Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

The protonated β-iminoamine 1,3-bis(2-methylanilino)-1-phenylbutane(1+) hexafluorophosphate

Najoua Belhaj Mbarek Elmkacher,[a]* Mohamed Rzaigui[b] and Faouzi Bouachir[a]

[a]Département de Chimie, Faculté des Sciences, 5019 Monastir, Tunisia, and [b]Département de Chimie, Faculté des Sciences, 7021 Bizerte, Tunisia
Correspondence e-mail: najouahaj@yahoo.fr

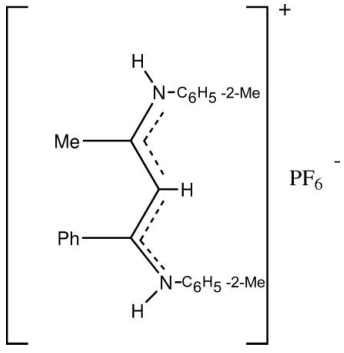
Received 3 May 2007; accepted 29 May 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.011 Å; R factor = 0.051; wR factor = 0.145; data-to-parameter ratio = 7.0.

The title compound, $C_{24}H_{25}N_2^+\cdot PF_6^-$, is a bis(imininium) hexafluorophosphate salt with interionic interactions. Significant delocalization within the π-system of the N—C—C—C—N backbone is suggested.

Related literature

For related literature, see: Allen *et al.* (1992); Bourget-Merle *et al.* (2002); Holm & O'Connor (1971); Landolsi *et al.* (2002).



Experimental

Crystal data

$C_{24}H_{25}N_2^+\cdot F_6P^-$
M_r = 486.43
Orthorhombic, $Pc2_1b$
a = 6.5352 (2) Å
b = 17.8580 (3) Å
c = 20.4249 (3) Å
V = 2383.70 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 293 (2) K
0.35 × 0.23 × 0.23 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Absorption correction: none
4127 measured reflections
2170 independent reflections
1221 reflections with $I > 2\sigma(I)$
R_{int} = 0.069
2 standard reflections
frequency: 120 min
intensity decay: 2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.145
S = 1.01
2170 reflections
310 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter: 0.1 (3)

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.317 (8)	C3—C5	1.492 (9)
N1—C18	1.436 (8)	C4—C1	1.491 (8)
C3—N2	1.340 (9)	N2—C11	1.434 (9)
C3—C2	1.387 (9)	C1—C2	1.388 (9)
C1—N1—C18	123.8 (6)	N1—C1—C2	117.8 (6)
N2—C3—C2	120.5 (6)	N1—C1—C4	115.4 (6)
N2—C3—C5	115.9 (6)	C3—C2—C1	130.2 (6)
C3—N2—C11	121.7 (5)		

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank Chtioui Ahlem for the structure resolution.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AV3093).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bourget-Merle, L., Lappert, M. F. & Severn, J. R. (2002). *Chem. Rev.* **102**, 3031–3065.
Enraf–Nonius (1994). *CAD-4 EXPRESS*. Version 5.1/1.2. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Holm, R. H. & O'Connor, M. J. (1971). *Prog. Inorg. Chem.* **14**, 241–401.
Landolsi, K., Rzaigui, M. & Bouachir, F. (2002). *Tetrahedron Lett.* **43**, 9463–9466.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.

 doi:10.1107/S1600536807026232

supplementary materials

Acta Cryst. (2007). E**63**, o3075 [**doi:10.1107/S1600536807026232**]

The protonated β-iminoamine 1,3-bis(2-methylanilino)-1-phenylbutane(1+) hexafluorophosphate

N. B. M. Elmkacher, M. Rzaigui and F. Bouachir

Comment

Recent years have witnessed an impressive revival of interest in bidentate β-diketiminate ligands, which have been known for more than four decades (Holm & O'Connor, 1971). β-Diketiminates are important spectator ligands by virtue of their strong binding to metals, their tunable and extensive steric demands, and their diversity of bonding modes (Bourget-Merle *et al.*, 2002). For example, their steric and electronic properties can be readily tuned by an appropriate choice of starting materials used in their synthesis. They can form a conjugated π-system due to essential electron delocalization along the ligand. Recently, we have been interested in the synthesis of the new nonsymmetrical β-iminoamines and their coordination in their neutral form as β-diimine nickel complexes (Landolsi *et al.*, 2002).

The crystal structure is composed of a cation (β-iminoamineH) and hexafluorophosphate anion with interionic interaction. The shortest F—C distance is F2—C13 [3.551 Å]. The hexafluorophosphate anion possesses an octahedral geometry, with P—F distances ranging from 1.523 to 1.585 Å. The cation adopts an open configuration with intramolecular interaction. The distance H2—N2 (2.366 Å) and H2—N1 (2.487 Å) are shorter than the sum of their van der Waals radii. The N—C [N1—C1 1.317 and N2—C3 1.340 Å] and the C—C [C2—C3 1.387 and C2—C1 1.388 Å] bond distances lie intermediate between the corresponding single and double-bond distances, which suggest significant delocalization within the π-system of the N—C—C—C—N backbone (Allen *et al.*, 1992). The methyl and phenyl groups of the backbone adopt a *syn* orientation; the two aryl rings adopt a synperiplanar arrangement in order to minimize steric crowding.

Experimental

Compound (I) was obtained after recristallization of the cationic methallyl β-diimine Nickel complexes in methylene chloride with traces of acid. In fact the β-diimine precursors were synthesized by acid-catalysed condensation of benzoylacteone and 2-methylaniline in toluene using a Dean Stark apparatus. Crystals were obtained from a diluted solution in methylene chloride /n-hexane at 243 K.

Refinement

Hydrogen atoms H2, HN1 and HN2 were located in a Fourier map and refined freely. All the other H atoms were placed in calculated positions and allowed to ride on their parent atoms. U_{iso} of H atoms are equal to 1.2 U_{iso} of the parent atom. We chose the non standard space group because when we chose the standard space group, we found problems in the structure resolution.

Figures

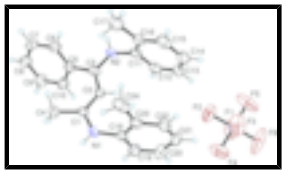


Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by circles of arbitrary size.

1,3-bis(2-methylanilino)-1-phenylbutane(1+) hexafluorophosphate

Crystal data

$C_{24}H_{25}N_2^+ \cdot F_6P^-$	F_{000} = 1008
M_r = 486.43	D_x = 1.355 Mg m^{-3}
Orthorhombic, $Pc2_1b$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P -2bc -2c	Cell parameters from 0 reflections
a = 6.5352 (2) Å	θ = 0–0º
b = 17.8580 (3) Å	μ = 0.18 mm^{-1}
c = 20.4249 (3) Å	T = 293 (2) K
V = 2383.70 (9) Å^3	Prism, colourless
Z = 4	0.35 × 0.23 × 0.23 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer	R_{int} = 0.069
Radiation source: fine-focus sealed tube	θ_{max} = 25.0º
Monochromator: graphite	θ_{min} = 2.3º
T = 293(2) K	h = −7→7
non–profiled ω scans	k = 0→21
Absorption correction: none	l = 0→24
4127 measured reflections	2 standard reflections
2170 independent reflections	every 120 min
1221 reflections with $I > 2\sigma(I)$	intensity decay: −2%

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.051	$w = 1/[\sigma^2(F_o^2) + (0.073P)^2 + 0.2103P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.145	$(\Delta/\sigma)_{max}$ = 0.026
S = 1.01	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
2170 reflections	$\Delta\rho_{min}$ = −0.23 e Å^{-3}

310 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), with how many Friedel pairs?
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.1 (3)
Secondary atom site location: difference Fourier map	

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^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
P1	0.4127 (3)	1.09449 (11)	0.65597 (9)	0.0592 (5)
F1	0.1705 (6)	1.0943 (4)	0.6594 (3)	0.122 (2)
F2	0.4234 (8)	1.0619 (4)	0.7256 (2)	0.116 (2)
F3	0.6520 (7)	1.0964 (4)	0.6521 (3)	0.130 (2)
F4	0.4089 (11)	1.0144 (3)	0.6304 (3)	0.145 (3)
F5	0.4123 (12)	1.1747 (3)	0.6844 (5)	0.183 (4)
F6	0.3998 (11)	1.1268 (6)	0.5861 (3)	0.201 (4)
N1	0.9600 (9)	0.7527 (3)	0.8552 (3)	0.0527 (15)
HN1	1.017 (11)	0.710 (4)	0.846 (3)	0.063*
N2	0.7305 (8)	0.9378 (3)	0.9982 (3)	0.0537 (15)
HN2	0.690 (10)	0.954 (4)	1.037 (4)	0.064*
C1	0.8882 (10)	0.7642 (3)	0.9146 (3)	0.0460 (15)
C2	0.8214 (10)	0.8358 (3)	0.9301 (3)	0.0471 (16)
H2	0.835 (10)	0.872 (4)	0.903 (3)	0.057*
C3	0.7419 (10)	0.8638 (4)	0.9881 (3)	0.0531 (17)
C4	0.9014 (12)	0.6988 (4)	0.9598 (3)	0.0604 (19)
H4A	0.7756	0.6711	0.9582	0.073*
H4B	0.9246	0.7162	1.0037	0.073*
H4C	1.0125	0.6670	0.9467	0.073*
C5	0.6616 (10)	0.8156 (4)	1.0419 (3)	0.0518 (17)
C6	0.7487 (12)	0.8162 (5)	1.1027 (3)	0.070 (2)
H6	0.8540	0.8495	1.1120	0.084*
C7	0.6804 (15)	0.7672 (5)	1.1508 (3)	0.085 (3)
H7	0.7430	0.7667	1.1917	0.102*
C8	0.5230 (14)	0.7200 (5)	1.1382 (4)	0.077 (2)
H8	0.4765	0.6876	1.1706	0.092*
C9	0.4328 (12)	0.7202 (5)	1.0780 (4)	0.076 (2)

H9	0.3247	0.6878	1.0696	0.091*
C10	0.4996 (12)	0.7680 (4)	1.0291 (3)	0.067 (2)
H10	0.4365	0.7681	0.9883	0.081*
C11	0.8208 (11)	0.9904 (4)	0.9537 (3)	0.0568 (18)
C12	0.7082 (13)	1.0115 (4)	0.8981 (4)	0.069 (2)
H12	0.5737	0.9955	0.8929	0.084*
C13	0.7985 (17)	1.0559 (4)	0.8513 (4)	0.079 (2)
H13	0.7266	1.0690	0.8137	0.095*
C14	0.9954 (18)	1.0810 (5)	0.8603 (5)	0.084 (3)
H14	1.0554	1.1114	0.8287	0.101*
C15	1.1061 (14)	1.0614 (4)	0.9158 (5)	0.079 (2)
H15	1.2383	1.0795	0.9216	0.095*
C16	1.0175 (12)	1.0140 (4)	0.9632 (3)	0.0581 (18)
C17	1.1384 (14)	0.9891 (5)	1.0219 (4)	0.088 (3)
H17A	1.0631	1.0003	1.0611	0.106*
H17B	1.2672	1.0149	1.0228	0.106*
H17C	1.1622	0.9361	1.0193	0.106*
C18	0.9586 (11)	0.8083 (3)	0.8044 (3)	0.0502 (17)
C19	0.7921 (12)	0.8119 (5)	0.7617 (4)	0.067 (2)
H19	0.6913	0.7752	0.7633	0.080*
C20	0.7763 (15)	0.8686 (6)	0.7179 (4)	0.088 (3)
H20	0.6637	0.8720	0.6903	0.106*
C21	0.9319 (17)	0.9217 (5)	0.7152 (4)	0.085 (3)
H21	0.9236	0.9607	0.6852	0.102*
C22	1.0939 (15)	0.9173 (4)	0.7556 (4)	0.074 (2)
H22	1.1956	0.9536	0.7525	0.088*
C23	1.1152 (12)	0.8606 (4)	0.8017 (3)	0.0617 (19)
C24	1.2965 (12)	0.8572 (5)	0.8484 (4)	0.089 (3)
H24A	1.4163	0.8761	0.8268	0.106*
H24B	1.3195	0.8062	0.8613	0.106*
H24C	1.2679	0.8870	0.8864	0.106*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C24	0.063 (5)	0.078 (6)	0.125 (8)	−0.021 (4)	0.007 (5)	−0.029 (6)
P1	0.0545 (11)	0.0530 (10)	0.0701 (12)	−0.0028 (12)	−0.0011 (10)	0.0105 (10)
F1	0.057 (3)	0.132 (4)	0.176 (5)	0.000 (4)	−0.009 (3)	0.062 (4)
N1	0.066 (4)	0.033 (3)	0.059 (4)	0.001 (3)	0.006 (3)	0.000 (3)
C3	0.050 (4)	0.052 (4)	0.057 (4)	−0.008 (3)	−0.003 (3)	−0.011 (4)
C4	0.079 (5)	0.046 (4)	0.057 (4)	0.005 (4)	0.002 (4)	0.002 (3)
N2	0.058 (4)	0.043 (3)	0.060 (3)	−0.009 (3)	0.013 (3)	−0.016 (3)
C23	0.073 (5)	0.051 (4)	0.061 (4)	−0.006 (4)	0.022 (4)	−0.016 (4)
C9	0.069 (5)	0.079 (5)	0.079 (6)	−0.021 (5)	0.006 (4)	0.011 (5)
C1	0.049 (4)	0.043 (4)	0.046 (4)	−0.007 (3)	0.005 (3)	−0.004 (3)
F2	0.103 (4)	0.164 (6)	0.080 (3)	−0.022 (4)	−0.016 (3)	0.041 (3)
F3	0.058 (3)	0.158 (5)	0.175 (5)	−0.005 (4)	0.012 (3)	0.058 (5)
C15	0.080 (5)	0.060 (5)	0.098 (6)	−0.014 (5)	0.026 (5)	−0.013 (5)

C16	0.062 (5)	0.048 (4)	0.064 (4)	−0.007 (4)	0.003 (4)	−0.011 (3)
C6	0.090 (6)	0.068 (5)	0.052 (4)	−0.016 (5)	−0.004 (4)	−0.009 (4)
C10	0.074 (5)	0.071 (5)	0.056 (4)	−0.016 (5)	0.000 (4)	0.011 (4)
C13	0.122 (8)	0.052 (4)	0.063 (5)	0.011 (5)	−0.008 (5)	0.001 (4)
C21	0.130 (9)	0.071 (6)	0.054 (5)	0.010 (6)	0.030 (6)	0.016 (4)
C8	0.108 (7)	0.072 (5)	0.051 (5)	−0.015 (5)	0.020 (4)	−0.003 (4)
F4	0.166 (7)	0.095 (4)	0.175 (6)	0.007 (4)	−0.019 (5)	−0.051 (4)
C19	0.073 (5)	0.072 (5)	0.055 (5)	−0.007 (4)	0.001 (4)	0.000 (4)
C14	0.121 (7)	0.060 (6)	0.071 (6)	0.000 (6)	0.026 (5)	−0.001 (4)
C18	0.061 (5)	0.045 (4)	0.044 (4)	−0.001 (3)	0.019 (3)	−0.008 (3)
C20	0.092 (7)	0.109 (7)	0.064 (5)	0.007 (6)	−0.004 (5)	0.018 (5)
C2	0.061 (4)	0.037 (3)	0.043 (4)	−0.003 (3)	0.015 (3)	−0.001 (3)
C22	0.098 (6)	0.057 (5)	0.065 (5)	−0.017 (5)	0.032 (5)	−0.004 (4)
C5	0.056 (4)	0.051 (4)	0.049 (4)	−0.010 (3)	0.009 (3)	−0.008 (3)
C12	0.076 (5)	0.050 (4)	0.082 (5)	0.008 (4)	0.000 (4)	−0.018 (4)
C11	0.068 (5)	0.041 (4)	0.062 (4)	0.002 (4)	−0.001 (4)	−0.012 (4)
C17	0.078 (6)	0.085 (6)	0.100 (7)	−0.012 (5)	−0.012 (5)	−0.009 (5)
C7	0.127 (8)	0.084 (6)	0.043 (4)	−0.004 (6)	−0.012 (5)	−0.017 (5)
F5	0.178 (8)	0.073 (4)	0.299 (10)	−0.005 (5)	−0.020 (7)	−0.062 (6)
F6	0.132 (5)	0.342 (13)	0.129 (5)	−0.037 (7)	−0.016 (4)	0.148 (7)

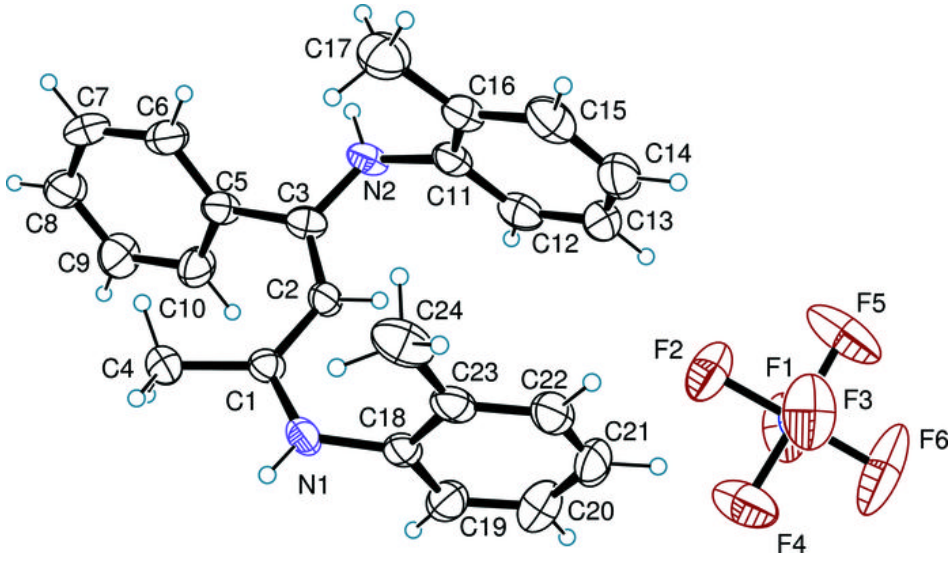
Geometric parameters (Å, °)

C24—C23	1.522 (11)	C15—H15	0.9300
C24—H24A	0.9600	C16—C11	1.367 (10)
C24—H24B	0.9600	C16—C17	1.504 (10)
C24—H24C	0.9600	C6—C5	1.367 (9)
P1—F4	1.523 (6)	C6—C7	1.389 (11)
P1—F2	1.539 (5)	C6—H6	0.9300
P1—F6	1.541 (6)	C10—C5	1.382 (9)
P1—F5	1.547 (6)	C10—H10	0.9300
P1—F3	1.566 (5)	C13—C14	1.374 (12)
P1—F1	1.585 (5)	C13—C12	1.375 (11)
N1—C1	1.317 (8)	C13—H13	0.9300
N1—C18	1.436 (8)	C21—C22	1.344 (11)
N1—HN1	0.87 (7)	C21—C20	1.391 (13)
C3—N2	1.340 (9)	C21—H21	0.9300
C3—C2	1.387 (9)	C8—C7	1.354 (12)
C3—C5	1.492 (9)	C8—H8	0.9300
C4—C1	1.491 (8)	C19—C20	1.354 (11)
C4—H4A	0.9600	C19—C18	1.396 (10)
C4—H4B	0.9600	C19—H19	0.9300
C4—H4C	0.9600	C14—H14	0.9300
N2—C11	1.434 (9)	C20—H20	0.9300
N2—HN2	0.88 (7)	C2—H2	0.86 (7)
C23—C18	1.387 (9)	C22—H22	0.9300
C23—C22	1.390 (10)	C12—C11	1.404 (10)
C9—C8	1.364 (10)	C12—H12	0.9300
C9—C10	1.384 (9)	C17—H17A	0.9600

C9—H9	0.9300	C17—H17B	0.9600
C1—C2	1.388 (9)	C17—H17C	0.9600
C15—C14	1.389 (13)	C7—H7	0.9300
C15—C16	1.410 (10)		
C23—C24—H24A	109.5	C5—C6—C7	120.2 (7)
C23—C24—H24B	109.5	C5—C6—H6	119.9
H24A—C24—H24B	109.5	C7—C6—H6	119.9
C23—C24—H24C	109.5	C5—C10—C9	118.9 (7)
H24A—C24—H24C	109.5	C5—C10—H10	120.5
H24B—C24—H24C	109.5	C9—C10—H10	120.5
F4—P1—F2	87.9 (4)	C14—C13—C12	119.8 (8)
F4—P1—F6	91.9 (6)	C14—C13—H13	120.1
F2—P1—F6	179.4 (4)	C12—C13—H13	120.1
F4—P1—F5	177.7 (5)	C22—C21—C20	120.8 (8)
F2—P1—F5	90.2 (5)	C22—C21—H21	119.6
F6—P1—F5	90.1 (6)	C20—C21—H21	119.6
F4—P1—F3	91.1 (4)	C7—C8—C9	119.8 (7)
F2—P1—F3	90.5 (3)	C7—C8—H8	120.1
F6—P1—F3	90.0 (4)	C9—C8—H8	120.1
F5—P1—F3	90.0 (5)	C20—C19—C18	120.4 (8)
F4—P1—F1	89.8 (4)	C20—C19—H19	119.8
F2—P1—F1	90.2 (3)	C18—C19—H19	119.8
F6—P1—F1	89.2 (4)	C13—C14—C15	121.0 (8)
F5—P1—F1	89.1 (4)	C13—C14—H14	119.5
F3—P1—F1	178.8 (4)	C15—C14—H14	119.5
C1—N1—C18	123.8 (6)	C23—C18—N1	119.3 (7)
C1—N1—HN1	120 (5)	C19—C18—N1	119.3 (6)
C18—N1—HN1	116 (5)	C19—C20—C21	118.7 (9)
N2—C3—C2	120.5 (6)	C19—C20—H20	120.6
N2—C3—C5	115.9 (6)	C21—C20—H20	120.7
C2—C3—C5	123.5 (6)	C3—C2—C1	130.2 (6)
C1—C4—H4A	109.5	C3—C2—H2	108 (5)
C1—C4—H4B	109.5	C1—C2—H2	121 (5)
H4A—C4—H4B	109.5	C21—C22—C23	122.5 (8)
C1—C4—H4C	109.5	C21—C22—H22	118.8
H4A—C4—H4C	109.5	C23—C22—H22	118.8
H4B—C4—H4C	109.5	C6—C5—C10	119.7 (7)
C3—N2—C11	121.7 (5)	C6—C5—C3	121.2 (6)
C3—N2—HN2	118 (5)	C10—C5—C3	119.0 (6)
C11—N2—HN2	119 (5)	C13—C12—C11	119.4 (8)
C18—C23—C22	116.4 (8)	C13—C12—H12	120.3
C18—C23—C24	121.5 (7)	C11—C12—H12	120.3
C22—C23—C24	122.1 (7)	C16—C11—C12	121.7 (7)
C8—C9—C10	121.1 (8)	C16—C11—N2	119.9 (7)
C8—C9—H9	119.5	C12—C11—N2	118.2 (7)
C10—C9—H9	119.5	C16—C17—H17A	109.5
N1—C1—C2	117.8 (6)	C16—C17—H17B	109.5
N1—C1—C4	115.4 (6)	H17A—C17—H17B	109.5
C2—C1—C4	126.8 (6)	C16—C17—H17C	109.5

C14—C15—C16	119.8 (8)	H17A—C17—H17C	109.5
C14—C15—H15	120.1	H17B—C17—H17C	109.5
C16—C15—H15	120.1	C8—C7—C6	120.1 (7)
C11—C16—C15	118.3 (7)	C8—C7—H7	119.9
C11—C16—C17	121.0 (7)	C6—C7—H7	119.9
C15—C16—C17	120.6 (8)		

Fig. 1


C17
C16
C15
C14
C7
C6
C5
C3
N2
C11
C13
C8
C12
C9
C2
C24
C10
F5
F2
F1
C4
C23
C22
F3
F6
C1
C18
C21
N1
C20
C19
F4