[1,4]Ditellurino[2,3-b:5,6-b′]dipyrazine

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[1,4]Ditellurino[2,3-b:5,6-b′]dipyrazine represents the first reported [1,4]chalcogena[2,3-b:5,6-b′]dipyrazine containing a heavy chalcogens. The asymmetric unit consists of three molecules. In contrast to its sulfur analog, which is planar [Lynch et al. (1994) Cryst. Struct. Commun. 50,1470–1472], C₈H₄N₄Te₂ is folded along the Te···Te axis to accommodate the larger chalcogenide atoms. The dihedral angle between the two TeC₂ rings of the central ring is 57.9° (mean of three). C–Te bond lengths range from 2.1105 (16) Å to 2.1381 (17) Å, in good agreement with those predicted by their covalent radii. All Te atoms are involved in intermolecular Te···N contacts, with distances in the range 2.894 (2) to 2.963 (2) Å. These result in a spiral supramolecular assembly, forming helical columns.

Structure description

Heterocyclic tellurium compounds have found considerable attention due to their tendency to form supramolecular assemblies including molecular wires (Kremer et al., 2016), ribbons (Cozzolino et al., 2010) and rings (Ho et al., 2016, 2017). Such assemblies can give rise to materials with non-linear optical properties (Cozzolino et al., 2010), as well as novel phosphorescent organic emitters (Kremer et al., 2015). A ribbon motif resulting from secondary intermolecular N···Te bonding interactions of 2.767 (6) and 2.659 (6) Å was reported for 3,4-dicyano-1,2,5-telluradiazole (Cozzolino et al., 2010). Similarly, molecular wire motifs resulting from secondary intermolecular N···Te bonding were observed for 2-substituted benzo-1,3-tellurazoles, but with significantly longer N···Te distances. This is exemplified by 2-(2-furanyl) benzo-1,3-tellurazole, 3.17 Å (Kremer et al., 2016) and 1,3-benzotellurazol-2-ylacetonitrile, 3.16 Å (Sanford et al., 2017). Not all Te, N-containing heterocycles form supramolecular wires or ribbons. Thus, 10H-pyrazino[2,3-b][1,4]benzotellurazine (Smith et al., 2020), 2H-1,4-benzo-tellurazin-3(4H)-one and 2,3-dihydro-1,5-benzotellurazepin-4(5H)-one (Myers et al., 2016) lack this
The [1,4]dichalcogena[2,3-b:5,6-b']dipyrazines remain poorly explored and no examples containing heavy chalcogens were reported prior to this study.

The three molecules of the asymmetric unit are shown in Fig. 1, which illustrates their folded V shapes. The degree of folding along the Te···Te line can be described by \( \varphi \), the dihedral angle between the two C2Te2 moieties of the central ring. This dihedral angle has a value of 60.08 (5)° for the molecule containing Te1 and Te2, 57.16 (5)° for the Te3/Te4 molecule, and 56.54 (5)° for the Te5/Te6 molecule, with a mean value of 57.9°. A sulfur analog of the title compound has been structurally characterized (Lynch et al., 1994), but is planar rather than folded along the chalcogen–chalcogen axis. The corresponding selenium congener remains unreported. The shape of the title compound shows structural similarity to those of 9,10-dichalcogenanthracenes containing tellurium and one other chalcogen atom in the central ring (Dereu et al., 1981; Meyers et al., 1988), as well as to the recently characterized 10\( H \)-pyrazino[2,3-b][1,4]benzotellurazine (Smith et al., 2020).

The C—Te—C angles for the three independent molecules of the title compound range from 91.48 (6) to 93.80 (6)°, similar to those of 95.3 and 95.9°, respectively, previously reported for telluranthrene (Dereu et al., 1981). C—Te bond lengths range from 2.1105 (16) Å to 2.1381 (17) Å, in good agreement with those predicted by their covalent radii.

Intermolecular features are dominated by Te···N interactions involving all Te atoms, as shown in Fig. 2. The range of distances for these contacts is 2.894 (2) to 2.963 (2) Å. These fall between those of 2.767 (6) and 2.659 (6) Å reported for 3,4-dicyano-1,2,5-telluradiazole (Cozzolino et al., 2010), and those for benzo-1,3-tellurazoles, ranging from 2.985 Å for 2-(methylsulfanyl)-1,3-benzotellurazole (Ali et al., 2016) to 3.169 Å for 2-(2-furyl)-1,3-benzotellurazole (Kremer et al., 2016). In contrast, despite its structural similarity, 10\( H \)-pyrazino[2,3-b][1,4]benzotellurazine does not exhibit any supramolecular Te···N bonding but forms hydrogen-bonded dimers instead (Smith et al., 2020).

Each molecule of the title compound is involved in four Te···N contacts, forming helical chains, as shown in Figs. 3 and 4. The helices have approximate threefold helical symmetry.

**Figure 1**
The asymmetric unit of [1,4]ditellurino[2,3-b:5,6-b']dipyrazine with 50% ellipsoids.

**Figure 2**
The unit cell, showing intermolecular Te···N contacts.

**Figure 3**
A portion of the helical chain, side view.

**Figure 4**
View of chain along the helix axis.
with a three-molecule repeat period. The helical chains are in the [1T1] direction and have a repeat distance of 20.244 (2) Å.

The Hirshfeld surface enclosing the Te3/Te4 molecule was calculated with respect to $d_{e}$, $d_{i}$ and $d_{norm}$ using Crystal Explorer (Spackman et al., 2021), where $d_{e}$ and $d_{i}$ represent the nearest distance of external or internal nucleus from a point of interest on the iso-surface. The dominant N···Te interactions with the adjacent Te1/Te2 molecule can be seen as the bright red areas on the Hirshfeld surface. The two-dimensional fingerprint plot and a two-dimensional fingerprint highlighting close reciprocal N···Te contacts are shown in Fig. 5. These contacts include 14.6% of the surface area.

A search of the Cambridge Structural Database (May 2021 update; Groom et al., 2016) for similar organotellurocen heterocycles yielded 9,10-dichalcogenaanthracenes, C$_7$H$_6$(X,Y) = (O, Te), (S, Te), (Se, Te) and (Te, Te): PXTELL (Smith et al., 1973), VEHVUZ (Meyers et al., 1988), VEHWEK (Meyers et al., 1988), and BAVJIR (Dereu et al., 1981), respectively. A further comparison was carried out with the sulfur analog of the title compound, WIBWEJ (Lynch et al., 1994), as well as with benzo[1,4]tellurazoles OLUQIX (Junk et al., 1993), UGIHIEL (Smith et al., 2020) and BUTNOV (Myers et al., 2016). A comparison with other Te, N-containing heterocycles known to undergo supramolecular interactions with the adjacent Te1/Te2 molecule can be seen as the bright red areas on the Hirshfeld surface. The two-dimensional fingerprint plot and a two-dimensional fingerprint plot highlighting close reciprocal N···Te contacts are shown in Fig. 5.

### Table 1

| Table 1 | Experimental details. |
|---------|-----------------------|
| Crystal data | C$_{8}$H$_{4}$N$_{4}$Te$_{2}$ |
| Chemical formula | 411.35 |
| Temperature (K) | 90 |
| a, b, c (Å) | 7.6531 (8), 11.7862 (12), 16.8371 (18) |
| V (Å$^{3}$) | 158610, 158610, 145750 |
| Z | 6 |
| Radiation type | Mo Kα |
| μ (mm$^{-1}$) | 5.88 |
| Crystal size (mm$^{3}$) | 0.19 × 0.17 × 0.16 |
| Data collection | Bruker Kappa APEXII DUO CCD |
| Absorption correction | Multi-scan (SADABS; Krause et al., 2015) |
| T$_{min}$, T$_{max}$ | 0.362, 0.453 |
| No. of measured, independent and observed [I > 2σ(I)] reflections | 158610 |
| R$_{int}$ | 0.025 |
| R$_{cryst}$ | 0.950 |
| Refinement | |
| R$_{cryst}$ | 0.024, 0.058, 1.10 |
| No. of reflections | 381 |
| No. of parameters | 158610 |
| H-atom treatment | H-atom parameters constrained |
| Δρ$_{max}$, Δρ$_{min}$ (e Å$^{-3}$) | 2.18, −0.97 |

#### Synthesis and crystallization

**Preparation of [1,4]ditellurino[2,3-b:5,6-b']dipyrazine**: a 100 ml round-bottom flask equipped with mechanical stirring and inert gas inlet was charged with tellurium powder (200 mesh, 1.28 g, 10 mmol), sodium hydride (0.6 g of 60% emulsion in mineral oil, 15 mmol) and dry N-methyl-2-pyrrolidone (12 ml). The mixture was purged with nitrogen, placed in a Wood’s metal bath and heated to 453 K with mechanical stirring for two hours. 2,3-Dichloropyrazine (1.49 g, 10 mmol) was then added, followed by continued stirring at 453 K. The mixture was allowed to cool and diluted with water (100 ml). Solids were collected by filtration and dried. They were subsequently extracted with 2 × 10 ml of chloroform. The combined extracts were chromatographed on a 1.5 × 10 cm column (silica gel, neutral, 200 mesh) using chloroform as mobile phase, followed by chloroform: acetonitrile (10:1 v/v). A yellow band eluted first and was identified as bis[pyrazin-2-yl]tellurium by mass spectrometry. This was followed by a blue band, identified as bis(3-chloropyrazin-2-yl)ditellurium. The following yellow band contained the title compound. Crystallization from chloroform solution furnished yellow crystals, m.p. 413–415 K, yield 46 mg (2.2%).

**Properties**: $^1$H NMR (CDCl$_3$, p.p.m.): 8.31 (s, 4H). $^{13}$C NMR (CDCl$_3$, p.p.m.): 1443.46, 154.32. The compound slowly oxidizes when exposed to air in solution. A sample suitable for X-ray crystallography was obtained by evaporation of a solution in chloroform.

#### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. In the later stages of refinement, a small amount of twinning was detected, by 180° rotation about the reciprocal 110 direction. Final refinement was as a twin-component twin using an HKL5 file prepared by ROTAX (Parsons et al., 2003). The BASF parameter is 0.0250 (4).

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*Figure 5*

(a) Hirshfeld surface mapped over $d_{norm}$, (b) two-dimensional fingerprint plot, (c) two-dimensional fingerprint plot with reciprocal N···Te contacts highlighted.
data reports

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full crystallographic data

IUCrData (2022). 7, x220622  [https://doi.org/10.1107/S2414314622006228]

[1,4]Ditellurino[2,3-b:5,6-b′]dipyazine

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[1,4]Ditellurino[2,3-b:5,6-b′]dipyazine

Crystal data

C₈H₄N₄Te₂  

\[ Z = 6 \]

\[ F(000) = 1104 \]

\[ D_x = 2.771 \text{ Mg m}^{-3} \]

Mo Kα radiation, λ = 0.71073 Å

Cell parameters from 9342 reflections

\[ \theta = 2.8–42.1° \]

\[ \mu = 5.88 \text{ mm}^{-1} \]

\[ T = 90 \text{ K} \]

Fragment, yellow

\[ 0.19 \times 0.17 \times 0.16 \text{ mm} \]

Data collection

Bruker Kappa APEXII DUO CCD diffractometer

158610 measured reflections

158610 independent reflections

145750 reflections with \( I > 2\sigma(I) \)

\[ R_{\text{int}} = 0.025 \]

\[ \theta_{\text{max}} = 42.5°, \theta_{\text{min}} = 1.2° \]

\[ h = -14 \rightarrow 14 \]

\[ k = -22 \rightarrow 22 \]

\[ l = -31 \rightarrow 31 \]

Refinement

Refinement on \( F^2 \)

Least-squares matrix: full

\[ R[F^2 > 2\sigma(F^2)] = 0.024 \]

\[ wR(F^2) = 0.058 \]

\[ S = 1.10 \]

158610 reflections

381 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

\[ w = 1/[\sigma^2(F_c^2) + (0.0009P)^2 + 1.6438P] \]

where \( P = (F_c^2 + 2F_s^2)/3 \)

\( (\Delta\sigma)_{\text{max}} = 0.002 \)

\( \Delta\rho_{\text{max}} = 2.18 \text{ e Å}^{-3} \)

\( \Delta\rho_{\text{min}} = -0.97 \text{ e Å}^{-3} \)

Extinction correction: SHELXL-2018/1 (Sheldrick 2015b),

\[ F_c^\alpha = kF_c[1+0.001xFe^\alpha\lambda^3/\sin(2θ)]^{-1/4} \]

Extinction coefficient: 0.00036 (7)
**Special details**

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement.** Refined as a two-component twin using an HKL5 file prepared by ROTAX (Parsons et al., 2003). The BASF parameter is 0.0250 (4). All H atoms were located in difference maps and then treated as riding in geometrically idealized positions with C—H distances 0.95 Å and with $U_{iso}(H) = 1.2U_{eq}$ for the attached C atom.

**Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\AA^2$)**

|      | x        | y        | z        | $U_{iso}*/U_{eq}$ |
|------|----------|----------|----------|-------------------|
| Te1  | 0.49841 (2) | 0.50998 (2) | 0.85722 (2) | 0.01013 (2)       |
| Te2  | 0.50106 (2) | 0.49957 (2) | 0.63430 (2) | 0.00816 (2)       |
| N1   | 0.4741 (2)  | 0.75856 (14) | 0.79682 (9)  | 0.0131 (3)        |
| N2   | 0.4700 (2)  | 0.75553 (14) | 0.63202 (9)  | 0.0113 (2)        |
| N3   | 0.8440 (2)  | 0.35839 (14) | 0.83665 (9)  | 0.0103 (2)        |
| N4   | 0.8595 (2)  | 0.37038 (14) | 0.66970 (9)  | 0.0104 (2)        |
| C1   | 0.4830 (2)  | 0.65832 (15) | 0.76698 (10) | 0.0098 (3)        |
| C2   | 0.4806 (2)  | 0.65701 (15) | 0.68373 (10) | 0.0090 (2)        |
| C3   | 0.4596 (3)  | 0.85524 (16) | 0.66225 (11) | 0.0131 (3)        |
| H3   | 0.450785    | 0.926470   | 0.626760   | 0.016*            |
| C4   | 0.4615 (3)  | 0.85661 (17) | 0.74470 (11) | 0.0139 (3)        |
| H4   | 0.453565    | 0.928841   | 0.764348   | 0.017*            |
| C5   | 0.7087 (2)  | 0.41601 (15) | 0.79341 (10) | 0.0086 (2)        |
| C6   | 0.7142 (2)  | 0.41927 (15) | 0.70924 (10) | 0.0084 (2)        |
| C7   | 0.9955 (2)  | 0.31457 (16) | 0.71338 (11) | 0.0118 (3)        |
| H7   | 1.100495    | 0.280085   | 0.687036   | 0.014*            |
| C8   | 0.9850 (2)  | 0.30641 (17) | 0.79687 (11) | 0.0118 (3)        |
| H8   | 1.080803    | 0.262596   | 0.826477   | 0.014*            |
| Te3  | 0.02141 (2) | 0.96211 (2)  | 0.37609 (2)  | 0.00927 (2)       |
| Te4  | 0.45479 (2) | 0.80313 (2)  | 0.45840 (2)  | 0.00845 (2)       |
| N5   | −0.1035 (2) | 0.76067 (14) | 0.47346 (9)  | 0.0109 (2)        |
| N6   | 0.2130 (2)  | 0.64559 (13) | 0.53966 (9)  | 0.0094 (2)        |
| N7   | 0.2250 (2)  | 0.92573 (13) | 0.22221 (8)  | 0.0094 (2)        |
| N8   | 0.5463 (2)  | 0.81350 (15) | 0.28562 (9)  | 0.0116 (2)        |
| C9   | 0.0482 (2)  | 0.80356 (15) | 0.45639 (10) | 0.0087 (2)        |
| C10  | 0.2078 (2)  | 0.74554 (15) | 0.48943 (9)  | 0.0084 (2)        |
| C11  | 0.0613 (2)  | 0.60249 (16) | 0.55555 (10) | 0.0111 (3)        |
| H11  | 0.061189    | 0.531090   | 0.590301   | 0.013*            |
| C12  | −0.0961 (2) | 0.65951 (17) | 0.52251 (11) | 0.0120 (3)        |
| H12  | −0.201159  | 0.625984   | 0.534990   | 0.014*            |
| C13  | 0.2442 (2)  | 0.90429 (15) | 0.30184 (10) | 0.0085 (2)        |
| C14  | 0.4045 (2)  | 0.84565 (15) | 0.33377 (10) | 0.0088 (2)        |
| C15  | 0.5256 (2)  | 0.83823 (18) | 0.20617 (11) | 0.0134 (3)        |
| H15  | 0.623674    | 0.818218   | 0.170301   | 0.016*            |
| C16  | 0.3656 (2)  | 0.89205 (16) | 0.17491 (10) | 0.0111 (3)        |
| H16  | 0.355508    | 0.905375   | 0.118238   | 0.013*            |
### Atomic displacement parameters ($\AA^2$)

|   | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|---|--------------|--------------|--------------|--------------|--------------|--------------|
| Te1| 0.01103 (4)  | 0.00946 (4)  | 0.00761 (4)  | 0.00239 (3)  | 0.00198 (3)  | 0.00057 (3)  |
| Te2| 0.00895 (4)  | 0.00699 (4)  | 0.00847 (4)  | $-0.00041$ (3) | $-0.00201$ (3) | $-0.00098$ (3) |
| N1 | 0.0182 (7)   | 0.0093 (6)   | 0.0112 (6)   | $-0.0003$ (5) | 0.0013 (5)   | $-0.0026$ (5) |
| N2 | 0.0145 (6)   | 0.0085 (6)   | 0.0105 (5)   | $-0.0016$ (5) | $-0.0021$ (5) | 0.0004 (4)   |
| N3 | 0.0089 (5)   | 0.0111 (6)   | 0.0099 (5)   | 0.0000 (5)    | $-0.0007$ (4) | $-0.0002$ (5) |
| N4 | 0.0096 (6)   | 0.0105 (6)   | 0.0112 (5)   | $-0.0001$ (5) | $-0.0001$ (4) | $-0.0036$ (5) |
| C1 | 0.0107 (6)   | 0.0087 (6)   | 0.0089 (6)   | 0.0004 (5)    | 0.0004 (5)   | $-0.0005$ (5) |
| C2 | 0.0096 (6)   | 0.0075 (6)   | 0.0094 (6)   | $-0.0007$ (5) | $-0.0006$ (5) | 0.0000 (5)   |
| C3 | 0.0173 (8)   | 0.0082 (7)   | 0.0133 (7)   | $-0.0022$ (6) | $-0.0014$ (6) | 0.0003 (5)   |
| C4 | 0.0188 (8)   | 0.0092 (7)   | 0.0136 (7)   | $-0.0013$ (6) | 0.0008 (6)   | $-0.0026$ (5) |
| C5 | 0.0081 (6)   | 0.0078 (6)   | 0.0093 (6)   | $-0.0006$ (5) | 0.0001 (5)   | $-0.0002$ (5) |
| C6 | 0.0086 (6)   | 0.0071 (6)   | 0.0094 (6)   | $-0.0008$ (5) | $-0.0010$ (5) | $-0.0014$ (5) |
| C7 | 0.0100 (6)   | 0.0122 (7)   | 0.0130 (6)   | 0.0000 (5)    | $-0.0003$ (5) | $-0.0034$ (5) |
| C8 | 0.0090 (6)   | 0.0128 (7)   | 0.0126 (6)   | 0.0013 (5)    | $-0.0012$ (5) | $-0.0009$ (5) |
| Te3| 0.00845 (4)  | 0.00910 (4)  | 0.00846 (4)  | 0.00204 (3)   | 0.00024 (3)  | 0.00044 (3)  |
| Te4| 0.00689 (4)  | 0.00985 (4)  | 0.00835 (4)  | $-0.0025$ (3) | $-0.00212$ (3) | 0.00166 (3)  |
| N5 | 0.0080 (5)   | 0.0141 (6)   | 0.0107 (5)   | $-0.0020$ (5) | 0.0006 (4)   | $-0.0018$ (5) |
| N6 | 0.0103 (6)   | 0.0087 (6)   | 0.0089 (5)   | $-0.0019$ (5) | $-0.0009$ (4) | 0.0003 (4)   |
| N7 | 0.0099 (6)   | 0.0096 (6)   | 0.0083 (5)   | $-0.0003$ (5) | $-0.0007$ (4) | $-0.0009$ (4) |
| N8 | 0.0082 (6)   | 0.0145 (7)   | 0.0113 (6)   | $-0.0006$ (5) | 0.0000 (4)   | $-0.0011$ (5) |
| C9 | 0.0078 (6)   | 0.0099 (6)   | 0.0080 (5)   | $-0.0007$ (5) | $-0.0003$ (4) | $-0.0008$ (5) |
| C10| 0.0081 (6)   | 0.0089 (6)   | 0.0081 (5)   | $-0.0019$ (5) | $-0.0005$ (5) | $-0.0004$ (5) |
| C11| 0.0126 (7)   | 0.0110 (7)   | 0.0099 (6)   | $-0.0042$ (6) | 0.0010 (5)   | 0.0001 (5)   |
| C12| 0.0099 (6)   | 0.0139 (7)   | 0.0127 (6)   | $-0.0042$ (6) | 0.0006 (5)   | $-0.0015$ (6) |
| C13| 0.0088 (6)   | 0.0082 (6)   | 0.0082 (5)   | $-0.0008$ (5) | $-0.0001$ (5) | $-0.0006$ (5) |
| C14| 0.0077 (6)   | 0.0089 (6)   | 0.0094 (6)   | $-0.0018$ (5) | $-0.0007$ (5) | 0.0001 (5)   |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| C15 | 0.0097 (7) | 0.0182 (8) | 0.0112 (6) | 0.0002 (6) | 0.0017 (5) | −0.0019 (6) |
| C16 | 0.0109 (7) | 0.0130 (7) | 0.0090 (6) | −0.0010 (5) | −0.0001 (5) | −0.0011 (5) |
| Te5 | 0.00776 (4) | 0.01048 (5) | 0.00853 (4) | −0.00312 (3) | −0.00108 (3) | 0.00122 (3) |
| Te6 | 0.00945 (4) | 0.00712 (4) | 0.00926 (4) | −0.00022 (3) | −0.00264 (3) | −0.00145 (3) |
| N9  | 0.0172 (7) | 0.0121 (7) | 0.0120 (6) | −0.0066 (5) | −0.0009 (5) | −0.0015 (5) |
| N10 | 0.0157 (7) | 0.0108 (6) | 0.0091 (5) | −0.0012 (5) | −0.0026 (5) | −0.0022 (5) |
| N11 | 0.0072 (5) | 0.0115 (6) | 0.0106 (5) | 0.0000 (5) | −0.0007 (4) | −0.0004 (5) |
| N12 | 0.0103 (6) | 0.0116 (6) | 0.0103 (5) | −0.0034 (5) | −0.0002 (4) | −0.0023 (5) |
| C17 | 0.0091 (6) | 0.0108 (7) | 0.0086 (6) | −0.0028 (5) | −0.0009 (5) | −0.0008 (5) |
| C18 | 0.0097 (6) | 0.0090 (6) | 0.0091 (6) | −0.0013 (5) | −0.0011 (5) | −0.0019 (5) |
| C19 | 0.0207 (8) | 0.0139 (8) | 0.0096 (6) | −0.0043 (6) | −0.0030 (6) | −0.0028 (6) |
| C20 | 0.0216 (9) | 0.0142 (8) | 0.0133 (7) | −0.0083 (7) | −0.0019 (6) | −0.0040 (6) |
| C21 | 0.0067 (6) | 0.0098 (6) | 0.0086 (6) | −0.0010 (5) | −0.0006 (4) | −0.0010 (5) |
| C22 | 0.0086 (6) | 0.0087 (6) | 0.0082 (6) | −0.0009 (5) | −0.0011 (5) | −0.0020 (5) |
| C23 | 0.0090 (6) | 0.0140 (7) | 0.0130 (6) | −0.0036 (5) | −0.0003 (5) | −0.0029 (6) |
| C24 | 0.0072 (6) | 0.0144 (7) | 0.0124 (6) | −0.0005 (5) | −0.0011 (5) | −0.0016 (5) |

**Geometric parameters (Å, °)**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| Te1—C5 | 2.1185 (17) | N8—C15 | 1.341 (2) |
| Te1—C1 | 2.1301 (17) | N8—C14 | 1.345 (2) |
| Te2—C2 | 2.1237 (17) | C9—C10 | 1.405 (2) |
| Te2—C6 | 2.1381 (17) | C11—C12 | 1.388 (3) |
| N1—C4 | 1.336 (3) | C11—H11 | 0.9500 |
| N1—C1 | 1.342 (2) | C12—H12 | 0.9500 |
| N2—C2 | 1.337 (2) | C13—C14 | 1.405 (2) |
| N2—C3 | 1.338 (2) | C15—C16 | 1.383 (3) |
| N3—C8 | 1.337 (2) | C15—H15 | 0.9500 |
| N3—C5 | 1.338 (2) | C16—H16 | 0.9500 |
| N4—C7 | 1.339 (2) | Te5—C21 | 2.1105 (16) |
| N4—C6 | 1.345 (2) | Te5—C17 | 2.1332 (16) |
| C1—C2 | 1.406 (2) | Te6—C18 | 2.1209 (17) |
| C3—C4 | 1.392 (3) | Te6—C22 | 2.1281 (17) |
| C3—H3 | 0.9500 | N9—C17 | 1.337 (2) |
| C4—H4 | 0.9500 | N9—C20 | 1.337 (3) |
| C5—C6 | 1.410 (2) | N10—C19 | 1.336 (2) |
| C7—C8 | 1.392 (3) | N10—C18 | 1.338 (2) |
| C7—H7 | 0.9500 | N11—C21 | 1.334 (2) |
| C8—H8 | 0.9500 | N11—C24 | 1.335 (2) |
| Te3—C13 | 2.1211 (17) | N12—C23 | 1.338 (2) |
| Te3—C9 | 2.1248 (17) | N12—C22 | 1.339 (2) |
| Te4—C10 | 2.1180 (16) | C17—C18 | 1.409 (2) |
| Te4—C14 | 2.1302 (16) | C19—C20 | 1.386 (3) |
| N5—C9 | 1.338 (2) | C19—H19 | 0.9500 |
| N5—C12 | 1.340 (2) | C20—H20 | 0.9500 |
| N6—C11 | 1.337 (2) | C21—C22 | 1.408 (2) |
| N6—C10 | 1.339 (2) | C23—C24 | 1.386 (3) |
| N7—C16 | 1.334 (2) | C23—H23 | 0.9500 |
| Bond                  | Length [Å] | Bond                  | Length [Å] | Bond                  | Length [Å] |
|----------------------|------------|----------------------|------------|----------------------|------------|
| N7—C13               | 1.340 (2)  | C24—H24              | 0.9500     |                      |            |
| C5—Te1—C1           | 92.54 (6)  | N5—C12—C11           | 121.60 (16)|                      |            |
| C2—Te2—C6           | 91.48 (6)  | N5—C12—H12           | 119.2      |                      |            |
| C4—N1—C1            | 117.64 (16)| C11—C12—H12          | 119.2      |                      |            |
| C2—N2—C3            | 117.78 (15)| N7—C13—C14           | 121.05 (15)|                      |            |
| C8—N3—C5            | 117.52 (15)| N7—C13—Te3           | 116.77 (12)|                      |            |
| C7—N4—C6            | 117.69 (15)| C14—C13—Te3          | 122.17 (12)|                      |            |
| N1—C1—C2            | 120.90 (16)| N8—C14—C13           | 121.25 (15)|                      |            |
| N1—C1—Te1           | 113.35 (12)| N8—C14—Te4           | 113.13 (12)|                      |            |
| C2—C1—Te1           | 125.74 (13)| C13—C14—Te4          | 125.59 (12)|                      |            |
| N2—C2—C1            | 120.98 (16)| N8—C15—C16           | 121.90 (16)|                      |            |
| N2—C2—Te2           | 117.13 (12)| N8—C15—H15           | 119.0      |                      |            |
| C1—C2—Te2           | 121.87 (12)| C16—C15—H15          | 119.0      |                      |            |
| N2—C3—C4            | 121.26 (17)| N7—C16—C15           | 121.76 (16)|                      |            |
| N2—C3—H3            | 119.4      | N7—C16—H16           | 119.1      |                      |            |
| C4—C3—H3            | 119.4      | C15—C16—H16          | 119.1      |                      |            |
| N1—C4—C3            | 121.43 (17)| C21—Te5—C17          | 93.44 (6)  |                      |            |
| N1—C4—H4            | 119.3      | C18—Te6—C22          | 93.72 (6)  |                      |            |
| C3—C4—H4            | 119.3      | C17—N9—C20           | 117.07 (16)|                      |            |
| N3—C5—C6            | 120.83 (15)| C19—N10—C18          | 117.32 (16)|                      |            |
| N3—C5—Te1           | 116.33 (12)| C21—N11—C24          | 117.52 (16)|                      |            |
| C6—C5—Te1           | 122.70 (12)| C23—N12—C22          | 117.19 (16)|                      |            |
| N4—C6—C5            | 120.95 (15)| N9—C17—C18           | 121.22 (15)|                      |            |
| N4—C6—Te2           | 114.60 (12)| N9—C17—Te5           | 113.16 (12)|                      |            |
| C5—C6—Te2           | 124.45 (12)| C18—C17—Te5          | 125.57 (12)|                      |            |
| N4—C7—C8            | 120.88 (16)| N10—C18—C17          | 120.98 (15)|                      |            |
| N4—C7—H7            | 119.6      | N10—C18—Te6          | 116.55 (12)|                      |            |
| C8—C7—H7            | 119.6      | C17—C18—Te6          | 122.48 (12)|                      |            |
| N3—C8—C7            | 121.98 (17)| N10—C19—C20          | 121.55 (17)|                      |            |
| N3—C8—H8            | 119.0      | N10—C19—H19          | 119.2      |                      |            |
| C7—C8—H8            | 119.0      | C20—C19—H19          | 119.2      |                      |            |
| C13—Te3—C9          | 93.30 (6)  | N9—C20—C19           | 121.84 (17)|                      |            |
| C10—Te4—C14         | 93.80 (6)  | N9—C20—H20           | 119.1      |                      |            |
| C9—N5—C12           | 117.13 (16)| C19—C20—H20          | 119.1      |                      |            |
| C11—N6—C10          | 117.26 (15)| N11—C21—C22          | 121.09 (15)|                      |            |
| C16—N7—C13          | 117.26 (15)| N11—C21—Te5          | 115.58 (12)|                      |            |
| C15—N8—C14          | 116.70 (16)| C22—C21—Te5          | 123.27 (12)|                      |            |
| N5—C9—C10           | 121.28 (16)| N12—C22—C21          | 120.99 (15)|                      |            |
| N5—C9—Te3           | 113.77 (12)| N12—C22—Te6          | 113.90 (12)|                      |            |
| C10—C9—Te3          | 124.94 (12)| C21—C22—Te6          | 125.11 (12)|                      |            |
| N6—C10—C9           | 121.09 (15)| N12—C23—C24          | 121.65 (16)|                      |            |
| N6—C10—Te4          | 115.90 (12)| N12—C23—H23          | 119.2      |                      |            |
| C9—C10—Te4          | 122.91 (12)| C24—C23—H23          | 119.2      |                      |            |
| N6—C11—C12          | 121.62 (16)| N11—C24—C23          | 121.50 (16)|                      |            |
| N6—C11—H11          | 119.2      | N11—C24—H24          | 119.3      |                      |            |
| C12—C11—H11         | 119.2      | C23—C24—H24          | 119.3      |                      |            |
C4—N1—C1—C2  0.5 (3)  
C4—N1—C1—Te1  −179.04 (14)  
C3—N2—C2—C1  −0.8 (3)  
C3—N2—C2—Te2  −179.06 (13)  
N1—C1—C2—N2  0.2 (3)  
Te1—C1—C2—N2  179.73 (13)  
N1—C1—C2—Te2  178.42 (13)  
Te1—C1—C2—Te2  −2.1 (2)  
C2—N2—C3—C4  0.6 (3)  
C1—N1—C4—C3  −0.7 (3)  
N2—C3—C4—N1  0.2 (3)  
C8—N3—C5—C6  1.3 (2)  
C8—N3—C5—Te1  −174.55 (13)  
C7—N4—C6—C5  2.7 (2)  
C7—N4—C6—Te2  −177.44 (13)  
N3—C5—C6—N4  −3.9 (3)  
Te1—C5—C6—N4  171.65 (12)  
N3—C5—C6—Te2  176.25 (12)  
Te1—C5—C6—Te2  −8.2 (2)  
C6—N4—C7—C8  0.8 (3)  
C5—N3—C8—C7  2.3 (3)  
N4—C7—C8—N3  −3.5 (3)  
C12—N5—C9—C10  −0.8 (2)  
C12—N5—C9—Te3  178.70 (13)  
C11—N6—C10—C9  1.4 (2)  
C11—N6—C10—Te4  −175.06 (12)  
N5—C9—C10—N6  −0.5 (3)  
Te3—C9—C10—N6  −179.93 (12)  
N5—C9—C10—Te4  175.68 (12)  
Te3—C9—C10—Te4  −3.8 (2)  
C10—N6—C11—C12  −1.0 (3)  
C9—N5—C12—C11  1.2 (3)  
N6—C11—C12—N5  −0.3 (3)  
C16—N7—C13—C14  −1.8 (2)  
C16—N7—C13—Te3  178.54 (13)  
C15—N8—C14—C13  −1.2 (3)  
C15—N8—C14—Te4  −179.44 (14)  
N7—C13—C14—N8  2.9 (3)  
Te3—C13—C14—N8  −177.51 (13)  
N7—C13—C14—Te4  −179.14 (12)  
Te3—C13—C14—Te4  0.5 (2)  
C14—N8—C15—C16  −1.3 (3)  
C13—N7—C16—C15  −0.7 (3)  
N8—C15—C16—N7  2.3 (3)  
C20—N9—C17—C18  1.5 (3)  
C20—N9—C17—Te5  −176.06 (14)  
C19—N10—C18—C17  −0.2 (3)  
C19—N10—C18—Te6  179.91 (14)  
N9—C17—C18—N10  −1.2 (3)  
Te5—C17—C18—N10  176.06 (13)  
N9—C17—C18—Te6  178.68 (13)  
Te5—C17—C18—Te6  −4.1 (2)  
C18—N10—C21—C22  2.7 (2)  
C18—N10—C21—Te5  −174.54 (13)  
C23—N12—C22—C21  −1.2 (2)  
C23—N12—C22—Te6  178.49 (12)  
N11—C21—C22—N12  −1.3 (2)  
Te5—C21—C22—N12  175.69 (12)  
C11—N12—C23—C24  2.2 (3)  
C11—N12—C23—Te6  −3.9 (2)  
C21—N11—C24—C23  −1.7 (3)  
N12—C23—C24—N11  −0.8 (3)