Deep-ultraviolet transparent alkali metal-rare earth metal sulfate $NaY(SO_4)_2 \cdot H_2O$ as a nonlinear optical crystal: synthesis and characterization

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CONTENTS

Table S1. Selected bond distances (Å) and angles (deg) for $NaY(SO_4)_2 \cdot H_2O$.[a]

Y(1)-O(2)#1	2.355(5)	Y(1)-O(2)#2	2.355(5)
Y(1)-O(1W)	2.386(11)	Y(1)-O(4)#3	2.393(6)
Y(1)-O(4)#4	2.393(6)	Y(1)-O(1)#5	2.441(5)
Y(1)-O(1)	2.441(5)	Y(1)-O(3)#5	2.474(5)
Y(1)-O(3)	2.474(5)	S(1)-O(4)	1.461(5)
S(1)-O(2)	1.471(5)	S(1)-O(3)	1.473(5)
S(1)-O(1)	1.482(5)	Na(1)-O(3)#9	2.356(6)
Na(1)-O(3)	2.356(6)	Na(1)-O(1)#10	2.415(6)
Na(1)-O(1)#4	2.415(6)	Na(1)-O(4)#11	2.533(5)
Na(1)-O(4)#2	2.533(5)	Na(1)-O(2)#2	2.888(5)
Na(1)-O(2)#11	2.888(5)		
O(4)-S(1)-O(2)	107.8(3)	O(4)-S(1)-O(3)	112.0(3)
O(2)-S(1)-O(3)	111.4(3)	O(4)-S(1)-O(1)	111.1(3)
O(2)-S(1)-O(1)	109.7(3)	O(3)-S(1)-O(1)	104.8(3)

[a]Symmetry codes: #1 y, x-1, -z; #2 -x+y+1, -x+1, z-1/3; #3 -x+y+1, -x, z-1/3; #4 y+1, x, -z; #5 x-y, -y, -z-1/3; #6 -y+1, x-y, z+1/3; #7 x, y-1, z; #8 -y, x-y-1, z+1/3; #9 y, x, -z; #10 x, y+1, z; #11 -x+1, -x+y+1, -z+1/3.

Table S2. Atomic coordinates ($\times 10^4$), equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) of $NaY(SO_4)_2 \cdot H_2O$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	Wyck.	x	y	z	$U_{eq}(\text{Å}^2)$
Y(1)	6*c*	5631(1)	0	-1667	8(1)
S(1)	6*c*	5573(3)	139(3)	741(1)	8(1)
Na(1)	3*a*	4716(6)	4716(6)	0	17(1)
O(1)	6*c*	6164(8)	-1250(9)	56(4)	14(1)
O(2)	6*c*	7573(8)	1742(9)	1350(4)	14(1)
O(3)	6*c*	4848(10)	1328(9)	9(3)	14(1)
O(4)	6*c*	3790(9)	-1277(10)	1486(4)	15(1)
O(1W)	6*c*	9131(16)	0	-1667	39(3)

Table S3. Hydrogen-bonding interactions for NaY(SO$_4$)$_2$·H$_2$O.

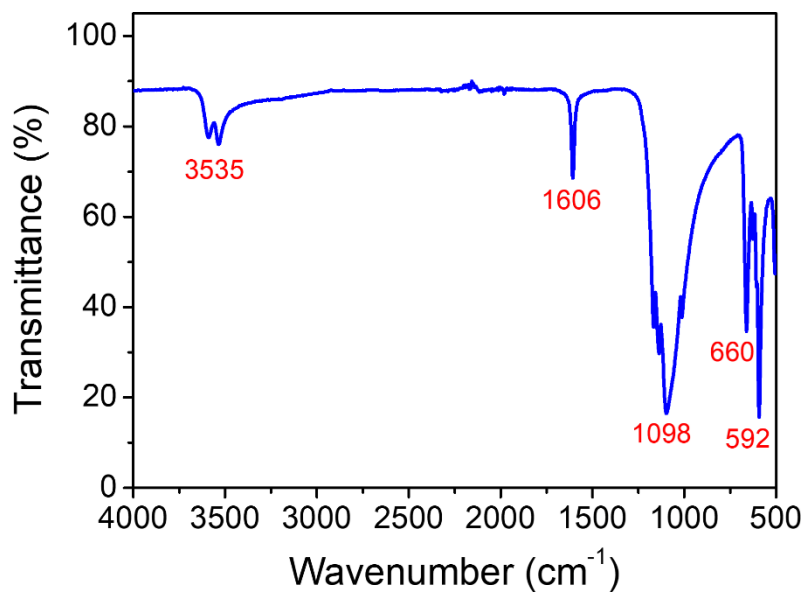| D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(DHA)
O1W-H1···O1	0.7600	2.4700	3.2274	173.00
O1W-H1···O2	0.7600	2.4800	3.0032	128.00

Figure S1. IR spectrum of $NaY(SO_4)_2 \cdot H_2O$.