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# Tetrakis(1,3,4,6,7,8-hexahydro-2*H*-pyrimido[1,2-*a*]pyrimidin-9-ido-$\kappa^2N^1,N^9$)niobium(V) hexafluoridophosphate

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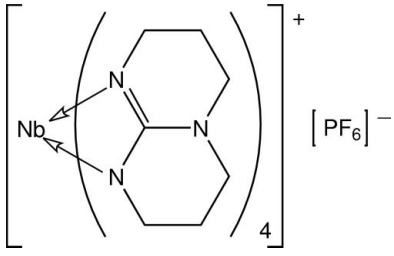
Key indicators: single-crystal X-ray study; $T$ = 213 K; mean $\sigma$(C–C) = 0.008 Å; $R$ factor = 0.050; $wR$ factor = 0.145; data-to-parameter ratio = 14.9.

The title complex, $[Nb(C_7H_{12}N_3)_4]PF_6$, features chelating hpp anions (hpp is 1,3,4,6,7,8-hexahydro-2*H*-pyrimido[1,2-*a*]-pyrimidine) that define a distorted dodecahedral coordination geometry based on an $N_8$ donor set. The Nb atom is situated on a site of symmetry $\overline{4}$, and the $PF_6^-$ anion has crystallographic fourfold symmetry.

## Related literature

For background literature, see: Cotton *et al.* (1998, 2005). For related structures, see: Cotton *et al.* (2000); Coles & Hitchcock (2001).




## Experimental

### Crystal data

$[Nb(C_7H_{12}N_3)_4]PF_6$
$M_r$ = 790.66
Tetragonal, $P4/n$
$a$ = 13.531 (6) Å
$c$ = 9.159 (4) Å
$V$ = 1676.9 (13) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.48 mm$^{-1}$
$T$ = 213 (2) K
0.20 × 0.15 × 0.10 mm

### Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min}$ = 0.910, $T_{max}$ = 0.953
10356 measured reflections
1655 independent reflections
1381 reflections with $I > 2\sigma(I)$

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.144
$S$ = 1.05
1655 reflections
111 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976); 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: LX2067).

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# supporting information

*Acta Cryst.* (2008). E**64**, m1197 [doi:10.1107/S1600536808026627]

## Tetrakis(1,3,4,6,7,8-hexahydro-2*H*-pyrimido[1,2-*a*]pyrimidin-9-ido-$\kappa^2N^1,N^9$)niobium(V) hexafluoridophosphate

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### S1. Comment

The title complex, $[Nb(hpp)_4][PF_6]$ (I), feaures a $[Nb(hpp)_4]^+$ cation, with the Nb atom located on a site of symmetry $\bar{4}$, and a $[PF_6]^-$ anion, with fourfold symmetry; where hpp is 1,3,4,6,7,8-hexahydro-2*H*-pyrimido(1,2 - a)pyrimidine. The Nb atom is chelated four hpp ligands and the $N_8$ donor set defines an approximate dodecahedral coordination environment (Fig. 1).

The conformations of the N1- and N-2 containing six-membered rings is twisted chair. Such a binding mode as observed in (I) is uncommon for the hpp ligand, which normally acts as a bridging group in various paddlewheel complexes (Cotton *et al.*, 2005). A related example of hpp acting as a chelating ligand is $[Ta(hpp)_4][Ta(CO)_6]$ (Cotton *et al.*, 2000). Both complexes were obtained by oxidizing the precursors $Nb_2(hpp)_4$ and $[Et_4N][Ta(CO)_6]$, respectively. The chelating mode of hpp is also found in some Ti complexes (Coles & Hitchcok, 2001).

### S2. Experimental

The title complex (I) was obtained unintentionally in an attempt to oxidize the paddlewheel complex $Nb_2(hpp)_4$ with $[Cp_2Fe][PF_6]$ in $CH_2Cl_2$. X-ray quality crystals were obtained by slow diffusion of hexanes into a $CH_2Cl_2$ solution of (I) at room temperature.

### S3. Refinement

The H atoms were geometrically placed (C—H = 0.98 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

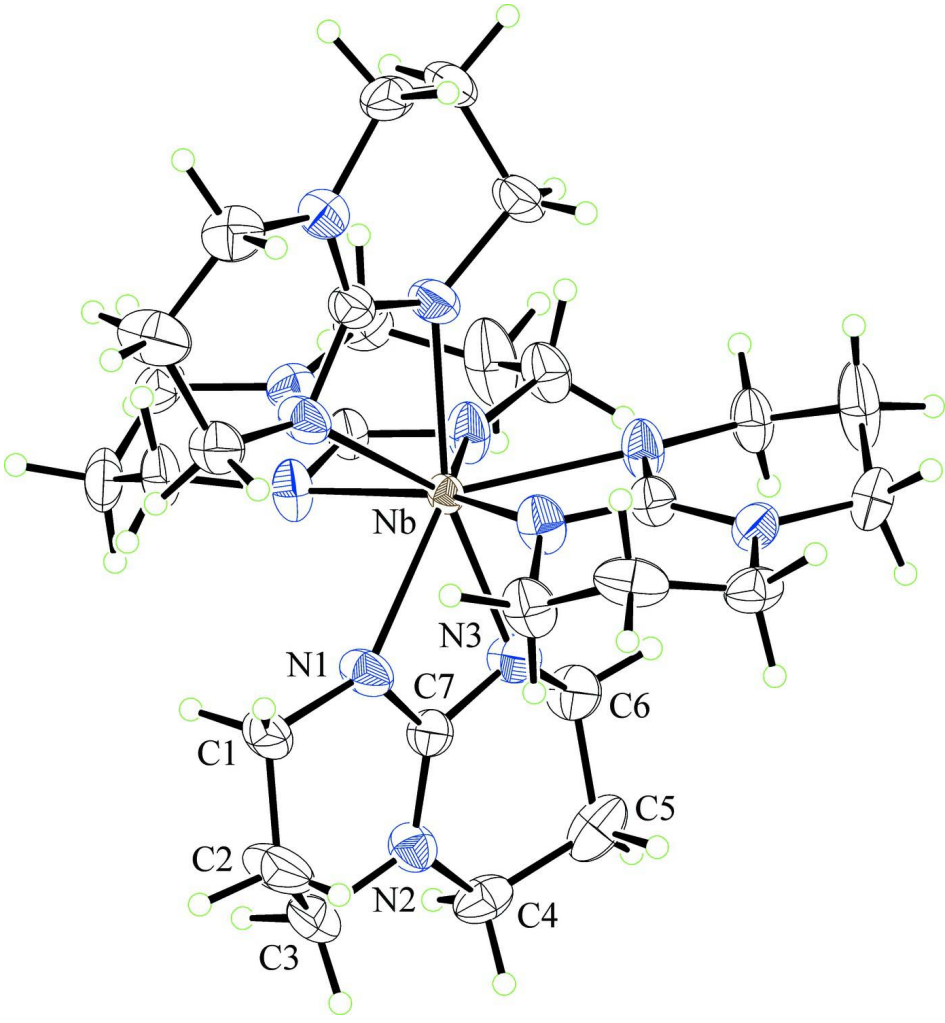


**Figure 1**

Molecular structure of the cation in (I) showing the crystallographic numbering scheme. Displacement ellipsoids are shown at the 35% probability level. The Nb atom is located on a site of symmetry $\overline{4}$.

**Tetrakis(1,3,4,6,7,8-hexahydro-2*H*-pyrimido[1,2-*a*]pyrimidin-9-ido- $\kappa^2N^1,N^9$)niobium(V) hexafluoridophosphate**

*Crystal data*

$[Nb(C_7H_{12}N_3)_4]PF_6$
$M_r = 790.66$
Tetragonal, $P4/n$
Hall symbol: -P 4a
$a = 13.531\ (6)$ Å
$c = 9.159\ (4)$ Å
$V = 1676.9\ (13)$ Å$^3$
$Z = 2$
$F(000) = 820$
$D_x = 1.566$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 10356 reflections
$\theta = 2.1–27.5°$
$\mu = 0.48$ mm$^{-1}$
$T = 213$ K
Block, yellow
0.20 × 0.15 × 0.10 mm

*Data collection*

Bruker SMART 1K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10 pixels mm$^{-1}$
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min}$ = 0.910, $T_{max}$ = 0.953
10356 measured reflections
1655 independent reflections
1381 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 2.1°
$h$ = −17→12
$k$ = −17→16
$l$ = −10→11

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.144
$S$ = 1.05
1655 reflections
111 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.067P)^2 + 3.4248P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.69 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$

*Special details*

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

**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 $F^2 > 2$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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Nb | 0.7500 | 0.2500 | 0.5000 | 0.0388 (2) |
| N1 | 0.6548 (3) | 0.1964 (3) | 0.3195 (4) | 0.0670 (11) |
| N2 | 0.6131 (3) | 0.1782 (3) | 0.5468 (4) | 0.0677 (11) |
| N3 | 0.4885 (3) | 0.1508 (3) | 0.3731 (4) | 0.0598 (9) |
| C1 | 0.6352 (4) | 0.1994 (4) | 0.1664 (5) | 0.0730 (14) |
| H1A | 0.6931 | 0.1747 | 0.1137 | 0.088* |
| H1B | 0.6245 | 0.2682 | 0.1370 | 0.088* |
| C2 | 0.5483 (5) | 0.1405 (7) | 0.1244 (6) | 0.116 (3) |
| H2A | 0.5295 | 0.1587 | 0.0247 | 0.139* |
| H2B | 0.5675 | 0.0706 | 0.1231 | 0.139* |
| C3 | 0.4618 (4) | 0.1511 (4) | 0.2179 (6) | 0.0783 (15) |
| H3A | 0.4158 | 0.0967 | 0.1985 | 0.094* |
| H3B | 0.4281 | 0.2132 | 0.1945 | 0.094* |
| C4 | 0.4136 (3) | 0.1333 (4) | 0.4827 (6) | 0.0694 (14) |
| H4A | 0.3720 | 0.0777 | 0.4523 | 0.083* |
| H4B | 0.3713 | 0.1919 | 0.4909 | 0.083* |

| | | | | |
|---|---|---|---|---|
| C5 | 0.4580 (4) | 0.1111 (4) | 0.6279 (6) | 0.0839 (18) |
| H5A | 0.4830 | 0.0431 | 0.6279 | 0.101* |
| H5B | 0.4067 | 0.1159 | 0.7032 | 0.101* |
| C6 | 0.5406 (4) | 0.1802 (4) | 0.6648 (5) | 0.0745 (14) |
| H6A | 0.5149 | 0.2474 | 0.6772 | 0.089* |
| H6B | 0.5718 | 0.1599 | 0.7566 | 0.089* |
| C7 | 0.5805 (3) | 0.1735 (3) | 0.4103 (5) | 0.0549 (10) |
| P1 | 0.2500 | 0.2500 | 0.9214 (2) | 0.0475 (5) |
| F1 | 0.13862 (19) | 0.2132 (2) | 0.9219 (3) | 0.0772 (9) |
| F2 | 0.2500 | 0.2500 | 0.7468 (5) | 0.0695 (14) |
| F3 | 0.2500 | 0.2500 | 1.0963 (5) | 0.0562 (11) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Nb | 0.0438 (3) | 0.0438 (3) | 0.0288 (4) | 0.000 | 0.000 | 0.000 |
| N1 | 0.056 (2) | 0.107 (3) | 0.0386 (18) | −0.013 (2) | −0.0009 (16) | −0.0025 (19) |
| N2 | 0.061 (2) | 0.095 (3) | 0.0472 (19) | −0.019 (2) | 0.0110 (18) | −0.003 (2) |
| N3 | 0.051 (2) | 0.067 (2) | 0.062 (2) | 0.0073 (17) | −0.0030 (17) | 0.0021 (19) |
| C1 | 0.077 (3) | 0.099 (4) | 0.043 (2) | −0.014 (3) | −0.009 (2) | 0.005 (2) |
| C2 | 0.084 (4) | 0.217 (8) | 0.047 (3) | −0.053 (5) | −0.014 (3) | 0.001 (4) |
| C3 | 0.061 (3) | 0.096 (4) | 0.078 (3) | −0.001 (3) | −0.023 (3) | 0.010 (3) |
| C4 | 0.048 (2) | 0.055 (3) | 0.105 (4) | −0.0021 (19) | 0.012 (3) | −0.006 (3) |
| C5 | 0.090 (4) | 0.072 (3) | 0.089 (4) | −0.004 (3) | 0.054 (3) | 0.000 (3) |
| C6 | 0.076 (3) | 0.101 (4) | 0.047 (2) | −0.013 (3) | 0.018 (2) | 0.000 (3) |
| C7 | 0.055 (2) | 0.065 (3) | 0.045 (2) | −0.005 (2) | 0.0064 (18) | 0.0035 (19) |
| P1 | 0.0530 (7) | 0.0530 (7) | 0.0365 (10) | 0.000 | 0.000 | 0.000 |
| F1 | 0.0582 (15) | 0.112 (2) | 0.0619 (17) | −0.0192 (15) | 0.0028 (13) | −0.0233 (16) |
| F2 | 0.087 (2) | 0.087 (2) | 0.035 (2) | 0.000 | 0.000 | 0.000 |
| F3 | 0.0660 (18) | 0.0660 (18) | 0.036 (2) | 0.000 | 0.000 | 0.000 |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Nb—N2 | 2.135 (4) | C2—H2B | 0.9800 |
| Nb—N2$^{i}$ | 2.135 (4) | C3—H3A | 0.9800 |
| Nb—N1 | 2.218 (4) | C3—H3B | 0.9800 |
| Nb—N1$^{i}$ | 2.218 (4) | C4—C5 | 1.490 (8) |
| Nb—C7 | 2.648 (4) | C4—H4A | 0.9800 |
| Nb—C7$^{i}$ | 2.648 (4) | C4—H4B | 0.9800 |
| N1—C7 | 1.341 (5) | C5—C6 | 1.496 (8) |
| N1—C1 | 1.428 (5) | C5—H5A | 0.9800 |
| N2—C7 | 1.328 (6) | C5—H5B | 0.9800 |
| N2—C6 | 1.460 (6) | C6—H6A | 0.9800 |
| N3—C7 | 1.326 (5) | C6—H6B | 0.9800 |
| N3—C4 | 1.447 (6) | P1—F1 | 1.587 (3) |
| N3—C3 | 1.466 (6) | P1—F1$^{ii}$ | 1.587 (3) |
| C1—C2 | 1.472 (7) | P1—F1$^{iii}$ | 1.587 (3) |
| C1—H1A | 0.9800 | P1—F1$^{iv}$ | 1.587 (3) |

| | | | |
|---|---|---|---|
| C1—H1B | 0.9800 | P1—F2 | 1.600 (5) |
| C2—C3 | 1.457 (8) | P1—F3 | 1.602 (5) |
| C2—H2A | 0.9800 | | |

| | | | |
|---|---|---|---|
| N2—Nb—N2$^{i}$ | 156.8 (2) | C7—N1—C1 | 118.4 (4) |
| N2—Nb—N2$^{v}$ | 92.31 (4) | C7—N1—Nb | 92.8 (3) |
| N2$^{i}$—Nb—N2$^{v}$ | 92.31 (4) | C1—N1—Nb | 146.2 (3) |
| N2—Nb—N2$^{vi}$ | 92.31 (4) | C7—N2—C6 | 118.3 (4) |
| N2$^{i}$—Nb—N2$^{vi}$ | 92.31 (4) | C7—N2—Nb | 97.0 (3) |
| N2$^{v}$—Nb—N2$^{vi}$ | 156.8 (2) | C6—N2—Nb | 136.4 (3) |
| N2—Nb—N1 | 59.80 (14) | C7—N3—C4 | 121.1 (4) |
| N2$^{i}$—Nb—N1 | 143.38 (14) | C7—N3—C3 | 118.7 (4) |
| N2$^{v}$—Nb—N1 | 80.23 (16) | C4—N3—C3 | 120.0 (4) |
| N2$^{vi}$—Nb—N1 | 82.54 (17) | N1—C1—C2 | 112.9 (4) |
| N2—Nb—N1$^{v}$ | 82.54 (17) | N1—C1—H1A | 109.0 |
| N2$^{i}$—Nb—N1$^{v}$ | 80.23 (16) | C2—C1—H1A | 109.0 |
| N2$^{v}$—Nb—N1$^{v}$ | 59.80 (14) | N1—C1—H1B | 109.0 |
| N2$^{vi}$—Nb—N1$^{v}$ | 143.38 (14) | C2—C1—H1B | 109.0 |
| N1—Nb—N1$^{v}$ | 123.75 (12) | H1A—C1—H1B | 107.8 |
| N2—Nb—N1$^{vi}$ | 80.23 (16) | C3—C2—C1 | 115.7 (6) |
| N2$^{i}$—Nb—N1$^{vi}$ | 82.54 (17) | C3—C2—H2A | 108.3 |
| N2$^{v}$—Nb—N1$^{vi}$ | 143.38 (14) | C1—C2—H2A | 108.3 |
| N2$^{vi}$—Nb—N1$^{vi}$ | 59.80 (14) | C3—C2—H2B | 108.3 |
| N1—Nb—N1$^{vi}$ | 123.75 (12) | C1—C2—H2B | 108.3 |
| N1$^{v}$—Nb—N1$^{vi}$ | 83.6 (2) | H2A—C2—H2B | 107.4 |
| N2—Nb—N1$^{i}$ | 143.38 (14) | C2—C3—N3 | 111.8 (4) |
| N2$^{i}$—Nb—N1$^{i}$ | 59.80 (14) | C2—C3—H3A | 109.3 |
| N2$^{v}$—Nb—N1$^{i}$ | 82.54 (17) | N3—C3—H3A | 109.3 |
| N2$^{vi}$—Nb—N1$^{i}$ | 80.23 (16) | C2—C3—H3B | 109.3 |
| N1—Nb—N1$^{i}$ | 83.6 (2) | N3—C3—H3B | 109.3 |
| N1$^{v}$—Nb—N1$^{i}$ | 123.75 (12) | H3A—C3—H3B | 107.9 |
| N1$^{vi}$—Nb—N1$^{i}$ | 123.75 (12) | N3—C4—C5 | 111.7 (4) |
| N2—Nb—C7 | 29.86 (14) | N3—C4—H4A | 109.3 |
| N2$^{i}$—Nb—C7 | 172.73 (14) | C5—C4—H4A | 109.3 |
| N2$^{v}$—Nb—C7 | 89.57 (16) | N3—C4—H4B | 109.3 |
| N2$^{vi}$—Nb—C7 | 83.26 (16) | C5—C4—H4B | 109.3 |
| N1—Nb—C7 | 30.39 (13) | H4A—C4—H4B | 107.9 |
| N1$^{v}$—Nb—C7 | 106.74 (15) | C4—C5—C6 | 112.1 (4) |
| N1$^{vi}$—Nb—C7 | 100.07 (15) | C4—C5—H5A | 109.2 |
| N1$^{i}$—Nb—C7 | 113.57 (13) | C6—C5—H5A | 109.2 |
| N2—Nb—C7$^{vi}$ | 89.57 (15) | C4—C5—H5B | 109.2 |
| N2$^{i}$—Nb—C7$^{vi}$ | 83.26 (16) | C6—C5—H5B | 109.2 |
| N2$^{v}$—Nb—C7$^{vi}$ | 172.73 (14) | H5A—C5—H5B | 107.9 |
| N2$^{vi}$—Nb—C7$^{vi}$ | 29.86 (14) | N2—C6—C5 | 108.9 (4) |
| N1—Nb—C7$^{vi}$ | 106.74 (15) | N2—C6—H6A | 109.9 |
| N1$^{v}$—Nb—C7$^{vi}$ | 113.57 (13) | C5—C6—H6A | 109.9 |
| N1$^{vi}$—Nb—C7$^{vi}$ | 30.39 (13) | N2—C6—H6B | 109.9 |
| N1$^{i}$—Nb—C7$^{vi}$ | 100.07 (15) | C5—C6—H6B | 109.9 |

| | | | |
|---|---|---|---|
| C7—Nb—C7$^{vi}$ | 95.53 (5) | H6A—C6—H6B | 108.3 |
| N2—Nb—C7$^{v}$ | 83.26 (16) | N3—C7—N2 | 124.4 (4) |
| N2$^{i}$—Nb—C7$^{v}$ | 89.57 (15) | N3—C7—N1 | 126.7 (4) |
| N2$^{v}$—Nb—C7$^{v}$ | 29.86 (14) | N2—C7—N1 | 108.8 (4) |
| N2$^{vi}$—Nb—C7$^{v}$ | 172.73 (14) | N3—C7—Nb | 169.6 (3) |
| N1—Nb—C7$^{v}$ | 100.07 (15) | N2—C7—Nb | 53.2 (2) |
| N1$^{v}$—Nb—C7$^{v}$ | 30.39 (13) | N1—C7—Nb | 56.8 (2) |
| N1$^{vi}$—Nb—C7$^{v}$ | 113.57 (13) | F1—P1—F1$^{ii}$ | 90.000 (2) |
| N1$^{i}$—Nb—C7$^{v}$ | 106.74 (15) | F1—P1—F1$^{iii}$ | 179.7 (2) |
| C7—Nb—C7$^{v}$ | 95.53 (5) | F1$^{ii}$—P1—F1$^{iii}$ | 90.000 (2) |
| C7$^{vi}$—Nb—C7$^{v}$ | 143.83 (18) | F1—P1—F1$^{iv}$ | 90.000 (1) |
| N2—Nb—C7$^{i}$ | 172.73 (14) | F1$^{ii}$—P1—F1$^{iv}$ | 179.7 (2) |
| N2$^{i}$—Nb—C7$^{i}$ | 29.86 (14) | F1$^{iii}$—P1—F1$^{iv}$ | 90.000 (2) |
| N2$^{v}$—Nb—C7$^{i}$ | 83.26 (16) | F1—P1—F2 | 90.16 (12) |
| N2$^{vi}$—Nb—C7$^{i}$ | 89.57 (16) | F1$^{ii}$—P1—F2 | 90.16 (12) |
| N1—Nb—C7$^{i}$ | 113.57 (13) | F1$^{iii}$—P1—F2 | 90.16 (12) |
| N1$^{v}$—Nb—C7$^{i}$ | 100.07 (15) | F1$^{iv}$—P1—F2 | 90.16 (12) |
| N1$^{vi}$—Nb—C7$^{i}$ | 106.74 (15) | F1—P1—F3 | 89.84 (12) |
| N1$^{i}$—Nb—C7$^{i}$ | 30.39 (13) | F1$^{ii}$—P1—F3 | 89.84 (12) |
| C7—Nb—C7$^{i}$ | 143.83 (18) | F1$^{iii}$—P1—F3 | 89.84 (12) |
| C7$^{vi}$—Nb—C7$^{i}$ | 95.53 (5) | F1$^{iv}$—P1—F3 | 89.84 (12) |
| C7$^{v}$—Nb—C7$^{i}$ | 95.53 (5) | F2—P1—F3 | 180.000 (2) |

| | | | |
|---|---|---|---|
| N2—Nb—N1—C7 | 7.7 (3) | N3—C4—C5—C6 | 45.0 (6) |
| N2$^{i}$—Nb—N1—C7 | −173.2 (3) | C7—N2—C6—C5 | 39.2 (7) |
| N2$^{v}$—Nb—N1—C7 | 106.2 (3) | Nb—N2—C6—C5 | 179.1 (4) |
| N2$^{vi}$—Nb—N1—C7 | −89.4 (3) | C4—C5—C6—N2 | −54.6 (6) |
| N1$^{v}$—Nb—N1—C7 | 63.0 (4) | C4—N3—C7—N2 | 3.0 (7) |
| N1$^{vi}$—Nb—N1—C7 | −43.6 (4) | C3—N3—C7—N2 | 178.2 (5) |
| N1$^{i}$—Nb—N1—C7 | −170.3 (4) | C4—N3—C7—N1 | −176.2 (5) |
| C7$^{vi}$—Nb—N1—C7 | −71.7 (3) | C3—N3—C7—N1 | −1.0 (7) |
| C7$^{v}$—Nb—N1—C7 | 83.7 (2) | C4—N3—C7—Nb | −70.1 (19) |
| C7$^{i}$—Nb—N1—C7 | −175.65 (18) | C3—N3—C7—Nb | 105.1 (17) |
| N2—Nb—N1—C1 | 165.9 (7) | C6—N2—C7—N3 | −14.1 (7) |
| N2$^{i}$—Nb—N1—C1 | −15.0 (8) | Nb—N2—C7—N3 | −167.5 (4) |
| N2$^{v}$—Nb—N1—C1 | −95.6 (7) | C6—N2—C7—N1 | 165.2 (5) |
| N2$^{vi}$—Nb—N1—C1 | 68.8 (7) | Nb—N2—C7—N1 | 11.8 (4) |
| N1$^{v}$—Nb—N1—C1 | −138.8 (6) | C6—N2—C7—Nb | 153.4 (5) |
| N1$^{vi}$—Nb—N1—C1 | 114.6 (6) | C1—N1—C7—N3 | 1.6 (8) |
| N1$^{i}$—Nb—N1—C1 | −12.1 (6) | Nb—N1—C7—N3 | 168.0 (4) |
| C7—Nb—N1—C1 | 158.2 (9) | C1—N1—C7—N2 | −177.7 (5) |
| C7$^{vi}$—Nb—N1—C1 | 86.5 (7) | Nb—N1—C7—N2 | −11.3 (4) |
| C7$^{v}$—Nb—N1—C1 | −118.0 (7) | C1—N1—C7—Nb | −166.4 (5) |
| C7$^{i}$—Nb—N1—C1 | −17.4 (7) | N2—Nb—C7—N3 | 80.4 (17) |
| N2$^{i}$—Nb—N2—C7 | 173.5 (3) | N2$^{v}$—Nb—C7—N3 | 175.8 (17) |
| N2$^{v}$—Nb—N2—C7 | −85.1 (3) | N2$^{vi}$—Nb—C7—N3 | −26.3 (17) |
| N2$^{vi}$—Nb—N2—C7 | 72.2 (3) | N1—Nb—C7—N3 | −113.0 (18) |
| N1—Nb—N2—C7 | −7.8 (3) | N1$^{v}$—Nb—C7—N3 | 117.6 (17) |

| | | | |
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| N1$^{v}$—Nb—N2—C7 | −144.2 (3) | N1$^{vi}$—Nb—C7—N3 | 31.3 (18) |
| N1$^{vi}$—Nb—N2—C7 | 131.0 (3) | N1$^{i}$—Nb—C7—N3 | −102.5 (17) |
| N1$^{i}$—Nb—N2—C7 | −4.5 (5) | C7$^{vi}$—Nb—C7—N3 | 1.0 (17) |
| C7$^{vi}$—Nb—N2—C7 | 101.9 (3) | C7$^{v}$—Nb—C7—N3 | 146.5 (18) |
| C7$^{v}$—Nb—N2—C7 | −113.6 (3) | C7$^{i}$—Nb—C7—N3 | −106.3 (18) |
| N2$^{i}$—Nb—N2—C6 | 28.4 (5) | N2$^{v}$—Nb—C7—N2 | 95.4 (3) |
| N2$^{v}$—Nb—N2—C6 | 129.7 (6) | N2$^{vi}$—Nb—C7—N2 | −106.7 (3) |
| N2$^{vi}$—Nb—N2—C6 | −73.0 (5) | N1—Nb—C7—N2 | 166.6 (5) |
| N1—Nb—N2—C6 | −153.0 (6) | N1$^{v}$—Nb—C7—N2 | 37.2 (3) |
| N1$^{v}$—Nb—N2—C6 | 70.6 (5) | N1$^{vi}$—Nb—C7—N2 | −49.1 (3) |
| N1$^{vi}$—Nb—N2—C6 | −14.2 (5) | N1$^{i}$—Nb—C7—N2 | 177.1 (3) |
| N1$^{i}$—Nb—N2—C6 | −149.7 (5) | C7$^{v}$—Nb—C7—N2 | 66.1 (3) |
| C7—Nb—N2—C6 | −145.2 (7) | C7$^{i}$—Nb—C7—N2 | 173.3 (3) |
| C7$^{vi}$—Nb—N2—C6 | −43.3 (5) | N2—Nb—C7—N1 | −166.6 (5) |
| C7$^{v}$—Nb—N2—C6 | 101.2 (5) | N2$^{v}$—Nb—C7—N1 | −71.2 (3) |
| C7—N1—C1—C2 | −22.7 (8) | N2$^{vi}$—Nb—C7—N1 | 86.7 (3) |
| Nb—N1—C1—C2 | −177.8 (5) | N1$^{v}$—Nb—C7—N1 | −129.3 (3) |
| N1—C1—C2—C3 | 44.3 (9) | N1$^{vi}$—Nb—C7—N1 | 144.4 (3) |
| C1—C2—C3—N3 | −43.2 (8) | N1$^{i}$—Nb—C7—N1 | 10.5 (4) |
| C7—N3—C3—C2 | 21.6 (8) | C7$^{vi}$—Nb—C7—N1 | 114.0 (3) |
| C4—N3—C3—C2 | −163.1 (5) | C7$^{v}$—Nb—C7—N1 | −100.5 (3) |
| C7—N3—C4—C5 | −19.0 (6) | C7$^{i}$—Nb—C7—N1 | 6.8 (3) |
| C3—N3—C4—C5 | 165.8 (5) | | |

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