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## Structure Reports

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## 1-Methyl-1-azonia-3,5-diaza-7-phosphatricyclo[3.3.1.1]decane 7-oxide triiodide

Alexander M. Kirillov,<sup>a</sup> Piotr Smoleński,<sup>a</sup> M. Fátima C. Guedes da Silva<sup>a,b,\*</sup> and Armando J. L. Pombeiro<sup>a</sup><sup>a</sup>Centro de Química Estrutural, Complexo Interdisciplinar, Instituto Superior Técnico, TU Lisbon, Avenida Rovisco Pais, 1049-001 Lisbon, Portugal, and <sup>b</sup>Universidade Lusófona de Humanidades e Tecnologias, ULHT Lisbon, Avenida do Campo Grande 376, 1749-024 Lisbon, Portugal

Correspondence e-mail: fatima.guedes@ist.utl.pt

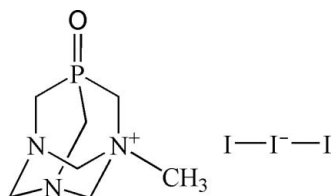
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Key indicators: single-crystal X-ray study;  $T = 150$  K; mean  $\sigma(\text{N}-\text{C}) = 0.009$  Å; some non-H atoms missing;  $R$  factor = 0.042;  $wR$  factor = 0.103; data-to-parameter ratio = 16.2.

The title compound,  $\text{C}_7\text{H}_{15}\text{N}_3\text{OP}^+\cdot\text{I}_3^-$ , is a derivative of the well known water-soluble aminophosphine 1,3,5-triaza-7-phosphaadamantane (PTA). The crystal structure is composed of a cage-like 1-methyl-1-azonia-3,5-diaza-7-phosphatricyclo[3.3.1.1]decane 7-oxide cation and a triiodide anion. The  $N$ -methylation of the PTA cage results in a slight elongation of the corresponding C–N bonds, while the oxidation of the P atom leads to a slight shortening of the C–P bonds in comparison with those of PTA. In general, most of the bonding parameters are comparable with those reported for related compounds bearing the PTA core. Two intermolecular C–H $\cdots$ O hydrogen bonds between methylene groups and the P=O group are responsible for the linkage of neighbouring cations into linear one-dimensional hydrogen-bonded chains.

## Related literature

For a comprehensive review of PTA chemistry, see: Phillips *et al.* (2004). For general background, see: Kirillov *et al.* (2007); Smoleński & Pombeiro (2008). For synthesis of PTA and its  $N$ -methylated derivative, see: Daigle *et al.* (1974); Daigle (1998). For related structures, see: Forward *et al.* (1996a,b); Otto *et al.* (2005); Frost *et al.* (2006); Marsh *et al.* (2002).



## Experimental

## Crystal data

$\text{C}_7\text{H}_{15}\text{N}_3\text{OP}^+\cdot\text{I}_3^-$   
 $M_r = 568.89$   
 Monoclinic,  $P2_1/n$   
 $a = 7.1570$  (8) Å  
 $b = 8.2257$  (8) Å  
 $c = 25.903$  (3) Å  
 $\beta = 92.472$  (7)°

$V = 1523.5$  (3) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 6.24$  mm<sup>-1</sup>  
 $T = 150$  (2) K  
 $0.13 \times 0.10 \times 0.10$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.497$ ,  $T_{\max} = 0.574$   
 (expected range = 0.464–0.536)

11526 measured reflections  
 2789 independent reflections  
 2214 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.040$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.102$   
 $S = 1.12$   
 2789 reflections  
 172 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 2.44$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -1.03$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

C1–N1	1.479 (8)	C12–N2	1.467 (10)
C1–P1	1.821 (8)	C23–N2	1.440 (9)
C2–N2	1.486 (8)	C23–N3	1.550 (9)
C2–P1	1.799 (7)	C31–N1	1.441 (9)
C3–N3	1.495 (9)	C31–N3	1.551 (9)
C3–P1	1.825 (8)	O1–P1	1.483 (5)
C4–N3	1.496 (9)	I1–I3	2.9067 (8)
C12–N1	1.462 (9)	I1–I2	2.9127 (7)
I3–I1–I2	172.41 (2)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C23–H23A $\cdots$ O1 <sup>1</sup>	0.99 (10)	2.26 (11)	3.161 (9)	150 (9)
C31–H31A $\cdots$ O1 <sup>1</sup>	0.97 (10)	2.23 (10)	3.160 (9)	161 (8)

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

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: WinGX (Version 1.70.01; Farrugia, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: Mercury (Macrae *et al.*, 2006); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2159).

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## supporting information

*Acta Cryst.* (2008). E64, o496–o497 [doi:10.1107/S1600536808001426]

## 1-Methyl-1-azonia-3,5-diaza-7-phosphatricyclo[3.3.1.1]decane 7-oxide triiodide

Alexander M. Kirillov, Piotr Smoleński, M. Fátima C. Guedes da Silva and Armando J. L. Pombeiro

### S1. Comment

Within our ongoing research (Kirillov *et al.*, 2007; Smoleński & Pombeiro, 2008) on the synthesis of transition metal complexes with PTA or derived ligands, we have attempted the reaction of a copper<sup>(II)</sup> salt with *N*-methyl-1,3,5-triaza-7-phospha-adamantane iodide, which resulted in the formation of the title compound, (I), as a by-product. Its crystal structure is reported herein.

The molecular structure of (I) (Fig. 1) bears a cage-like cation  $[C_7H_{15}N_3OP]^+$  and a tri-iodide anion, with the shortest cation⋯anion separation of *ca* 4.0 Å. The *N*-methylation of the PTA cage results in a slight elongation of the C—N bonds around N3 atom [*avg.* 1.53 (1) Å] in comparison with the C—N bonds around N1 and N2 atoms [*avg.* 1.46 (1) Å] (Table 1). The oxidation of P1 atom also slightly affects the C—P bonds [*avg.* 1.82 (1) Å] which are somewhat shorter than those in PTA [*avg.* 1.86 (1) Å]. The tri-iodide anion with the I2—I1—I3 angle of 172.41 (2)° deviates from the linear geometry. In general, most of the bonding parameters of (I) agree within values reported for the related compound,  $[C_7H_{15}N_3OP][BPh_4]$  (Forward *et al.*, 1996a,b), possessing similar cation, as well as for other *N*-alkylated (Otto *et al.*, 2005; Forward *et al.*, 1996a,b) or *P*-oxidized (Frost *et al.*, 2006; Marsh *et al.*, 2002) PTA derivatives.

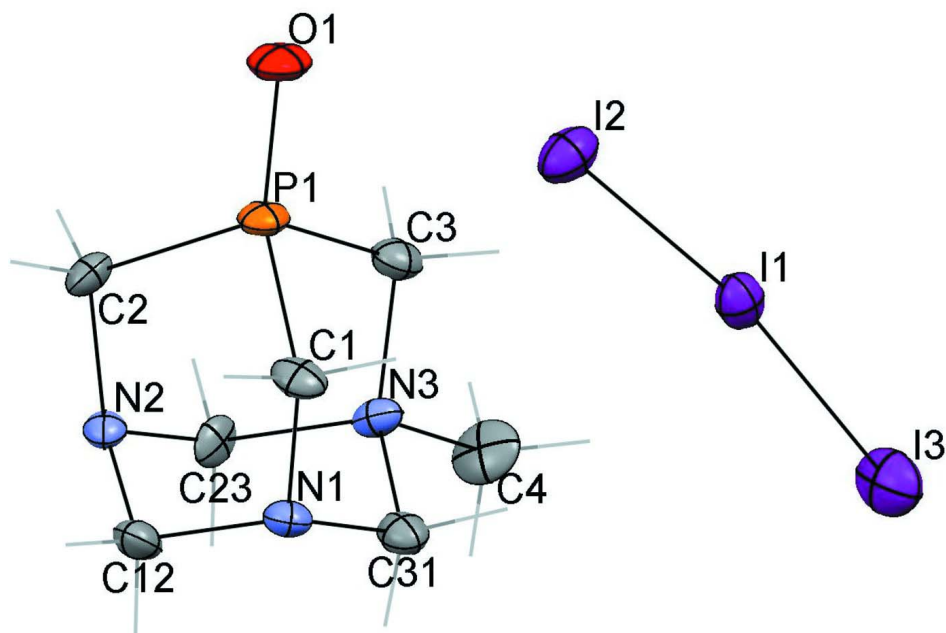
In (I), the neighbouring cationic units are combined into the linear one-dimensional H-bonded chains (Fig. 2) by means of two intermolecular C—H⋯O hydrogen bonds [C23—H23A⋯O1<sup>i</sup> 1.00 (11) Å, 2.26 (11) Å, 3.161 (9) Å, 150 (9)°; C31—H31A⋯O1<sup>i</sup> 0.97 (10) Å, 2.23 (10) Å, 3.160 (9) Å, 161 (8)°; symmetry code: 1 + *x*, *y*, *z*], which link the methylene groups (C23, C31) with the O1 atom of the P=O moiety.

### S2. Experimental

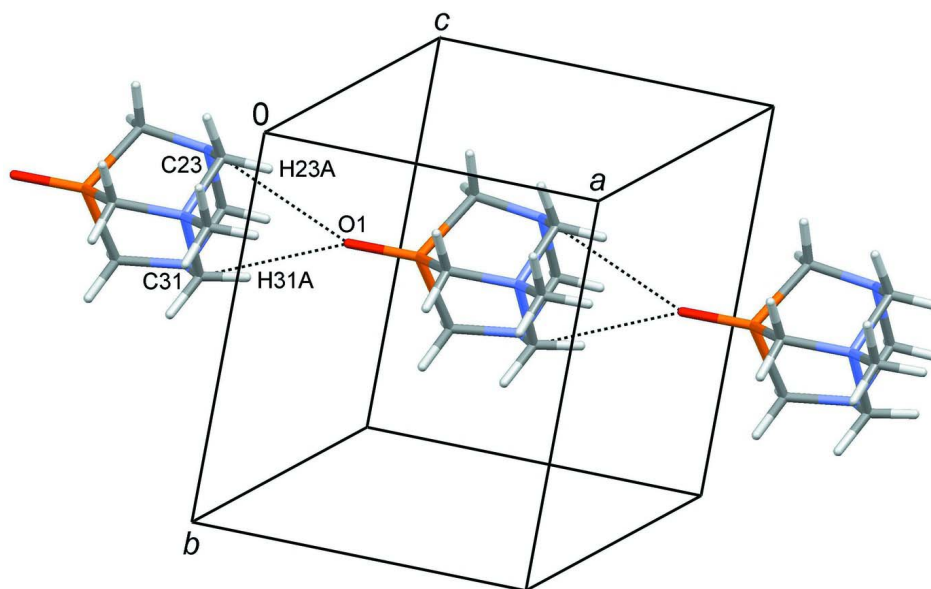
The aqueous solutions (5 ml each) of  $Cu(NO_3)_2 \cdot 2.5 H_2O$  (116 mg, 0.50 mmol) and *N*-methyl-1,3,5-triaza-7-phosphaadamantane iodide,  $[C_7H_{15}N_3P]I$  (299 mg, 1.00 mmol) [for the synthesis of this compound, see: Daigle *et al.* (1974); Daigle (1998)], were combined and left stirring in air at ambient temperature for 1 h. The resulting white suspension containing mainly a Cu<sup>I</sup> aminophosphine compound was filtered off. The colourless filtrate was left to evaporate in a beaker in air for two weeks, leading to the formation of a small crop of red X-ray quality crystals of compound (I) as a by-product (it is typically contaminated by a colourless crystalline material). FT–IR (KBr pellet),  $cm^{-1}$ : 2967 w, 2939 w, 1449 m, 1384 s, 1304 m, 1279 w, 1246 w, 1195 s [ $\nu(P=O)$ ], 1108 w, 1091 w, 1066 w, 1019 m, 983 m, 934 m, 900 w, 876 w, 816 m, 792 w, 752 m, 544 w, 441 w, 408 w. FAB-MS<sup>+</sup> (*m*-nitrobenzylalcohol), *m/z*: 188  $[C_7H_{15}N_3OP]^+$ .

### S3. Refinement

All hydrogen atoms were located except from H4A, H4B and H4C which were inserted in calculated positions.

**Figure 1**

The molecular structure of the title compound with the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as grey sticks. C, grey; N, blue; P, orange; O, red; I, purple.

**Figure 2**

Fragment of the crystal packing diagram of (I) showing the generation of a one-dimensional linear chain from the neighbouring cations *via* intermolecular C—H...O hydrogen bonds (dotted lines). Tri-iodide anions are omitted for clarity. C, grey; N, blue; P, orange; O, red; H, pale grey.

## 1-Methyl-1-azonia-3,5-diaza-7-phosphatricyclo[3.3.1.1]decane 7-oxide triiodide

## Crystal data

$C_7H_{15}N_3OP^+I_3^-$   
 $M_r = 568.89$   
 Monoclinic,  $P2_1/n$   
 Hall symbol:  $-P2_1n$   
 $a = 7.1570$  (8) Å  
 $b = 8.2257$  (8) Å  
 $c = 25.903$  (3) Å  
 $\beta = 92.472$  (7)°  
 $V = 1523.5$  (3) Å<sup>3</sup>  
 $Z = 4$

$F(000) = 1040$   
 $D_x = 2.480$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation,  $\lambda = 0.71069$  Å  
 Cell parameters from 2835 reflections  
 $\theta = 2.6$ – $27.9$ °  
 $\mu = 6.24$  mm<sup>-1</sup>  
 $T = 150$  K  
 Plate, red  
 $0.13 \times 0.10 \times 0.10$  mm

## Data collection

Bruker SMART CCD area-detector  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.497$ ,  $T_{\max} = 0.574$

11526 measured reflections  
 2789 independent reflections  
 2214 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.040$   
 $\theta_{\max} = 25.4$ °,  $\theta_{\min} = 2.9$ °  
 $h = -8 \rightarrow 8$   
 $k = -9 \rightarrow 9$   
 $l = -29 \rightarrow 31$

## Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.102$   
 $S = 1.12$   
 2789 reflections  
 172 parameters  
 0 restraints  
 0 constraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 6.2243P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.017$   
 $\Delta\rho_{\max} = 2.44$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -1.03$  e Å<sup>-3</sup>

## 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.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.5522 (9)	0.4541 (10)	0.1979 (3)	0.0186 (16)
C2	0.5510 (9)	0.1132 (8)	0.1974 (3)	0.0156 (15)
C3	0.5535 (10)	0.2823 (10)	0.1042 (3)	0.0188 (15)
C4	0.8586 (11)	0.2823 (11)	0.0631 (3)	0.0294 (18)

H4A	0.9942	0.2819	0.0701	0.044*
H4B	0.8230	0.3796	0.0432	0.044*
H4C	0.8222	0.1851	0.0432	0.044*
C12	0.8197 (10)	0.2815 (10)	0.2227 (3)	0.0192 (15)
C23	0.8255 (10)	0.1301 (8)	0.1442 (3)	0.0162 (15)
C31	0.8255 (10)	0.4347 (10)	0.1446 (3)	0.0192 (16)
N1	0.7565 (7)	0.4292 (7)	0.1960 (2)	0.0169 (13)
N2	0.7569 (7)	0.1334 (7)	0.1956 (2)	0.0141 (12)
N3	0.7614 (8)	0.2828 (7)	0.1131 (2)	0.0168 (12)
O1	0.2300 (7)	0.2825 (7)	0.1582 (2)	0.0268 (12)
P1	0.4367 (2)	0.2827 (2)	0.16547 (7)	0.0168 (4)
I1	0.42016 (7)	0.78153 (6)	0.088953 (18)	0.02270 (15)
I2	0.14227 (7)	0.78170 (6)	0.16786 (2)	0.02691 (16)
I3	0.73414 (8)	0.78543 (8)	0.02143 (2)	0.03606 (18)
H1A	0.517 (12)	0.452 (11)	0.232 (4)	0.043*
H1B	0.498 (12)	0.558 (11)	0.183 (3)	0.043*
H2A	0.501 (12)	0.108 (11)	0.232 (4)	0.043*
H2B	0.521 (12)	0.008 (12)	0.182 (3)	0.050*
H3A	0.512 (14)	0.190 (12)	0.084 (4)	0.060*
H3B	0.522 (14)	0.380 (13)	0.085 (4)	0.060*
H12A	0.948 (16)	0.286 (12)	0.225 (4)	0.060*
H12B	0.793 (14)	0.282 (11)	0.256 (4)	0.050*
H23A	0.964 (15)	0.135 (13)	0.147 (4)	0.060*
H23B	0.769 (13)	0.034 (13)	0.127 (4)	0.060*
H31A	0.959 (14)	0.414 (12)	0.147 (4)	0.060*
H31B	0.768 (13)	0.538 (13)	0.126 (4)	0.060*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.010 (3)	0.026 (5)	0.020 (4)	0.005 (3)	0.001 (3)	-0.003 (3)
C2	0.014 (3)	0.011 (4)	0.022 (4)	-0.002 (3)	0.006 (3)	0.000 (3)
C3	0.013 (3)	0.021 (4)	0.023 (4)	0.002 (3)	-0.003 (3)	0.000 (3)
C4	0.027 (4)	0.041 (5)	0.022 (4)	-0.001 (4)	0.017 (3)	-0.007 (4)
C12	0.016 (4)	0.021 (4)	0.020 (4)	-0.001 (3)	-0.006 (3)	0.000 (3)
C23	0.018 (4)	0.006 (4)	0.026 (4)	0.004 (3)	0.005 (3)	0.002 (3)
C31	0.012 (4)	0.027 (5)	0.019 (4)	0.001 (3)	0.002 (3)	0.001 (3)
N1	0.011 (3)	0.020 (3)	0.019 (3)	-0.001 (2)	-0.002 (2)	0.000 (3)
N2	0.009 (3)	0.017 (3)	0.017 (3)	0.001 (2)	0.002 (2)	0.002 (2)
N3	0.014 (3)	0.020 (3)	0.016 (3)	-0.005 (3)	0.002 (2)	-0.004 (3)
O1	0.009 (2)	0.029 (3)	0.042 (3)	0.000 (2)	-0.002 (2)	0.002 (3)
P1	0.0075 (8)	0.0187 (9)	0.0244 (10)	0.0007 (7)	0.0003 (7)	-0.0004 (8)
I1	0.0282 (3)	0.0183 (3)	0.0215 (3)	0.0009 (2)	-0.00114 (19)	-0.0002 (2)
I2	0.0230 (3)	0.0207 (3)	0.0376 (3)	0.0000 (2)	0.0081 (2)	0.0000 (2)
I3	0.0341 (3)	0.0527 (4)	0.0218 (3)	0.0017 (3)	0.0054 (2)	-0.0023 (3)

*Geometric parameters (Å, °)*

C1—N1	1.479 (8)	C12—N1	1.462 (9)
C1—P1	1.821 (8)	C12—N2	1.467 (10)
C1—H1A	0.94 (9)	C12—H12A	0.92 (11)
C1—H1B	1.01 (9)	C12—H12B	0.90 (11)
C2—N2	1.486 (8)	C23—N2	1.440 (9)
C2—P1	1.799 (7)	C23—N3	1.550 (9)
C2—H2A	0.98 (9)	C23—H23A	0.99 (10)
C2—H2B	0.97 (10)	C23—H23B	0.99 (10)
C3—N3	1.495 (9)	C31—N1	1.441 (9)
C3—P1	1.825 (8)	C31—N3	1.551 (9)
C3—H3A	0.96 (10)	C31—H31A	0.97 (10)
C3—H3B	0.96 (11)	C31—H31B	1.06 (10)
C4—N3	1.496 (9)	O1—P1	1.483 (5)
C4—H4A	0.9800	I1—I3	2.9067 (8)
C4—H4B	0.9800	I1—I2	2.9127 (7)
C4—H4C	0.9800		
N1—C1—P1	107.9 (5)	N2—C23—H23A	108 (6)
N1—C1—H1A	109 (5)	N3—C23—H23A	106 (6)
P1—C1—H1A	107 (6)	N2—C23—H23B	107 (6)
N1—C1—H1B	118 (5)	N3—C23—H23B	107 (6)
P1—C1—H1B	109 (5)	H23A—C23—H23B	117 (8)
H1A—C1—H1B	105 (7)	N1—C31—N3	110.8 (6)
N2—C2—P1	109.3 (5)	N1—C31—H31A	109 (6)
N2—C2—H2A	116 (5)	N3—C31—H31A	99 (6)
P1—C2—H2A	106 (5)	N1—C31—H31B	108 (5)
N2—C2—H2B	107 (5)	N3—C31—H31B	108 (5)
P1—C2—H2B	114 (5)	H31A—C31—H31B	122 (8)
H2A—C2—H2B	104 (7)	C31—N1—C12	110.7 (6)
N3—C3—P1	110.8 (5)	C31—N1—C1	114.0 (5)
N3—C3—H3A	112 (6)	C12—N1—C1	112.6 (6)
P1—C3—H3A	109 (6)	C23—N2—C12	110.4 (6)
N3—C3—H3B	106 (6)	C23—N2—C2	113.9 (5)
P1—C3—H3B	110 (6)	C12—N2—C2	111.2 (6)
H3A—C3—H3B	109 (8)	C4—N3—C3	111.3 (6)
N3—C4—H4A	109.5	C4—N3—C31	108.6 (5)
N3—C4—H4B	109.5	C3—N3—C31	110.7 (6)
H4A—C4—H4B	109.5	C4—N3—C23	108.0 (6)
N3—C4—H4C	109.5	C3—N3—C23	110.4 (6)
H4A—C4—H4C	109.5	C31—N3—C23	107.8 (5)
H4B—C4—H4C	109.5	O1—P1—C2	119.2 (3)
N1—C12—N2	112.4 (5)	O1—P1—C1	119.3 (3)
N1—C12—H12A	107 (6)	C2—P1—C1	101.5 (3)
N2—C12—H12A	111 (6)	O1—P1—C3	112.4 (3)
N1—C12—H12B	112 (6)	C2—P1—C3	100.5 (4)
N2—C12—H12B	113 (6)	C1—P1—C3	100.8 (4)

H12A—C12—H12B	100 (9)	I3—I1—I2	172.41 (2)
N2—C23—N3	111.1 (5)		
N3—C31—N1—C12	57.7 (7)	N1—C31—N3—C4	-172.0 (6)
N3—C31—N1—C1	-70.5 (8)	N1—C31—N3—C3	65.6 (7)
N2—C12—N1—C31	-59.3 (8)	N1—C31—N3—C23	-55.2 (7)
N2—C12—N1—C1	69.6 (8)	N2—C23—N3—C4	172.4 (6)
P1—C1—N1—C31	65.5 (7)	N2—C23—N3—C3	-65.7 (7)
P1—C1—N1—C12	-61.6 (7)	N2—C23—N3—C31	55.3 (7)
N3—C23—N2—C12	-57.4 (7)	N2—C2—P1—O1	174.7 (4)
N3—C23—N2—C2	68.6 (7)	N2—C2—P1—C1	-52.0 (5)
N1—C12—N2—C23	59.1 (7)	N2—C2—P1—C3	51.4 (5)
N1—C12—N2—C2	-68.4 (7)	N1—C1—P1—O1	-175.4 (4)
P1—C2—N2—C23	-64.0 (7)	N1—C1—P1—C2	51.3 (6)
P1—C2—N2—C12	61.6 (6)	N1—C1—P1—C3	-51.8 (6)
P1—C3—N3—C4	179.9 (5)	N3—C3—P1—O1	179.9 (5)
P1—C3—N3—C31	-59.2 (7)	N3—C3—P1—C2	-52.2 (6)
P1—C3—N3—C23	60.0 (7)	N3—C3—P1—C1	51.8 (6)

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>
C23—H23 <i>A</i> ...O1 <sup>i</sup>	0.99 (10)	2.26 (11)	3.161 (9)	150 (9)
C31—H31 <i>A</i> ...O1 <sup>i</sup>	0.97 (10)	2.23 (10)	3.160 (9)	161 (8)

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