

Pyridine-3-carboxamide–telluric acid (1/1)

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In the title structure, $C_6H_6N_2O \cdot H_6O_6Te$, the pyridine-3-carboxamide and telluric acid molecules are interconnected by conventional $O-H \cdots N$, $N-H \cdots O$ and $O-H \cdots O$ hydrogen bonds of moderate strength as well as by $\pi-\pi$ interactions between the pyridine rings. The strongest hydrogen bond in the structure is formed between a hydroxyl group of the H_6TeO_6 molecule and the *N*-pyrimidine N atom. The structure is unusual because of presence of the alternating sheets, which contain H_6TeO_6 and pyridine-3-carboxamide molecules, respectively. These sheets are aligned parallel to (001).

1. Chemical context

The motivation for the title structure determination follows from the fact that there are relatively a few structure determinations of molecular crystals containing the telluric acid molecule H_6TeO_6 (Groom *et al.*, 2016). These structure determinations are summarized in Table 1.

H_6TeO_6 is a weak acid with $pK_a = 7.68$ (1st degree; CRC Handbook, 2017) at room temperature. At the same time, the pK_a value for pyridine-3-carboxamide is 3.3 (CRC Handbook, 2009). $\Delta pK_a = pK_a(\text{base}) - pK_a(\text{acid}) = 4.4$, which indicates that the crystalline product would rather be a co-crystal (Childs *et al.*, 2007). In all the cases listed in Table 1, the H_6TeO_6 molecules are fully protonated. All of these known structures are co-crystals except for ZARGII where H_6TeO_6 is an additive molecule in the salt structure.

In most of the listed structures, the molecules of H_6TeO_6 form columns which are interconnected by $O-H \cdots O$ hydrogen bonds. Such a situation takes place in KUTBUW (the columns are parallel to the *a* axis), UREATE, UREATE01, UREATE02 (parallel to the *c* axis) and VALTUX (parallel to the *c* axis). Analogous columns parallel to the *a* axis are present in GUNQUB; however, these columns are formed together with water molecules. In the other two structures, the constituent molecules are surrounded by each other. None of the structures in Table 1 contains a hydrogen bond with disordered hydrogen atoms in which the hydroxyl groups of the telluric acid are involved. Interestingly, neutron diffraction experiments revealed that the cubic form of H_6TeO_6 (Cohen-Addad, 1971) possesses disordered hydrogen atoms, in contrast to the monoclinic form (Lindqvist & Lehmann, 1973). The H_6TeO_6 molecule can be considered as an interesting building block for crystal engineering because it can offer each of its six hydroxyl groups for the formation of hydrogen bonds with neighbouring molecules.

3-Pyridinecarboxamide (nicotinamide) is a biologically important molecule which is an active part of the vitamin B3

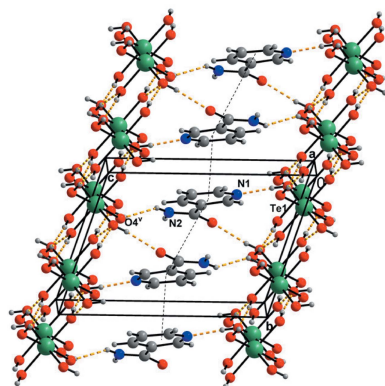


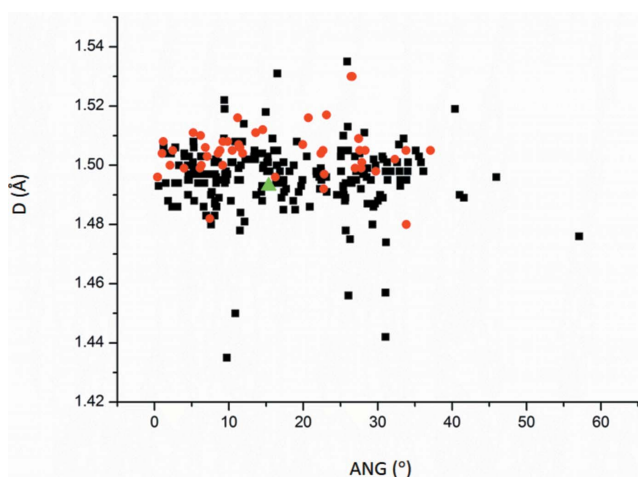
Table 1

 Overview of the known structure determinations of molecular crystals containing the H_6TeO_6 molecule.

Refcode	Reference	Important functional groups present in the structure
BINFAP	Tran Qui <i>et al.</i> (1982) ^a	H_3N^+ , COO^-
BINFAP01	Andersen <i>et al.</i> (1983) ^a	H_3N^+ , COO^-
BINFAP02	Tran Qui <i>et al.</i> (1987) ^a	H_3N^+ , COO^-
BINFAP10	Tran Qui <i>et al.</i> (1984) ^a	H_3N^+ , COO^-
GUNQUB	Driess <i>et al.</i> (2001) ^b	N, NH, NH_2
KUTBUW	Ilczyszyn <i>et al.</i> (1992) ^c	$(H_3C)N^+$, COO^-
UREATE	Loub <i>et al.</i> (1979) ^d	NH_2 , CO
UREATE01	Loub & Dušek (1986) ^d	NH_2 , CO
UREATE02	Averbuch-Pouchot & Durif (1989) ^d	NH_2 , CO
VALTUX	Averbuch-Pouchot (1988) ^e	$R_2H_2N^+$, COO^-
ZARGII	Císařová <i>et al.</i> (1995) ^f	R_3NH , COO^-

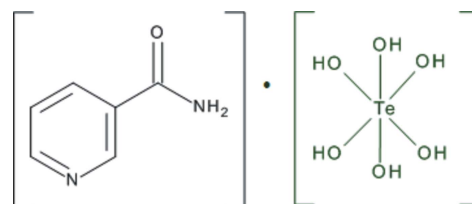
Notes: (a) bis(glycine) hexahydroxytellurium monohydrate; (b) bis(adenine) hexahydroxytellurium tetrahydrate; (c) bis(betaïne) telluric acid; (d) bis(urea) orthotelluric acid; (e) sarcosine telluric acid; (f) disodium hexahydroxytelluric acid dihydrogenethylenediaminetetraacetate dihydrate.

and nicotinamide adenine dinucleotide (NAD) [see for example Wald (1991) and Williamson *et al.* (1967)]. The interplanar angles *ANG* between the pyridine and the amide groups in the 3-pyridinecarboxamide or 3-carbamoylpyridin-1-ium molecules span a large angle because these two moieties are connected by a single C—C bond (bond *D*, Fig. 1). (This single bond corresponds to the bond C1—C6 in the title structure.) Thus 3-pyridinecarboxamide as well as 3-carbamoylpyridin-1-ium molecules can easily accommodate to the environment for optimization of the amide interactions. It seems that the bond length *D* tends to be longer in the 3-carbamoylpyridin-1-ium molecules than in 3-pyridinecarboxamide molecules. This phenomenon can easily be explained by the elongation of the C—NH⁺ bonds in


Figure 1

Dependence of the C—C bond distance *D*, which interconnects the pyridine and the amide groups, on the interplanar angle (*ANG*) between these groups in 3-pyridinecarboxamide molecules (black squares) or 3-carbamoylpyridin-1-ium molecules (red circles). The interplanar angle has been calculated from the non-hydrogen atoms of these groups. The title structure, which belongs among 3-pyridinecarboxamide molecules, is depicted by a green triangle.

comparison to the the C—N bonds in the conjugated bonds system present in the pyridine rings, and thus by a tendency to a slight elongation of bond *D*.



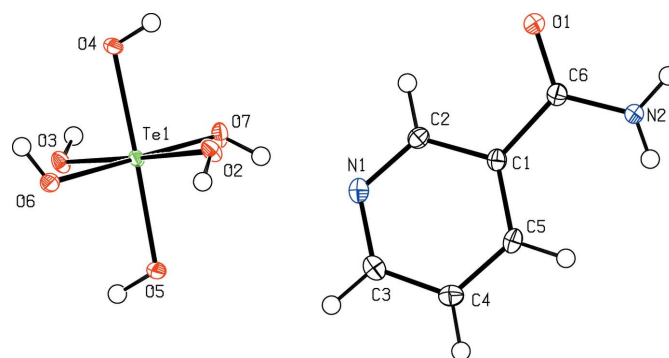
2. Structural commentary

The title molecules are shown in Fig. 2. The interplanar angle between the pyridine non-hydrogen atoms and the non-hydrogen amide atoms is 15.25 (8)°.

Table 2 lists the hydrogen bonds present in the title structure. The parameters of these hydrogen bonds place them in the category of moderate hydrogen bonds (Gilli & Gilli, 2009). The sheets composed of the telluric acid molecules only are held together by O—H...O hydrogen bonds (Fig. 3). These sheets alternate with the 3-pyridinecarboxamide molecules, which are interconnected by hydrogen bonds as well as by π -electron... π -electron ring interactions (Figs. 3–5). These sheets are parallel to (001). The presence of these sheets is so far unique among the known structures of molecular crystals with H_6TeO_6 (see also the *Chemical context* section).

The secondary amine nitrogen is the acceptor of the strongest hydrogen bond present in the structure (O7—H1O7...N1; Table 2). The primary amine hydrogen H1N2 is donated to one of the hydroxyl oxygen atoms of the telluric acid while H2N2 is donated to the oxygen atom of the amide group (O4).

The most important piece of knowledge derived from the study of the title structure is the functionality of the telluric acid molecule, which can become a constitutional part of the hydrogen-bonding pattern. This property of the telluric acid molecule has not been so far studied in depth in molecular crystals because of scarcity of relevant structural data.


Figure 2

The title molecule with anisotropic atomic displacements shown at the 50% probability level (*PLATON*; Spek, 2009).

Table 2
 Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N2-H1N2\cdots O1^i$	0.83 (2)	2.11 (2)	2.9359 (18)	174.8 (19)
$N2-H2N2\cdots O4^{ii}$	0.81 (2)	2.26 (2)	2.9847 (17)	149.2 (18)
$O2-H1O2\cdots O6^{iii}$	0.81 (2)	1.92 (2)	2.7215 (15)	170 (2)
$O3-H1O3\cdots O7^{iv}$	0.78 (2)	1.93 (2)	2.6988 (15)	168 (2)
$O4-H1O4\cdots O2^v$	0.80 (2)	1.97 (2)	2.7621 (15)	171 (2)
$O5-H1O5\cdots O3^{vi}$	0.81 (2)	1.92 (2)	2.7237 (15)	170 (2)
$O6-H1O6\cdots O1^v$	0.79 (2)	2.02 (2)	2.7548 (15)	156 (2)
$O7-H1O7\cdots N1$	0.82 (1)	1.79 (2)	2.6038 (16)	175 (2)

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x, y, z+1$; (iii) $-x, -y+1, -z$; (iv) $-x+1, -y, -z$; (v) $-x+1, -y+1, -z$; (vi) $-x, -y, -z$.

3. Supramolecular features

The telluric acid molecules H_6TeO_6 form sheets (Fig. 3) parallel to (001). Each telluric acid molecule donates four hydrogen atoms to four symmetry-equivalent telluric acid molecules and accepts four hydrogen atoms from these molecules. These hydrogen bonds are arranged in centrosymmetric graph-set motifs $R_2^2(8)$ (Etter *et al.*, 1990): $Te1/O3/\cdots H1O5^{vi}/O5^{vi}/Te1^{vi}/O3^{vi}\cdots H1O5/O5$; $Te1/O7/\cdots H1O3^{iv}/O3^{iv}/Te1^{iv}/O7^{iv}\cdots H1O3/O3$; $Te1/O6/\cdots H1O2^{iii}/O2^{iii}/Te1^{iii}/O6^{iii}\cdots H1O2/O2$; $Te1/O2/\cdots H1O2/O4^v/Te1^v/O2^v\cdots H1O4/O4$ (symmetry codes as in Table 2).

Another hydrogen atom of the telluric acid is donated to atom N1, thus forming a chain with graph-set motif $C(3)$. The

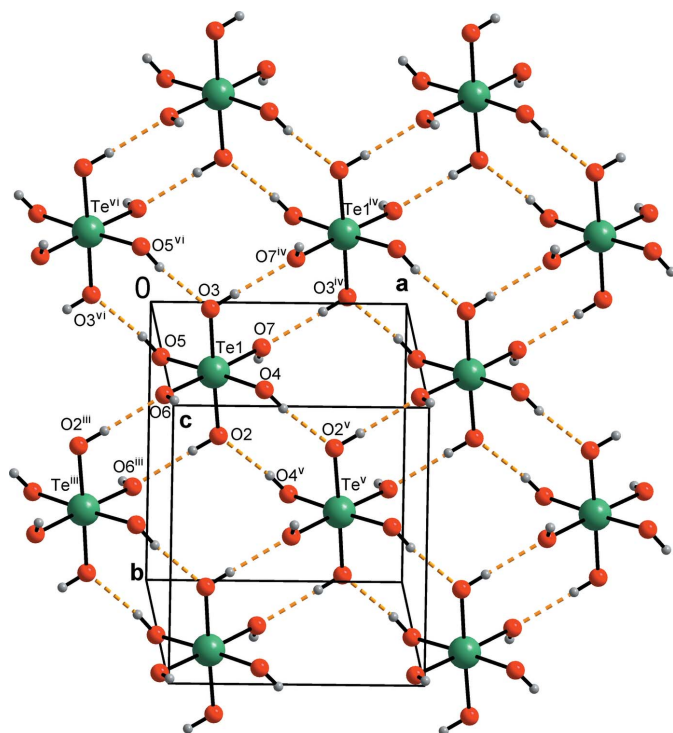


Figure 3
 View (DIAMOND; Brandenburg & Putz, 2005) of a sheet composed of H_6TeO_6 molecules only. H, O and Te atoms are represented by small grey, red and green circles, respectively. Hydrogen bonds are shown as yellow dashed lines. Symmetry codes as in Table 2.

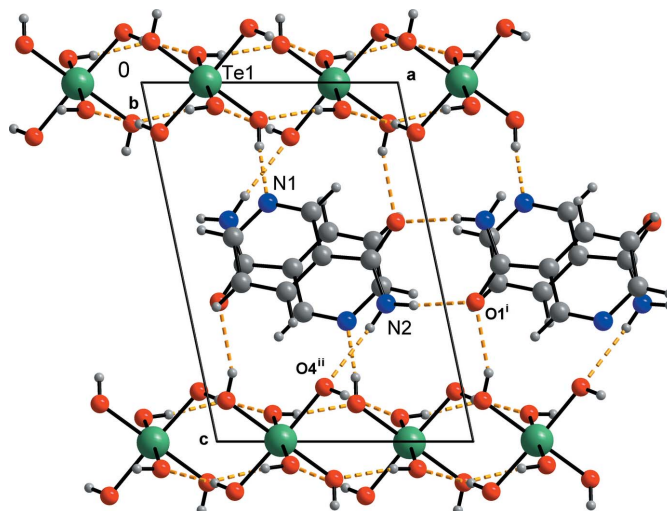


Figure 4
 View (DIAMOND; Brandenburg & Putz, 2005) of the title structure along the b axis. C, H, N, O and Te atoms are represented by grey, small grey, blue, red and green circles, respectively. Hydrogen bonds are shown as yellow dashed lines. Symmetry codes as in Table 2

chain is composed of the atoms $O7-H1O7\cdots N1$ (Figs. 4 and 5) and this hydrogen bond is the strongest of all the hydrogen bonds present in the title structure (Table 2).

The primary amine hydrogen atom H1N2 is involved in the hydrogen bond $N2-H1N2\cdots O4^{ii}$ (symmetry codes as in Table 2). The other primary amine hydrogen atom, H2N2,

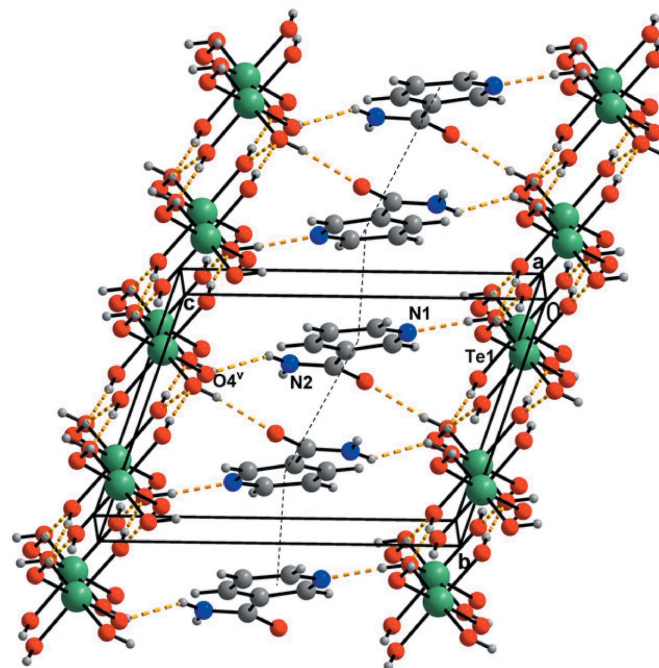


Figure 5
 View (DIAMOND; Brandenburg & Putz, 2005) of the title structure along the a axis. C, H, N, O and Te atoms are represented by grey, small grey, blue, red and green circles, respectively. Hydrogen bonds are shown as yellow dashed lines. The π - π electron-ring interactions are indicated by black dashed lines.

takes part in the centrosymmetric pair with an $R_2^2(8)$ graph-set motif composed of the the atoms $O1/C6/N2/H2N2 \cdots O2^i/C6^i/N2^i/H2N2^i$ (symmetry codes as in Table 2; Figs. 4 and 5).

The closest centroid–centroid distance [3.4101 (9) Å] indicates the presence of π – π interactions between adjacent pyridine rings (at x, y, z and $-x + 1, -y, -z + 1$) (Fig. 5).

4. Synthesis and crystallization

Equimolar amounts of 3-pyridinecarboxamide (0.40 g) and telluric acid (0.75 g) were dissolved in water (10 ml). Colourless crystals of the title compound were obtained by slow evaporation over the course of three weeks.

5. Database survey

The applied crystallographic databases were the Cambridge Crystallographic Database (version 5.39 with updates up to May 2018; Groom *et al.*, 2016) and the Inorganic Crystal Structure Database (ICSD-Web, June 2018; FIZ Karlsruhe, 2018).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All hydrogen atoms were discernible in the difference electron-density map. The constraints $C_{\text{aryl}}-H_{\text{aryl}} = 0.95 \text{ \AA}$ and $U_{\text{iso}}(H_{\text{aryl}}) = 1.2U_{\text{eq}}(C_{\text{aryl}})$ were applied to the aryl H atoms. The positional parameters of the primary amine hydrogens H1N2 and H2N2 were refined freely, $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(N2)$. The positional parameters of the hydroxyl groups of H_6TeO_6 were refined with the distance restraints 0.84 \AA with elasticities 0.02 \AA (Müller, 2009); $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(O_{\text{telluric acid}})$. The reason for these restraints follows from quite short O–H distances, which spanned the interval $0.66(2)$ – $0.75(2) \text{ \AA}$ if no restraint was applied. Reflection 011 was masked by the backstop and omitted from the refinement.

Acknowledgements

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Table 3
Experimental details.

Crystal data	
Chemical formula	$C_6H_6N_2O \cdot H_6O_6Te$
M_r	351.8
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	120
a, b, c (Å)	7.0094 (3), 7.5750 (3), 10.6149 (5)
α, β, γ (°)	70.945 (4), 78.748 (4), 89.901 (4)
V (Å ³)	521.32 (4)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	2.88
Crystal size (mm)	0.31 × 0.21 × 0.09
Data collection	
Diffractometer	Rigaku Oxford Diffraction Xcalibur, AtlasS2, Gemini ultra
Absorption correction	Analytical <i>CrysAlis PRO</i> (Rigaku OD, 2018)
$T_{\text{min}}, T_{\text{max}}$	0.618, 0.816
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6995, 2408, 2254
R_{int}	0.019
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.671
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.012, 0.032, 1.08
No. of reflections	2408
No. of parameters	170
No. of restraints	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.42, -0.35

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *SIR2014* (Burla *et al.*, 2015), *SHELXL* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *DIAMOND* (Brandenburg & Putz, 2005).

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supporting information

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Pyridine-3-carboxamide–telluric acid (1/1)

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2018); cell refinement: *CrysAlis PRO* (Rigaku OD, 2018); data reduction: *CrysAlis PRO* (Rigaku OD, 2018); program(s) used to solve structure: *SIR2014* (Burla *et al.*, 2015); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009) and *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *SHELXL* (Sheldrick, 2015).

Pyridine-3-carboxamide–telluric acid (1/1)

Crystal data

$C_6H_6N_2O \cdot H_6O_6Te$

$M_r = 351.8$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.0094$ (3) Å

$b = 7.5750$ (3) Å

$c = 10.6149$ (5) Å

$\alpha = 70.945$ (4)°

$\beta = 78.748$ (4)°

$\gamma = 89.901$ (4)°

$V = 521.32$ (4) Å³

$Z = 2$

$F(000) = 340$

$D_x = 2.241$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5013 reflections

$\theta = 3.3$ – 28.4 °

$\mu = 2.88$ mm⁻¹

$T = 120$ K

Prism, colourless

$0.31 \times 0.21 \times 0.09$ mm

Data collection

Rigaku Oxford Diffraction Xcalibur, AtlasS2,

Gemini ultra

diffractometer

Radiation source: X-ray tube

Graphite monochromator

Detector resolution: 10.3567 pixels mm⁻¹

ω scans

Absorption correction: analytical

CrysAlisPro (Rigaku OD, 2018)

$T_{\min} = 0.618$, $T_{\max} = 0.816$

6995 measured reflections

2408 independent reflections

2254 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\max} = 28.5$ °, $\theta_{\min} = 2.9$ °

$h = -9 \rightarrow 8$

$k = -10 \rightarrow 9$

$l = -14 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.012$

$wR(F^2) = 0.032$

$S = 1.08$

2408 reflections

170 parameters

6 restraints

24 constraints

H atoms treated by a mixture of independent

and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0117P)^2 + 0.2806P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.003$

$\Delta\rho_{\max} = 0.42$ e Å⁻³

$\Delta\rho_{\min} = -0.35$ e Å⁻³

Extinction correction: SHELXL2014
 (Sheldrick, 2015),
 $F_c^* = kF_c [1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0185 (6)

Special details

Refinement. The unrestrained refinement of the H atoms of the OH groups of the telluric acid resulted in too short O—H distances: O2 H1O2 0.70 (2) Å, O3 H1O3 0.66 (2) Å, O4 H1O4 0.70 (2) Å, O5 H1O5 0.72 (2) Å, O6 H1O6 0.70 (2) Å, O7 H1O7 0.75 (2) Å.

Therefore the restrained refinement has been applied. The O—H distances were restrained as 0.84 Å with elasticity 0.02 Å.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
O1	0.87715 (15)	0.43054 (16)	0.38915 (10)	0.0154 (2)
N1	0.39465 (19)	0.18273 (18)	0.33548 (12)	0.0137 (3)
N2	0.7726 (2)	0.3530 (2)	0.61605 (13)	0.0159 (3)
H1N2	0.872 (3)	0.409 (3)	0.6196 (19)	0.019*
H2N2	0.687 (3)	0.314 (3)	0.683 (2)	0.019*
C1	0.5627 (2)	0.2754 (2)	0.48208 (14)	0.0115 (3)
C2	0.5568 (2)	0.2446 (2)	0.36022 (14)	0.0125 (3)
H1C2	0.6729	0.2686	0.2922	0.015*
C3	0.2306 (2)	0.1498 (2)	0.43111 (16)	0.0147 (3)
H1C3	0.1135	0.1124	0.4115	0.018*
C4	0.2249 (2)	0.1682 (2)	0.55750 (15)	0.0148 (3)
H1C4	0.1080	0.1379	0.6250	0.018*
C5	0.3941 (2)	0.2320 (2)	0.58308 (15)	0.0132 (3)
H1C5	0.3945	0.2459	0.6688	0.016*
C6	0.7492 (2)	0.3584 (2)	0.49361 (15)	0.0121 (3)
Te1	0.24981 (2)	0.25172 (2)	−0.00312 (2)	0.00795 (5)
O2	0.26677 (16)	0.45520 (15)	0.06561 (11)	0.0126 (2)
H1O2	0.164 (2)	0.503 (3)	0.072 (2)	0.019*
O3	0.24036 (16)	0.05185 (15)	−0.07618 (11)	0.0118 (2)
H1O3	0.335 (2)	−0.002 (3)	−0.073 (2)	0.018*
O4	0.46392 (15)	0.36909 (16)	−0.15123 (11)	0.0122 (2)
H1O4	0.533 (3)	0.429 (3)	−0.127 (2)	0.018*
O5	0.02924 (16)	0.14607 (16)	0.13902 (11)	0.0135 (2)
H1O5	−0.040 (3)	0.081 (3)	0.117 (2)	0.020*
O6	0.07017 (15)	0.37675 (16)	−0.11412 (11)	0.0122 (2)
H1O6	0.119 (3)	0.429 (3)	−0.1913 (15)	0.018*
O7	0.42559 (16)	0.12206 (16)	0.10483 (11)	0.0131 (2)
H1O7	0.409 (3)	0.141 (3)	0.1777 (16)	0.020*

Atomic displacement parameters (Å²)

	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
O1	0.0120 (5)	0.0219 (6)	0.0120 (5)	−0.0006 (4)	−0.0017 (4)	−0.0055 (4)
N1	0.0173 (7)	0.0122 (6)	0.0135 (6)	0.0022 (5)	−0.0058 (5)	−0.0053 (5)

N2	0.0112 (6)	0.0252 (7)	0.0113 (6)	-0.0033 (5)	-0.0013 (5)	-0.0066 (5)
C1	0.0125 (7)	0.0114 (7)	0.0113 (6)	0.0030 (5)	-0.0046 (5)	-0.0035 (5)
C2	0.0135 (7)	0.0121 (7)	0.0117 (7)	0.0019 (5)	-0.0022 (5)	-0.0039 (6)
C3	0.0141 (7)	0.0126 (7)	0.0185 (7)	0.0014 (6)	-0.0058 (6)	-0.0052 (6)
C4	0.0126 (7)	0.0145 (7)	0.0159 (7)	0.0015 (6)	-0.0014 (6)	-0.0040 (6)
C5	0.0161 (7)	0.0133 (7)	0.0113 (7)	0.0028 (6)	-0.0038 (6)	-0.0051 (6)
C6	0.0116 (7)	0.0130 (7)	0.0127 (7)	0.0040 (5)	-0.0038 (5)	-0.0052 (6)
Te1	0.00632 (6)	0.01029 (6)	0.00892 (6)	0.00042 (3)	-0.00173 (4)	-0.00533 (4)
O2	0.0086 (5)	0.0145 (5)	0.0193 (5)	0.0023 (4)	-0.0034 (4)	-0.0117 (4)
O3	0.0098 (5)	0.0137 (5)	0.0164 (5)	0.0022 (4)	-0.0040 (4)	-0.0100 (4)
O4	0.0081 (5)	0.0171 (6)	0.0124 (5)	-0.0035 (4)	0.0006 (4)	-0.0079 (4)
O5	0.0104 (5)	0.0189 (6)	0.0117 (5)	-0.0047 (4)	0.0006 (4)	-0.0075 (4)
O6	0.0085 (5)	0.0168 (5)	0.0106 (5)	0.0021 (4)	-0.0023 (4)	-0.0036 (4)
O7	0.0132 (5)	0.0181 (6)	0.0134 (5)	0.0066 (4)	-0.0071 (4)	-0.0100 (4)

Geometric parameters (Å, °)

O1—C6	1.2450 (18)	C5—H1C5	0.9500
N1—C2	1.3337 (19)	Te1—O7	1.8994 (11)
N1—C3	1.340 (2)	Te1—O5	1.9007 (11)
N2—C6	1.3290 (19)	Te1—O3	1.9197 (10)
N2—H1N2	0.83 (2)	Te1—O4	1.9198 (11)
N2—H2N2	0.81 (2)	Te1—O2	1.9212 (10)
C1—C5	1.390 (2)	Te1—O6	1.9279 (11)
C1—C2	1.3955 (19)	O2—H1O2	0.806 (15)
C1—C6	1.495 (2)	O3—H1O3	0.781 (15)
C2—H1C2	0.9500	O4—H1O4	0.796 (15)
C3—C4	1.387 (2)	O5—H1O5	0.812 (15)
C3—H1C3	0.9500	O6—H1O6	0.789 (15)
C4—C5	1.388 (2)	O7—H1O7	0.818 (14)
C4—H1C4	0.9500		
C2—N1—C3	118.72 (13)	O7—Te1—O5	92.47 (5)
C6—N2—H1N2	117.2 (13)	O7—Te1—O3	90.08 (5)
C6—N2—H2N2	122.0 (14)	O5—Te1—O3	92.84 (5)
H1N2—N2—H2N2	120.0 (18)	O7—Te1—O4	90.50 (5)
C5—C1—C2	118.11 (14)	O5—Te1—O4	176.85 (4)
C5—C1—C6	124.29 (13)	O3—Te1—O4	88.21 (5)
C2—C1—C6	117.58 (13)	O7—Te1—O2	89.74 (5)
N1—C2—C1	122.63 (14)	O5—Te1—O2	89.02 (5)
N1—C2—H1C2	118.7	O3—Te1—O2	178.14 (4)
C1—C2—H1C2	118.7	O4—Te1—O2	89.94 (5)
N1—C3—C4	122.59 (14)	O7—Te1—O6	178.29 (4)
N1—C3—H1C3	118.7	O5—Te1—O6	87.35 (5)
C4—C3—H1C3	118.7	O3—Te1—O6	88.22 (5)
C3—C4—C5	118.47 (14)	O4—Te1—O6	89.72 (5)
C3—C4—H1C4	120.8	O2—Te1—O6	91.96 (5)
C5—C4—H1C4	120.8	Te1—O2—H1O2	110.5 (15)

C4—C5—C1	119.35 (13)	Te1—O3—H1O3	110.6 (15)
C4—C5—H1C5	120.3	Te1—O4—H1O4	109.1 (15)
C1—C5—H1C5	120.3	Te1—O5—H1O5	110.4 (15)
O1—C6—N2	122.04 (14)	Te1—O6—H1O6	114.5 (15)
O1—C6—C1	119.44 (13)	Te1—O7—H1O7	111.3 (14)
N2—C6—C1	118.52 (13)		
C3—N1—C2—C1	0.4 (2)	C2—C1—C5—C4	-2.8 (2)
C5—C1—C2—N1	2.7 (2)	C6—C1—C5—C4	175.27 (14)
C6—C1—C2—N1	-175.51 (13)	C5—C1—C6—O1	-164.04 (14)
C2—N1—C3—C4	-3.4 (2)	C2—C1—C6—O1	14.1 (2)
N1—C3—C4—C5	3.2 (2)	C5—C1—C6—N2	15.8 (2)
C3—C4—C5—C1	0.0 (2)	C2—C1—C6—N2	-166.14 (14)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H1N2...O1 ⁱ	0.83 (2)	2.11 (2)	2.9359 (18)	174.8 (19)
N2—H2N2...O4 ⁱⁱ	0.81 (2)	2.26 (2)	2.9847 (17)	149.2 (18)
O2—H1O2...O6 ⁱⁱⁱ	0.81 (2)	1.92 (2)	2.7215 (15)	170 (2)
O3—H1O3...O7 ^{iv}	0.78 (2)	1.93 (2)	2.6988 (15)	168 (2)
O4—H1O4...O2 ^v	0.80 (2)	1.97 (2)	2.7621 (15)	171 (2)
O5—H1O5...O3 ^{vi}	0.81 (2)	1.92 (2)	2.7237 (15)	170 (2)
O6—H1O6...O1 ^v	0.79 (2)	2.02 (2)	2.7548 (15)	156 (2)
O7—H1O7...N1	0.82 (1)	1.79 (2)	2.6038 (16)	175 (2)

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x, y, z+1$; (iii) $-x, -y+1, -z$; (iv) $-x+1, -y, -z$; (v) $-x+1, -y+1, -z$; (vi) $-x, -y, -z$.