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# N-[6-(Dimethylamino)-9-phenyl-3H-telluroxanthene-3-ylidene]-N-methylmethanaminium hexafluorophosphate monoclinic polymorph<sup>1</sup>

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<sup>1</sup> This paper is dedicated to the late Professor Michael R. Detty.

‡ Both authors contributed equally to this work

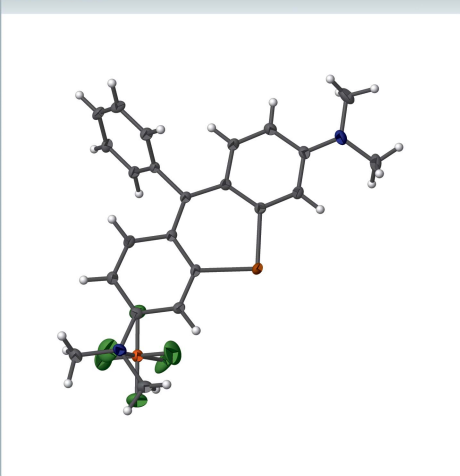
Keywords: xanthene; dye; rhodamine; telluroxanthene; crystal structure; polymorph.

CCDC reference: 2085596

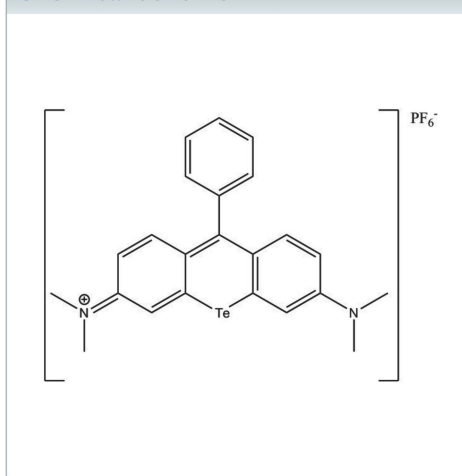
Structural data: full structural data are available from iucrdata.iucr.org

The title compound  $C_{23}H_{23}N_2Te^+ \cdot PF_6^-$ , is a monoclinic polymorph of the previously reported triclinic structure [Calitree *et al.* (2007). *Organometallics*, **26**, 6248–6257]. In the crystal, parallel offset  $\pi$ – $\pi$  stacking [shortest centroid–centroid separation = 3.9620 (9) Å] and ionic interactions help to establish the packing.

## 3D view



## Chemical scheme



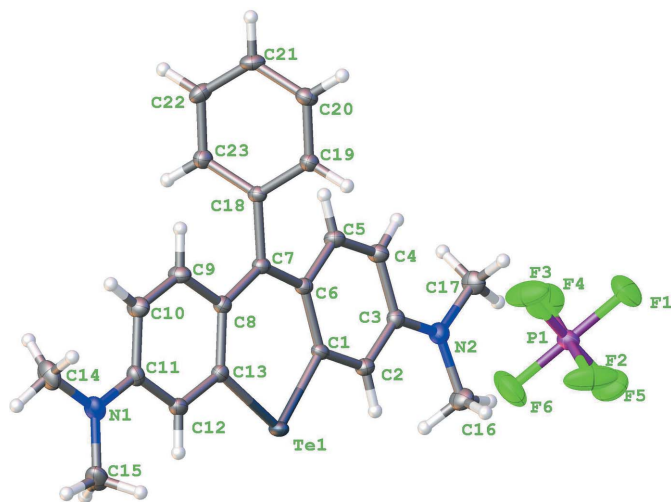
## Structure description

Chalcogen dyes with near-infrared absorption are used in the targeting of mitochondria of tumors (Detty *et al.*, 1990; Leonard *et al.*, 1999) and enhancing the sensitivity of medical imaging (Bedics *et al.*, 2015; Kryman *et al.*, 2016). The title compound crystallizes with a single  $C_{23}H_{23}N_2Te^+$  telluroxanthene cation and its  $PF_6^-$  counter-ion in the asymmetric unit (Fig. 1). The present monoclinic structure is a polymorph of the previously reported triclinic phase (Calitree *et al.*, 2007; Cambridge Structural Database refcode CIRPAV), which was recrystallized from the mixed solvents of acetonitrile and ether.

The mean plane of the pendant phenyl ring (C19–C23) is nearly orthogonal to the plane of the central telluroxanthene ring (C1/C6/C7/C8/C13/Te1), which subtends a dihedral angle of 70.40 (6)°. The amine bonds (C3–N2 and C11–N1) on either side of the nearly planar telluroxanthene core (r.m.s. deviation = 0.035 Å) are almost the same length [1.343 (3) and 1.347 (3) Å, respectively] indicating delocalization of the positive charge of the cation. The crystal packing is shown in Fig. 2. The telluroxanthene cations form centrosymmetric dimer pairs, which  $\pi$ -stack to form columns propagating parallel to [100]. Neighboring columns interact along [010] to form a herringbone pattern when viewed parallel to [001] (Fig. 3).



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**Figure 1**  
Asymmetric unit of the title compound with displacement ellipsoids drawn at 50%.

## Synthesis and crystallization

The synthesis of title compound was previously reported (Calitree *et al.*, 2007). The title compound was dissolved in a solution of ethanol and water (70/30) and recrystallized by slow evaporation to give metallic green prisms suitable for X-ray diffraction.

## Refinement

Crystal data, data collection, and refinement details are summarized in Table 1.

## Funding information

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## References

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**Table 1**

Experimental details.

|                                                                            |                                       |
|----------------------------------------------------------------------------|---------------------------------------|
| Crystal data                                                               |                                       |
| Chemical formula                                                           | $C_{23}H_{23}N_2Te^+ \cdot PF_6^-$    |
| $M_r$                                                                      | 600.00                                |
| Crystal system, space group                                                | Monoclinic, $P2_1/n$                  |
| Temperature (K)                                                            | 90                                    |
| $a, b, c$ (Å)                                                              | 8.7763 (6), 23.9606 (17), 10.8738 (8) |
| $\beta$ (°)                                                                | 99.256 (2)                            |
| $V$ (Å <sup>3</sup> )                                                      | 2256.8 (3)                            |
| $Z$                                                                        | 4                                     |
| Radiation type                                                             | Mo $K\alpha$                          |
| $\mu$ (mm <sup>-1</sup> )                                                  | 1.45                                  |
| Crystal size (mm)                                                          | 0.6 × 0.5 × 0.05                      |
| Data collection                                                            |                                       |
| Diffractometer                                                             | Bruker APEXII CCD                     |
| Absorption correction                                                      | Multi-scan (SADABS; Bruker, 2018)     |
| $T_{min}, T_{max}$                                                         | 0.689, 0.746                          |
| No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections | 56521, 8157, 6766                     |
| $R_{int}$                                                                  | 0.071                                 |
| $(\sin \theta/\lambda)_{max}$ (Å <sup>-1</sup> )                           | 0.767                                 |
| Refinement                                                                 |                                       |
| $R[F^2 > 2\sigma(F^2)], wR(F^2), S$                                        | 0.034, 0.078, 1.02                    |
| No. of reflections                                                         | 8157                                  |
| No. of parameters                                                          | 302                                   |
| H-atom treatment                                                           | H-atom parameters constrained         |
| $\Delta\rho_{max}, \Delta\rho_{min}$ (e Å <sup>-3</sup> )                  | 0.67, -0.59                           |

Computer programs: APEX3 and SAINT (Bruker, 2018), SHELXT2014/5 (Sheldrick, 2015a), SHELXL (Sheldrick, 2015b), and OLEX2 (Dolomanov *et al.*, 2009).

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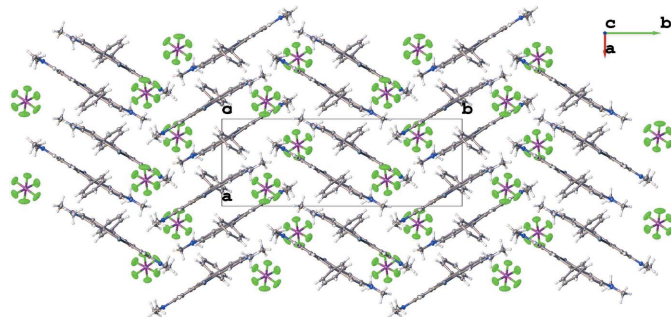
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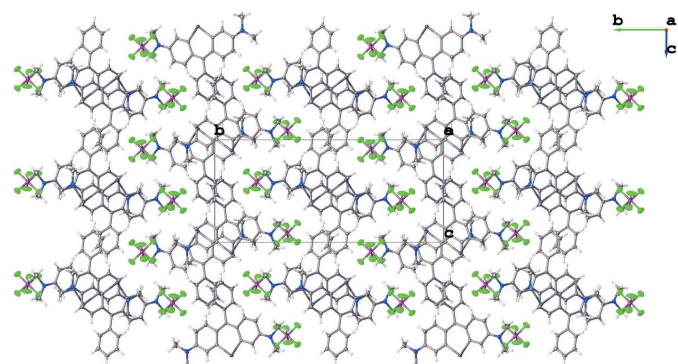
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**Figure 2**  
Crystal packing of the title compound viewed along [001].



**Figure 3**  
Crystal packing of the title compound viewed along [100].

## full crystallographic data

*IUCrData* (2021). 6, x210545 [https://doi.org/10.1107/S2414314621005459]

***N*-[6-(Dimethylamino)-9-phenyl-3*H*-telluroxanthen-3-ylidene]-*N*-methylmethanaminium hexafluorophosphate monoclinic polymorph**

Shea Myers, Patrick Johnson and Jason B. Benedict

*N*-[6-(Dimethylamino)-9-phenyl-3*H*-telluroxanthen-3-ylidene]-*N*-methylmethanaminium hexafluorophosphate

*Crystal data*

$C_{23}H_{23}N_2Te^+ \cdot PF_6^-$

$M_r = 600.00$

Monoclinic,  $P2_1/n$

$a = 8.7763$  (6) Å

$b = 23.9606$  (17) Å

$c = 10.8738$  (8) Å

$\beta = 99.256$  (2)°

$V = 2256.8$  (3) Å<sup>3</sup>

$Z = 4$

$F(000) = 1184$

$D_x = 1.766$  Mg m<sup>-3</sup>

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

Cell parameters from 9937 reflections

$\theta = 2.5$ – $30.3^\circ$

$\mu = 1.45$  mm<sup>-1</sup>

$T = 90$  K

Plate, metallic green

$0.6 \times 0.5 \times 0.05$  mm

*Data collection*

Bruker APEXII CCD  
diffractometer

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Bruker, 2018)

$T_{\min} = 0.689$ ,  $T_{\max} = 0.746$

56521 measured reflections

8157 independent reflections

6766 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.071$

$\theta_{\max} = 33.0^\circ$ ,  $\theta_{\min} = 1.7^\circ$

$h = -13 \rightarrow 12$

$k = -36 \rightarrow 36$

$l = -16 \rightarrow 16$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.078$

$S = 1.01$

8157 reflections

302 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0237P)^2 + 2.0434P]$

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

$(\Delta/\sigma)_{\max} = 0.005$

$\Delta\rho_{\max} = 0.67$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.59$  e Å<sup>-3</sup>

*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.

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

|      | <i>x</i>    | <i>y</i>     | <i>z</i>      | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|-------------|--------------|---------------|----------------------------------|
| Tel  | 0.37770 (2) | 0.57306 (2)  | 0.60576 (2)   | 0.01836 (4)                      |
| P1   | 0.20110 (7) | 0.81612 (2)  | 0.40997 (5)   | 0.02187 (11)                     |
| F3   | 0.1105 (2)  | 0.77039 (8)  | 0.32013 (17)  | 0.0596 (6)                       |
| F4   | 0.3481 (2)  | 0.80903 (9)  | 0.34268 (19)  | 0.0567 (5)                       |
| N2   | 0.6606 (2)  | 0.74434 (7)  | 0.42304 (17)  | 0.0210 (3)                       |
| F5   | 0.2897 (2)  | 0.86218 (8)  | 0.49805 (18)  | 0.0576 (5)                       |
| F2   | 0.0542 (2)  | 0.82231 (11) | 0.47618 (17)  | 0.0693 (7)                       |
| F1   | 0.1372 (3)  | 0.86213 (8)  | 0.30973 (18)  | 0.0595 (5)                       |
| F6   | 0.2649 (3)  | 0.77015 (8)  | 0.50973 (19)  | 0.0644 (6)                       |
| N1   | 0.0763 (2)  | 0.37834 (8)  | 0.56622 (18)  | 0.0248 (4)                       |
| C13  | 0.2664 (2)  | 0.50923 (8)  | 0.49838 (18)  | 0.0164 (3)                       |
| C7   | 0.3079 (2)  | 0.55013 (8)  | 0.29042 (18)  | 0.0156 (3)                       |
| C1   | 0.4416 (2)  | 0.61632 (8)  | 0.45709 (17)  | 0.0156 (3)                       |
| C6   | 0.4000 (2)  | 0.59734 (8)  | 0.33084 (18)  | 0.0155 (3)                       |
| C5   | 0.4606 (2)  | 0.63079 (8)  | 0.24046 (19)  | 0.0189 (4)                       |
| H5   | 0.441068    | 0.619248     | 0.155810      | 0.023*                           |
| C12  | 0.2101 (2)  | 0.46640 (8)  | 0.56335 (19)  | 0.0191 (4)                       |
| H12  | 0.225645    | 0.467975     | 0.651777      | 0.023*                           |
| C11  | 0.1301 (2)  | 0.42024 (8)  | 0.5026 (2)    | 0.0190 (4)                       |
| C19  | 0.1629 (2)  | 0.57900 (8)  | 0.08336 (19)  | 0.0188 (4)                       |
| H19  | 0.119627    | 0.608620     | 0.124457      | 0.023*                           |
| C18  | 0.2679 (2)  | 0.54247 (8)  | 0.15202 (17)  | 0.0154 (3)                       |
| C4   | 0.5441 (2)  | 0.67792 (9)  | 0.26909 (19)  | 0.0199 (4)                       |
| H4   | 0.580399    | 0.698301     | 0.204645      | 0.024*                           |
| C3   | 0.5786 (2)  | 0.69747 (8)  | 0.39471 (19)  | 0.0171 (4)                       |
| C9   | 0.1639 (2)  | 0.46274 (9)  | 0.30664 (19)  | 0.0207 (4)                       |
| H9   | 0.145827    | 0.461284     | 0.218177      | 0.025*                           |
| C8   | 0.2473 (2)  | 0.50933 (8)  | 0.36550 (18)  | 0.0163 (3)                       |
| C2   | 0.5249 (2)  | 0.66452 (8)  | 0.48724 (19)  | 0.0186 (4)                       |
| H2   | 0.546799    | 0.675927     | 0.571915      | 0.022*                           |
| C10  | 0.1088 (3)  | 0.42026 (9)  | 0.3704 (2)    | 0.0231 (4)                       |
| H10  | 0.055233    | 0.390205     | 0.325641      | 0.028*                           |
| C20  | 0.1214 (3)  | 0.57237 (9)  | −0.04422 (19) | 0.0212 (4)                       |
| H20  | 0.049254    | 0.597224     | −0.090058     | 0.025*                           |
| C23  | 0.3309 (2)  | 0.49957 (9)  | 0.08981 (19)  | 0.0195 (4)                       |
| H23  | 0.402725    | 0.474487     | 0.135230      | 0.023*                           |
| C22  | 0.2894 (3)  | 0.49323 (9)  | −0.0381 (2)   | 0.0229 (4)                       |
| H22  | 0.332861    | 0.463846     | −0.079840     | 0.027*                           |
| C17  | 0.7068 (3)  | 0.77967 (9)  | 0.3255 (2)    | 0.0259 (4)                       |
| H17A | 0.758035    | 0.756767     | 0.269628      | 0.039*                           |
| H17B | 0.778070    | 0.808576     | 0.363729      | 0.039*                           |
| H17C | 0.615117    | 0.797316     | 0.277811      | 0.039*                           |
| C16  | 0.6824 (3)  | 0.76688 (10) | 0.5492 (2)    | 0.0278 (5)                       |
| H16A | 0.582395    | 0.778526     | 0.569750      | 0.042*                           |
| H16B | 0.751810    | 0.799123     | 0.554501      | 0.042*                           |

|      |            |              |               |            |
|------|------------|--------------|---------------|------------|
| H16C | 0.727487   | 0.738145     | 0.608176      | 0.042*     |
| C21  | 0.1849 (3) | 0.52966 (9)  | −0.10492 (19) | 0.0224 (4) |
| H21  | 0.156722   | 0.525308     | −0.192469     | 0.027*     |
| C15  | 0.0866 (3) | 0.38130 (10) | 0.7010 (2)    | 0.0307 (5) |
| H15A | 0.195362   | 0.381323     | 0.739952      | 0.046*     |
| H15B | 0.034410   | 0.348939     | 0.730416      | 0.046*     |
| H15C | 0.036942   | 0.415640     | 0.723435      | 0.046*     |
| C14  | 0.0003 (3) | 0.32985 (10) | 0.5022 (3)    | 0.0327 (5) |
| H14A | −0.104010  | 0.340189     | 0.462121      | 0.049*     |
| H14B | −0.006029  | 0.299921     | 0.562561      | 0.049*     |
| H14C | 0.059824   | 0.316883     | 0.438780      | 0.049*     |

*Atomic displacement parameters ( $\text{\AA}^2$ )*

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Te1 | 0.02524 (7) | 0.01836 (7) | 0.01140 (6) | −0.00151 (5) | 0.00277 (5)  | 0.00012 (4)  |
| P1  | 0.0231 (3)  | 0.0232 (3)  | 0.0192 (3)  | −0.0027 (2)  | 0.0032 (2)   | 0.0013 (2)   |
| F3  | 0.0821 (14) | 0.0652 (12) | 0.0340 (9)  | −0.0458 (11) | 0.0166 (9)   | −0.0173 (9)  |
| F4  | 0.0367 (9)  | 0.0773 (14) | 0.0610 (12) | 0.0056 (9)   | 0.0226 (9)   | −0.0010 (10) |
| N2  | 0.0213 (8)  | 0.0186 (8)  | 0.0219 (9)  | −0.0039 (6)  | 0.0003 (7)   | −0.0002 (7)  |
| F5  | 0.0738 (13) | 0.0491 (11) | 0.0467 (11) | −0.0247 (10) | −0.0002 (10) | −0.0150 (9)  |
| F2  | 0.0339 (9)  | 0.146 (2)   | 0.0308 (9)  | −0.0007 (11) | 0.0147 (7)   | −0.0149 (11) |
| F1  | 0.0782 (14) | 0.0536 (11) | 0.0438 (10) | 0.0231 (10)  | 0.0010 (10)  | 0.0201 (9)   |
| F6  | 0.0841 (15) | 0.0490 (11) | 0.0559 (12) | 0.0037 (10)  | −0.0014 (11) | 0.0296 (9)   |
| N1  | 0.0276 (9)  | 0.0207 (8)  | 0.0274 (9)  | −0.0028 (7)  | 0.0082 (8)   | 0.0048 (7)   |
| C13 | 0.0176 (8)  | 0.0161 (8)  | 0.0159 (8)  | 0.0018 (7)   | 0.0036 (7)   | −0.0004 (7)  |
| C7  | 0.0162 (8)  | 0.0173 (8)  | 0.0130 (8)  | 0.0011 (7)   | 0.0015 (7)   | 0.0000 (7)   |
| C1  | 0.0171 (8)  | 0.0174 (8)  | 0.0123 (8)  | 0.0022 (7)   | 0.0026 (7)   | 0.0021 (6)   |
| C6  | 0.0154 (8)  | 0.0172 (8)  | 0.0136 (8)  | 0.0009 (7)   | 0.0016 (7)   | 0.0003 (7)   |
| C5  | 0.0201 (9)  | 0.0219 (9)  | 0.0150 (9)  | −0.0005 (7)  | 0.0041 (7)   | −0.0002 (7)  |
| C12 | 0.0235 (9)  | 0.0189 (9)  | 0.0156 (9)  | 0.0030 (7)   | 0.0052 (7)   | 0.0013 (7)   |
| C11 | 0.0198 (9)  | 0.0166 (9)  | 0.0211 (9)  | 0.0011 (7)   | 0.0050 (7)   | 0.0030 (7)   |
| C19 | 0.0217 (9)  | 0.0191 (9)  | 0.0157 (9)  | 0.0019 (7)   | 0.0030 (7)   | 0.0011 (7)   |
| C18 | 0.0169 (8)  | 0.0164 (8)  | 0.0130 (8)  | −0.0024 (7)  | 0.0024 (7)   | 0.0002 (6)   |
| C4  | 0.0212 (9)  | 0.0218 (9)  | 0.0166 (9)  | −0.0026 (7)  | 0.0032 (7)   | 0.0011 (7)   |
| C3  | 0.0156 (8)  | 0.0166 (8)  | 0.0186 (9)  | 0.0010 (7)   | 0.0016 (7)   | 0.0003 (7)   |
| C9  | 0.0233 (10) | 0.0236 (10) | 0.0146 (9)  | −0.0043 (8)  | 0.0010 (7)   | −0.0005 (7)  |
| C8  | 0.0167 (8)  | 0.0166 (8)  | 0.0155 (8)  | 0.0004 (7)   | 0.0019 (7)   | 0.0005 (7)   |
| C2  | 0.0223 (9)  | 0.0181 (9)  | 0.0149 (8)  | 0.0000 (7)   | 0.0018 (7)   | −0.0011 (7)  |
| C10 | 0.0268 (11) | 0.0212 (10) | 0.0209 (10) | −0.0062 (8)  | 0.0024 (8)   | −0.0010 (8)  |
| C20 | 0.0225 (10) | 0.0251 (10) | 0.0156 (9)  | 0.0014 (8)   | 0.0018 (7)   | 0.0031 (7)   |
| C23 | 0.0207 (9)  | 0.0198 (9)  | 0.0179 (9)  | 0.0024 (7)   | 0.0029 (7)   | 0.0000 (7)   |
| C22 | 0.0241 (10) | 0.0252 (10) | 0.0199 (10) | 0.0004 (8)   | 0.0052 (8)   | −0.0069 (8)  |
| C17 | 0.0277 (11) | 0.0231 (10) | 0.0272 (11) | −0.0077 (8)  | 0.0056 (9)   | 0.0013 (9)   |
| C16 | 0.0341 (12) | 0.0243 (10) | 0.0239 (11) | −0.0074 (9)  | 0.0012 (9)   | −0.0056 (8)  |
| C21 | 0.0242 (10) | 0.0304 (11) | 0.0125 (9)  | −0.0024 (8)  | 0.0022 (7)   | −0.0024 (8)  |
| C15 | 0.0397 (13) | 0.0275 (11) | 0.0291 (12) | 0.0046 (10)  | 0.0188 (10)  | 0.0083 (9)   |
| C14 | 0.0342 (12) | 0.0215 (10) | 0.0410 (14) | −0.0079 (9)  | 0.0015 (11)  | 0.0078 (10)  |

*Geometric parameters (Å, °)*

|            |             |             |             |
|------------|-------------|-------------|-------------|
| Te1—C13    | 2.0711 (19) | C19—C20     | 1.386 (3)   |
| Te1—C1     | 2.0723 (19) | C18—C23     | 1.393 (3)   |
| P1—F3      | 1.5930 (17) | C4—H4       | 0.9500      |
| P1—F4      | 1.5911 (18) | C4—C3       | 1.430 (3)   |
| P1—F5      | 1.5813 (17) | C3—C2       | 1.418 (3)   |
| P1—F2      | 1.5816 (18) | C9—H9       | 0.9500      |
| P1—F1      | 1.5877 (17) | C9—C8       | 1.429 (3)   |
| P1—F6      | 1.5838 (18) | C9—C10      | 1.363 (3)   |
| N2—C3      | 1.343 (3)   | C2—H2       | 0.9500      |
| N2—C17     | 1.464 (3)   | C10—H10     | 0.9500      |
| N2—C16     | 1.458 (3)   | C20—H20     | 0.9500      |
| N1—C11     | 1.347 (3)   | C20—C21     | 1.382 (3)   |
| N1—C15     | 1.456 (3)   | C23—H23     | 0.9500      |
| N1—C14     | 1.460 (3)   | C23—C22     | 1.388 (3)   |
| C13—C12    | 1.382 (3)   | C22—H22     | 0.9500      |
| C13—C8     | 1.428 (3)   | C22—C21     | 1.385 (3)   |
| C7—C6      | 1.419 (3)   | C17—H17A    | 0.9800      |
| C7—C18     | 1.501 (3)   | C17—H17B    | 0.9800      |
| C7—C8      | 1.430 (3)   | C17—H17C    | 0.9800      |
| C1—C6      | 1.436 (3)   | C16—H16A    | 0.9800      |
| C1—C2      | 1.378 (3)   | C16—H16B    | 0.9800      |
| C6—C5      | 1.435 (3)   | C16—H16C    | 0.9800      |
| C5—H5      | 0.9500      | C21—H21     | 0.9500      |
| C5—C4      | 1.355 (3)   | C15—H15A    | 0.9800      |
| C12—H12    | 0.9500      | C15—H15B    | 0.9800      |
| C12—C11    | 1.416 (3)   | C15—H15C    | 0.9800      |
| C11—C10    | 1.419 (3)   | C14—H14A    | 0.9800      |
| C19—H19    | 0.9500      | C14—H14B    | 0.9800      |
| C19—C18    | 1.397 (3)   | C14—H14C    | 0.9800      |
| C13—Te1—C1 | 95.27 (8)   | N2—C3—C4    | 121.10 (19) |
| F4—P1—F3   | 90.36 (11)  | N2—C3—C2    | 122.01 (18) |
| F5—P1—F3   | 179.21 (12) | C2—C3—C4    | 116.88 (18) |
| F5—P1—F4   | 89.82 (11)  | C8—C9—H9    | 118.2       |
| F5—P1—F2   | 90.94 (12)  | C10—C9—H9   | 118.2       |
| F5—P1—F1   | 90.93 (11)  | C10—C9—C8   | 123.63 (19) |
| F5—P1—F6   | 89.14 (11)  | C13—C8—C7   | 125.81 (18) |
| F2—P1—F3   | 88.88 (11)  | C13—C8—C9   | 114.86 (17) |
| F2—P1—F4   | 179.18 (13) | C9—C8—C7    | 119.29 (18) |
| F2—P1—F1   | 91.36 (12)  | C1—C2—C3    | 121.47 (18) |
| F2—P1—F6   | 88.73 (12)  | C1—C2—H2    | 119.3       |
| F1—P1—F3   | 88.30 (12)  | C3—C2—H2    | 119.3       |
| F1—P1—F4   | 88.93 (11)  | C11—C10—H10 | 119.5       |
| F6—P1—F3   | 91.63 (12)  | C9—C10—C11  | 121.0 (2)   |
| F6—P1—F4   | 90.98 (12)  | C9—C10—H10  | 119.5       |
| F6—P1—F1   | 179.88 (14) | C19—C20—H20 | 119.9       |

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| C3—N2—C17       | 121.19 (18)  | C21—C20—C19     | 120.11 (19)  |
| C3—N2—C16       | 120.66 (18)  | C21—C20—H20     | 119.9        |
| C16—N2—C17      | 117.25 (17)  | C18—C23—H23     | 119.8        |
| C11—N1—C15      | 120.73 (19)  | C22—C23—C18     | 120.46 (19)  |
| C11—N1—C14      | 121.3 (2)    | C22—C23—H23     | 119.8        |
| C15—N1—C14      | 117.96 (19)  | C23—C22—H22     | 120.0        |
| C12—C13—Te1     | 115.80 (14)  | C21—C22—C23     | 120.09 (19)  |
| C12—C13—C8      | 121.69 (18)  | C21—C22—H22     | 120.0        |
| C8—C13—Te1      | 122.50 (14)  | N2—C17—H17A     | 109.5        |
| C6—C7—C18       | 115.97 (16)  | N2—C17—H17B     | 109.5        |
| C6—C7—C8        | 127.88 (18)  | N2—C17—H17C     | 109.5        |
| C8—C7—C18       | 116.15 (17)  | H17A—C17—H17B   | 109.5        |
| C6—C1—Te1       | 121.88 (14)  | H17A—C17—H17C   | 109.5        |
| C2—C1—Te1       | 115.68 (14)  | H17B—C17—H17C   | 109.5        |
| C2—C1—C6        | 122.44 (18)  | N2—C16—H16A     | 109.5        |
| C7—C6—C1        | 126.39 (17)  | N2—C16—H16B     | 109.5        |
| C7—C6—C5        | 119.26 (17)  | N2—C16—H16C     | 109.5        |
| C5—C6—C1        | 114.35 (17)  | H16A—C16—H16B   | 109.5        |
| C6—C5—H5        | 118.2        | H16A—C16—H16C   | 109.5        |
| C4—C5—C6        | 123.68 (19)  | H16B—C16—H16C   | 109.5        |
| C4—C5—H5        | 118.2        | C20—C21—C22     | 120.00 (19)  |
| C13—C12—H12     | 118.9        | C20—C21—H21     | 120.0        |
| C13—C12—C11     | 122.21 (19)  | C22—C21—H21     | 120.0        |
| C11—C12—H12     | 118.9        | N1—C15—H15A     | 109.5        |
| N1—C11—C12      | 122.1 (2)    | N1—C15—H15B     | 109.5        |
| N1—C11—C10      | 121.37 (19)  | N1—C15—H15C     | 109.5        |
| C12—C11—C10     | 116.57 (18)  | H15A—C15—H15B   | 109.5        |
| C18—C19—H19     | 119.7        | H15A—C15—H15C   | 109.5        |
| C20—C19—H19     | 119.7        | H15B—C15—H15C   | 109.5        |
| C20—C19—C18     | 120.53 (19)  | N1—C14—H14A     | 109.5        |
| C19—C18—C7      | 119.16 (17)  | N1—C14—H14B     | 109.5        |
| C23—C18—C7      | 122.02 (17)  | N1—C14—H14C     | 109.5        |
| C23—C18—C19     | 118.82 (18)  | H14A—C14—H14B   | 109.5        |
| C5—C4—H4        | 119.5        | H14A—C14—H14C   | 109.5        |
| C5—C4—C3        | 121.07 (19)  | H14B—C14—H14C   | 109.5        |
| C3—C4—H4        | 119.5        |                 |              |
| Te1—C13—C12—C11 | 179.33 (15)  | C18—C7—C6—C5    | −6.0 (3)     |
| Te1—C13—C8—C7   | 3.9 (3)      | C18—C7—C8—C13   | −177.95 (18) |
| Te1—C13—C8—C9   | −178.28 (14) | C18—C7—C8—C9    | 4.3 (3)      |
| Te1—C1—C6—C7    | 3.0 (3)      | C18—C19—C20—C21 | −0.5 (3)     |
| Te1—C1—C6—C5    | −176.93 (13) | C18—C23—C22—C21 | 0.0 (3)      |
| Te1—C1—C2—C3    | 178.68 (15)  | C4—C3—C2—C1     | −0.9 (3)     |
| N2—C3—C2—C1     | −179.61 (19) | C8—C13—C12—C11  | −0.2 (3)     |
| N1—C11—C10—C9   | −179.8 (2)   | C8—C7—C6—C1     | −5.3 (3)     |
| C13—C12—C11—N1  | 179.5 (2)    | C8—C7—C6—C5     | 174.64 (19)  |
| C13—C12—C11—C10 | −0.6 (3)     | C8—C7—C18—C19   | 108.2 (2)    |
| C7—C6—C5—C4     | 177.11 (19)  | C8—C7—C18—C23   | −71.0 (2)    |

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| C7—C18—C23—C22  | 179.00 (19)  | C8—C9—C10—C11   | 0.8 (3)      |
| C1—C6—C5—C4     | −3.0 (3)     | C2—C1—C6—C7     | −176.38 (19) |
| C6—C7—C18—C19   | −71.2 (2)    | C2—C1—C6—C5     | 3.7 (3)      |
| C6—C7—C18—C23   | 109.6 (2)    | C10—C9—C8—C13   | −1.5 (3)     |
| C6—C7—C8—C13    | 1.4 (3)      | C10—C9—C8—C7    | 176.5 (2)    |
| C6—C7—C8—C9     | −176.38 (19) | C20—C19—C18—C7  | −178.77 (19) |
| C6—C1—C2—C3     | −1.9 (3)     | C20—C19—C18—C23 | 0.5 (3)      |
| C6—C5—C4—C3     | 0.4 (3)      | C23—C22—C21—C20 | −0.1 (3)     |
| C5—C4—C3—N2     | −179.61 (19) | C17—N2—C3—C4    | 5.2 (3)      |
| C5—C4—C3—C2     | 1.6 (3)      | C17—N2—C3—C2    | −176.13 (19) |
| C12—C13—C8—C7   | −176.66 (19) | C16—N2—C3—C4    | 174.0 (2)    |
| C12—C13—C8—C9   | 1.2 (3)      | C16—N2—C3—C2    | −7.3 (3)     |
| C12—C11—C10—C9  | 0.3 (3)      | C15—N1—C11—C12  | 5.5 (3)      |
| C19—C18—C23—C22 | −0.2 (3)     | C15—N1—C11—C10  | −174.4 (2)   |
| C19—C20—C21—C22 | 0.4 (3)      | C14—N1—C11—C12  | −177.2 (2)   |
| C18—C7—C6—C1    | 174.05 (18)  | C14—N1—C11—C10  | 3.0 (3)      |

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