# *Supporting Information*

## $Ag_2[TeO_2(OH)_4]$: A Nonlinear Optical Tellurate with Balanced Comprehensive Performance

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**Table S1.** Space group, synthetic method, basic building blocks (BBBs) of anions, and connection methods of the anionic group of the material containing $TeO_{6-x}(OH)_x$ (x=1-6) anionic group.

| Material | Space group | Synthetic method | BBBs of anions | Connection | Ref. |
|---|---|---|---|---|---|
| $H_6TeO_6$ | $F4_132$ | Aqueous solution | $Te(OH)_6$ | Isolated | 1 |
| $KIO_3{\cdot}Te(OH)_6$ | $Pna2_1$ | Aqueous solution | $Te(OH)_6$ | Isolated | 2 |
| $Te(OH)_6{\cdot}(NH_4)_2SO_4$ | $Cc$ | Aqueous solution | $Te(OH)_6$ | Isolated | 3 |
| $K_2SeO_4{\cdot}Te(OH)_6$ | $Cc$ | Aqueous solution | $Te(OH)_6$ | Isolated | 4 |
| $Na_2SeO_4{\cdot}Te(OH)_6{\cdot}H_2O$ | $P2_1/c$ | Aqueous solution | $Te(OH)_6$ | Isolated | 5 |
| $Cs_2SO_4{\cdot}Te(OH)_6$ | $R3$ | Aqueous solution | $Te(OH)_6$ | Isolated | 6 |
| $Cs_2SeO_4{\cdot}Te(OH)_6$ | $P2_1/c$ | Aqueous solution | $Te(OH)_6$ | Isolated | 6 |
| $Hg^{I}_2(H_4Te^{VI}O_6)(H_6Te^{VI}O_6){\cdot}2H_2O$ | $P\text{-}1$ | Aqueous solution | $Te(OH)_6$<br>$TeO_2(OH)_4$ | Isolated | 7 |
| $Na[TeO(OH)_5]$ | $P4_2/n$ | Aqueous solution | $TeO(OH)_5$ | Isolated | 8 |
| $K[TeO(OH)_5]{\cdot}H_2O$ | $P2_1/c$ | / | $TeO(OH)_5$ | Isolated | 9 |
| $Na_2[TeO_2(OH)_4]$ | $C2/c$ | Aqueous solution<br>Hydrothermal method | $TeO_2(OH)_4$ | Isolated | 8 |
| $(NH_4)_2TeO_2(OH)_4$ | $C2/m$ | Hydrothermal method (Unstable) | $TeO_2(OH)_4$ | Isolated | 10 |

| | | | | | |
|---|---|---|---|---|---|
| $Hg^{II}(H_4Te^{VI}O_6)$ | *Pna*$2_1$ | Aqueous solution | $TeO_2(OH)_4$ | Isolated | [7] |
| $K_2[TeO_2(OH)_4]$ | *P*-1 | Hydrothermal method | $TeO_2(OH)_4^{2-}$ | Isolated | [11] |
| $Ag_2[TeO_2(OH)_4]$ | *Fdd2* | Aqueous solution | $TeO_2(OH)_4^{2-}$ | Isolated | [12-13] This work |
| $Cs_2[Te_2O_{10}H_6][Te(OH)_6]$ | *P*-1 | Aqueous solution | $TeO_3(OH)_3$ | Dimer; $[Te_2O_{10}H_6]^{2-}$ | [14] |
| | | | $Te(OH)_6$ | Isolated | |
| $Cs_3[Te_2O_{10}H_5]\cdot 4H_2O$ | *P*-1 | Aqueous solution | $TeO_3(OH)_3$ | Dimer; $[Te_2O_{10}H_5]^{3-}$ | [14] |
| | | | $Te(OH)_6$ | Isolated | |
| $Cs_4[Te_2O_{10}H_4]\cdot 8H_2O$ | *P*-1 | Aqueous solution (Unstable) | $TeO_4(OH)_2$ | Dimer; $[Te_2O_{10}H_4]^{4-}$ | [14] |
| $K_4[Te_2O_{10}H_4]\cdot 8H_2O$ | *C*2/*c* | Aqueous solution (Unstable) | $TeO_4(OH)_2$ | Dimer; $[Te_2O_{10}H_4]^{4-}$ | [14] |
| $K_4[Te_2O_6(OH)_4]\cdot 7.3H_2O$ | *C*2/*c* | Aqueous solution | $TeO_4(OH)_2$ | Dimer; $[Te_2O_6(OH)_4]^{4-}$ | [15] |
| $KTeO_3(OH)$ | *P*$2_1$/*c* | Aqueous solution | $TeO_4(OH)_2$ | Chain; $[TeO_3(OH)]_n^{n-}$ | [16] |
| $Rb_4[Te_2O_{10}H_4]\cdot 10H_2O$ | *P*-1 | Aqueous solution (Unstable) | $TeO_4(OH)_2$ | Dimer; $[Te_2O_{10}H_4]^{4-}$ | [14] |
| $K_2[Te_3O_8(OH)_4]$ | *Fdd*2 | Hydrothermal method | $TeO_4(OH)_2$<br>$TeO_5(OH)$ | Chain; $(Te_3O_{12})^{6-}$ | [17] |
| $K_6[Te_2O_{10}H_4][TeO_6H_4]\cdot 12H_2O$ | *P*-1 | Aqueous solution (Unstable) | $TeO_4(OH)_2$ | Dimer; $[Te_2O_{10}H_4]^{4-}$ | [14] |
| | | | $TeO_2(OH)_4$ | Isolated | |
| | | | $Te(OH)_6$ | Isolated | |
| $K_2[Te_4O_8(OH)_{10}]$ | *P*$2_1$/*c* | Hydrothermal method | $TeO_4(OH)_2$<br>$TeO_3(OH)_3$ | Tetramer; $[Te_4O_8(OH)_{10}]^{2-}$ | [18] |
| $Rb[Te_2O_4(OH)_5]$ | *P*$2_1$/*c* | Hydrothermal method | $TeO_4(OH)_2$<br>$TeO_3(OH)_3$ | Tetramer; $(Te_4O_{18}H_{10})^{2-}$ | [17] |
| $Te_2O_4(OH)_2$ | *Pna*$2_1$ | Hydrothermal method | $TeO_4(OH)_2$<br>$TeO_4$ | Chain; Te(VI) chain | [19] |

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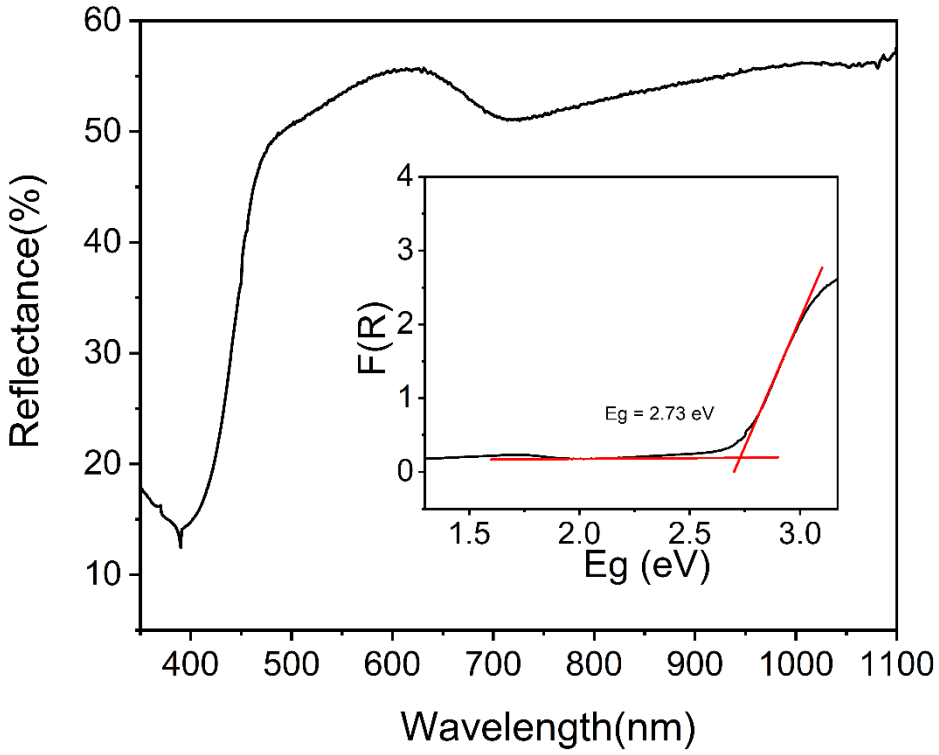
|---|---|---|---|---|---|
| $K_{8\cdot5}[Te_6O_{27}H_9]\cdot0.5H_3O\cdot17H_2O$ | *C*2 | Aqueous solution (Unstable) | $TeO_4(OH)_2$<br>$TeO_5(OH)$ | Ring; $[Te_6O_{27}H_9]^{9-}$ | 14 |
| $NH_4TeO_3(OH)$ | *P*-1 | Hydrothermal method | $TeO_4(OH)_2$ | Chain | 20 |
| $Na_4[Te_2O_6(OH)_4]\cdot6H_2O$ | *P*-1 | Aqueous solution | $TeO_4(OH)_2$ | Dimer; $[Te_2O_6(OH)_4]^{4-}$ | 8 |
| $Na_2K_4[Te_2O_8(OH)_2](H_2O)_{14}$ | *I*2/*m* | Aqueous solution | $TeO_5(OH)$ | Dimer; $[Te_2O_8(OH)_2]^{6-}$ | 21 |
| $NH_4[Te^{IV}Te^{VI}O_5(OH)]$ | *Pnma* | Hydrothermal method | $TeO_5(OH)$ | Chain; $[Te^{IV}Te^{VI}O_5(OH)]^-$ | 22 |
| $Cs_2[Te_3O_8(OH)_4]$ | *Fdd*2 | Hydrothermal method | $TeO_5(OH)$<br>$TeO_4(OH)_2$ | Chain; $[Te_3O_8(OH)_4]^{2-}$ | 23 |
| $K_2[Te_3O_8(OH)_4]$ | *Fdd*2 | Hydrothermal method | $TeO_5(OH)$<br>$TeO_4(OH)_2$ | Chain; $[Te_3O_8(OH)_4]^{2-}$ | 17 |
| $Na_2[Te_3O_8(OH)_4]$ | *Fdd*2 | Hydrothermal method | $TeO_5(OH)$<br>$TeO_4(OH)_2$ | Chain; $[Te_3O_8(OH)_4]^{2-}$ | 23 |
| $Rb_2[Te_3O_8(OH)_4]$ | *Fdd*2 | Hydrothermal method | $TeO_5(OH)$<br>$TeO_4(OH)_2$ | Chain; $[Te_3O_8(OH)_4]^{2-}$ | 23 |
| $K_8Te_6O_{17}(OH)_{10}\cdot1/2KOH\cdot16H_2O$ | *C*2 | Aqueous solution<br>(Unstable) | $TeO_5(OH)$<br>$TeO_4(OH)_2$ | Ring; $[Te_6O_{17}(OH)_{10}]^{8-}$ | 24 |

**Figure S1.** UV−vis−NIR transmittance spectrum on a single crystal of $Ag_2[TeO_2(OH)_4]$.




## REFERENCES


(1) Zilber, R.; Durif, A.; Averbuch-Pouchot, M. T., Structure of potassium sulfate tellurate: $Te(OH)_6$. *Acta Crystallogr B.* **1980,** *36* (11), 2743-2745.

(2) Wu, H.; Yu, H.; Zhang, W.; Cantwell, J.; Poeppelmeier, K. R.; Pan, S.; Halasyamani, P. S., Crystal Growth and Linear and Nonlinear Optical Properties of $KIO_3{\cdot}Te(OH)_6$. *Cryst. Growth Des.* **2017,** *17* (8), 4405-4412.

(3) Zilber, R.; Durif, A.; Averbuch-Pouchot, M. T., Structure of ammonium sulfate tellurate $Te(OH)_6{\cdot}(NH_4)_2SO_4$. *Acta Crystallogr B.* **1981,** *37* (3), 650-652. (37) Dammak, M.; Khemakhem, H.; Mhiri, T.; Kolsi, A. W.; Daoud, A., Structural and Vibrational Study of $K_2SeO_4{\cdot}Te(OH)_6$ Material. *J. Solid State Chem.* **1999,** *145* (2), 612-618.

(4) Dammak, M.; Litaiem, H.; Mhiri, T., Structural, thermal and dielectric studies in $Na_2SeO_4{\cdot}Te(OH)_6{\cdot}H_2O$. *J. Alloys Compd.* **2006,** *416* (1), 228-235.

(5) Dammak, M.; Mhiri, T.; Jaud, J.; Savariault, J. M., Structural study of the two new caesium sulfate and selenate tellurate $Cs_2SO_4{\cdot}Te(OH)_6$ and $Cs_2SeO_4{\cdot}Te(OH)_6$. *Int. J. Inorg. Mater.* **2001,** *3* (7), 861-873.

(6) Weil, M., Preparation and Crystal Structures of the Hydrous Mercury Tellurates, $Hg^{II}(H_4Te^{VI}O_6)$ and $Hg^{I}_2(H_4Te^{VI}O_6)(H_6Te^{VI}O_6){\cdot}2H_2O$. *Z. Anorg. Allg. Chem.* **2004,** *630* (7), 1048-1053.

(7) Weil, M.; Stöger, B.; Larvor, C.; Raih, I.; Gierl-Mayer, C., The Hydrous Sodium Oxotellurates(VI) $Na[TeO(OH)_5]$, $Na_2[TeO_2(OH)_4]$, $Na_4[Te_2O_6(OH)_4](H_2O)_6$, and a Third Polymorph of Anhydrous $Na_2[TeO_4]$. *Z. Anorg. Allg. Chem.* **2017,** *643* (23), 1888-1897.

(8) Raman S. Crystal Structure of $KTeO(OH)_5{\cdot}H_2O$. *Inorg. Chem.*, **1964**, *3*(5), 634-638.

(9) Johansson, G. B.; Lindqvist, O.; Moret, J., Diammonium tellurium(VI) dioxide tetrahydroxide. *Acta Crystallogr B.* **1979,** *35* (7), 1684-1686.

(10) He, H.; Li, Y.; Albrecht, R.; Ruck, M., Oxohydroxo-Tellurates(VI) $K_2[TeO_2(OH)_4]$ and $K_2[Fe_2TeO_6(OH)_2] \cdot 2H_2O$ from Alkaline Hydroflux. *Z. Anorg. Allg. Chem.* **2023,** *649* (22), e202300170.

(11) Churakov, A. V.; Ustinova, E. A.; Prikhodchenko, P. V.; Tripol'skaya, T. A.; Howard, J. A. K., Synthesis and crystal structure of new alkali metal hydrogen tellurates. *Russ. J. Inorg. Chem.* **2007,** *52* (10), 1503-1510.

(12) Yun, G.; Hwang, Y.; Yun, H.; Do, J.; Jacobson, A. J., A Vanadium Tellurate, $(NH_4)_2[VO_2]_2[TeO_4(OH)_2]$, Containing Two Edge-Shared Square-Pyramidal $VO_5$ Groups. *Inorg. Chem.* **2010,** *49* (1), 229-233.

(12) EfTenberger, H.; Tillmanns, E., The crystal structure of $K_2\{Cu[TeO_4(OH)_2]\}$ $H_2O$. *Z. Krist-Cryst. Mater*. **1993,** *205* (1-2), 41-54.

(13) Lindqvist O, Lundgren G. The crystal structure of potassium tellurate (VI). *Acta Chem. Scand.* **1966**, *20*: 2138-2155.

(14) Lindqvist O. A redetermination of the crystal structure of $KTeO_3(OH)$. *Acta Chem. Scand.* **1972**, *26*: 4109-4120.

(15) Levason, W.; Spicer, M. D.; Webster, M., Co-ordination chemistry of higher oxidation states. Part 26. Spectroscopic studies of tellurate complexes of the trivalent Group 1B metals. X-Ray structure of $Na_5[Cu\{TeO_4(OH)_2\}_2]\cdot 16H_2O$. *J. Chem. Soc. Dalton.* **1988,** (5), 1377-1381.

(16) Hector, A. L.; Hill, N. J.; Levason, W.; Webster, M., X-Ray Crystal Structures of Hexa-oxotellurate Complexes of Ruthenium(VI) and Silver(III): $Na_6[RuO_2\{TeO_4(OH)_2\}_2]\cdot 16H_2O$ and $Na_5[Ag\{TeO_4(OH)_2\}_2]\cdot 16H_2O$. *Z. Anorg. Allg. Chem.* **2002,** *628* (4), 815-818.

(17) Levason, W.; Webster, M., Pentasodium Bis[dihydroxytetraoxotellurium(VI)]gold(III) Hexadecahydrate. *Acta Crystallogr C.* **1998,** *54* (12), 1729-1731.

(18) An, Y.; Mosbah, A.; Le Gal La Salle, A.; Guyomard, D.; Verbaere, A.; Piffard, Y., $K_2[Te_4O_8(OH)_{10}]$: synthesis, crystal structure and thermal behavior. *Solid State Sci.* **2001,** *3* (1), 93-101.

(19) Benmiloud, L.; Moret, J.; Maurin, M.; Philippot, E., Structure d'un tellurate d'ammonium: $NH_4TeO_3(OH)$. *Acta Crystallogr B.* **1980,** *36* (1), 139-141.

(20) Lindqvist, O., Lundgren, G., Mark, W., Lundström, H., Borch, G., & Craig, J. C. The Crystal Structure of the Tellurate $Na_2K_4[Te_2O_8(OH)_2](H_2O)_{14}$. *Acta Chem. Scand.* **1969**, *23*: 3062-3070.

(21) Philippot, E. T. I. E. N. N. E., Benmiloud, L. E. I. L. A., Maurin, M., & Moret, J. Pentacoordination de l'atome de tellure (IV) par les atomes d'oxygène. Etude cristallochimique d'un oxotellurate mixte: NH4 $[Te^{IV}Te^{VI}O_5(OH)]$. *Acta. Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.* **1979**, *35*(9), 1986-1989.

(22) Minimol, M. P., & Vidyasagar, K. Hydrothermal synthesis and characterization of new one-dimensional tellurates, $A_2[Te_3O_8(OH)_4]$ (A = Cs, Rb, K, Na). *Indian Journal of Chemistry - Section A*, **2003**, *42(A)*, 2244-2249.

(23) Puder, A.; Fuchs, J.; Lentz, D.; Roth, K., Das erste cyclische Isopolyoxoanion aus Oktaederbausteinen. Synthese und Strukturbestimmung von Kaliumhexatellurat(VI) $K_8Te_6O_{17}(OH)_{10}$ 1/2 $KOH\cdot 6H_2O$. Z. Naturforsch. B. **1995,** *50* (1), 91-93.