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A square-planar tellurium(II) complex with Te, Te' -chelating ligands

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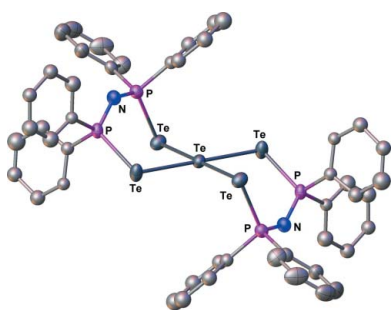
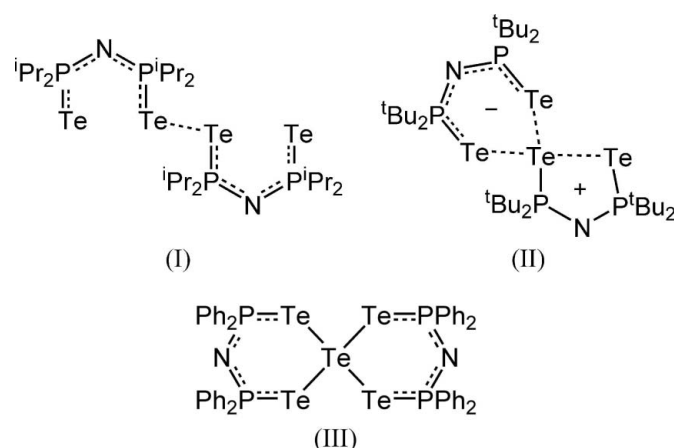
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While exploring the chemistry of tellurium-containing dichalcogenidoimido-diphosphinate ligands, the first all-tellurium member of a series of related square-planar $E^{II}(E')_4$ complexes (E and E' are group 16 elements), namely bis(P, P, P', P' -tetraphenylditelluridoimidodiphosphinato- $\kappa^2 Te, Te'$)tellurium(II) (systematic name: 2,2,4,4,8,8,10,10-octaphenyl-1 $\lambda^3, 5, 6\lambda^4, 7\lambda^3, 11$ -pentatellura-3,9-diaza-2 $\lambda^5, 4\lambda^5, 8\lambda^5, 10\lambda^5$ -tetraphosphaspiro[5.5]undeca-1,3,7,9-tetraene), $C_{48}H_{40}N_2P_4Te_5$, was obtained unexpectedly. The formally Te^{II} centre is situated on a crystallographic inversion centre and is Te, Te' -chelated to two anionic $[(TePPh_2)_2N]^-$ ligands in an *anti* conformation. The central $Te^{II}(Te)_4$ unit is approximately square planar [$Te-Te-Te = 93.51(3)$ and $86.49(3)^\circ$], with $Te-Te$ bond lengths of 2.9806 (6) and 2.9978 (9) Å.

1. Introduction

Dichalcogenidoimidodiphosphinates, $[(EPR_2)_2N]^-$ ($E = O, S, Se, Te; R = \text{alkyl, aryl}$), are versatile ligands that can coordinate to elements from the main group (Silvestru & Drake, 2001), *d*-block (Ly & Woollins, 1998) and *f*-block (Glover *et al.*, 2007). These species can be viewed as flexible inorganic analogues of planar β -diketonate ligands, and many derivatives are known owing to the varying identities possible for the chalcogen and the organic substituents on phosphorus. In keeping with this versatility, these ligands have demonstrated a wealth of different coordination modes and solid-state structures in combination with metal atoms.



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We have been exploring the chemistry of the rarer tellurium-containing ligands since reporting a route to the synthesis of their sodium salts (Briand *et al.*, 2002). In addition to studying their coordination chemistry (Chivers *et al.*, 2010), the one-electron chemical oxidation of these anions with

Table 1
 Experimental details.

Crystal data	
Chemical formula	$C_{48}H_{40}N_2P_4Te_5$
M_r	1406.70
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, b, c (Å)	11.021 (2), 14.950 (3), 15.893 (3)
β (°)	113.47 (3)
V (Å ³)	2402.2 (10)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	3.17
Crystal size (mm)	0.02 × 0.02 × 0.02
Data collection	
Diffractometer	Nonius KappaCCD diffractometer
Absorption correction	Integration (SCALEPACK; Otwinowski & Minor, 1997)
T_{min}, T_{max}	0.939, 0.939
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8246, 4216, 3159
R_{int}	0.033
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.034, 0.083, 1.08
No. of reflections	4216
No. of parameters	253
No. of restraints	12
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.60, -0.71

Computer programs: COLLECT (Nonius, 2001), DENZO (Otwinowski & Minor, 1997), SHELXS97 (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015) and OLEX2 (Dolomanov *et al.*, 2009).

iodine was pursued in the context of forming ditelluride dimers. The isopropyl-substituted ligand forms a symmetric dimer, (I) (see Scheme), with an unusually long Te—Te distance (Chivers *et al.*, 2005), while the *tert*-butyl analogue forms an asymmetric dimer, (II) (Ritch *et al.*, 2007), resembling a contact ion pair between a cation and an anion. In this work, an unexpected product, obtained by the oxidation of the phenyl-substituted ligand [(TePPh₂)₂N][−] is reported, namely bis(*P,P,P',P'*-tetraphenylditelluridoimidodiphosphinato- κ^2 Te,Te')tellurium(II), Te[(TePPh₂)₂N]₂, (III) (Fig. 1).

2. Experimental

2.1. Synthesis and crystallization

To a solution of Na(tmeda)[(TePPh₂)₂N] (tmeda is tetramethylethylenediamine; 285 mg, 0.366 mmol) in tetrahydrofuran (THF) at 195 K was added a solution of one-half molar equivalent of I₂ (45 mg, 0.177 mmol) in THF at 195 K. The resulting mixture was stirred cold for 30 min and then warmed to room temperature for an additional 30 min. The volatiles were removed under vacuum and the residual material was extracted with toluene and filtered through a 0.45 μm pore size PTFE filter disk. Removal of the volatiles afforded a red solid (60 mg), which was shown to be a complicated mixture of phosphorus-containing compounds (ten resonances in the ³¹P NMR spectrum). A few X-ray-quality red block-like crystals of Te[(TePPh₂)₂N]₂, (III), were obtained from a THF solution

layered with *n*-hexane and stored at 278 K. All solvents were dried (THF and toluene with sodium/benzophenone, and *n*-hexane with sodium), distilled and stored over 4 Å molecular sieves prior to use, and all manipulations were conducted under argon using a glove-box or Schlenk line.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Three of the four phenyl rings in the asymmetric unit exhibit positional disorder and were modelled as isotropic mixtures over two positions. The occupancy factors for the disordered atoms were determined by free variable refinement and yielded values of *ca* 0.5. The planarity of the half-occupancy phenyl rings was maintained by the application of restraints on the geometric parameters. H atoms were placed in calculated positions, with C—H = 0.95 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, and treated with a riding-model approximation.

3. Results and discussion

The complex mixture obtained in the oxidation of the phenyl-substituted ditelluridoimidodiphosphinate anion is in contrast to the alkyl-substituted derivatives ($R = {}^i$ Pr, ^tBu), for which the corresponding reactions with iodine were quite clean (Chivers *et al.*, 2005; Ritch *et al.*, 2007). The red crystals obtained from this mixture possess a molecular spirocyclic square-planar Te^{II}(Te)₄ motif (Fig. 2), of which only a few examples are known.

Some extended structures exhibit square-planar Te₅ units, such as the anions in the previously reported salt [NMe₄]₂[As₂Te₅], which contains alternating Te₅^{6−} and As₂⁴⁺ groups in one-dimensional chains (Warren *et al.*, 1994). A spirocyclic

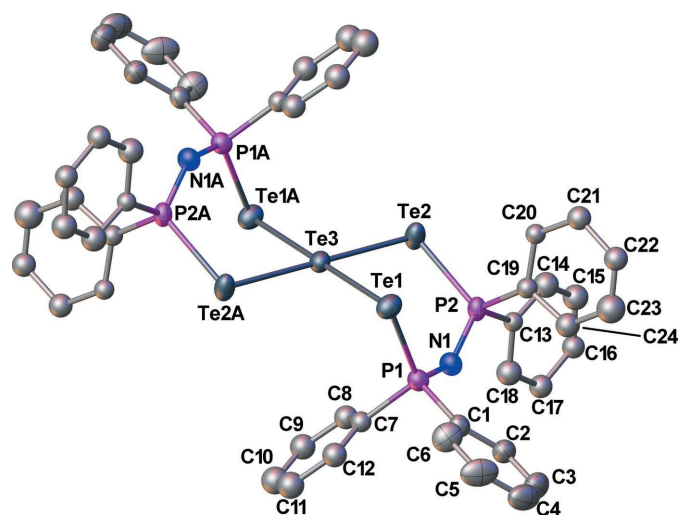


Figure 1
 Displacement ellipsoid plot (50% probability level) of the structure of (III). H atoms have been omitted for clarity and spheres indicate isotropic C atoms from one orientation of the disordered phenyl rings. Symmetry-equivalent atoms are related by an inversion centre at Te3. [Symmetry code: (A) $-x + 2, -y + 1, -z$.]

Te_8^{2-} anion is seen in the structure of $[\text{K}(\text{18-crown-5})_2]_2[\text{Te}_8]$ (Schreiner *et al.*, 1993). More recently, the Te_5 unit was observed in $[\text{Na}(\text{tmeda})_2][\text{tBuN}(\text{Te})\text{P}(\mu\text{-N}^t\text{Bu})_2\text{P}(\text{Te})\text{N}^t\text{Bu}]_2\text{-}\mu_4\text{-Te}]$, (IV) (tmrdheider *et al.*, 2015), which can be described as a Te^{2+} cation bound by two *Te,Te'*-chelating dianionic ligands. In this structure, the Te–Te distances range from 3.014 (2) to 3.027 (2) Å and, while the Te_5 unit is planar, the *cis*-Te–Te–Te bond angles range from 74.47 (4) to 105.61 (5)°.

The title compound, (III), features slightly shorter bond lengths, with Te1–Te3 and Te2–Te3 distances of 2.9806 (6) and 2.9978 (9) Å, respectively, which are still significantly longer than the distances observed in organic ditellurides [*e.g.* 2.712 (2) Å in Ph_2Te_2 ; Llabres *et al.*, 1972]. The geometry in (III) is also much closer to ideal square planar; the two unique *cis*-Te–Te–Te bond angles are 93.51 (3) and 86.49 (3)°. Compared to the dianionic ligands in (IV), which feature rigid P_2N_2 rings, the $[(\text{TePPh}_2)_2\text{N}]^-$ ligands in (III) are considerably more flexible, as can be seen from the Te–P–N–P torsion angles [–9.3 (5) and 67.9 (4)°]. This flexibility may be the reason the geometry of the $\text{Te}(\text{Te})_4$ core in (III) is closer to ideal square planar than that in (IV).

The bonding parameters of the $[(\text{TePPh}_2)_2\text{N}]^-$ ligands are indicative of delocalization of π -electron density within the TePNPTe fragment. The P–Te distances of 2.4278 (16) and 2.4331 (15) Å are equal within experimental error, and are significantly longer than a formal P=Te double bond, *e.g.* a distance of 2.3798 (8) Å is observed in the monotelluridoimidodiphosphinate, $\text{TeP}^i\text{Pr}_2\text{NP}(\text{H})^i\text{Pr}_2$ (Chivers *et al.*, 2005). The P–N–P bond angle of (III) is 134.1 (3)° and the interatomic P–N distances of 1.593 (5) and 1.594 (5) Å are shorter than the formally single P–N bonds observed in the diselenoimidodiphosphinate ($\text{SePPh}_2)_2\text{NH}$ [1.678 (4) and 1.686 (3) Å; Bhattacharyya *et al.*, 1995]. Together, these data suggest partial multiple-bond character throughout the ligand backbone, which is consistent with other structures containing $[(\text{EPR})_2\text{N}]^-$ anions ($E = \text{O}, \text{S}, \text{Se}, \text{Te}$; $R = \text{alkyl}, \text{aryl}$).

Square-planar $\text{Te}(\text{E})_4$ ($E = \text{S}, \text{Se}$) complexes involving dichalcogenoimidodiphosphinates have been observed previously [*e.g.* TeS_4 (Bjørnrvåg *et al.*, 1982; Birdsall *et al.*, 2000; Necas *et al.*, 2001), TeSe_4 (Novosad *et al.*, 1998; Birdsall *et al.*, 2000) and TeS_2Se_2 (Sekar & Ibers, 2003)], however, compound (III) is the first example of a $\text{Te}^{\text{II}}(\text{Te})_4$ imidodiphosphinate complex. Similar to the previously reported complexes, the

two ligands in (III) are in an *anti* conformation with respect to each other.

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Computing details

Data collection: *COLLECT* (Nonius, 2001); cell refinement: *DENZO* (Nonius, 2001); data reduction: *DENZO* (Nonius, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

2,2,4,4,8,8,10,10-Octaphenyl-1 λ^3 ,5,6 λ^4 ,7 λ^3 ,11-pentatellura-3,9-diaza-2 λ^5 ,4 λ^5 ,8 λ^5 ,10 λ^5 -tetraphoshaspiro[5.5]undeca-1,3,7,9-tetraene

Crystal data

C₄₈H₄₀N₂P₄Te₅

$M_r = 1406.70$

Monoclinic, $P2_1/c$

$a = 11.021$ (2) Å

$b = 14.950$ (3) Å

$c = 15.893$ (3) Å

$\beta = 113.47$ (3)°

$V = 2402.2$ (10) Å³

$Z = 2$

$F(000) = 1324$

$D_x = 1.945$ Mg m⁻³

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

Cell parameters from 41094 reflections

$\theta = 2.7$ – 25.0 °

$\mu = 3.17$ mm⁻¹

$T = 173$ K

Block, red

$0.02 \times 0.02 \times 0.02$ mm

Data collection

Nonius KappaCCD
diffractometer

Graphite monochromator

φ and ω scans

Absorption correction: integration

(*SCALEPACK*; Otwinowski & Minor, 1997)

$T_{\min} = 0.939$, $T_{\max} = 0.939$

8246 measured reflections

4216 independent reflections

3159 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\max} = 25.0$ °, $\theta_{\min} = 2.7$ °

$h = -13 \rightarrow 13$

$k = -17 \rightarrow 17$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

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

$wR(F^2) = 0.083$

$S = 1.08$

4216 reflections

253 parameters

12 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0334P)^2 + 3.8459P]$

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

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.60$ e Å⁻³

$\Delta\rho_{\min} = -0.71$ e Å⁻³

Special details

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

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Te1	1.04321 (4)	0.36828 (3)	0.15000 (3)	0.04004 (13)	
Te2	1.26616 (4)	0.58511 (3)	0.09597 (3)	0.04165 (13)	
Te3	1.0000	0.5000	0.0000	0.03290 (14)	
P1	1.05091 (14)	0.48895 (9)	0.25423 (10)	0.0310 (3)	
P2	1.29607 (13)	0.56634 (9)	0.25510 (9)	0.0302 (3)	
N1	1.1666 (4)	0.5605 (3)	0.2763 (3)	0.0344 (11)	
C1	1.0619 (5)	0.4377 (4)	0.3609 (4)	0.0324 (13)	
C2	1.1378 (6)	0.4791 (4)	0.4437 (4)	0.0431 (15)	
H2	1.1827	0.5334	0.4439	0.052*	
C3	1.1476 (7)	0.4415 (5)	0.5252 (5)	0.0582 (19)	
H3	1.2020	0.4691	0.5814	0.070*	
C4	1.0799 (8)	0.3644 (5)	0.5263 (5)	0.062 (2)	
H4	1.0859	0.3397	0.5829	0.074*	
C5	1.0031 (8)	0.3234 (4)	0.4444 (5)	0.060 (2)	
H5	0.9566	0.2699	0.4447	0.072*	
C6	0.9936 (7)	0.3599 (4)	0.3621 (5)	0.0515 (17)	
H6	0.9401	0.3316	0.3060	0.062*	
C7	0.898 (2)	0.5566 (13)	0.2135 (9)	0.028 (7)*	0.507 (13)
C8	0.9012 (13)	0.6397 (8)	0.1819 (8)	0.036 (3)*	0.507 (13)
H8	0.9815	0.6634	0.1823	0.044*	0.507 (13)
C9	0.7878 (12)	0.6901 (9)	0.1490 (8)	0.042 (3)*	0.507 (13)
H9	0.7900	0.7486	0.1263	0.050*	0.507 (13)
C10	0.6738 (18)	0.6578 (12)	0.1483 (9)	0.050 (5)*	0.507 (13)
H10	0.5960	0.6934	0.1259	0.059*	0.507 (13)
C11	0.6700 (13)	0.5693 (9)	0.1816 (9)	0.047 (4)*	0.507 (13)
H11	0.5898	0.5457	0.1813	0.056*	0.507 (13)
C12	0.7852 (11)	0.5183 (8)	0.2144 (8)	0.039 (3)*	0.507 (13)
H12	0.7858	0.4592	0.2366	0.046*	0.507 (13)
C7A	0.897 (2)	0.5446 (15)	0.2063 (10)	0.026 (7)*	0.493 (13)
C8A	0.8894 (14)	0.6383 (9)	0.2152 (9)	0.044 (4)*	0.493 (13)
H8A	0.9684	0.6718	0.2447	0.052*	0.493 (13)
C9A	0.7678 (15)	0.6824 (10)	0.1812 (9)	0.050 (4)*	0.493 (13)
H9A	0.7643	0.7454	0.1872	0.060*	0.493 (13)
C10A	0.6512 (16)	0.6335 (11)	0.1383 (9)	0.037 (4)*	0.493 (13)
H10A	0.5681	0.6631	0.1165	0.044*	0.493 (13)
C11A	0.6563 (12)	0.5465 (8)	0.1282 (8)	0.040 (3)*	0.493 (13)
H11A	0.5770	0.5138	0.0972	0.048*	0.493 (13)
C12A	0.7759 (11)	0.5025 (8)	0.1621 (8)	0.035 (3)*	0.493 (13)
H12A	0.7754	0.4394	0.1549	0.042*	0.493 (13)

C13	1.3903 (19)	0.6627 (12)	0.3096 (12)	0.025 (6)*	0.47 (4)
C14	1.5141 (16)	0.6797 (11)	0.3150 (16)	0.043 (5)*	0.47 (4)
H14	1.5523	0.6401	0.2857	0.051*	0.47 (4)
C15	1.5863 (16)	0.7525 (10)	0.3617 (15)	0.042 (5)*	0.47 (4)
H15	1.6723	0.7626	0.3632	0.051*	0.47 (4)
C16	1.5365 (19)	0.8087 (11)	0.4047 (10)	0.033 (5)*	0.47 (4)
H16	1.5892	0.8571	0.4386	0.040*	0.47 (4)
C17	1.412 (2)	0.7985 (10)	0.4014 (10)	0.035 (4)*	0.47 (4)
H17	1.3763	0.8393	0.4314	0.042*	0.47 (4)
C18	1.336 (2)	0.7235 (16)	0.3506 (15)	0.042 (7)*	0.47 (4)
H18	1.2477	0.7155	0.3452	0.050*	0.47 (4)
C13A	1.3736 (17)	0.6690 (12)	0.3191 (12)	0.027 (5)*	0.53 (4)
C14A	1.5115 (14)	0.6797 (10)	0.3414 (13)	0.038 (4)*	0.53 (4)
H14A	1.5595	0.6363	0.3234	0.046*	0.53 (4)
C15A	1.5741 (15)	0.7563 (10)	0.3906 (13)	0.042 (4)*	0.53 (4)
H15A	1.6660	0.7654	0.4072	0.051*	0.53 (4)
C16A	1.499 (2)	0.8196 (10)	0.4153 (10)	0.037 (4)*	0.53 (4)
H16A	1.5396	0.8723	0.4475	0.045*	0.53 (4)
C17A	1.365 (2)	0.8045 (9)	0.3923 (9)	0.038 (4)*	0.53 (4)
H17A	1.3135	0.8470	0.4085	0.046*	0.53 (4)
C18A	1.308 (2)	0.7299 (11)	0.3472 (12)	0.031 (5)*	0.53 (4)
H18A	1.2173	0.7194	0.3344	0.037*	0.53 (4)
C19	1.4013 (15)	0.4821 (11)	0.3088 (12)	0.028 (6)*	0.478 (19)
C20	1.4711 (12)	0.4284 (8)	0.2699 (8)	0.026 (3)*	0.478 (19)
H20	1.4557	0.4380	0.2073	0.031*	0.478 (19)
C21	1.5617 (14)	0.3617 (9)	0.3181 (9)	0.037 (4)*	0.478 (19)
H21	1.6077	0.3277	0.2897	0.044*	0.478 (19)
C22	1.5817 (15)	0.3474 (10)	0.4103 (11)	0.037 (5)*	0.478 (19)
H22	1.6396	0.3009	0.4440	0.044*	0.478 (19)
C23	1.5227 (14)	0.3964 (11)	0.4504 (13)	0.054 (4)*	0.478 (19)
H23	1.5422	0.3870	0.5136	0.065*	0.478 (19)
C24	1.4321 (12)	0.4618 (10)	0.4031 (10)	0.038 (4)*	0.478 (19)
H24	1.3887	0.4943	0.4344	0.046*	0.478 (19)
C19A	1.4201 (15)	0.4712 (9)	0.3069 (10)	0.026 (5)*	0.522 (19)
C20A	1.5171 (14)	0.4543 (9)	0.2756 (8)	0.042 (3)*	0.522 (19)
H20A	1.5204	0.4853	0.2244	0.051*	0.522 (19)
C21A	1.6107 (15)	0.3895 (9)	0.3224 (8)	0.046 (4)*	0.522 (19)
H21A	1.6786	0.3754	0.3020	0.055*	0.522 (19)
C22A	1.6070 (15)	0.3472 (9)	0.3946 (9)	0.036 (4)*	0.522 (19)
H22A	1.6743	0.3052	0.4263	0.044*	0.522 (19)
C23A	1.5020 (14)	0.3639 (10)	0.4264 (10)	0.046 (4)*	0.522 (19)
H23A	1.4973	0.3316	0.4765	0.055*	0.522 (19)
C24A	1.4088 (13)	0.4290 (9)	0.3805 (9)	0.041 (3)*	0.522 (19)
H24A	1.3396	0.4439	0.3994	0.049*	0.522 (19)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Te1	0.0506 (3)	0.0344 (2)	0.0348 (2)	0.00087 (18)	0.01672 (19)	-0.00028 (17)
Te2	0.0320 (2)	0.0580 (3)	0.0303 (2)	-0.00880 (18)	0.00750 (17)	0.00862 (18)
Te3	0.0310 (3)	0.0380 (3)	0.0280 (3)	0.0006 (2)	0.0099 (2)	-0.0024 (2)
P1	0.0284 (8)	0.0322 (8)	0.0328 (8)	-0.0008 (6)	0.0126 (6)	0.0018 (6)
P2	0.0248 (7)	0.0330 (8)	0.0279 (7)	-0.0034 (6)	0.0053 (6)	0.0040 (6)
N1	0.030 (2)	0.036 (3)	0.037 (3)	-0.005 (2)	0.013 (2)	-0.001 (2)
C1	0.028 (3)	0.035 (3)	0.033 (3)	0.004 (2)	0.012 (2)	0.007 (3)
C2	0.038 (3)	0.058 (4)	0.034 (3)	0.004 (3)	0.015 (3)	0.004 (3)
C3	0.055 (4)	0.082 (5)	0.036 (4)	0.013 (4)	0.017 (3)	0.011 (4)
C4	0.077 (5)	0.069 (5)	0.052 (5)	0.027 (4)	0.038 (4)	0.025 (4)
C5	0.094 (6)	0.037 (4)	0.070 (5)	0.005 (4)	0.054 (5)	0.018 (4)
C6	0.065 (4)	0.038 (4)	0.054 (4)	-0.005 (3)	0.026 (4)	0.004 (3)

Geometric parameters (\AA , $^\circ$)

Te1—Te3	2.9806 (6)	C11A—C12A	1.376 (16)
Te1—P1	2.4278 (16)	C12A—H12A	0.9500
Te2—Te3	2.9978 (9)	C13—C14	1.36 (2)
Te2—P2	2.4331 (15)	C13—C18	1.39 (3)
Te3—Te1 ⁱ	2.9806 (6)	C14—H14	0.9500
Te3—Te2 ⁱ	2.9979 (9)	C14—C15	1.38 (2)
P1—N1	1.593 (5)	C15—H15	0.9500
P1—C1	1.820 (6)	C15—C16	1.33 (2)
P1—C7	1.85 (2)	C16—H16	0.9500
P1—C7A	1.77 (2)	C16—C17	1.36 (2)
P2—N1	1.594 (5)	C17—H17	0.9500
P2—C13	1.786 (18)	C17—C18	1.44 (3)
P2—C13A	1.851 (17)	C18—H18	0.9500
P2—C19	1.695 (19)	C13A—C14A	1.43 (2)
P2—C19A	1.917 (17)	C13A—C18A	1.34 (3)
C1—C2	1.392 (8)	C14A—H14A	0.9500
C1—C6	1.390 (8)	C14A—C15A	1.40 (2)
C2—H2	0.9500	C15A—H15A	0.9500
C2—C3	1.376 (9)	C15A—C16A	1.41 (2)
C3—H3	0.9500	C16A—H16A	0.9500
C3—C4	1.377 (10)	C16A—C17A	1.39 (2)
C4—H4	0.9500	C17A—H17A	0.9500
C4—C5	1.382 (10)	C17A—C18A	1.34 (2)
C5—H5	0.9500	C18A—H18A	0.9500
C5—C6	1.383 (9)	C19—C20	1.41 (2)
C6—H6	0.9500	C19—C24	1.43 (2)
C7—C8	1.35 (2)	C20—H20	0.9500
C7—C12	1.38 (2)	C20—C21	1.402 (16)
C8—H8	0.9500	C21—H21	0.9500
C8—C9	1.372 (17)	C21—C22	1.41 (2)

C9—H9	0.9500	C22—H22	0.9500
C9—C10	1.34 (2)	C22—C23	1.30 (2)
C10—H10	0.9500	C23—H23	0.9500
C10—C11	1.43 (2)	C23—C24	1.39 (2)
C11—H11	0.9500	C24—H24	0.9500
C11—C12	1.393 (17)	C19A—C20A	1.37 (2)
C12—H12	0.9500	C19A—C24A	1.38 (2)
C7A—C8A	1.41 (3)	C20A—H20A	0.9500
C7A—C12A	1.39 (2)	C20A—C21A	1.394 (17)
C8A—H8A	0.9500	C21A—H21A	0.9500
C8A—C9A	1.40 (2)	C21A—C22A	1.33 (2)
C9A—H9A	0.9500	C22A—H22A	0.9500
C9A—C10A	1.40 (2)	C22A—C23A	1.46 (2)
C10A—H10A	0.9500	C23A—H23A	0.9500
C10A—C11A	1.31 (2)	C23A—C24A	1.392 (18)
C11A—H11A	0.9500	C24A—H24A	0.9500
P1—Te1—Te3	90.34 (4)	C10A—C11A—C12A	120.4 (13)
P2—Te2—Te3	100.37 (4)	C12A—C11A—H11A	119.8
Te1—Te3—Te1 ⁱ	180.0	C7A—C12A—H12A	118.0
Te1—Te3—Te2	93.51 (3)	C11A—C12A—C7A	124.0 (13)
Te1—Te3—Te2 ⁱ	86.49 (3)	C11A—C12A—H12A	118.0
Te1 ⁱ —Te3—Te2	86.49 (3)	C14—C13—P2	123.9 (14)
Te1 ⁱ —Te3—Te2 ⁱ	93.51 (3)	C14—C13—C18	117.3 (17)
Te2—Te3—Te2 ⁱ	180.0	C18—C13—P2	118.7 (15)
N1—P1—Te1	117.19 (18)	C13—C14—H14	118.9
N1—P1—C1	109.1 (3)	C13—C14—C15	122.3 (17)
N1—P1—C7	104.3 (6)	C15—C14—H14	118.9
N1—P1—C7A	109.0 (7)	C14—C15—H15	119.8
C1—P1—Te1	107.11 (19)	C16—C15—C14	120.4 (15)
C1—P1—C7	105.7 (5)	C16—C15—H15	119.8
C7—P1—Te1	112.9 (4)	C15—C16—H16	119.2
C7A—P1—Te1	106.8 (6)	C15—C16—C17	121.7 (15)
C7A—P1—C1	107.3 (5)	C17—C16—H16	119.2
N1—P2—Te2	117.66 (18)	C16—C17—H17	121.3
N1—P2—C13	109.8 (7)	C16—C17—C18	117.4 (16)
N1—P2—C13A	100.7 (7)	C18—C17—H17	121.3
N1—P2—C19	110.1 (6)	C13—C18—C17	120.8 (18)
N1—P2—C19A	114.4 (5)	C13—C18—H18	119.6
C13—P2—Te2	102.9 (6)	C17—C18—H18	119.6
C13A—P2—Te2	108.5 (5)	C14A—C13A—P2	116.3 (13)
C13A—P2—C19A	106.6 (6)	C18A—C13A—P2	123.5 (13)
C19—P2—Te2	113.1 (7)	C18A—C13A—C14A	120.2 (17)
C19—P2—C13	101.9 (7)	C13A—C14A—H14A	121.0
C19A—P2—Te2	108.1 (5)	C15A—C14A—C13A	118.0 (14)
P1—N1—P2	134.1 (3)	C15A—C14A—H14A	121.0
C2—C1—P1	119.0 (4)	C14A—C15A—H15A	120.4
C6—C1—P1	122.0 (5)	C14A—C15A—C16A	119.3 (13)

C6—C1—C2	118.9 (5)	C16A—C15A—H15A	120.4
C1—C2—H2	120.0	C15A—C16A—H16A	120.1
C3—C2—C1	120.0 (6)	C17A—C16A—C15A	119.9 (13)
C3—C2—H2	120.0	C17A—C16A—H16A	120.1
C2—C3—H3	119.5	C16A—C17A—H17A	120.2
C2—C3—C4	120.9 (7)	C18A—C17A—C16A	119.6 (15)
C4—C3—H3	119.5	C18A—C17A—H17A	120.2
C3—C4—H4	120.3	C13A—C18A—H18A	118.5
C3—C4—C5	119.5 (6)	C17A—C18A—C13A	123.0 (17)
C5—C4—H4	120.3	C17A—C18A—H18A	118.5
C4—C5—H5	119.9	C20—C19—P2	125.7 (13)
C4—C5—C6	120.1 (7)	C20—C19—C24	113.2 (15)
C6—C5—H5	119.9	C24—C19—P2	121.0 (14)
C1—C6—H6	119.8	C19—C20—H20	118.1
C5—C6—C1	120.5 (6)	C21—C20—C19	123.9 (12)
C5—C6—H6	119.8	C21—C20—H20	118.1
C8—C7—P1	118.9 (15)	C20—C21—H21	121.3
C8—C7—C12	123.1 (18)	C20—C21—C22	117.4 (12)
C12—C7—P1	118.1 (13)	C22—C21—H21	121.3
C7—C8—H8	120.2	C21—C22—H22	119.3
C7—C8—C9	119.7 (15)	C23—C22—C21	121.4 (15)
C9—C8—H8	120.2	C23—C22—H22	119.3
C8—C9—H9	119.5	C22—C23—H23	119.2
C10—C9—C8	120.9 (14)	C22—C23—C24	121.6 (16)
C10—C9—H9	119.5	C24—C23—H23	119.2
C9—C10—H10	120.2	C19—C24—H24	118.8
C9—C10—C11	119.6 (15)	C23—C24—C19	122.5 (15)
C11—C10—H10	120.2	C23—C24—H24	118.8
C10—C11—H11	120.4	C20A—C19A—P2	120.4 (12)
C12—C11—C10	119.3 (13)	C20A—C19A—C24A	124.9 (15)
C12—C11—H11	120.4	C24A—C19A—P2	114.5 (12)
C7—C12—C11	117.5 (13)	C19A—C20A—H20A	121.6
C7—C12—H12	121.3	C19A—C20A—C21A	116.9 (13)
C11—C12—H12	121.3	C21A—C20A—H20A	121.6
C8A—C7A—P1	120.6 (15)	C20A—C21A—H21A	119.3
C12A—C7A—P1	124.7 (15)	C22A—C21A—C20A	121.5 (14)
C12A—C7A—C8A	114.6 (17)	C22A—C21A—H21A	119.3
C7A—C8A—H8A	119.5	C21A—C22A—H22A	119.3
C9A—C8A—C7A	121.1 (15)	C21A—C22A—C23A	121.5 (13)
C9A—C8A—H8A	119.5	C23A—C22A—H22A	119.3
C8A—C9A—H9A	120.1	C22A—C23A—H23A	121.3
C8A—C9A—C10A	119.8 (13)	C24A—C23A—C22A	117.3 (12)
C10A—C9A—H9A	120.1	C24A—C23A—H23A	121.3
C9A—C10A—H10A	120.0	C19A—C24A—C23A	117.9 (13)
C11A—C10A—C9A	120.1 (14)	C19A—C24A—H24A	121.1
C11A—C10A—H10A	120.0	C23A—C24A—H24A	121.1
C10A—C11A—H11A	119.8		

Te1—P1—N1—P2	-9.3 (5)	C7—P1—C1—C2	-95.2 (7)
Te1—P1—C1—C2	144.2 (4)	C7—P1—C1—C6	82.8 (8)
Te1—P1—C1—C6	-37.9 (5)	C7—C8—C9—C10	0.4 (6)
Te1—P1—C7—C8	-107.5 (7)	C8—C7—C12—C11	-0.7 (11)
Te1—P1—C7—C12	70.5 (8)	C8—C9—C10—C11	-0.6 (11)
Te1—P1—C7A—C8A	-144.4 (7)	C9—C10—C11—C12	0.2 (14)
Te1—P1—C7A—C12A	38.9 (10)	C10—C11—C12—C7	0.4 (13)
Te2—P2—N1—P1	67.9 (4)	C12—C7—C8—C9	0.3 (6)
Te2—P2—C13—C14	-63.3 (17)	C7A—P1—N1—P2	-130.7 (6)
Te2—P2—C13—C18	118.0 (15)	C7A—P1—C1—C2	-101.4 (9)
Te2—P2—C13A—C14A	-76.0 (12)	C7A—P1—C1—C6	76.5 (9)
Te2—P2—C13A—C18A	106.4 (15)	C7A—C8A—C9A—C10A	0.5 (5)
Te2—P2—C19—C20	2.3 (9)	C8A—C7A—C12A—C11A	0.5 (11)
Te2—P2—C19—C24	179.3 (7)	C8A—C9A—C10A—C11A	-1.5 (11)
P1—C1—C2—C3	-179.9 (5)	C9A—C10A—C11A—C12A	2.0 (14)
P1—C1—C6—C5	-179.2 (5)	C10A—C11A—C12A—C7A	-1.6 (14)
P1—C7—C8—C9	178.2 (8)	C12A—C7A—C8A—C9A	0.0 (5)
P1—C7—C12—C11	-178.6 (8)	C13—P2—N1—P1	-175.0 (7)
P1—C7A—C8A—C9A	-177.1 (9)	C13—P2—C19—C20	-107.4 (11)
P1—C7A—C12A—C11A	177.4 (9)	C13—P2—C19—C24	69.6 (11)
P2—C13—C14—C15	-176.6 (13)	C13—C14—C15—C16	1 (3)
P2—C13—C18—C17	175.2 (14)	C14—C13—C18—C17	-4 (3)
P2—C13A—C14A—C15A	-179.4 (11)	C14—C15—C16—C17	-3 (2)
P2—C13A—C18A—C17A	-179.0 (13)	C15—C16—C17—C18	1 (2)
P2—C19—C20—C21	177.1 (9)	C16—C17—C18—C13	2 (3)
P2—C19—C24—C23	-176.7 (9)	C18—C13—C14—C15	2 (3)
P2—C19A—C20A—C21A	174.3 (7)	C13A—P2—N1—P1	-174.5 (6)
P2—C19A—C24A—C23A	-175.1 (8)	C13A—C14A—C15A—C16A	-1 (2)
N1—P1—C1—C2	16.4 (5)	C14A—C13A—C18A—C17A	4 (2)
N1—P1—C1—C6	-165.6 (5)	C14A—C15A—C16A—C17A	1 (2)
N1—P1—C7—C8	20.8 (7)	C15A—C16A—C17A—C18A	0 (2)
N1—P1—C7—C12	-161.2 (7)	C16A—C17A—C18A—C13A	-3 (2)
N1—P1—C7A—C8A	-16.9 (8)	C18A—C13A—C14A—C15A	-2 (2)
N1—P1—C7A—C12A	166.4 (8)	C19—P2—N1—P1	-63.6 (7)
N1—P2—C13—C14	170.6 (15)	C19—P2—C13—C14	54.0 (18)
N1—P2—C13—C18	-8.0 (17)	C19—P2—C13—C18	-124.7 (16)
N1—P2—C13A—C14A	159.8 (11)	C19—C20—C21—C22	1.0 (5)
N1—P2—C13A—C18A	-17.7 (15)	C20—C19—C24—C23	0.7 (11)
N1—P2—C19—C20	136.2 (8)	C20—C21—C22—C23	-2.7 (12)
N1—P2—C19—C24	-46.8 (9)	C21—C22—C23—C24	3.5 (16)
C1—P1—N1—P2	112.5 (4)	C22—C23—C24—C19	-2.4 (15)
C1—P1—C7—C8	135.7 (6)	C24—C19—C20—C21	-0.1 (5)
C1—P1—C7—C12	-46.3 (8)	C19A—P2—N1—P1	-60.7 (6)
C1—P1—C7A—C8A	101.1 (8)	C19A—P2—C13A—C14A	40.1 (14)
C1—P1—C7A—C12A	-75.7 (10)	C19A—P2—C13A—C18A	-137.4 (14)
C1—C2—C3—C4	-2.1 (10)	C19A—C20A—C21A—C22A	-1.0 (5)
C2—C1—C6—C5	-1.3 (9)	C20A—C19A—C24A—C23A	-0.5 (11)
C2—C3—C4—C5	1.3 (11)	C20A—C21A—C22A—C23A	2.5 (11)

C3—C4—C5—C6	-0.5 (11)	C21A—C22A—C23A—C24A	-2.9 (13)
C4—C5—C6—C1	0.5 (11)	C22A—C23A—C24A—C19A	1.8 (12)
C6—C1—C2—C3	2.1 (9)	C24A—C19A—C20A—C21A	0.0 (5)
C7—P1—N1—P2	-134.9 (5)		

Symmetry code: (i) $-x+2, -y+1, -z$.