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## 3-(8-Methoxyquinolin-2-ylmethyl)-1methyl-3*H*-1-imidazolium hexafluorophosphate

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Key indicators: single-crystal X-ray study; T = 291 K; mean  $\sigma$ (C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.058; wR factor = 0.170; data-to-parameter ratio = 10.5.

In the cation of the title compound,  $C_{15}H_{17}N_3O^+ \cdot PF_6^-$ , the dihedral angle between the mean planes of the quinoline and imidazole groups is 78.02 (7)°. In the crystal structure,  $\pi - \pi$  stacking interactions, with a ring centroid separation of 3.752 (2) Å, link the molecules into centrosymmetric dimers. In addition, weak intermolecular  $C-H \cdot \cdot \cdot F$  and  $C-H \cdot \cdot \cdot O$  interactions help to stabilize the crystal structure. The F atoms of the anion are disordered over two sites in a ratio of approximately 0.86:0.14.

#### **Related literature**

For related literature, see: Bortolini *et al.* (2003); Dibrov & Kochi (2006); Pretti *et al.* (2006).



#### **Experimental**

Crystal data  $C_{15}H_{17}N_3O^+ \cdot F_6P^ M_r = 400.29$ 

Monoclinic, C2/c*a* = 12.2183 (11) Å b = 21.3444 (19) Åc = 14.4056 (13) Å $\beta = 112.059 (1)^{\circ}$  $V = 3481.9 (5) \text{ Å}^{3}$ Z = 8

#### Data collection

Bruker SMART CCD area-detector	12564 measured reflections
diffractometer	3087 independent reflections
Absorption correction: multi-scan	2808 reflections with $I > 2\sigma(I)$
(SADABS; Sheldrick, 1996)	$R_{\rm int} = 0.108$
$T_{\min} = 0.947, \ T_{\max} = 0.964$	

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.059$ 108 restraints $wR(F^2) = 0.170$ H-atom parameters constrainedS = 1.05 $\Delta \rho_{max} = 1.13 \text{ e } \text{\AA}^{-3}$ 3087 reflections $\Delta \rho_{min} = -0.67 \text{ e } \text{\AA}^{-3}$ 293 parameters $\Delta \rho_{min} = -0.67 \text{ e } \text{\AA}^{-3}$ 

#### Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$C12-H12\cdots F1^{i}$ $C9-H9A\cdots F2^{ii}$ $C3-H3\cdots O1^{iii}$	0.93 0.97 0.93	2.46 2.49 2.27	3.204 (5) 3.244 (4) 3.122 (3)	137 135 152
Symmetry codes: $-x + 1, y, -z + \frac{1}{2}$ .	(i) $-x + \frac{1}{2}$	$y + \frac{1}{2}, -z + \frac{3}{2};$	(ii) $x + \frac{1}{2}, y$	$+\frac{1}{2}, z-1;$ (iii)

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *SHELXTL* (Bruker, 1998).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2402).

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Mo  $K\alpha$  radiation  $\mu = 0.23 \text{ mm}^{-1}$ 

 $0.24 \times 0.18 \times 0.16$  mm

T = 291 (2) K

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#### 3-(8-Methoxyquinolin-2-ylmethyl)-1-methyl-3H-1-imidazolium hexafluorophosphate

### Y.-L. Zhu, Z.-F. Zhong, Q.-F. Yin and W. Liu

#### Comment

Room-temperature ionic liquids are attracting significant interest owing to their chemical characteristics and potentially useful solvent properties (Dibrov & Kochi, 2006) and imidazolium salts, which are regarded as a type of ionic liquids, have an extensive application in organic synthesis (Pretti *et al.*, 2006).

The molecular structure of (I) is shown in Fig. 1. The dihedral angle between the quinoline plane and imidazole plane is 78.02 (7) °. In the crystal structure,  $\pi$ - $\pi$  stacking internactions link molecules into centrosymmetric dimers. In addition, weak intermolecular C—H···F and C—H····F and C—H···F and C—H···F and C—H···F and C—H···F and C—H···F and C—H····F and C—H····F and C—H····F and C—H····F and C—H···F and C—H····F and C—H

#### Experimental

The title compound was synthesized according to the literature procedure (Bortolini et al., 2003).

#### Refinement

All H atoms were included in calculated positions and refined as riding (C—H = 0.93–0.97 Å; N—H = 0.88 Å), with  $U_{iso}(H)$  =  $1.5U_{eq}(C)$  for methyl and  $1.2U_{eq}(C,N)$  for all other H atoms. The largest peak in the final difference Fourier of 1.33 e Å<sup>-3</sup> is 0.83 Å from atom H7. The F atoms of the anion are disordered over two sites with refined occupancies 0.859 (6) and 0.141 (6) for the major and minor components.

#### **Figures**



Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids. Hydrogen atoms and the minor component of disorder have been omitted.



Fig. 2. : The packing of the title compound, viewed down the *b* axis.

## 3-(8-Methoxyquinolin-2-ylmethyl)-1-methyl-3H-1-imidazolium hexafluorophosphate

### Crystal data

$C_{15}H_{17}N_3O^+ \cdot F_6P^-$	Z = 8
$M_r = 400.29$	$F_{000} = 1640$
Monoclinic, C2/c	$D_{\rm x} = 1.527 {\rm Mg} {\rm m}^{-3}$
Hall symbol: -C 2yc	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
<i>a</i> = 12.2183 (11) Å	$\mu = 0.23 \text{ mm}^{-1}$
b = 21.3444 (19)  Å	T = 291 (2)  K
c = 14.4056 (13)  Å	Block, colourless
$\beta = 112.059 (1)^{\circ}$	$0.24\times0.18\times0.16~mm$
$V = 3481.9 (5) \text{ Å}^3$	

### Data collection

3087 independent reflections
2808 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.108$
$\theta_{\text{max}} = 25.0^{\circ}$
$\theta_{\min} = 1.9^{\circ}$
$h = -14 \rightarrow 13$
$k = -25 \rightarrow 25$
$l = -16 \rightarrow 17$

#### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.059$	H-atom parameters constrained
$wR(F^2) = 0.170$	$w = 1/[\sigma^2(F_o^2) + (0.0848P)^2 + 6.8821P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{\rm max} = 0.001$
3087 reflections	$\Delta \rho_{max} = 1.13 \text{ e } \text{\AA}^{-3}$
293 parameters	$\Delta \rho_{min} = -0.67 \text{ e } \text{\AA}^{-3}$
108 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct	

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.0026 (5)

#### 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  $F^2 > 2 \operatorname{sigma}(F^2)$  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  $(A^2)$ 

	x	у	Ζ	$U_{\rm iso}$ */ $U_{\rm eq}$	Occ. (<1)
P1	0.01910 (7)	0.33923 (4)	0.99358 (6)	0.0431 (3)	
F1	0.0575 (5)	0.3561 (2)	1.1098 (3)	0.092 (2)	0.859 (6)
F2	0.0141 (3)	0.26827 (11)	1.0220 (2)	0.0687 (9)	0.859 (6)
F3	-0.1135 (2)	0.3483 (2)	0.9796 (3)	0.0951 (13)	0.859 (6)
F4	0.0294 (4)	0.41165 (15)	0.9733 (3)	0.1144 (16)	0.859 (6)
F5	0.1552 (2)	0.33103 (19)	1.0130 (3)	0.0916 (12)	0.859 (6)
F6	-0.0185 (5)	0.3223 (3)	0.8809 (3)	0.118 (3)	0.859 (6)
F1'	0.0459 (14)	0.3516 (7)	1.1049 (6)	0.038 (6)	0.141 (6)
F2'	-0.0984 (11)	0.3001 (8)	0.9825 (10)	0.080 (6)	0.141 (6)
F3'	-0.0593 (16)	0.3991 (6)	0.9584 (11)	0.089 (7)	0.141 (6)
F4'	0.1291 (12)	0.3739 (9)	0.9927 (12)	0.113 (9)	0.141 (6)
F5'	0.0894 (16)	0.2751 (6)	1.0179 (12)	0.117 (9)	0.141 (6)
F6'	-0.0142 (12)	0.3222 (7)	0.8752 (7)	0.046 (6)	0.141 (6)
N1	0.35973 (18)	0.67281 (10)	0.14547 (16)	0.0286 (5)	
N2	0.51217 (19)	0.55385 (10)	0.12278 (15)	0.0297 (5)	
H2	0.5699	0.5799	0.1455	0.036*	
N3	0.29978 (19)	0.68579 (10)	0.26701 (16)	0.0324 (5)	
01	0.73297 (16)	0.51432 (9)	0.21731 (16)	0.0406 (5)	
C1	0.5310(2)	0.49095 (12)	0.13432 (18)	0.0302 (6)	
C2	0.4026 (2)	0.57384 (13)	0.07571 (19)	0.0326 (6)	
C3	0.3228 (2)	0.64369 (12)	0.20928 (19)	0.0305 (6)	
H3	0.3143	0.6006	0.2130	0.037*	
C4	0.3047 (2)	0.53339 (14)	0.0384 (2)	0.0403 (7)	
H4	0.2290	0.5494	0.0063	0.048*	
C5	0.6489 (2)	0.46864 (12)	0.1842 (2)	0.0336 (6)	
C6	0.3226 (3)	0.47019 (14)	0.0499 (2)	0.0407 (7)	
Н6	0.2588	0.4429	0.0260	0.049*	
C7	0.4631 (3)	0.38144 (13)	0.1118 (2)	0.0410 (7)	
H7	0.4025	0.3522	0.0882	0.049*	
C8	0.4378 (2)	0.44646 (13)	0.09821 (19)	0.0338 (6)	
C9	0.3866 (3)	0.64389 (13)	0.0633 (2)	0.0360 (6)	
H9A	0.4582	0.6624	0.0612	0.043*	
H9B	0.3229	0.6528	0.0000	0.043*	

C10	0.3589 (3)	0.73643 (13)	0.1622 (2)	0.0385 (6)
H10	0.3799	0.7680	0.1275	0.046*
C11	0.6706 (3)	0.40540 (13)	0.1961 (2)	0.0407 (7)
H11	0.7475	0.3910	0.2284	0.049*
C12	0.3219 (3)	0.74401 (13)	0.2382 (2)	0.0401 (7)
H12	0.3130	0.7820	0.2663	0.048*
C13	0.5766 (3)	0.36226 (13)	0.1594 (2)	0.0436 (7)
H13	0.5927	0.3196	0.1680	0.052*
C14	0.2529 (3)	0.67183 (15)	0.3445 (2)	0.0460 (7)
H14A	0.1684	0.6752	0.3166	0.069*
H14B	0.2846	0.7011	0.3987	0.069*
H14C	0.2750	0.6300	0.3690	0.069*
C15	0.8535 (3)	0.49475 (17)	0.2664 (3)	0.0613 (10)
H15A	0.8622	0.4725	0.3266	0.092*
H15B	0.9040	0.5309	0.2827	0.092*
H15C	0.8749	0.4678	0.2226	0.092*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
P1	0.0324 (5)	0.0473 (5)	0.0488 (5)	-0.0030 (3)	0.0140 (3)	0.0112 (3)
F1	0.112 (4)	0.076 (3)	0.066 (3)	0.004 (3)	0.009 (2)	-0.017 (2)
F2	0.092 (2)	0.0408 (13)	0.0805 (18)	-0.0165 (13)	0.0406 (16)	-0.0023 (12)
F3	0.0347 (14)	0.126 (3)	0.115 (3)	0.0141 (16)	0.0167 (14)	-0.015 (2)
F4	0.113 (3)	0.068 (2)	0.128 (3)	-0.0150 (19)	0.006 (2)	0.0528 (19)
F5	0.0423 (15)	0.118 (3)	0.122 (3)	-0.0103 (16)	0.0385 (16)	0.007 (2)
F6	0.125 (5)	0.168 (5)	0.057 (3)	-0.007 (4)	0.029 (3)	0.003 (3)
F1'	0.047 (8)	0.035 (9)	0.034 (9)	0.004 (6)	0.019 (7)	0.015 (7)
F2'	0.082 (10)	0.101 (11)	0.067 (8)	-0.024 (8)	0.039 (7)	0.009 (7)
F3'	0.102 (11)	0.073 (9)	0.094 (10)	0.033 (8)	0.039 (8)	0.015 (7)
F4'	0.100 (12)	0.111 (12)	0.134 (13)	-0.018 (9)	0.052 (9)	0.002 (9)
F5'	0.114 (12)	0.101 (12)	0.116 (12)	0.033 (9)	0.021 (9)	-0.005 (9)
F6'	0.037 (8)	0.083 (11)	0.033 (9)	-0.009(7)	0.032 (7)	0.002 (7)
N1	0.0253 (10)	0.0285 (11)	0.0319 (11)	0.0030 (8)	0.0105 (8)	0.0018 (8)
N2	0.0319 (11)	0.0288 (11)	0.0321 (11)	-0.0008 (9)	0.0165 (9)	-0.0039 (9)
N3	0.0322 (11)	0.0332 (11)	0.0325 (11)	0.0028 (9)	0.0130 (9)	-0.0019 (9)
O1	0.0328 (10)	0.0339 (10)	0.0514 (12)	0.0035 (8)	0.0113 (9)	-0.0043 (9)
C1	0.0380 (14)	0.0310 (13)	0.0274 (12)	0.0017 (10)	0.0190 (11)	-0.0021 (10)
C2	0.0354 (13)	0.0364 (14)	0.0305 (13)	0.0051 (11)	0.0174 (11)	-0.0016 (11)
C3	0.0335 (13)	0.0269 (12)	0.0314 (13)	0.0033 (10)	0.0124 (10)	0.0017 (10)
C4	0.0318 (14)	0.0500 (17)	0.0410 (15)	0.0025 (12)	0.0159 (12)	-0.0058 (13)
C5	0.0377 (14)	0.0323 (14)	0.0337 (13)	0.0018 (11)	0.0166 (11)	-0.0033 (10)
C6	0.0378 (15)	0.0461 (17)	0.0433 (15)	-0.0078 (12)	0.0210 (12)	-0.0107 (13)
C7	0.0544 (18)	0.0345 (14)	0.0419 (15)	-0.0075 (12)	0.0270 (14)	-0.0057 (12)
C8	0.0418 (14)	0.0340 (14)	0.0323 (13)	-0.0042 (11)	0.0215 (11)	-0.0052 (11)
С9	0.0391 (14)	0.0381 (15)	0.0357 (14)	0.0082 (11)	0.0195 (12)	0.0039 (11)
C10	0.0421 (15)	0.0278 (13)	0.0478 (16)	-0.0030 (11)	0.0193 (13)	0.0012 (12)
C11	0.0483 (16)	0.0335 (14)	0.0420 (15)	0.0088 (12)	0.0190 (13)	0.0016 (12)

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C12	0.0465 (16)	0.0276 (13)	0.0471 (16)	0.0012 (11)	0.0183 (13)	-0.0052 (12)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C13	0.0627 (19)	0.0275 (13)	0.0463 (16)	0.0018 (13)	0.0271 (15)	0.0005 (12)
C15         0.031 (16)         0.051 (2)         0.084 (3)         0.0072 (14)         0.0059 (16) $-0.0075 (18)$ Geometric parameters (Å, ?)                 P1—F1         1.534 (8)         C2—C3         1.510 (4)           0.0075 (18)           P1—F2         1.553 (8)         C4—C6         1.367 (4)          9.000            P1—F3         1.558 (3)         C4—H4         0.9300           9.001            P1—F2         1.576 (2)         CS—C11         1.374 (4)           9.000          9.001          9.001          9.001         9.001          9.001	C14	0.0552 (18)	0.0516 (18)	0.0409 (16)	0.0011 (14)	0.0290 (14)	-0.0024 (13)
Geometric parameters (Å. ?)PI-FI'1.534 (8)C2-C41.409 (4)PI-F4'1.539 (8)C2-C51.510 (4)PI-F51.563 (8)C4-C61.367 (4)PI-F21.563 (8)C4-C61.367 (4)PI-F21.568 (3)C4-H40.9300PI-F21.568 (3)C4-H40.9300PI-F21.584 (8)C6-C81.409 (4)PI-F41.587 (3)C6-H60.9300PI-F51.589 (3)C7-C131.358 (5)PI-F11.601 (4)C7-C81.420 (4)PI-F21.616 (8)C7-H70.9300PI-F41.639 (8)C9-H9A0.9700NI-C31.322 (3)C10-H100.9300NI-C41.332 (3)C10-H100.9300N2-C11.332 (3)C10-H100.9300N2-C21.323 (3)C11-H110.9300N2-C11.324 (3)C11-H110.9300N2-C21.324 (3)C13-H130.9300N3-C121.366 (4)C15-H15A0.9600O1-C51.366 (3)C14-H14A0.9600O1-C51.436 (4)C15-H15A0.9600C1-C81.429 (4)C15-H15A0.9600C1-C81.429 (4)C15-H15A0.9600C1-C51.436 (4)C15-H15A0.9600C1-C51.436 (4)C15-H15A0.9600C1-C61.429 (4)C15-H15A0.9600C1-C71.832 (2)C1-H141.252 (2)F1-P1-F4 <td< td=""><td>C15</td><td>0.0341 (16)</td><td>0.051 (2)</td><td>0.084 (3)</td><td>0.0072 (14)</td><td>0.0059 (16)</td><td>-0.0075 (18)</td></td<>	C15	0.0341 (16)	0.051 (2)	0.084 (3)	0.0072 (14)	0.0059 (16)	-0.0075 (18)
Geometric parameters (Å, °)         PIFI       1.534 (8)       C2-C4       1.409 (4)         PIF4       1.539 (8)       C2-C9       1.510 (4)         PIF4       1.555 (4)       C3-H3       0.9300         PIF3       1.568 (3)       C4-C6       1.367 (4)         PIF3       1.566 (2)       C5-C11       1.374 (4)         PIF3       1.587 (3)       C6-H6       0.9300         PIF4       1.587 (3)       C7-C13       1.585 (5)         PIF1       1.601 (4)       C7-C3       1.420 (4)         PIF2       1.616 (8)       C7-H7       0.9300         PI-F2       1.616 (8)       C7-H7       0.9300         PI-F2       1.638 (3)       C10-C12       1.313 (4)         NI-C3       1.322 (3)       C10-H10       0.9300         NI-C4       1.362 (3)       C11-H11       0.9300         N2-C2       1.323 (3)       C12-H112       0.9300         N2-C1       1.366 (3)       C14-H14A       0.9600         N2-H2       0.8600       C12-H112       0.9300         N3-C12       1.366 (3)       C14-H14A       0.9600         N3-C14       1.446 (3)       C14-H14A <t< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td></t<>							
P Fl'1.534 (8)C2C41.409 (4)P F4'1.539 (8)C2C91.510 (4)P F4'1.539 (8)C4C61.367 (4)P -F31.568 (3)C4H40.9300P -F21.568 (3)C4C61.409 (4)P -F31.588 (3)C6C81.409 (4)P -F41.587 (3)C6-H60.9300P -F51.584 (8)C6C131.358 (5)P -F11.601 (4)C7C31.420 (4)P -F2'1.616 (8)C7H70.9300P -F6'1.639 (8)C9-H9B0.9700NI-C31.222 (3)C0-H19A0.9300NI-C101.380 (3)C10-C121.343 (4)N1-C91.478 (3)C10-H100.9300N2-C11.322 (3)C11-H110.9300N2-C21.232 (3)C11-H110.9300N2-C11.324 (3)C13-H1130.9300N3-C121.369 (4)C14-H14A0.9600O1-C51.366 (3)C14-H14A0.9600O1-C51.366 (3)C14-H14C0.9600O1-C151.436 (4)C15-H15A0.9600C1-C81.429 (4)C15-H15A0.9600C1-C81.429 (4)C15-H15A0.9600C1-C81.429 (4)C15-H15A0.9600C1-C71.336 (5)C1-N2-H212.9F1-P1-F6'9.96 (5)C1-N2-H212.9F4-P1-F5'9.5 (5)C1-N2-H212.9F4-P1-F5'9.5 (5)C1-N2-H2	Geometric pa	arameters (Å, °)					
PI-F4'1.539 (8)C2-C91.510 (4)PI-F2'1.553 (4)C3-H30.9300PI-F21.556 (8)C4-C61.367 (4)PI-F31.568 (3)C4-H40.9300PI-F21.576 (C)C5-C111.374 (4)PI-F5'1.584 (8)C6-C81.409 (4)PI-F41.587 (3)C6-H60.9300PI-F51.589 (3)C7-C131.358 (5)PI-F6'1.601 (4)C7-C81.420 (4)PI-F6'1.639 (8)C9-H9A0.9700NI-C101.320 (3)C10-C121.343 (4)NI-C201.320 (3)C10-H100.9300N2-C21.323 (3)C10-H100.9300N2-C21.323 (3)C11-H110.9300N2-C21.326 (3)C11-H110.9300N2-C21.326 (3)C11-H110.9300N3-C31.324 (3)C13-H130.9300N3-C121.366 (4)C14-H14A0.9600O1-C51.366 (4)C14-H14A0.9600O1-C51.436 (4)C15-H15A0.9600C1-C51.436 (4)C15-H15A0.9600C1-C51.436 (4)C15-H15A0.9600C1-C51.436 (5)C1-M1-C9124 7 (2)F1-P1-F4'9.76 (6)C10-N1-C9124 7 (2)F1-P1-F59.56 (5)C1-N2-H2120.9F4-P1-F59.56 (5)C1-N2-H2120.9F4-P1-F59.56 (5)C1-N2-H2120.9F4-P1-F59.56 (6)C1-N3-C14 <td< td=""><td>P1—F1'</td><td></td><td>1.534 (8)</td><td>C2—</td><td>C4</td><td>1.40</td><td>09 (4)</td></td<>	P1—F1'		1.534 (8)	C2—	C4	1.40	09 (4)
P1-F6         1.555 (4)         C3-H3         0.9300           P1-F3'         1.563 (8)         C4-C6         1.367 (4)           P1-F3         1.566 (3)         C4-H4         0.9300           P1-F2         1.576 (2)         C5-C11         1.374 (4)           P1-F5         1.584 (8)         C6-C8         1.409 (4)           P1-F5         1.587 (3)         C6-H6         0.9300           P1-F1         1.601 (4)         C7-C13         1.358 (5)           P1-F1         1.601 (4)         C7-C7         0.9300           P1-F2         1.616 (8)         C9-H9A         0.9700           N1-C3         1.322 (3)         C10-C12         1.333 (4)           N1-C0         1.380 (3)         C10-C12         1.334 (4)           N2-C2         1.323 (3)         C11-C13         1.411 (4)           N2-C1         1.362 (3)         C11-H11         0.9300           N3-C12         1.360 (4)         C14-H14B         0.9600           N3-C14         1.464 (3)         C14-H14B         0.9600           O1-C15         1.360 (4)         C15-H15C         0.9600           C1-C48         1.423 (4)         C15-H15C         0.9600           C1	P1—F4'		1.539 (8)	C2—	С9	1.51	10 (4)
P1-F3'1.563 (8)C4-C61.367 (4)P1-F21.568 (3)C4-H40.9300P1-F21.576 (2)C5-C111.374 (4)P1-F51.584 (8)C6-C81.409 (4)P1-F41.587 (3)C6-H60.9300P1-F51.589 (3)C7-C131.358 (5)P1-F11.601 (4)C7-C81.420 (4)P1-F2'1.616 (8)C7-H70.9300P1-F6'1.639 (8)C9-H9A0.9700N1-C101.380 (3)C10-C121.343 (4)N1-C21.323 (3)C11-C131.411 (4)N2-C21.323 (3)C11-C131.411 (4)N2-C11.362 (3)C11-H110.9300N2-C21.324 (3)C11-H110.9300N3-C121.369 (4)C14-H14A0.9600N3-C121.366 (3)C14-H14A0.9600N3-C121.366 (3)C14-H14A0.9600O1-C51.366 (3)C14-H14A0.9600C1-C51.366 (3)C14-H14A0.9600C1-C51.429 (4)C15-H15B0.9600C1-C51.429 (4)C15-H15B0.9600C1-C51.429 (4)C15-H15B0.9600C1-C51.429 (4)C15-H15B0.9600C1-C51.429 (4)C15-H15B0.9600C1-C51.429 (4)C15-H15B0.9600C1-C51.429 (4)C15-H15B0.9600C1-C51.429 (4)C15-H15B0.9600C1-C51.429 (4)C15-H15B0.9600<	P1—F6		1.555 (4)	С3—	H3	0.93	300
P1-F31.568 (3)C4-H40.9300P1-F21.576 (2)C5-C111.374 (4)P1-F5'1.584 (8)C6-C81.400 (4)P1-F41.587 (3)C6-H60.9300P1-F51.589 (3)C7-C131.358 (5)P1-F11.601 (4)C7-C81.420 (4)P1-F2'1.616 (8)C7-H70.9300P1-F6'1.639 (8)C9-H9R0.9700N1-C31.322 (3)C10-H100.9300N1-C101.380 (3)C10-C121.343 (4)N1-C91.478 (3)C10-H100.9300N2-C11.323 (3)C11-C131.411 (4)N2-C11.323 (3)C11-H110.9300N2-C21.323 (3)C13-H130.9300N3-C121.369 (4)C14-H1480.9600N3-C121.369 (4)C14-H1480.9600O1-C51.366 (3)C14-H1480.9600O1-C51.436 (4)C15-H1580.9600C1-C51.429 (7)C-N2-H2120.9 <td>P1—F3'</td> <td></td> <td>1.563 (8)</td> <td>C4—</td> <td>C6</td> <td>1.30</td> <td>67 (4)</td>	P1—F3'		1.563 (8)	C4—	C6	1.30	67 (4)
P1F21.576 (2)C5C111.374 (4)P1F21.584 (8)C6C81.409 (4)P1F5'1.587 (3)C6H60.9300P1F51.589 (3)C7C131.358 (5)P1F11.601 (4)C7C81.420 (4)P1F2'1.616 (8)C7H70.9300N1C31.322 (3)C9H9A0.9700N1C101.380 (3)C10C121.343 (4)N1C21.323 (3)C10C121.343 (4)N2C21.323 (3)C11H110.9300N2C21.323 (3)C11H110.9300N2C11.362 (3)C11H110.9300N3C31.324 (3)C13H130.9300N3C121.369 (4)C14H14A0.9600O1C51.366 (3)C14H14B0.9600O1C51.436 (4)C15H15A0.9600C1C81.423 (4)C15H15A0.9600C1C51.429 (4)C15H15A0.9600C1C51.429 (4)C15H15A0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C1-NC141.25 (2)F4	P1—F3		1.568 (3)	C4—	H4	0.93	300
P1—F5'         1.584 (8)         C6—C8         1.409 (4)           P1—F4         1.587 (3)         C6—H6         0.9300           P1—F5         1.589 (3)         C7—C13         1.358 (5)           P1—F1         1.601 (4)         C7—C8         1.420 (4)           P1—F2'         1.616 (8)         C7—H7         0.9300           P1—F6'         1.639 (8)         C9—H9A         0.9700           N1—C10         1.380 (3)         C10—C12         1.343 (4)           N1—C2         1.323 (3)         C10—H10         0.9300           N2—C2         1.323 (3)         C11—C13         1.411 (4)           N2—C1         1.366 (3)         C14—H14         0.9300           N2—C2         1.324 (3)         C13—H13         0.9300           N3—C14         1.464 (3)         C14—H14A         0.9600           O1—C15         1.366 (3)         C14—H14B         0.9600           O1—C15         1.423 (4)         C15—H15A         0.9600           C1—C2         1.429 (4)         C15—H15A         0.9600           C1—C1         1.423 (4)         C15—H15A         0.9600           C1—C2         1.429 (4)         C15—H15A         0.9600 <td< td=""><td>P1—F2</td><td></td><td>1.576 (2)</td><td>C5—</td><td>C11</td><td>1.37</td><td>74 (4)</td></td<>	P1—F2		1.576 (2)	C5—	C11	1.37	74 (4)
P1-F41.587 (3)C6-H60.9300P1-F51.589 (3)C7-C131.358 (5)P1-F11.601 (4)C7-C81.420 (4)P1-F2'1.616 (8)C7-H70.9300P1-F6'1.639 (8)C9-H9A0.9700N1-C31.322 (3)C9-H9B0.9700N1-C101.380 (3)C10-C121.343 (4)N1-C91.478 (3)C10-H100.9300N2-C21.323 (3)C11-C131.411 (4)N2-H20.8600C12-H120.9300N3-C11.324 (3)C13-H130.9300N3-C211.369 (4)C14-H14A0.9600N3-C141.464 (3)C14-H14B0.9600O1-C51.366 (3)C14-H14C0.9600O1-C51.436 (4)C15-H15A0.9600C1-C81.423 (4)C15-H15B0.9600C1-C81.423 (4)C15-H15B0.9600C1-C71.429 (4)C15-H15B0.9600C1-C81.423 (4)C15-H15B0.9600C1-C71.423 (4)C15-H15B0.9600C1-C81.423 (4)C1-N1-C91.82 (2)F1'-P1-F393.6 (5)C1-N2-H2120.9F4'-P1-F691.2 (7)C2-N2-C11.82 (2)F4'-P1-F691.2 (7)C3-N3-C14125.5 (2)F4'-P1-F390.5 (2)N2-C1-C51.86 (2)F4'-P1-F390.5 (2)N2-C1-C51.86 (2)F4'-P1-F390.5 (2)N2-C1-C51.86 (2)F4'-P1-F39.5 (2)	P1—F5'		1.584 (8)	С6—	C8	1.40	09 (4)
P1-F51.589 (3)C7-C131.538 (5)P1-F11.601 (4)C7-C81.420 (4)P1-F2'1.616 (8)C7-H70.9300P1-F6'1.639 (8)C9-H9A0.9700N1-C31.322 (3)C9-H9B0.9700N1-C101.380 (3)C10-C121.343 (4)N1-C21.323 (3)C10-H100.9300N2-C21.323 (3)C11-H110.9300N2-C21.323 (3)C11-H110.9300N2-C11.362 (3)C13-H130.9300N3-C31.324 (3)C13-H130.9300N3-C31.324 (3)C14-H14A0.9600N3-C141.464 (3)C14-H14B0.9600O1-C51.366 (3)C14-H14B0.9600O1-C51.429 (4)C15-H15A0.9600C1-C51.429 (4)C15-H15A0.9600C1-C51.429 (4)C15-H15A0.9600C1-C51.429 (4)C15-H15C0.9600C1-C51.429 (4)C15-H15C0.9600C1-C51.429 (4)C15-H15C0.9600C1-C51.423 (4)C15-H15C0.9600C1-C51.423 (4)C15-H15C0.9600C1-C51.423 (4)C15-H15C0.9600C1-C51.423 (4)C15-H15C0.9600C1-C51.436 (8)C1-N3-C14125.2 (2)F4-P1-F69.12 (7)C2-N2-H2120.9F4-P1-F79.5 (5)C1-N3-C14125.2 (2)F4-P1-F39.5 (2)N2-C1-C5118	P1—F4		1.587 (3)	С6—	H6	0.93	300
P1F11.601 (4)C7C81.420 (4)P1F2'1.616 (8)C7H70.9300P1F6'1.639 (8)C9-H9A0.9700N1C31.320 (3)C10C121.343 (4)N1C101.380 (3)C10C121.343 (4)N1C91.478 (3)C10H100.9300N2C21.323 (3)C11C131.411 (4)N2C11.362 (3)C11H110.9300N2C21.363 (3)C13H130.9300N2C11.364 (3)C14H1480.9600N3C121.364 (3)C14H1480.9600N3C121.366 (3)C14H1480.9600O1C51.436 (4)C15H15A0.9600C1C51.436 (4)C15H15A0.9600C1C51.436 (4)C15H15B0.9600C1C51.429 (4)C15H15B0.9600C1C51.429 (4)C15H15B0.9600C1C51.429 (4)C15H15C0.9600F1'-P1-F4'94.7 (6)C2-N2C1118.2 (2)F4'-P1-F5'9.36 (5)C1-N3C14125.2 (2)F4'-P1-F5'9.36 (5)C1-N2-H2120.9F4'-P1-F3'9.50 (2)N2-C1C5118.8 (2)F4'-P1-F39.51 (7)N2-C1-C5118.8 (2)F4'-P1-F39.57 (8)N2-C2-C4123.3 (3)F4'-P1-F39.57 (8)N2-C2-C4123.3 (3)F4'-P1-F39.57 (8)N2-C2-C4125.2 (2)F4'-P1-F59.13 (2)N2-C2-	P1—F5		1.589 (3)	С7—	C13	1.35	58 (5)
P1—F2'         1.616 (8)         C7—H7         0.9300           P1—F6'         1.639 (8)         C9—H9A         0.9700           N1—C3         1.322 (3)         C9—H9B         0.9700           N1—C10         1.380 (3)         C10—C12         1.343 (4)           N1—C9         1.478 (3)         C10—H10         0.9300           N2—C2         1.323 (3)         C11—C13         1.411 (4)           N2—C1         1.362 (3)         C13—H13         0.9300           N3—C3         1.324 (3)         C14—H14A         0.9600           N3—C12         1.366 (3)         C14—H14B         0.9600           O1—C15         1.436 (4)         C15—H15A         0.9600           O1—C5         1.436 (4)         C15—H15A         0.9600           C1—C8         1.423 (4)         C15—H15A         0.9600           C1—C5         1.429 (4)         C15—H15A         0.9600           C1—C5         1.436 (6)         C1—N2—C1         1.82 (2) <t< td=""><td>P1—F1</td><td></td><td>1.601 (4)</td><td>С7—</td><td>C8</td><td>1.42</td><td>20 (4)</td></t<>	P1—F1		1.601 (4)	С7—	C8	1.42	20 (4)
P1—F6         1.639 (8)         C9—H9A         0.9700           N1—C3         1.322 (3)         C9—H9B         0.9700           N1—C10         1.380 (3)         C10—C12         1.343 (4)           N1—C9         1.478 (3)         C10—H10         0.9300           N2—C2         1.323 (3)         C11—H11         0.9300           N2—C2         1.324 (3)         C13—H12         0.9300           N2—C1         1.360 (4)         C14—H14A         0.9600           N3—C12         1.366 (3)         C14—H14A         0.9600           N3—C14         1.446 (3)         C14—H14B         0.9600           O1—C5         1.366 (3)         C14—H14B         0.9600           C1—C5         1.436 (4)         C15—H15A         0.9600           C1—C5         1.443 (4)         C15—H15A         0.9600           C1—C5         1.442 (4)         C15—H15A         0.9600           C1—C5         1.442 (4)         C15—H15A         0.9600           C1—C4         1.443 (4)         C16—N1—C9         124.7 (2)           F1—P1—F4         94.7 (6)         C1—N2—C1         118.2 (2)           F4—P1—F5         92.0 (6)         C3—N3—C14         125.2 (2)	P1—F2'		1.616 (8)	С7—	H7	0.93	300
N1-C31.322 (3)C9-H9B0.9700N1-C101.380 (3)C10-C121.343 (4)N1-C91.478 (3)C10-H100.9300N2-C21.323 (3)C11-C131.411 (4)N2-C11.362 (3)C11-H110.9300N2-H20.8600C12-H120.9300N3-C31.324 (3)C13-H130.9300N3-C121.369 (4)C14-H14A0.9600O1-C51.366 (3)C14-H14B0.9600O1-C51.436 (4)C15-H15A0.9600C1-C151.435 (4)C15-H15A0.9600C1-C51.429 (4)C15-H15C0.9600C1-C51.429 (4)C15-H15C0.9600C1-C51.429 (4)C15-H15C0.9600C1-C51.429 (4)C15-H15C0.9600C1-C51.429 (4)C15-H15C0.9600C1-C51.429 (4)C15-H15C0.9600C1-C51.429 (4)C15-H15C0.9600C1-C51.429 (4)C15-H15C0.9600C1-P1-F4'94.7 (6)C2-N2-C1118.2 (2)F4'-P1-F593.6 (5)C1-N3-C14125.2 (2)F4'-P1-F590.5 (2)N2-C1-C5118.6 (2)F4'-P1-F31.43.4 (8)C5-O1-C15117.5 (2)F6-P1-F390.5 (2)N2-C1-C5118.8 (2)F4'-P1-F31.43.4 (8)C5-O1-C15118.8 (2)F4'-P1-F31.43.2 (7)C4-C2-C9116.2 (2)F3'-P1-F31.3 (2)N2-C1-C5118.8 (2)F4'-P	P1—F6'		1.639 (8)	С9—	H9A	0.97	700
N1C101.380 (3)C10C121.343 (4)N1C91.478 (3)C10H100.9300N2C21.323 (3)C11C131.411 (4)N2C11.362 (3)C11H110.9300N2H20.8600C12H120.9300N3C31.324 (3)C13H130.9300N3C121.369 (4)C14H14A0.9600N3C141.464 (3)C14H14B0.9600O1C51.366 (3)C14H14C0.9600O1C51.366 (4)C15H15A0.9600C1-C41.423 (4)C15H15A0.9600C1-C51.429 (4)C15H15A0.9600C1-C51.429 (4)C15H15C0.9600C1-C51.429 (4)C15H15A0.9600C1-C51.429 (4)C15H15C0.9600C1-C51.429 (4)C15H15C0.9600C1-C51.429 (4)C15H15C0.9600C1-C51.429 (4)C15H15C0.9600C1-C51.429 (4)C15H15C0.9600C1-C51.82 (2)P1P1-F39.3 (5)F4P1-F691.2 (7)C2N2C118.8 (2)F4P1-F39.2 0.6C3N3C14125.2 (2)F4P1-F39.0 5 (2)N2C1-C5118.8 (2)F4P1-F39.0 5 (2)N2C1-C5118.8 (2)F4P1-F39.0 5 (2)N2C1-C5118.8 (2)F4P1-F39.1 3 (2)N2C2-C4123.3 (3)F6-P1-F29.1 3 (2)N2C2-C91	N1—C3		1.322 (3)	С9—	H9B	0.97	700
N1C91.478 (3)C10H100.9300N2C21.323 (3)C11C131.411 (4)N2C11.362 (3)C11H110.9300N2H20.8600C12H120.9300N3C31.324 (3)C13H130.9300N3C121.369 (4)C14H14A0.9600N3C141.464 (3)C14H14B0.9600O1C51.366 (3)C14H14C0.9600O1C51.436 (4)C15H15A0.9600C1C81.423 (4)C15H15B0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C10N1C9124.7 (2)F1'P1F61.74.1 (6)C2N2C1118.2 (2)F4'P1F691.2 (7)C2N2H2120.9F1'P1F592.0 (6)C3N3C14125.2 (2)F4'P1F385.3 (6)C12N3C14125.2 (2)F4'P1-F385.3 (6)C12-N3C14125.6 (2)F4'P1-F39.05 (2)N2C1C8122.6 (2)F3'P1-F39.05 (2)N2C1-C5118.8 (2)F1'P1-F284.7 (6)C8C1C5118.6 (2)F4'P1-F2125.7 (8)N2C2Q9162.2 (2)F3'P1-F29.1 (2)N2C2Q9162.2 (2)F3'P1-F29.1 (2)N2C2Q9162.2 (2)F3'P1-F29.1 (2)N2C2Q9162.2 (2)F3'P1-F29.1 (2)N2C2Q9162.2 (2) </td <td>N1-C10</td> <td></td> <td>1.380 (3)</td> <td>C10–</td> <td>C12</td> <td>1.34</td> <td>43 (4)</td>	N1-C10		1.380 (3)	C10–	C12	1.34	43 (4)
N2C21.323 (3)C11C131.411 (4)N2C11.362 (3)C11H110.9300N2H20.8600C12H120.9300N3C31.324 (3)C13H130.9300N3C121.369 (4)C14H14A0.9600N3C121.369 (4)C14H14B0.9600O1C51.366 (3)C14H14B0.9600O1C51.366 (3)C14H14C0.9600O1C51.366 (3)C14H14C0.9600C1C81.423 (4)C15H15B0.9600C1C51.429 (4)C15H15B0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600F1'-P1F691.2 (7)C2-N2C1118.2 (2)F4'-P1-F691.2 (7)C2-N2-H2120.9F4'-P1-F385.3 (6)C12-N3C14125.5 (2)F4'-P1-F393.5 (5)N2C1C5118.8 (2)F4'-P1-F394.3 (8)C5-O1C15117.5 (2)F6-P1-F390.5 (2)N2C1C5118.6 (2)F4'-P1-F351.7 (7)N2C1C5118.6 (2)F4'-P1-F2125.7 (8)N2C2C	N1—C9		1.478 (3)	C10-	-H10	0.93	300
N2C11.362 (3)C11H110.9300N2H20.8600C12H120.9300N3C31.324 (3)C13H130.9300N3C121.369 (4)C14H14A0.9600N3C141.464 (3)C14H14B0.9600O1C51.366 (3)C14H14C0.9600O1C51.436 (4)C15H15A0.9600C1C81.423 (4)C15H15A0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600C1C51.429 (4)C15H15C0.9600F1'-P1F6174.1 (6)C2N2C1118.2 (2)F4'-P1-F691.2 (7)C2N2H2120.9F1'-P1-F393.6 (5)C1-N2H2120.9F4'-P1-F3'92.0 (6)C3-N3C14125.2 (2)F4'-P1-F385.3 (6)C12N3C14125.2 (2)F1'-P1-F385.3 (6)C12-N3C14125.6 (2)F4'-P1-F390.5 (2)N2C1-C5118.8 (2)F4'-P1-F390.5 (2)N2-C1-C5118.8 (2)F1'-P1-F213.3 (2)N2-C2-C4123.3 (3)F6-P1-F291.3 (2)N2-C2-C9116.2 (2)F3'-P1-F291.3 (2)N2-C2-C9116.2 (2)F3'-P1-F290.7 (19)N1-C3-N3109.0 (2)F1'-P1-F5'91.8 (5)N1-C3-H3125.5	N2—C2		1.323 (3)	C11-	C13	1.41	11 (4)
N2-H20.8600C12-H120.9300N3-C31.324 (3)C13-H130.9300N3-C121.369 (4)C14-H14A0.9600N3-C141.464 (3)C14-H14B0.9600O1-C51.366 (3)C14-H14C0.9600O1-C51.366 (3)C14-H14C0.9600C1-C81.423 (4)C15-H15A0.9600C1-C51.429 (4)C15-H15B0.9600C1-C51.429 (4)C15-H15C0.9600C1-C51.429 (4)C15-H15C0.9600C1-C51.429 (4)C15-H15C0.9600F1'-P1-F6174.1 (6)C2-N2-C1118.2 (2)F4'-P1-F691.2 (7)C2-N2-H2120.9F1'-P1-F593.6 (5)C1-N2-H2120.9F4'-P1-F393.6 (5)C1-N2-H2120.9F4'-P1-F393.6 (5)C12-N3-C14125.2 (2)F4'-P1-F385.3 (6)C12-N3-C14125.5 (2)F4'-P1-F3143.4 (8)C5-O1-C15117.5 (2)F6-P1-F390.5 (2)N2-C1-C5118.8 (2)F1'-P1-F2143.4 (8)C5-O1-C15118.6 (2)F4'-P1-F213.3 (3)F6-P1-F213.3 (3)F6-P1-F291.3 (2)N2-C2-C4123.3 (3)F6-P1-F291.3 (2)N2-C2-C9116.2 (2)F3'-P1-F2142.3 (7)C4-C2-C9120.5 (2)F3'-P1-F290.9 (6)N1-C3-H3109.0 (2)F1'-P1-F5'90.8 (5)N1-C3-H3125.5	N2—C1		1.362 (3)	C11-	-H11	0.93	300
N3-C31.324 (3)C13-H130.9300N3-C121.369 (4)C14-H14A0.9600N3-C141.464 (3)C14-H14B0.9600O1-C51.366 (3)C14-H14C0.9600O1-C151.436 (4)C15-H15A0.9600C1-C81.423 (4)C15-H15B0.9600C1-C51.429 (4)C15-H15C0.9600C1-C51.429 (4)C15-H15C0.9600F1'-P1-F4'94.7 (6)C10-N1-C9124.7 (2)F1'-P1-F6174.1 (6)C2-N2-C1118.2 (2)F4'-P1-F691.2 (7)C2-N2-H2120.9F1'-P1-F3'93.6 (5)C1-N2-H2120.9F4'-P1-F3'92.0 (6)C3-N3-C12108.3 (2)F6-P1-F3'87.0 (7)C3-N3-C14125.2 (2)F1'-P1-F5143.4 (8)C5-O1-C15117.5 (2)F6-P1-F390.5 (2)N2-C1-C5118.8 (2)F1'-P1-F2125.7 (8)N2-C2-C4123.3 (3)F6-P1-F291.3 (2)C2-C2-C9116.2 (2)F4'-P1-F2125.7 (8)N2-C2-C9120.5 (2)F3'-P1-F2142.3 (7)C4-C2-C9120.5 (2)F3'-P1-F290.7 (19)N1-C3-N3109.0 (2)F1'-P1-F5'90.9 (6)N3-C3-H3125.5	N2—H2		0.8600	C12-	-H12	0.93	300
N3-C121.369 (4)C14-H14A0.9600N3-C141.464 (3)C14-H14B0.9600O1-C51.366 (3)C14-H14C0.9600O1-C151.436 (4)C15-H15A0.9600C1-C81.423 (4)C15-H15B0.9600C1-C51.429 (4)C15-H15C0.9600C1-C51.429 (4)C15-H15C0.9600F1'-P1-F4'94.7 (6)C10-N1-C9124.7 (2)F1'-P1-F6174.1 (6)C2-N2-C1118.2 (2)F4'-P1-F691.2 (7)C2-N2-H2120.9F1'-P1-F3'93.6 (5)C1-N2-H2120.9F4'-P1-F3'92.0 (6)C3-N3-C14125.2 (2)F1'-P1-F3'85.3 (6)C12-N3-C14125.2 (2)F1'-P1-F385.3 (6)C12-N3-C14126.5 (2)F4'-P1-F390.5 (2)N2-C1-C8122.6 (2)F3'-P1-F351.7 (7)N2-C1-C5118.8 (2)F1'-P1-F2125.7 (8)N2-C2-C4123.3 (3)F6-P1-F291.3 (2)N2-C2-C9116.2 (2)F3'-P1-F2143.3 (7)C4-C2-C9120.5 (2)F3'-P1-F290.74 (19)N1-C3-N3109.0 (2)F1'-P1-F5'91.8 (5)N1-C3-H3125.5	N3—C3		1.324 (3)	C13-	-H13	0.93	300
N3C141.464 (3)C14H14B0.9600O1C51.366 (3)C14H14C0.9600O1C151.436 (4)C15H15A0.9600C1C81.423 (4)C15H15B0.9600C1C51.429 (4)C15H15C0.9600F1'-P1F4'94.7 (6)C10N1C9124.7 (2)F1'-P1F6174.1 (6)C2N2C1118.2 (2)F4'-P1F691.2 (7)C2N2H2120.9F1'-P1F3'93.6 (5)C1N2H2108.3 (2)F6-P1F3'92.0 (6)C3N3C14125.2 (2)F1'-P1-F385.3 (6)C12N3C14126.5 (2)F4'-P1-F3143.4 (8)C5O1-C15117.5 (2)F6-P1-F390.5 (2)N2C1C8122.6 (2)F3'-P1-F351.7 (7)N2C1C5118.8 (2)F1'-P1-F213.2)N2C2C4123.3 (3)F6-P1-F291.3 (2)N2C2C9116.2 (2)F3'-P1-F2142.3 (7)C4C2C9120.9F3'-P1-F290.74 (19)N1-C3N3109.0 (2)F1'-P1-F5'91.8 (5)N1-C3H3125.5	N3—C12		1.369 (4)	C14-	-H14A	0.96	500
O1-C5 $1.366 (3)$ $C14-H14C$ $0.9600$ $O1-C15$ $1.436 (4)$ $C15-H15A$ $0.9600$ $C1-C8$ $1.423 (4)$ $C15-H15B$ $0.9600$ $C1-C5$ $1.429 (4)$ $C15-H15C$ $0.9600$ $F1'-P1-F4'$ $94.7 (6)$ $C10-N1-C9$ $124.7 (2)$ $F1'-P1-F6$ $174.1 (6)$ $C2-N2-C1$ $118.2 (2)$ $F4'-P1-F6$ $91.2 (7)$ $C2-N2-H2$ $120.9$ $F4'-P1-F3'$ $93.6 (5)$ $C1-N2-H2$ $108.3 (2)$ $F4'-P1-F3'$ $92.0 (6)$ $C3-N3-C12$ $108.3 (2)$ $F6-P1-F3'$ $87.0 (7)$ $C3-N3-C14$ $125.2 (2)$ $F4'-P1-F3$ $85.3 (6)$ $C12-N3-C14$ $126.5 (2)$ $F4'-P1-F3$ $90.5 (2)$ $N2-C1-C8$ $122.6 (2)$ $F4'-P1-F3$ $51.7 (7)$ $N2-C1-C5$ $118.8 (2)$ $F1'-P1-F2$ $84.7 (6)$ $C8-C1-C5$ $118.6 (2)$ $F1'-P1-F2$ $125.7 (8)$ $N2-C2-C4$ $123.3 (3)$ $F6-P1-F2$ $91.3 (2)$ $N2-C2-C9$ $162.2 (2)$ $F3'-P1-F2$ $142.3 (7)$ $C4-C2-C9$ $125.5 (2)$ $F3'-P1-F2$ $90.9 (6)$ $N3-C3-H3$ $109.0 (2)$	N3—C14		1.464 (3)	C14–	-H14B	0.90	500
O1-C15 $1.436$ (4) $C15-H15A$ $0.9600$ $C1-C8$ $1.423$ (4) $C15-H15B$ $0.9600$ $C1-C5$ $1.429$ (4) $C15-H15C$ $0.9600$ $F1'-P1-F4'$ $94.7$ (6) $C10-N1-C9$ $124.7$ (2) $F1'-P1-F6$ $174.1$ (6) $C2-N2-C1$ $118.2$ (2) $F4'-P1-F6$ $91.2$ (7) $C2-N2-H2$ $120.9$ $F1'-P1-F3'$ $93.6$ (5) $C1-N2-H2$ $120.9$ $F4'-P1-F3'$ $92.0$ (6) $C3-N3-C12$ $108.3$ (2) $F6-P1-F3'$ $87.0$ (7) $C3-N3-C14$ $125.2$ (2) $F1'-P1-F3$ $85.3$ (6) $C12-N3-C14$ $126.5$ (2) $F4'-P1-F3$ $143.4$ (8) $C5-O1-C15$ $117.5$ (2) $F6-P1-F3$ $90.5$ (2) $N2-C1-C8$ $122.6$ (2) $F3'-P1-F3$ $51.7$ (7) $N2-C1-C5$ $118.8$ (2) $F1'-P1-F2$ $84.7$ (6) $C8-C1-C5$ $118.6$ (2) $F4'-P1-F2$ $125.7$ (8) $N2-C2-C4$ $123.3$ (3) $F6-P1-F2$ $91.3$ (2) $N2-C2-C9$ $16.2$ (2) $F3'-P1-F2$ $142.3$ (7) $C4-C2-C9$ $120.5$ (2) $F3-P1-F2$ $90.74$ (19) $N1-C3-N3$ $109.0$ (2) $F1'-P1-F5'$ $91.8$ (5) $N1-C3-H3$ $125.5$ $F4'-P1-F5'$ $90.9$ (6) $N3-C3-H3$ $125.5$	O1—C5		1.366 (3)	C14–	-H14C	0.90	500
C1-C81.423 (4)C15-H15B0.9600C1-C51.429 (4)C15-H15C0.9600F1'-P1-F4'94.7 (6)C10-N1-C9124.7 (2)F1'-P1-F6174.1 (6)C2-N2-C1118.2 (2)F4'-P1-F691.2 (7)C2-N2-H2120.9F1'-P1-F3'93.6 (5)C1-N2-H2120.9F4'-P1-F3'92.0 (6)C3-N3-C12108.3 (2)F6-P1-F3'87.0 (7)C3-N3-C14125.2 (2)F1'-P1-F385.3 (6)C12-N3-C14126.5 (2)F4'-P1-F3143.4 (8)C5-O1-C15117.5 (2)F6-P1-F390.5 (2)N2-C1-C8122.6 (2)F3'-P1-F351.7 (7)N2-C1-C5118.8 (2)F1'-P1-F284.7 (6)C8-C1-C5118.6 (2)F4'-P1-F2125.7 (8)N2-C2-C4123.3 (3)F6-P1-F291.3 (2)N2-C2-C9116.2 (2)F3'-P1-F290.74 (19)N1-C3-N3109.0 (2)F1'-P1-F5'91.8 (5)N1-C3-H3125.5	O1—C15		1.436 (4)	C15-	-H15A	0.90	500
C1—C51.429 (4)C15—H15C0.9600F1'—P1—F4'94.7 (6)C10—N1—C9124.7 (2)F1'—P1—F6174.1 (6)C2—N2—C1118.2 (2)F4'—P1—F691.2 (7)C2—N2—H2120.9F1'—P1—F3'93.6 (5)C1—N2—H2120.9F4'—P1—F3'92.0 (6)C3—N3—C12108.3 (2)F6—P1—F3'87.0 (7)C3—N3—C14125.2 (2)F1'—P1—F385.3 (6)C12—N3—C14126.5 (2)F4'—P1—F3143.4 (8)C5—O1—C15117.5 (2)F6—P1—F390.5 (2)N2—C1—C8122.6 (2)F3'—P1—F351.7 (7)N2—C1—C5118.8 (2)F1'—P1—F284.7 (6)C8—C1—C5118.6 (2)F4'—P1—F2125.7 (8)N2—C2—C9116.2 (2)F3'—P1—F290.74 (19)N1—C3—N3109.0 (2)F1'—P1—F5'91.8 (5)N1—C3—H3125.5F4'—P1—F5'90.9 (6)N3—C3—H3125.5	C1—C8		1.423 (4)	C15-	-H15B	0.90	500
F1'-P1-F4'94.7 (6)C10-N1-C9124.7 (2)F1'-P1-F6174.1 (6)C2-N2-C1118.2 (2)F4'-P1-F691.2 (7)C2-N2-H2120.9F1'-P1-F3'93.6 (5)C1-N2-H2120.9F4'-P1-F3'92.0 (6)C3-N3-C12108.3 (2)F6-P1-F3'87.0 (7)C3-N3-C14125.2 (2)F1'-P1-F385.3 (6)C12-N3-C14126.5 (2)F4'-P1-F3143.4 (8)C5-O1-C15117.5 (2)F6-P1-F390.5 (2)N2-C1-C8122.6 (2)F3'-P1-F351.7 (7)N2-C1-C5118.8 (2)F1'-P1-F284.7 (6)C8-C1-C5118.6 (2)F4'-P1-F2125.7 (8)N2-C2-C4123.3 (3)F6-P1-F291.3 (2)N2-C2-C9116.2 (2)F3'-P1-F2142.3 (7)C4-C2-C9120.5 (2)F3-P1-F290.74 (19)N1-C3-N3109.0 (2)F1'-P1-F5'91.8 (5)N1-C3-H3125.5	C1—C5		1.429 (4)	C15–	-H15C	0.90	500
F1'-P1-F6174.1 (6)C2-N2-C1118.2 (2)F4'-P1-F691.2 (7)C2-N2-H2120.9F1'-P1-F3'93.6 (5)C1-N2-H2120.9F4'-P1-F3'92.0 (6)C3-N3-C12108.3 (2)F6-P1-F3'87.0 (7)C3-N3-C14125.2 (2)F1'-P1-F385.3 (6)C12-N3-C14126.5 (2)F4'-P1-F3143.4 (8)C5-O1-C15117.5 (2)F6-P1-F390.5 (2)N2-C1-C8122.6 (2)F3'-P1-F351.7 (7)N2-C1-C5118.8 (2)F1'-P1-F284.7 (6)C8-C1-C5118.6 (2)F4'-P1-F2125.7 (8)N2-C2-C4123.3 (3)F6-P1-F291.3 (2)N2-C2-C9116.2 (2)F3'-P1-F290.74 (19)N1-C3-N3109.0 (2)F1'-P1-F5'91.8 (5)N1-C3-H3125.5F4'-P1-F5'90.9 (6)N3-C3-H3125.5	F1'—P1—F4'		94.7 (6)	C10-	-N1-C9	124	.7 (2)
F4'-P1-F6 $91.2$ (7) $C2-N2-H2$ $120.9$ $F1'-P1-F3'$ $93.6$ (5) $C1-N2-H2$ $120.9$ $F4'-P1-F3'$ $92.0$ (6) $C3-N3-C12$ $108.3$ (2) $F6-P1-F3'$ $87.0$ (7) $C3-N3-C14$ $125.2$ (2) $F1'-P1-F3$ $85.3$ (6) $C12-N3-C14$ $126.5$ (2) $F4'-P1-F3$ $143.4$ (8) $C5-O1-C15$ $117.5$ (2) $F6-P1-F3$ $90.5$ (2) $N2-C1-C8$ $122.6$ (2) $F3'-P1-F3$ $51.7$ (7) $N2-C1-C5$ $118.8$ (2) $F1'-P1-F2$ $84.7$ (6) $C8-C1-C5$ $118.6$ (2) $F4'-P1-F2$ $125.7$ (8) $N2-C2-C4$ $123.3$ (3) $F6-P1-F2$ $91.3$ (2) $N2-C2-C9$ $116.2$ (2) $F3'-P1-F2$ $90.74$ (19) $N1-C3-N3$ $109.0$ (2) $F1'-P1-F5'$ $91.8$ (5) $N1-C3-H3$ $125.5$ $F4'-P1-F5'$ $90.9$ (6) $N3-C3-H3$ $125.5$	F1'—P1—F6		174.1 (6)	C2—	N2—C1	118	.2 (2)
F1'-P1-F3'93.6 (5) $C1-N2-H2$ 120.9 $F4'-P1-F3'$ 92.0 (6) $C3-N3-C12$ 108.3 (2) $F6-P1-F3'$ 87.0 (7) $C3-N3-C14$ 125.2 (2) $F1'-P1-F3$ 85.3 (6) $C12-N3-C14$ 126.5 (2) $F4'-P1-F3$ 143.4 (8) $C5-O1-C15$ 117.5 (2) $F6-P1-F3$ 90.5 (2) $N2-C1-C8$ 122.6 (2) $F3'-P1-F3$ 51.7 (7) $N2-C1-C5$ 118.8 (2) $F1'-P1-F2$ 84.7 (6) $C8-C1-C5$ 118.6 (2) $F4'-P1-F2$ 125.7 (8) $N2-C2-C4$ 123.3 (3) $F6-P1-F2$ 91.3 (2) $N2-C2-C9$ 116.2 (2) $F3'-P1-F2$ 142.3 (7) $C4-C2-C9$ 120.5 (2) $F3-P1-F2$ 90.74 (19) $N1-C3-N3$ 109.0 (2) $F1'-P1-F5'$ 91.8 (5) $N1-C3-H3$ 125.5 $F4'-P1-F5'$ 90.9 (6) $N3-C3-H3$ 125.5	F4'—P1—F6		91.2 (7)	C2—	N2—H2	120	.9
F4'-P1-F3'92.0 (6) $C3-N3-C12$ 108.3 (2) $F6-P1-F3'$ $87.0$ (7) $C3-N3-C14$ 125.2 (2) $F1'-P1-F3$ $85.3$ (6) $C12-N3-C14$ 126.5 (2) $F4'-P1-F3$ $143.4$ (8) $C5-O1-C15$ $117.5$ (2) $F6-P1-F3$ $90.5$ (2) $N2-C1-C8$ 122.6 (2) $F3'-P1-F3$ $51.7$ (7) $N2-C1-C5$ $118.8$ (2) $F1'-P1-F2$ $84.7$ (6) $C8-C1-C5$ $118.6$ (2) $F4'-P1-F2$ $125.7$ (8) $N2-C2-C4$ 123.3 (3) $F6-P1-F2$ $91.3$ (2) $N2-C2-C9$ $116.2$ (2) $F3'-P1-F2$ $90.74$ (19) $N1-C3-N3$ $109.0$ (2) $F1'-P1-F5'$ $91.8$ (5) $N1-C3-H3$ 125.5	F1'—P1—F3'		93.6 (5)	C1—	N2—H2	120	.9
F6-P1-F3' $87.0$ (7) $C3-N3-C14$ $125.2$ (2) $F1'-P1-F3$ $85.3$ (6) $C12-N3-C14$ $126.5$ (2) $F4'-P1-F3$ $143.4$ (8) $C5-O1-C15$ $117.5$ (2) $F6-P1-F3$ $90.5$ (2) $N2-C1-C8$ $122.6$ (2) $F3'-P1-F3$ $51.7$ (7) $N2-C1-C5$ $118.8$ (2) $F4'-P1-F2$ $84.7$ (6) $C8-C1-C5$ $118.6$ (2) $F4'-P1-F2$ $125.7$ (8) $N2-C2-C4$ $123.3$ (3) $F6-P1-F2$ $91.3$ (2) $N2-C2-C9$ $116.2$ (2) $F3'-P1-F2$ $142.3$ (7) $C4-C2-C9$ $120.5$ (2) $F3-P1-F2$ $90.74$ (19) $N1-C3-N3$ $109.0$ (2) $F1'-P1-F5'$ $91.8$ (5) $N1-C3-H3$ $125.5$	F4'—P1—F3'		92.0 (6)	С3—	N3—C12	108	.3 (2)
F1'-P1-F3 $85.3 (6)$ $C12-N3-C14$ $126.5 (2)$ $F4'-P1-F3$ $143.4 (8)$ $C5-O1-C15$ $117.5 (2)$ $F6-P1-F3$ $90.5 (2)$ $N2-C1-C8$ $122.6 (2)$ $F3'-P1-F3$ $51.7 (7)$ $N2-C1-C5$ $118.8 (2)$ $F1'-P1-F2$ $84.7 (6)$ $C8-C1-C5$ $118.6 (2)$ $F4'-P1-F2$ $125.7 (8)$ $N2-C2-C4$ $123.3 (3)$ $F6-P1-F2$ $91.3 (2)$ $N2-C2-C9$ $116.2 (2)$ $F3'-P1-F2$ $142.3 (7)$ $C4-C2-C9$ $120.5 (2)$ $F3-P1-F2$ $90.74 (19)$ $N1-C3-N3$ $109.0 (2)$ $F1'-P1-F5'$ $91.8 (5)$ $N1-C3-H3$ $125.5$	F6—P1—F3'		87.0 (7)	С3—	N3—C14	125	.2 (2)
F4'-P1-F3143.4 (8) $C5-O1-C15$ $117.5 (2)$ $F6-P1-F3$ $90.5 (2)$ $N2-C1-C8$ $122.6 (2)$ $F3'-P1-F3$ $51.7 (7)$ $N2-C1-C5$ $118.8 (2)$ $F1'-P1-F2$ $84.7 (6)$ $C8-C1-C5$ $118.6 (2)$ $F4'-P1-F2$ $125.7 (8)$ $N2-C2-C4$ $123.3 (3)$ $F6-P1-F2$ $91.3 (2)$ $N2-C2-C9$ $116.2 (2)$ $F3'-P1-F2$ $142.3 (7)$ $C4-C2-C9$ $120.5 (2)$ $F3-P1-F2$ $90.74 (19)$ $N1-C3-N3$ $109.0 (2)$ $F1'-P1-F5'$ $91.8 (5)$ $N1-C3-H3$ $125.5$	F1'—P1—F3		85.3 (6)	C12–	-N3-C14	126	.5 (2)
F6—P1—F390.5 (2)N2—C1—C8122.6 (2)F3'—P1—F3 $51.7$ (7)N2—C1—C5 $118.8$ (2)F1'—P1—F2 $84.7$ (6)C8—C1—C5 $118.6$ (2)F4'—P1—F2 $125.7$ (8)N2—C2—C4 $123.3$ (3)F6—P1—F2 $91.3$ (2)N2—C2—C9 $116.2$ (2)F3'—P1—F2 $142.3$ (7)C4—C2—C9 $120.5$ (2)F3—P1—F2 $90.74$ (19)N1—C3—N3 $109.0$ (2)F1'—P1—F5' $91.8$ (5)N1—C3—H3 $125.5$ F4'—P1—F5' $90.9$ (6)N3—C3—H3 $125.5$	F4'—P1—F3		143.4 (8)	С5—	O1—C15	117	.5 (2)
F3'—P1—F3 $51.7 (7)$ N2—C1—C5 $118.8 (2)$ F1'—P1—F2 $84.7 (6)$ $C8$ —C1—C5 $118.6 (2)$ F4'—P1—F2 $125.7 (8)$ $N2$ —C2—C4 $123.3 (3)$ F6—P1—F2 $91.3 (2)$ $N2$ —C2—C9 $116.2 (2)$ F3'—P1—F2 $142.3 (7)$ C4—C2—C9 $120.5 (2)$ F3—P1—F2 $90.74 (19)$ $N1$ —C3—N3 $109.0 (2)$ F1'—P1—F5' $91.8 (5)$ $N1$ —C3—H3 $125.5$ F4'—P1—F5' $90.9 (6)$ $N3$ —C3—H3 $125.5$	F6—P1—F3		90.5 (2)	N2—	-C1C8	122	.6 (2)
F1'-P1-F284.7 (6)C8-C1-C5118.6 (2)F4'-P1-F2125.7 (8)N2-C2-C4123.3 (3)F6-P1-F291.3 (2)N2-C2-C9116.2 (2)F3'-P1-F2142.3 (7)C4-C2-C9120.5 (2)F3-P1-F290.74 (19)N1-C3-N3109.0 (2)F1'-P1-F5'91.8 (5)N1-C3-H3125.5F4'-P1-F5'90.9 (6)N3-C3-H3125.5	F3'—P1—F3		51.7 (7)	N2—	-C1C5	118	.8 (2)
F4'-P1-F2125.7 (8)N2-C2-C4123.3 (3) $F6-P1-F2$ 91.3 (2)N2-C2-C9116.2 (2) $F3'-P1-F2$ 142.3 (7)C4-C2-C9120.5 (2) $F3-P1-F2$ 90.74 (19)N1-C3-N3109.0 (2) $F1'-P1-F5'$ 91.8 (5)N1-C3-H3125.5 $F4'-P1-F5'$ 90.9 (6)N3-C3-H3125.5	F1'—P1—F2		84.7 (6)	C8—	C1—C5	118	.6 (2)
F6—P1—F291.3 (2)N2—C2—C9116.2 (2)F3'—P1—F2142.3 (7)C4—C2—C9120.5 (2)F3—P1—F290.74 (19)N1—C3—N3109.0 (2)F1'—P1—F5'91.8 (5)N1—C3—H3125.5F4'—P1—F5'90.9 (6)N3—C3—H3125.5	F4'—P1—F2		125.7 (8)	N2—	-C2C4	123	.3 (3)
F3'-P1-F2142.3 (7)C4-C2-C9120.5 (2)F3-P1-F290.74 (19)N1-C3-N3109.0 (2)F1'-P1-F5'91.8 (5)N1-C3-H3125.5F4'-P1-F5'90.9 (6)N3-C3-H3125.5	F6—P1—F2		91.3 (2)	N2—	-C2C9	116	.2 (2)
F3—P1—F290.74 (19)N1—C3—N3109.0 (2)F1'—P1—F5'91.8 (5)N1—C3—H3125.5F4'—P1—F5'90.9 (6)N3—C3—H3125.5	F3'—P1—F2		142.3 (7)	C4—	C2—C9	120	.5 (2)
F1'P1F5'91.8 (5)N1C3H3125.5F4'P1F5'90.9 (6)N3C3H3125.5	F3—P1—F2		90.74 (19)	N1—	-C3—N3	109	.0 (2)
F4'—P1—F5' 90.9 (6) N3—C3—H3 125.5	F1'—P1—F5'		91.8 (5)	N1—	-С3—Н3	125	.5
	F4'—P1—F5'		90.9 (6)	N3—	-С3—Н3	125	.5

F6—P1—F5'	87.3 (7)	C6—C4—C2	118.9 (3)
F3'—P1—F5'	173.7 (7)	С6—С4—Н4	120.5
F3—P1—F5'	125.7 (8)	C2—C4—H4	120.5
F1'—P1—F4	91.4 (6)	O1C5C11	125.0 (3)
F4'—P1—F4	53.1 (8)	O1—C5—C1	114.9 (2)
F6—P1—F4	92.7 (3)	C11—C5—C1	120.1 (3)
F3—P1—F4	90.3 (2)	C4—C6—C8	120.0 (3)
F2—P1—F4	175.85 (18)	С4—С6—Н6	120.0
F5'—P1—F4	144.0 (8)	С8—С6—Н6	120.0
F1'—P1—F5	92.1 (6)	C13—C7—C8	119.5 (3)
F6—P1—F5	92.2 (2)	С13—С7—Н7	120.2
F3'—P1—F5	128.4 (7)	С8—С7—Н7	120.2
F3—P1—F5	177.34 (19)	C6—C8—C7	123.0 (3)
F2—P1—F5	89.34 (17)	C6—C8—C1	117.0 (3)
F5'—P1—F5	54.7 (8)	C7—C8—C1	119.9 (3)
F4—P1—F5	89.4 (2)	N1—C9—C2	112.1 (2)
F4'—P1—F1	89.2 (7)	N1—C9—H9A	109.2
F6—P1—F1	179.5 (3)	С2—С9—Н9А	109.2
F3'—P1—F1	93.3 (6)	N1—C9—H9B	109.2
F3—P1—F1	89.4 (2)	С2—С9—Н9В	109.2
F2—P1—F1	88.2 (2)	Н9А—С9—Н9В	107.9
F5'—P1—F1	92.4 (7)	C12-C10-N1	106.7 (2)
F4—P1—F1	87.8 (2)	С12—С10—Н10	126.6
F5—P1—F1	88.0 (2)	N1-C10-H10	126.6
F1'—P1—F2'	91.4 (5)	C5-C11-C13	120.2 (3)
F4'—P1—F2'	173.8 (6)	C5-C11-H11	119.9
F6—P1—F2'	82.7 (6)	C13—C11—H11	119.9
F3'—P1—F2'	88.6 (5)	C10-C12-N3	107.6 (2)
F2—P1—F2'	53.8 (7)	C10—C12—H12	126.2
F5'—P1—F2'	87.9 (5)	N3—C12—H12	126.2
F4—P1—F2'	127.9 (7)	C7—C13—C11	121.7 (3)
F5—P1—F2'	142.5 (7)	С7—С13—Н13	119.2
F1—P1—F2'	96.9 (6)	C11—C13—H13	119.2
F1'—P1—F6'	176.4 (6)	N3—C14—H14A	109.5
F4'—P1—F6'	88.6 (5)	N3—C14—H14B	109.5
F3'—P1—F6'	87.8 (5)	H14A—C14—H14B	109.5
F3—P1—F6'	93.0 (5)	N3—C14—H14C	109.5
F2—P1—F6'	92.2 (6)	H14A—C14—H14C	109.5
F5'—P1—F6'	86.6 (5)	H14B—C14—H14C	109.5
F4—P1—F6'	91.8 (6)	O1—C15—H15A	109.5
F5—P1—F6'	89.6 (5)	O1—C15—H15B	109.5
F1—P1—F6'	177.5 (6)	H15A—C15—H15B	109.5
F2'	85.3 (5)	01—C15—H15C	109.5
C3—N1—C10	108.4 (2)	H15A—C15—H15C	109.5
C3—N1—C9	126.7 (2)	H15B—C15—H15C	109.5
C2—N2—C1—C8	-0.2 (3)	C13—C7—C8—C6	-179.8 (3)
C2—N2—C1—C5	179.5 (2)	C13—C7—C8—C1	0.1 (4)
C1—N2—C2—C4	0.9 (4)	N2—C1—C8—C6	-0.7 (4)
C1—N2—C2—C9	-179.0 (2)	C5—C1—C8—C6	179.6 (2)

C10 N1 C2 N2	-0.8(2)	N2 C1 C9 C7	170.4(2)
C10— $N1$ — $C3$ — $N3$	-0.8 (3)	N2-CI-Co-C/	1/9.4 (2)
C9—N1—C3—N3	-175.3 (2)	C5-C1-C8-C7	-0.2 (4)
C12—N3—C3—N1	0.6 (3)	C3—N1—C9—C2	-16.9 (4)
C14—N3—C3—N1	177.7 (2)	C10-N1-C9-C2	169.4 (2)
N2-C2-C4-C6	-0.7 (4)	N2-C2-C9-N1	-93.1 (3)
C9—C2—C4—C6	179.3 (2)	C4—C2—C9—N1	87.0 (3)
C15—O1—C5—C11	1.4 (4)	C3—N1—C10—C12	0.7 (3)
C15—O1—C5—C1	-178.8 (3)	C9—N1—C10—C12	175.4 (2)
N2-C1-C5-O1	0.8 (3)	O1—C5—C11—C13	179.5 (2)
C8—C1—C5—O1	-179.4 (2)	C1—C5—C11—C13	-0.2 (4)
N2-C1-C5-C11	-179.4 (2)	N1-C10-C12-N3	-0.4 (3)
C8—C1—C5—C11	0.3 (4)	C3—N3—C12—C10	-0.1 (3)
C2—C4—C6—C8	-0.3 (4)	C14—N3—C12—C10	-177.2 (3)
C4—C6—C8—C7	-179.2 (3)	C8—C7—C13—C11	0.1 (4)
C4—C6—C8—C1	0.9 (4)	C5-C11-C13-C7	0.0 (4)

## Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	$D\!\!-\!\!\mathrm{H}\!\cdots\!\!A$
C12—H12···F1 <sup>i</sup>	0.93	2.46	3.204 (5)	137
C9—H9A…F2 <sup>ii</sup>	0.97	2.49	3.244 (4)	135
C3—H3···O1 <sup>iii</sup>	0.93	2.27	3.122 (3)	152

Symmetry codes: (i) -*x*+1/2, *y*+1/2, -*z*+3/2; (ii) *x*+1/2, *y*+1/2, *z*-1; (iii) -*x*+1, *y*, -*z*+1/2.



Fig. 1

