Supporting information

# Double Second-order Jahn-Teller Strategy Driven NLO Response in Sulfate Crystal $Nb_2O_2(TeO_3)_2(SO_4)$ with a Large Birefringence

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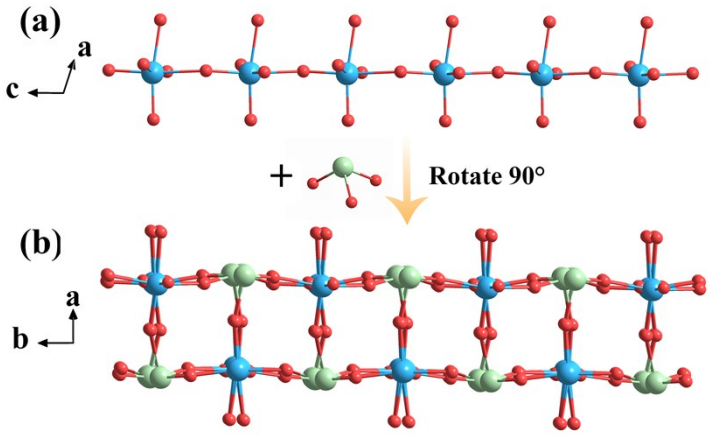


**Fig. S1** (a) 1D chain structure formed by the connection of [$NbO_6$] octahedra. (b) Layered structure constructed by the interweaving of [$NbO_6$] chains and [$TeO_3$] pyramids. Blue, green, and red spheres represent Nb, Te, and O atoms, respectively.

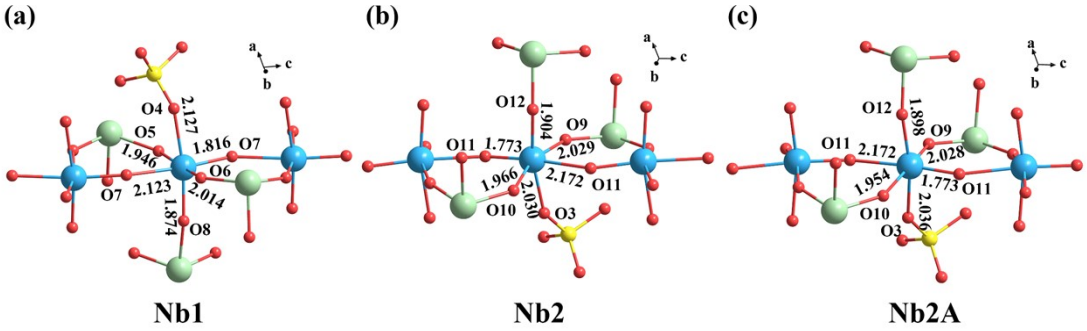


**Fig. S2** The coordination environments of [$NbO_6$] in $Nb_2O_2(TeO_3)_2(SO_4)$: (a) [$Nb1O_6$], (b) [$Nb2O_6$], and (c) [$Nb2AO_6$]. Blue, green, and red spheres represent Nb, Te, and O atoms, respectively.

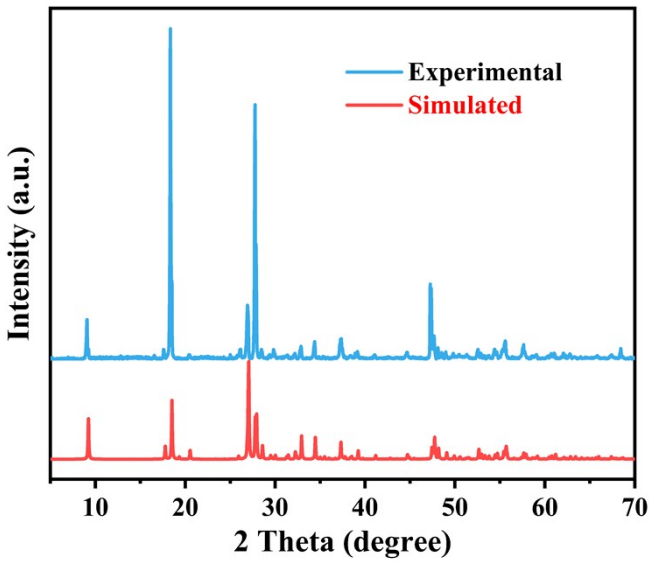


**Fig. S3** Powder X-ray diffraction patterns of $Nb_2O_2(TeO_3)_2(SO_4)$.

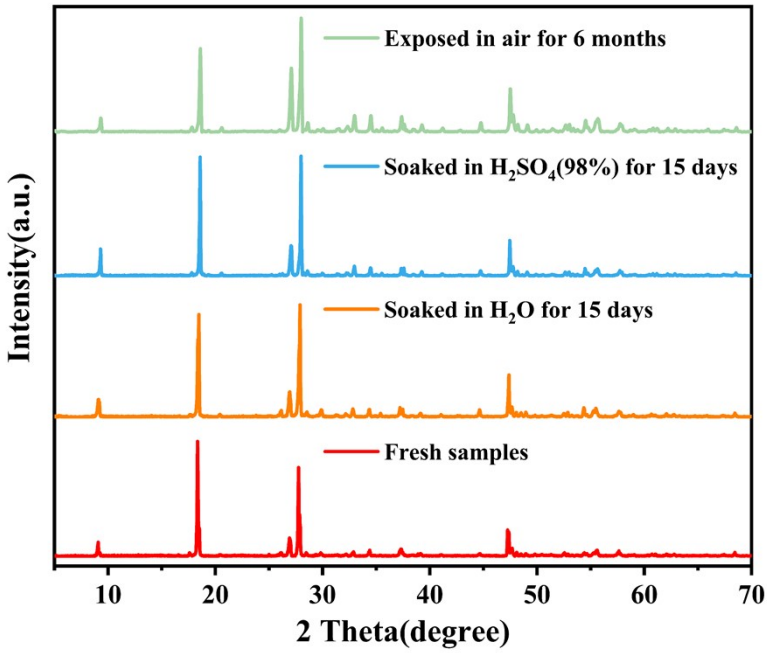


**Fig. S4** Powder X-ray diffraction patterns of $Nb_2O_2(TeO_3)_2(SO_4)$ of fresh samples, samples after soaked in water, $H_2SO_4$(98%) for 15 days, and exposed in air for 6 months.

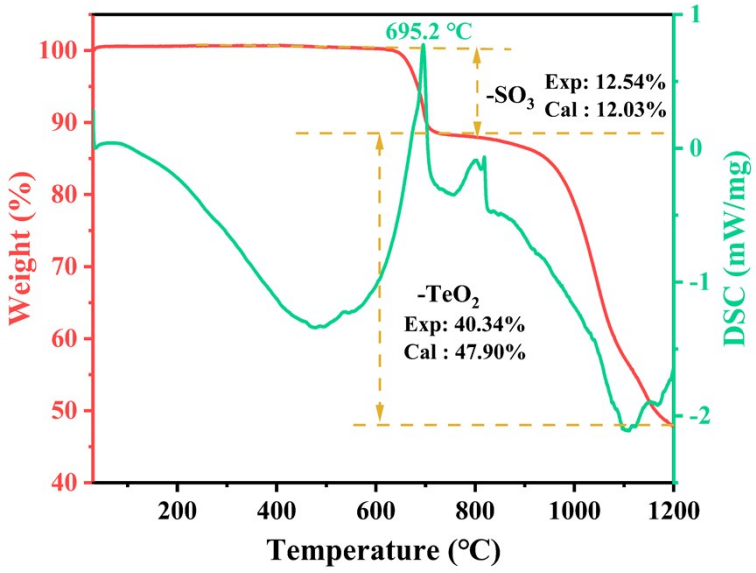


**Fig. S5** The TGA and DSC curves of $Nb_2O_2(TeO_3)_2(SO_4)$ under $N_2$ atmosphere.

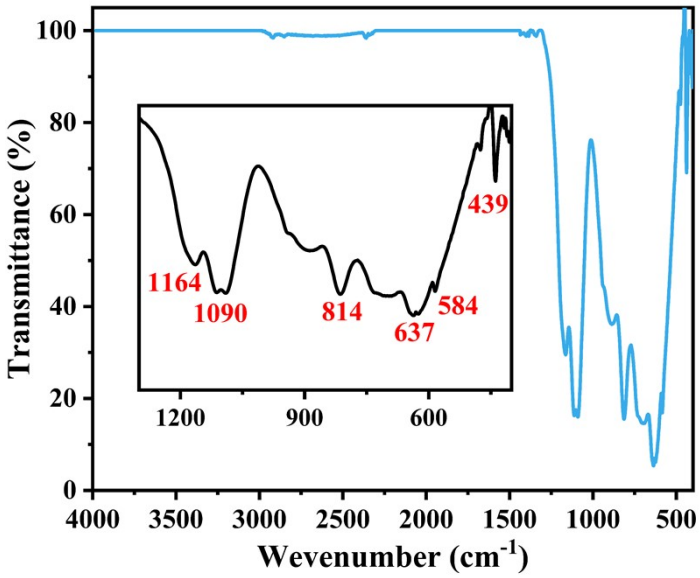


**Fig. S6** IR spectra of $Nb_2O_2(TeO_3)_2(SO_4)$.

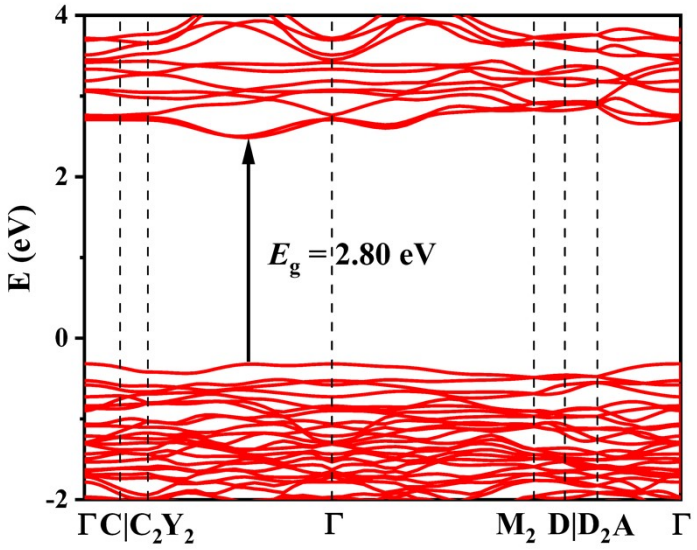


**Fig. S7** Calculated band structure for $Nb_2O_2(TeO_3)_2(SO_4)$.

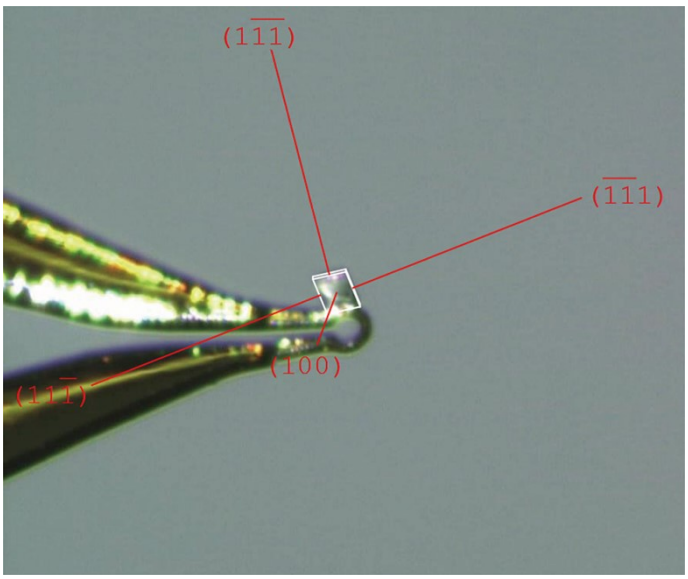


**Fig. S8** The crystal orientation of the naturally growing surface of $Nb_2O_2(TeO_3)_2(SO_4)$.

**Table S1.** Crystallographic data for $Nb_2O_2(TeO_3)_2(SO_4)$.

| Empirical formula | $Nb_2O_2(TeO_3)_2SO_4$ |
|---|---|
| Formula weight | 665.08 |
| Temperature (K) | 296.00 |
| Crystal system | Monoclinic |
| Space group | *Cc* |
| *Z* | 4 |
| *a* (Å) | 20.0326(7) |
| *b* (Å) | 6.5977(3) |
| *c* (Å) | 7.6438(2) |
| *α* (°) | 90 |
| *β* (°) | 107.220(2) |
| *γ* (°) | 90 |
| V (Å$^3$) | 964.99(6) |
| $D_c$ (Mg m$^{-3}$) | 4.578 |
| $\mu$ (mm$^{-1}$) | 8.581 |
| *F*(000) | 1192.0 |
| Radiation | Mo-K$\alpha$ ($\lambda$ = 0.71073) |
| 2$\vartheta$ range (°) | 4.258 to 61.008 |
| Reflections collected | 14713 |
| Indep. Reflns/ Rint | 2812/ 0.0491 |
| GOOF on $F^2$ | 1.008 |
| $R_1$, w$R_2$ ($I > 2\sigma(I)$)[a] | 0.0288, 0.0629 |
| $R_1$, w$R_2$ (all data) | 0.0359, 0.0662 |
| largest diff. peak and hole (e Å$^{-3}$) | 1.02, -0.67 |

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, [b] $wR_2 = \Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

**Table S2.** Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) and calculated Bond Valence Sum for $Nb_2O_2(TeO_3)_2(SO_4)$. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalized $U_{ij}$ tensor.

| Atom | *x* | *y* | *z* | $U_{eq}$ | BVS |
|---|---|---|---|---|---|
| Te1 | 2957.6(5) | 5313(3) | 4491.5(14) | 19.7(3) | 3.94 |
| Te2 | 5103.7(4) | 314(3) | 8784.1(14) | 18.7(3) | 3.73 |
| Nb1 | 4909.9(12) | 5058(5) | 6338(3) | 18.8(4) | 5.18 |
| Nb2 | 3157.6(17) | 9930(7) | 1908(10) | 17.4(9) | 5.27 |
| Nb2A | 3155(4) | 10089(16) | 2410(30) | 16.2(18) | 5.32 |
| S1 | 6522(5) | 6699(3) | 6630(11) | 22.1(4) | 6.10 |
| O1 | 6291(11) | 7940(30) | 5070(30) | 33(4) | 1.79 |
| O2 | 6829(11) | 7940(30) | 8330(20) | 34(4) | 1.65 |
| O3 | 7107(10) | 5370(30) | 6355(19) | 23(4) | 1.94 |
| O4 | 6012(11) | 5280(40) | 6890(20) | 31(4) | 2.20 |
| O5 | 4912(10) | 2120(30) | 10600(20) | 21(3) | 1.98 |
| O6 | 5057(9) | 2070(30) | 6846(19) | 20(4) | 2.13 |
| O7 | 4957(11) | 5710(30) | 8680(20) | 30(5) | 1.86 |
| O8 | 3937(10) | 4760(30) | 5470(20) | 27(4) | 2.28 |
| O9 | 3125(10) | 7060(30) | 2834(19) | 21(3) | 2.20 |
| O10 | 2985(10) | 7160(30) | 6430(20) | 27(4) | 1.98 |
| O11 | 3115(9) | 9270(30) | -371(19) | 21(4) | 1.95 |
| O12 | 4141(9) | 10240(30) | 2940(20) | 24(4) | 2.22 |

**Table S3.** Selected bond lengths (Å) for $Nb_2O_2(TeO_3)_2(SO_4)$.

| Selected bond | Length (Å) | Selected bond | Length (Å) |
|---|---|---|---|
| Te1-O8 | 1.916(19) | Nb2-O10$^{\#4}$ | 1.97(2) |
| Te1-O9 | 1.814(15) | Nb2-O11 | 1.773(16) |
| Te1-O10 | 1.907(16) | Nb2-O11$^{\#5}$ | 2.171(17) |
| Te2-O5 | 1.954(16) | Nb2-O12 | 1.903(18) |
| Te2-O6 | 1.860(16) | Nb2A-O3$^{\#3}$ | 2.04(2) |
| Te2-O12$^{\#1}$ | 1.881(19) | Nb2A-O9 | 2.03(2) |
| Nb1-O4 | 2.13(2) | Nb2A-O10$^{\#4}$ | 1.95(2) |
| Nb1-O5$^{\#2}$ | 1.944(19) | Nb2A-O11$^{\#5}$ | 1.77(3) |
| Nb1-O6 | 2.015(17) | Nb2A-O11 | 2.17(3) |
| Nb1-O7 | 1.816(16) | Nb2A-O12 | 1.90(2) |
| Nb1-O7$^{\#2}$ | 2.124(17) | S1-O1 | 1.409(19) |
| Nb1-O8 | 1.875(18) | S1-O2 | 1.504(19) |
| Nb2-O3$^{\#3}$ | 2.03(2) | S1-O3 | 1.53(2) |
| Nb2-O9 | 2.033(18) | S1-O4 | 1.44(2) |

$^{\#1}x$, 1-$y$, 1/2+$z$; $^{\#2}x$, 1-$y$, -1/2+$z$; $^{\#3}$-1/2+$x$, 3/2-$y$, -1/2+$z$; $^{\#4}x$, 2-$y$, -1/2+$z$; $^{\#5}x$, 2-$y$, 1/2+$z$

**Table S4.** Selected bond angles (°) for $Nb_2O_2(TeO_3)_2(SO_4)$.

| Selected bond angles | Angle (°) | Selected bond angles | Angle (°) |
|---|---|---|---|
| O9-Te1-O8 | 90.9(8) | O11-Nb2-O10$^{\#5}$ | 95.9(8) |
| O9-Te1-O10 | 99.8(8) | O11-Nb2-O11$^{\#4}$ | 175.3(11) |
| O10-Te1-O8 | 91.5(8) | O11-Nb2-O12 | 100.1(8) |
| O6-Te2-O5 | 102.3(7) | O12-Nb2-O3$^{\#3}$ | 168.2(8) |
| O6-Te2-O12$^{\#1}$ | 92.5(7) | O12-Nb2-O9 | 95.4(8) |
| O12$^{\#1}$-Te2-O5 | 88.1(8) | O12-Nb2-O10$^{\#5}$ | 94.2(8) |
| O5$^{\#2}$-Nb1-O4 | 84.2(8) | O12-Nb2-O11$^{\#4}$ | 84.7(7) |
| O5$^{\#2}$-Nb1-O6 | 168.5(6) | O3$^{\#3}$-Nb2A-O11 | 80.9(9) |
| O5$^{\#2}$-Nb1-O7$^{\#2}$ | 87.1(7) | O9-Nb2A-O3$^{\#3}$ | 80.9(9) |
| O6-Nb1-O4 | 86.9(8) | O9-Nb2A-O11 | 85.3(10) |
| O6-Nb1-O7$^{\#2}$ | 84.5(7) | O10$^{\#5}$-Nb2A-O3$^{\#3}$ | 86.8(9) |
| O7-Nb1-O4 | 92.4(8) | O10$^{\#5}$-Nb2A-O9 | 165.1(11) |
| O7$^{\#2}$-Nb1-O4 | 82.4(7) | O10$^{\#5}$-Nb2A-O11 | 84.6(10) |
| O7-Nb1-O5$^{\#2}$ | 93.0(8) | O11$^{\#4}$-Nb2A-O3$^{\#3}$ | 94.6(10) |
| O7-Nb1-O6 | 94.7(8) | O11$^{\#4}$-Nb2A-O9 | 94.0(9) |
| O7-Nb1-O7$^{\#2}$ | 174.8(12) | O11$^{\#4}$-Nb2A-O10$^{\#5}$ | 95.3(11) |
| O7-Nb1-O8 | 96.8(8) | O11$^{\#4}$-Nb2A-O11 | 175.5(11) |
| O8-Nb1-O4 | 170.8(7) | O11$^{\#4}$-Nb2A-O12 | 97.0(11) |
| O8-Nb1-O5$^{\#2}$ | 95.1(8) | O12-Nb2A-O3$^{\#3}$ | 168.1(15) |
| O8-Nb1-O6 | 92.5(8) | O12-Nb2A-O9 | 95.6(9) |
| O8-Nb1-O7$^{\#2}$ | 88.5(8) | O12-Nb2A-O10$^{\#5}$ | 94.8(9) |
| O3$^{\#3}$-Nb2-O9 | 81.0(8) | O12-Nb2A-O11 | 87.5(10) |
| O3$^{\#3}$-Nb2-O11$^{\#4}$ | 83.7(7) | O1-S1-O2 | 111.4(4) |
| O9-Nb2-O11$^{\#4}$ | 83.0(7) | O1-S1-O3 | 106.9(12) |
| O10$^{\#5}$-Nb2-O3$^{\#3}$ | 86.6(8) | O1-S1-O4 | 115.1(13) |
| O10$^{\#5}$-Nb2-O9 | 162.6(8) | O2-S1-O3 | 107.4(12) |
| O10$^{\#5}$-Nb2-O11$^{\#4}$ | 83.4(7) | O4-S1-O2 | 111.1(12) |
| O11-Nb2-O3$^{\#3}$ | 91.5(7) | O4-S1-O3 | 104.4(4) |
| O11-Nb2-O9 | 96.7(8) | | |

$^{\#1}$+*x*, 1-*y*, 1/2+*z*; $^{\#2}$+*x*, 1-*y*, -1/2+*z*; $^{\#3}$-1/2+*x*, 3/2-*y*, -1/2+*z*; $^{\#4}$+*x*, 2-*y*, 1/2+*z*; $^{\#5}$+*x*, 2-*y*, -1/2+*z*

**Table S5.** Space groups, starting weight loss temperature, band gap, and birefringence information of some sulfates.

| Compound | Space group | Weight loss temperature (℃) | Band gap (eV) | Birefringence | Reference |
|---|---|---|---|---|---|
| $Ti(TeO_3)(SO_4)$ | $P2_1$ | 560 | 2.75 | 0.145@visible | 1 |
| $Sb_2(TeO_3)(SO_4)_2$ | $P\bar{1}$ | 380 | 4.24 | 0.11@546 nm | 2 |
| $Sb_2(TeO_3)(SO_4)_2$ | $P2_1/c$ | 390 | 4.22 | 0.10@546 nm | 2 |
| $In_2(SO_4)(TeO_3)(OH)_2(H_2O)$ | $P2_1/n$ | 350 | 4.86 | 0.0561@1064 nm | 3 |
| $In_3(SO_4)(TeO_3)_2F_3(H_2O)$ | $P2_12_12_1$ | 350 | 4.10 | 0.0876@1064 nm | 3 |
| $Ga_2(TeO_3)(SO_4)(OH)_2$ | $P2_1/m$ | N/A | 4.23 | 0.1029@1064 nm | 4 |
| $In_2(TeO_3)_2(SO_4)(H_2O)$ | $C2/c$ | N/A | 4.86 | 0.0134@1064 nm | 4 |
| $Zn_4(Te_3O_7)_2(SO_4)_2(H_2O)$ | $C2/c$ | N/A | 4.13 | 0.0840@1064 nm | 4 |
| $Hg_3(Te_3O_8)(SO_4)$ | $P\bar{1}$ | N/A | 3.36 | 0.1667@1064 nm | 4 |
| $Y_3(TeO_3)_2(SO_4)_2(OH)(H_2O)$ | $P2_1/m$ | 434 | 4.40 | 0.0800@1064 nm | 5 |
| $Y_2(Te_4O_{10})(SO_4)$ | $P\bar{1}$ | 700 | 4.10 | 0.1243@1064 nm | 5 |
| $Hg_2(TeO_3)(SO_4)$ | $P2_1/c$ | 530 | 3.55 | 0.159@534 nm | 6 |
| $Hg_4(Te_2O_5)(SO_4)$ | $P2_1/c$ | 350 | 2.85 | 0.520@534 nm | 6 |
| $Nb_2O_2(TeO_3)_2(SO_4)$ | $Cc$ | 600 | 2.8 | 0.197@546 nm | This work |

**Table S6.** Calculated dipole moment component of $Nb_2O_2(TeO_3)_2(SO_4)$.

| Unit | Dipole moment (D = Debyes) | | | |
|---|---|---|---|---|
| | *x* | *y* | *z* | total magnitude |
| $Te(1)O_3$ | 8.19 | 8.41 | 2.58 | 12.01 |
| $Te(1)O_3$ | 8.19 | 8.41 | 2.58 | 12.01 |
| $Te(2)O_3$ | 7.76 | 7.02 | 3.43 | 11.02 |
| $Te(2)O_3$ | 7.76 | 7.02 | 3.43 | 11.02 |
| $TeO_3$ in the cell | 0.85 | 0.00 | 1.71 | 1.91 |
| $Nb(1)O_6$ | 1.21 | 0.39 | 0.83 | 1.52 |
| $Nb(1)O_6$ | 1.21 | 0.39 | 0.83 | 1.52 |
| $Nb(2)O_6$ | 3.41 | 0.41 | 1.05 | 3.59 |
| $Nb(2)O_6$ | 3.41 | 0.41 | 1.05 | 3.59 |
| $Nb(2A)O_6$ | 2.10 | 0.52 | 1.81 | 2.82 |
| $Nb(2A)O_6$ | 2.10 | 0.52 | 1.81 | 2.82 |
| $NbO_6$ in the cell | 3.82 | 0.00 | 0.85 | 3.91 |
| $SO_4$ | 2.55 | 1.93 | 0.02 | 3.20 |
| $SO_4$ | 2.55 | 1.93 | 0.02 | 3.20 |
| $SO_4$ in cell | 5.09 | 0.00 | 0.03 | 5.09 |
| Net dipole moment | 2.12 | 0.00 | 2.59 | 3.35 |

Symmetry transformations used to generate equivalent atoms: +*x*, -*y*, 0.5+*z*

**Table S7.** Space groups, SHG responses and birefringence information of some sulfates.

| Number | Compounds | Space Group | SHG Intensity (× KDP) | Birefringence | Reference |
|---|---|---|---|---|---|
| 1 | $CeF_2(SO_4)$ | $Pca2_1$ | 8 | 0.361@546 nm | 7 |
| 2 | $Ce(IO_3)_2SO_4$ | $P2_12_12_1$ | 3.5 | 0.259@546 nm | 8 |
| 3 | $Nb_2O_3(IO_3)_2(SO_4)$ | $P2_1$ | 6 | 0.220@1064 nm | 9 |
| 4 | $Nb_2O_2(TeO_3)_2(SO_4)$ | $Cc$ | 0.82 | 0.197@546 nm | This work |
| 5 | $Hg_2(IO_3)_2(SO_4)\cdot H_2O$ | $C2$ | 6 | 0.138@546 nm | 10 |
| 6 | $CsSbF_2SO_4$ | $Pna2_1$ | 3 | 0.112@1064 nm | 11 |
| 7 | $RbSbSO_4Cl_2$ | $P2_12_12_1$ | 2.7 | 0.11@1064 nm | 12 |
| 8 | $Hg_3O_2SO_4$ | $P3_221$ | 14 | 0.100@546 nm | 13 |
| 9 | $KBiCl_2SO_4$ | $P2_12_12_1$ | 1.7 | 0.098@1064 nm | 14 |
| 10 | $HgSO_4$ | $Pmn2_1$ | 11 | 0.093@546 nm | 15 |
| 11 | $In_3(SO_4)(TeO_3)_2F_3(H_2O)$ | $P2_12_12_1$ | 0.11 | 0.088@1064 nm | 16 |
| 12 | $[Ag(NH_3)_2]_2SO_4$ | $P\bar{4}2_1c$ | 1.4 | 0.080@589 nm | 17 |
| 13 | $K_4Sb(SO_4)_3Cl$ | $P6_1$ | 0.1 | 0.068@546 nm | 18 |
| 14 | $NaBi(SO_4)_2(H_2O)$ | $P3_22_1$ | 0.38 | 0.062@546 nm | 19 |
| 15 | $K_2Bi_2(SO_4)_2Cl_4$ | $P2_12_12_1$ | 5.5 | 0.056@1064 nm | 20 |
| 16 | $(NH_4)_2Bi_2(SO_4)_2Cl_4$ | $P2_12_12_1$ | 4.8 | 0.055@1064 nm | 20 |
| 17 | $Te(OH)_3(SO_4)\cdot H_2O$ | $P2_12_12_1$ | 3 | 0.052@546 nm | 21 |
| 18 | $Sb_6O_7(SO_4)_2$ | $Ccc2$ | 2 | 0.052@1064nm | 22 |
| 19 | $Rb_2Bi_2(SO_4)_2Cl_4$ | $P2_12_12_1$ | 5.3 | 0.047@1064 nm | 20 |
| 20 | $HfF_2(SO_4)$ | $Pca2_1$ | 2.5 | 0.045@546 nm | 23 |
| 21 | $ZrF_2(SO_4)$ | $Pca2_1$ | 3.2 | 0.044@546 nm | 23 |
| 22 | $Te_2O_3(SO_4)$ | $Pmn2_1$ | 6 | 0.043@546 nm | 21 |
| 23 | $NaHSO_4\cdot H_2O$ | $Cc$ | 1.5 | 0.042@546 nm | 24 |
| 24 | $NaCe(SO_4)_2(H_2O)$ | $P3_22_1$ | 0.2 | 0.039@546 nm | 25 |
| 25 | $La(NH_4)(SO_4)_2$ | $Pmn2_1$ | 2.4 | 0.03@1064 nm | 26 |
| 26 | $Li_8NaRb_3(SO_4)_6\cdot 2H_2O$ | $C2$ | 0.5 | 0.021@1064 nm | 27 |
| 27 | $Rb_3In(SO_4)_3$ | $R3c$ | 0.5 | 0.019@1064 nm | 28 |
| 28 | $Rb_6Sb_4(SO_4)_3F_{12}$ | $P3$ | 0.1 | 0.01@1064 nm | 29 |
| 29 | $NH_4NaLi_2(SO_4)_2$ | $C2$ | 1.1 | 0.009@546 nm | 30 |
| 30 | $(NH_4)_2Na_3Li_9(SO_4)_7$ | $P6_3$ | 0.5 | 0.008@1064 nm | 30 |
| 31 | $LiKSO_4$ | $P6_3$ | 4 | 0.0002@546 nm | 31 |

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