkali metal sulfates. (a) SO_2; (b) SO_3; (c) SO_4; (d) S_2O_7; (e) S_4O_{13}; (f) S_5O_{16}.