# Electronic Supplementary Information

## $(C_7H_3NO_4)_2Sb_2F_2{\cdot}2H_2O$: a pyridine-based compound shows large optical anisotropy

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### Contents

**Reagents**

$C_7H_5NO_4$ (99%), $SbF_3$ (98%) and HF(AR, ⩾40%) were purchased from Aladdin and used as received.

(Caution: Hydrofluoric acid is a great safety risk and must be protected and used with care)

**Synthesis of $(C_7H_3NO_4)_2Sb_2F_2{\cdot}2H_2O$ (CSF)**

Polycrystalline samples of **CSF** were synthesized by a simple evaporation technique of aqueous solution. The raw reactants of $C_7H_5NO_4$ (0.167 g, 1 mmol), $SbF_3$ (1.424 g, 8 mmol) and HF (5ml) were mixed together with deionized water (5 mL) in a plastic beaker. The solution was stirred with a magnetic mixer for 30 minutes, and then filtered through a filter paper to obtain a clear, transparent liquid. The beaker was sealed with perforated plastic wrap and left to stand at room temperature for about days. Colorless rod crystals were obtained at the bottom of beaker. The purity of the obtained product is confirmed by the powder X−ray diffraction (XRD) patterns, which were taken on a Rigaku MiniFlex II diffractometer (Cu $K\alpha$ radiation) in the range of $2\theta$ = 7°−70° with a step width of 0.01° and a sampling rate of 5° $min^{-1}$. The results agree well with the calculated XRD patterns from single−crystal XRD analyses (Figure 2c).

**Single−Crystal Structure Determination**

A colorless **CSF** crystal (0.09 × 0.08 × 0.07 $mm^3$) was selected using an optical microscope for single−crystal XRD analysis. The diffraction data were collected by using graphite−monochromatized Mo $K\alpha$ radiation ($\lambda$ = 0.71073 Å) at 200 (10) K on an Agilent SuperNova Dual diffractometer with an Atlas detector. The collection of the intensity data, cell refinement, and data reduction were carried out with the program CrysAlisPro.[1] Using Olex2,[2] the structure was solved with the olex2.solve[3] structure solution program using Charge Flipping and refined with the SHELXL[4] refinement package using Least Squares minimisation. Details of crystal parameters, data collection, and structure refinement are summarized in Table S1. The atomic coordinates and equivalent isotropic displacement parameters are listed in Table S2, and the anisotropic displacement parameters are listed in Table S3. The selected bond distances and angles are presented in Table S4−S5. Hydrogen Bonds are listed in Table S6. The torsion angles are listed in Table S7. The hydrogen atom coordinates and the isotropic displacement parameters are listed in Table S8.The Comparison of statistics for most birefringent compounds in recent years are listed in Table S9.

**Thermal Stability Analysis**

The thermogravimetric (TG) of **CSF** was carried out on a NETZSCH STA 449C simultaneous analyzer. About 16.7 mg of **CSF** was placed in $Al_2O_3$ crucibles, heated at a rate of 293 K $min^{-1}$ from room temperature to 773 K under flowing nitrogen.

**UV−Vis−NIR Diffuse Reflectance Spectroscopy**

The UV/Vis/NIR diffuse reflection data were collected on a PerkinElmer Lamda−1050 UV/vis/NIR spectrophotometer. A whiteboard provided by the merchant was used as a reference (100% reflectance) in the range from 220 nm to 800 nm. The measured results can be converted to absorption rate of light according to Kubelka−Munk function: $F(R) = (1-R)^2/2R$, where R is the reflectance.

**Infrared Spectroscopy**

Infrared spectrum was measured on a Nicolet iS50FT−IR spectrometer with KBr pellets as a standard in the range of 4000~400 $cm^{-1}$. The mixture of **CSF** and dried KBr (mass ratio = 1:100) was ground thoroughly in an agate mortar, and then pressed into a thin slice for measurement.

**Computational Methods**

The first−principles calculations for **CSF** were performed by CASTEP[5] on a plane−wave pseudopotential total energy package based density functional theory (DFT).[6] The functional developed by Perdew−Burke−Ernzerhof (PBE) functional within the generalized gradient approximation (GGA)[7–8] form was adopted to describe the exchange−correlation energy. The ultrasoft pseudopotentials were used to model the effective interaction between atom cores and valence electrons. H $1s^1$, C $2s^22p^2$, N $2s^22p^3$, O $2s^22p^4$, F $2s^22p^5$ and Sb $5s^25p^3$ electrons were treated as valence electrons. The kinetic energy cutoff of 489.80 eV and dense 2 × 1 × 2 Monkhorst−Pack[9] k−point meshes in the Brillouin zones were chosen. The linear optical properties were examined based on the dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$. The imaginary part of dielectric function $\varepsilon_2$ can be calculated based on the electronic structures and the real part is obtained by the Kramers−Kronig transformation, accordingly the refractive indices and the birefringence ($\Delta n$) can be calculated. The frequency−dependent refractive indices were calculated to demonstrate the validity of birefringence measurements.

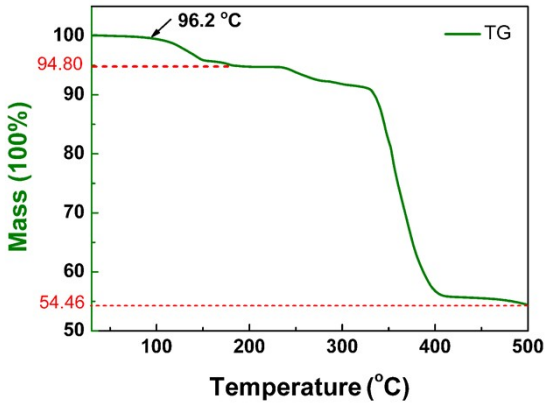


**Fig. S1.** Thermal stability analysis for **CSF**.

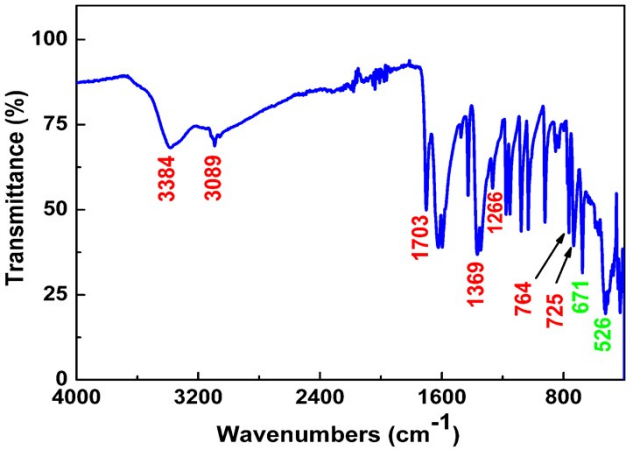


**Fig. S2.** Infrared spectrum of **CSF**.

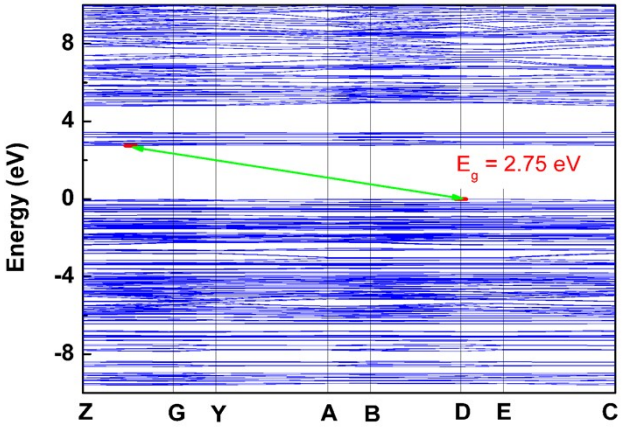


**Fig. S3.** Electronic band structure of **CSF**.

**Table S1. Crystal Data and Structural Refinement for $(C_7H_3NO_4)_2Sb_2F_2{\cdot}2H_2O$.**

| Empirical formula | $(C_7H_3NO_4)_2Sb_2F_2{\cdot}2H_2O$ |
|---|---|
| Formula weight | 647.74 |
| Temperature/K | 293(2) |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 8.6106(5) |
| b/Å | 22.0552(11) |
| c/Å | 10.2958(5) |
| α/° | 90 |
| β/° | 108.674(6) |
| γ/° | 90 |
| Volume/Å$^3$ | 1852.33(18) |
| Z | 4 |
| $\rho_{calc}$ g/cm$^3$ | 2.323 |
| μ/mm$^{-1}$ | 2.996 |
| F(000) | 1232.0 |
| Crystal size/mm$^3$ | 0.09 × 0.08 × 0.07 |
| Radiation | Mo Kα (λ = 0.71073 Å) |
| 2Θ range for data collection/° | 3.694 to 53.758 |
| Index ranges | $-10 \le h \le 8$, $-27 \le k \le 23$, $-9 \le l \le 13$ |
| Reflections collected | 9033 |
| Independent reflections | 3774 [$R_{int}$ = 0.0203, $R_{sigma}$ = 0.0311] |
| Data/restraints/parameters | 3774/6/284 |
| Goodness−of−fit on $F^2$ | 1.047 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0237, wR2 = 0.0511 |
| Final R indexes [all data] | R1 = 0.0279, wR2 = 0.0533 |

**Table S2. The Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for $(C_7H_3NO_4)_2Sb_2F_2·2H_2O$. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| Sb1 | 6763.4(2) | 5800.4(2) | 4861.0(2) | 23.03(7) |
| Sb2 | 8167.6(2) | 3896.4(2) | 4945.6(2) | 23.02(7) |
| F1 | 6314.5(19) | 3715.3(8) | 5558.4(17) | 37.2(4) |
| F2 | 8560.7(19) | 5645.7(8) | 4172.3(17) | 34.2(4) |
| O1 | 5880(3) | 7522.7(10) | 3059(3) | 66.5(9) |
| O2 | 6997(3) | 6739.6(9) | 4405(2) | 36.7(6) |
| O3 | 5881(2) | 4877.8(9) | 3736.3(19) | 32.2(5) |
| O4 | 4311(3) | 4436.6(10) | 1811(2) | 52.2(7) |
| O5 | 9206(3) | 6199.2(10) | 6729(2) | 46.3(7) |
| O6 | 9979(3) | 5207.0(9) | 8275(2) | 45.7(6) |
| O7 | 8324(2) | 4772.1(9) | 6364.2(19) | 31.9(5) |
| O8 | 6240(3) | 3483.9(10) | 2862(2) | 47.7(7) |
| O9 | 8637(2) | 2950.1(9) | 5092.0(18) | 33.4(5) |
| O10 | 9756(3) | 2156.0(9) | 6407(2) | 45.4(6) |
| N1 | 5312(3) | 5955.2(10) | 2669(2) | 24.8(6) |
| N2 | 9610(3) | 3704.3(10) | 7118(2) | 22.7(5) |
| C1 | 5062(4) | 6532.0(13) | 2240(3) | 30.9(7) |
| C2 | 3994(4) | 6674.7(15) | 971(3) | 40.3(9) |
| C3 | 3172(4) | 6209.7(17) | 129(3) | 45.5(10) |
| C4 | 3445(4) | 5618.4(15) | 565(3) | 37.3(8) |
| C5 | 4524(4) | 5504.1(14) | 1859(3) | 27.5(7) |
| C6 | 4926(4) | 4880.3(14) | 2495(3) | 32.7(8) |
| C7 | 6025(4) | 6980.3(14) | 3299(3) | 36.9(8) |
| C8 | 9416(4) | 4769.7(14) | 7539(3) | 29.7(7) |
| C9 | 10081(4) | 4141.7(13) | 8059(3) | 25.5(7) |
| C10 | 11117(4) | 4025.6(14) | 9359(3) | 33.5(8) |
| C11 | 11681(4) | 3437.5(15) | 9688(3) | 37.2(8) |
| C12 | 11176(4) | 2987.4(14) | 8715(3) | 34.6(8) |
| C13 | 10138(4) | 3136.3(13) | 7425(3) | 26.8(7) |
| C14 | 9495(4) | 2700.2(14) | 6254(3) | 29.9(7) |

**Table S3. Anisotropic Displacement Parameters ($Å^2×10^3$) for $(C_7H_3NO_4)_2Sb_2F_2·2H_2O$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| Sb1 | 21.54(12) | 20.46(13) | 24.63(12) | 0.63(8) | 3.97(9) | −0.94(8) |
| Sb2 | 22.35(12) | 21.47(13) | 22.59(12) | −0.05(8) | 3.49(9) | 0.98(8) |
| F1 | 25.4(10) | 43.7(12) | 45.0(11) | 5.8(9) | 14.9(9) | 0.1(9) |
| F2 | 24.3(10) | 42.1(11) | 38.2(10) | −0.6(8) | 13.0(8) | −0.8(8) |
| O1 | 76(2) | 22.7(14) | 68.5(17) | 4.2(12) | −22.9(15) | −2.7(13) |
| O2 | 36.5(13) | 22.5(12) | 38.5(13) | 1.8(10) | −5.8(10) | −4.4(10) |
| O3 | 34.1(12) | 25.5(12) | 27.2(11) | 2.9(9) | −3.8(9) | −5.0(10) |
| O4 | 60.8(18) | 23.4(13) | 45.2(14) | −5.7(11) | −21.2(12) | 0.1(12) |
| O5 | 62.5(17) | 25.2(14) | 34.2(14) | −3.0(10) | −8.5(12) | 0.9(13) |
| O6 | 66.4(16) | 21.3(12) | 32.0(13) | −6.3(10) | −8.4(11) | 1.8(12) |
| O7 | 33.1(12) | 27.2(12) | 26.0(11) | −0.7(9) | −3.8(9) | 6.5(10) |
| O8 | 53.0(17) | 28.9(15) | 41.7(14) | −0.5(11) | −12.1(12) | −2.7(12) |
| O9 | 40.9(13) | 22.1(12) | 28.7(12) | −3.3(9) | −0.7(10) | 2.8(10) |
| O10 | 61.8(16) | 20.2(12) | 44.0(14) | −0.7(10) | 2.7(12) | 5.7(12) |
| N1 | 26.2(14) | 19.6(13) | 25.1(13) | 0.0(10) | 3.4(11) | −1.7(11) |
| N2 | 24.8(13) | 19.3(13) | 21.2(12) | 0.4(10) | 3.2(10) | −2.4(11) |
| C1 | 31.7(19) | 21.0(17) | 34.2(17) | 2.8(13) | 2.6(14) | −1.3(14) |
| C2 | 47(2) | 25.4(19) | 38.1(19) | 7.8(15) | −0.3(17) | 1.0(16) |
| C3 | 50(2) | 44(2) | 29.6(19) | 6.3(15) | −5.6(17) | 3.0(18) |
| C4 | 43(2) | 31(2) | 27.3(17) | −2.1(14) | −3.0(15) | −2.6(16) |
| C5 | 27.3(17) | 26.2(17) | 26.2(16) | −0.2(13) | 4.8(13) | −0.3(14) |
| C6 | 34.1(19) | 27.6(18) | 29.2(17) | 1.0(14) | −0.2(14) | −2.5(15) |
| C7 | 37(2) | 22.6(18) | 40.5(19) | 2.5(15) | −3.0(16) | −3.1(15) |
| C8 | 36.6(19) | 25.7(18) | 22.1(15) | 1.3(13) | 3.1(13) | 6.9(15) |
| C9 | 27.5(17) | 23.4(17) | 23.3(15) | −0.9(12) | 4.9(13) | −0.8(13) |
| C10 | 38(2) | 28.8(18) | 25.7(17) | −1.5(14) | −0.6(15) | −0.3(16) |
| C11 | 42(2) | 33(2) | 29.3(17) | 6.8(14) | 1.2(15) | 4.4(16) |
| C12 | 39(2) | 26.3(18) | 32.6(18) | 7.6(14) | 2.9(15) | 1.6(15) |
| C13 | 29.0(18) | 22.4(17) | 28.0(16) | 1.5(13) | 7.8(14) | 0.2(14) |
| C14 | 31.8(18) | 23.6(18) | 31.1(17) | −0.9(13) | 5.8(14) | 0.7(14) |

**Table S4. Bond Lengths for $(C_7H_3NO_4)_2Sb_2F_2{\cdot}2H_2O$.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| Sb1 | F2 | 1.9279(16) | Sb2 | F1 | 1.9361(16) |
| Sb1 | O2 | 2.147(2) | Sb2 | O7 | 2.3991(19) |
| Sb1 | O3 | 2.3442(19) | Sb2 | O8 | 2.430(2) |
| Sb1 | O5 | 2.511(2) | Sb2 | O9 | 2.122(2) |
| Sb1 | N1 | 2.228(2) | Sb2 | N2 | 2.224(2) |
| O1 | C7 | 1.220(3) | O6 | C8 | 1.226(3) |
| O2 | C7 | 1.292(3) | O7 | C8 | 1.273(3) |
| O3 | C6 | 1.279(3) | O9 | C14 | 1.310(3) |
| O4 | C6 | 1.223(3) | O10 | C14 | 1.222(3) |
| N1 | C1 | 1.341(3) | N2 | C9 | 1.335(3) |
| N1 | C5 | 1.336(3) | N2 | C13 | 1.336(3) |
| C1 | C2 | 1.372(4) | C8 | C9 | 1.528(4) |
| C1 | C7 | 1.508(4) | C9 | C10 | 1.374(4) |
| C2 | C3 | 1.383(4) | C10 | C11 | 1.388(4) |
| C3 | C4 | 1.375(5) | C11 | C12 | 1.378(4) |
| C4 | C5 | 1.382(4) | C12 | C13 | 1.382(4) |
| C5 | C6 | 1.515(4) | C13 | C14 | 1.502(4) |

**Table S5. Bond Angles for $(C_7H_3NO_4)_2Sb_2F_2{\cdot}2H_2O$.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| F2 | Sb1 | O2 | 87.02(8) | F1 | Sb2 | O7 | 81.90(7) |
| F2 | Sb1 | O3 | 80.57(7) | F1 | Sb2 | O8 | 79.00(8) |
| F2 | Sb1 | O5 | 76.66(8) | F1 | Sb2 | O9 | 86.10(8) |
| F2 | Sb1 | N1 | 84.87(8) | F1 | Sb2 | N2 | 83.47(8) |
| O2 | Sb1 | O3 | 140.13(7) | O7 | Sb2 | O8 | 136.74(7) |
| O2 | Sb1 | O5 | 73.46(7) | O9 | Sb2 | O7 | 140.92(6) |
| O2 | Sb1 | N1 | 72.08(8) | O9 | Sb2 | O8 | 75.83(7) |
| O3 | Sb1 | O5 | 137.89(7) | O9 | Sb2 | N2 | 73.08(8) |
| N1 | Sb1 | O3 | 69.19(7) | N2 | Sb2 | O7 | 68.69(7) |
| N1 | Sb1 | O5 | 141.49(8) | N2 | Sb2 | O8 | 145.11(8) |
| C7 | O2 | Sb1 | 120.63(19) | C8 | O7 | Sb2 | 117.11(18) |
| C6 | O3 | Sb1 | 119.52(19) | C14 | O9 | Sb2 | 121.17(18) |
| C1 | N1 | Sb1 | 117.24(19) | C9 | N2 | Sb2 | 122.28(19) |
| C5 | N1 | Sb1 | 121.78(19) | C9 | N2 | C13 | 120.3(2) |
| C5 | N1 | C1 | 120.3(3) | C13 | N2 | Sb2 | 117.03(19) |
| N1 | C1 | C2 | 121.3(3) | O6 | C8 | O7 | 127.6(3) |
| N1 | C1 | C7 | 113.0(3) | O6 | C8 | C9 | 117.8(3) |

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| C2 | C1 | C7 | 125.7(3) | O7 | C8 | C9 | 114.6(3) |
| C1 | C2 | C3 | 118.7(3) | N2 | C9 | C8 | 114.1(3) |
| C4 | C3 | C2 | 119.9(3) | N2 | C9 | C10 | 121.6(3) |
| C3 | C4 | C5 | 118.7(3) | C10 | C9 | C8 | 124.3(3) |
| N1 | C5 | C4 | 121.1(3) | C9 | C10 | C11 | 118.6(3) |
| N1 | C5 | C6 | 114.0(3) | C12 | C11 | C10 | 119.4(3) |
| C4 | C5 | C6 | 124.9(3) | C11 | C12 | C13 | 118.9(3) |
| O3 | C6 | C5 | 114.9(3) | N2 | C13 | C12 | 121.1(3) |
| O4 | C6 | O3 | 126.4(3) | N2 | C13 | C14 | 113.6(2) |
| O4 | C6 | C5 | 118.7(3) | C12 | C13 | C14 | 125.3(3) |
| O1 | C7 | O2 | 125.3(3) | O9 | C14 | C13 | 114.8(3) |
| O1 | C7 | C1 | 120.0(3) | O10 | C14 | O9 | 123.9(3) |
| O2 | C7 | C1 | 114.8(3) | O10 | C14 | C13 | 121.4(3) |

**Table S6. Hydrogen Bonds for $(C_7H_3NO_4)_2Sb_2F_2\cdot 2H_2O$.**

| D | H | A | d(D−H)/Å | d(H−A)/Å | d(D−A)/Å | D−H−A/° |
|---|---|---|---|---|---|---|
| O5 | H5A | O6 | 0.850(17) | 1.833(18) | 2.663(3) | 165(3) |
| O5 | H5B | O10[1] | 0.837(17) | 1.973(19) | 2.800(3) | 169(4) |
| O8 | H8A | O4 | 0.863(17) | 1.829(18) | 2.682(3) | 170(4) |
| O8 | H8B | O1[2] | 0.867(17) | 1.94(2) | 2.760(3) | 158(3) |

(1) 2−X,1/2+Y,3/2−Z; [2]1−X,−1/2+Y,1/2−Z

**Table S7. Torsion Angles for $(C_7H_3NO_4)_2Sb_2F_2\cdot 2H_2O$.**

| A | B | C | D | Angle/° | A | B | C | D | Angle/° |
|---|---|---|---|---|---|---|---|---|---|
| Sb1 | O2 | C7 | O1 | 167.3(3) | Sb2 | O7 | C8 | O6 | 160.6(3) |
| Sb1 | O2 | C7 | C1 | −14.6(4) | Sb2 | O7 | C8 | C9 | −19.1(3) |
| Sb1 | O3 | C6 | O4 | −176.2(3) | Sb2 | O9 | C14 | O10 | 177.5(2) |
| Sb1 | O3 | C6 | C5 | 2.5(4) | Sb2 | O9 | C14 | C13 | −1.8(4) |
| Sb1 | N1 | C1 | C2 | −170.6(2) | Sb2 | N2 | C9 | C8 | 5.1(4) |
| Sb1 | N1 | C1 | C7 | 8.0(4) | Sb2 | N2 | C9 | C10 | −172.9(2) |
| Sb1 | N1 | C5 | C4 | 170.7(2) | Sb2 | N2 | C13 | C12 | 173.6(2) |
| Sb1 | N1 | C5 | C6 | −9.1(4) | Sb2 | N2 | C13 | C14 | −6.5(3) |
| N1 | C1 | C2 | C3 | −0.1(5) | O6 | C8 | C9 | N2 | −169.7(3) |
| N1 | C1 | C7 | O1 | −178.1(3) | O6 | C8 | C9 | C10 | 8.2(5) |
| N1 | C1 | C7 | O2 | 3.7(4) | O7 | C8 | C9 | N2 | 10.1(4) |
| N1 | C5 | C6 | O3 | 3.9(4) | O7 | C8 | C9 | C10 | −172.0(3) |
| N1 | C5 | C6 | O4 | −177.3(3) | N2 | C9 | C10 | C11 | 0.1(5) |
| C1 | N1 | C5 | C4 | 0.3(5) | N2 | C13 | C14 | O9 | 5.5(4) |
| C1 | N1 | C5 | C6 | −179.5(3) | N2 | C13 | C14 | O10 | −173.8(3) |
| C1 | C2 | C3 | C4 | −0.6(5) | C8 | C9 | C10 | C11 | −177.7(3) |
| C2 | C1 | C7 | O1 | 0.4(6) | C9 | N2 | C13 | C12 | 0.1(5) |
| C2 | C1 | C7 | O2 | −177.8(3) | C9 | N2 | C13 | C14 | 180.0(3) |
| C2 | C3 | C4 | C5 | 1.1(5) | C9 | C10 | C11 | C12 | −0.7(5) |
| C3 | C4 | C5 | N1 | −1.0(5) | C10 | C11 | C12 | C13 | 1.0(5) |
| C3 | C4 | C5 | C6 | 178.7(3) | C11 | C12 | C13 | N2 | −0.7(5) |
| C4 | C5 | C6 | O3 | −175.9(3) | C11 | C12 | C13 | C14 | 179.4(3) |
| C4 | C5 | C6 | O4 | 2.9(5) | C12 | C13 | C14 | O9 | −174.7(3) |
| C5 | N1 | C1 | C2 | 0.3(5) | C12 | C13 | C14 | O10 | 6.1(5) |
| C5 | N1 | C1 | C7 | 178.8(3) | C13 | N2 | C9 | C8 | 178.2(3) |
| C7 | C1 | C2 | C3 | −178.5(3) | C13 | N2 | C9 | C10 | 0.2(5) |

**Table S8. Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for $(C_7H_3NO_4)_2Sb_2F_2·2H_2O$.**

| Atom | *X* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H5A | 9510(50) | 5928(12) | 7340(30) | 70 |
| H5B | 9420(50) | 6514(10) | 7210(30) | 70 |
| H2 | 3826.15 | 7076.04 | 682.94 | 48 |
| H3 | 2436.12 | 6296.8 | −732.52 | 55 |
| H4 | 2913.54 | 5301.7 | 0.2 | 45 |
| H8A | 5560(40) | 3761(12) | 2440(30) | 72 |
| H8B | 5670(40) | 3156(11) | 2800(40) | 72 |
| H10 | 11434.09 | 4334.55 | 10004.78 | 40 |
| H11 | 12393.04 | 3348.1 | 10557.53 | 45 |
| H12 | 11527.63 | 2589.79 | 8922.68 | 42 |

**Table S9. Comparison of statistics for most birefringent compounds in recent years.**

| Number | substance | Birefringence | Reference |
|---|---|---|---|
| 1 | $(C_7H_3NO_4)_2Sb_2F_2·2H_2O$ | 0.40@550 nm | This work |
| 2 | $(C_6H_5N_2)HgCl_3$ | 0.36@546 nm | 10 |
| 3 | $[(H-cmpy)_4(Pb_3Br_{10})]$ | 0.315@550 nm | 11 |
| 4 | $[4-AP][3-pySO_3]$ | 0.296@546 nm | 12 |
| 5 | $(C_6H_6NO_2)(H_2PO_4)$ | 0.284@546 nm | 13 |
| 6 | $(C_5H_4N)NH(C_5H_4NH)Br·2H_2O$ | 0.28@550 nm | 14 |
| 7 | $Ag_2C_{14}H_{20}N_6O_6$ | 0.261@546.1 nm | 15 |
| 8 | $(C_5H_4N)$ $NH(C_5H_4NH)Cl·2H_2O$ | 0.25@550 nm | 14 |
| 9 | $(C_5H_6ON)^+(H_2PO_4)^-$ | 0.25@1064 nm | 16 |
| 10 | $[C_5H_6O_2N_3][HSO_4]·H2O$ | 0.25@1064 nm | 17 |
| 11 | $(C_4H_6N_3)^+(H_2PO_3)^-$ | 0.225@589.3 nm | 18 |
| 12 | $(C_3H_7N_6)_6(H_2PO_4)_4(HPO_4)·4H_2O$ | 0.22@1064 nm | 19 |
| 13 | $(C_5H_6NO)(CH_3SO_3)$ | 0.216@546 nm | 20 |
| 14 | $AgC_6H_8N_3O_3$ | 0.212@546.1 nm | 15 |
| 15 | $Te(CS(NH_2)_2)_4SO_4·2H_2O$ | 0.210@546.1 nm | 21 |
| 16 | $[(H_2-dpys)(PbBr_4)]$ | 0.192@550 nm | 20 |
| 17 | $(C_3H_7N_6)_2SO_4·2H_2O$ | 0.173@1064 nm | 19 |
| 18 | $(C_5H_6N)_2B_2O(HPO_4)_2$ | 0.156@547 nm | 22 |
| 19 | $[C(NH_2)_3]SbFPO_4·H_2O$ | 0.151@546 nm | 23 |
| 20 | $[Te(C_6H_5)_2][PO_3(OH)]_n$ | 0.133@550 nm | 24 |
| 21 | $C(NH_2)_3SO_3F$ | 0.133@1064 nm | 25 |
| 22 | $NaIn(C_2O_4)(HPO_4)(H_2O)_5$ | 0.098@546 nm | 10 |
| 23 | $[C(NH_2)_3]_6(PO_4)·3H_2O$ | 0.078@546 nm | 26 |
| 24 | $[(C(NH_2)_3]_3PO_4·2H_2O$ | 0.055@546 nm | 27 |

| | | | |
|---|---|---|---|
| 25 | $(C_5H_4NH)_2SBr_2$ | 0.048@550 nm | 11 |
| 26 | $[C(NH_2)_3]_2PO_3F$ | 0.039@532 nm | 10 |
| 27 | $[C(NH_2)_3]_2Sb_3F_3(HPO_3)_4$ | 0.027@546 nm | 23 |
| 28 | $[C(NH_2)_3]_2HPO_4{\cdot}H_2O$ | 0.014@532 nm | 10 |

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