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# Crystal structure of *fac*-trichlorido[tris(pyridin-2-yl-*N*)amine]chromium(III)

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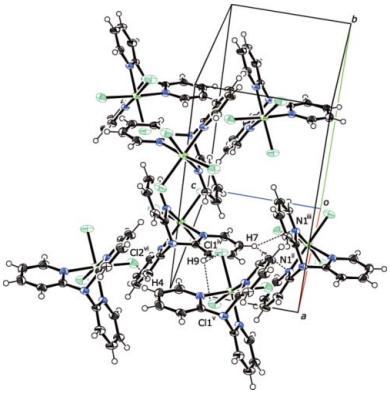
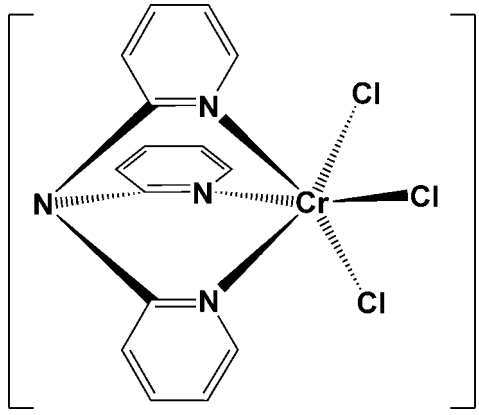
In the neutral complex molecule of the title compound, *fac*-[$CrCl_3$(tpa)] [tpa is tris(pyridin-2-yl)amine; $C_{15}H_{12}N_4$], the $Cr^{III}$ ion is bonded to three N atoms that are constrained to a *facial* arrangement by the tpa ligand and by three chloride ligands, leading to a distorted octahedral coordination sphere. The average Cr—N and Cr—Cl bond lengths are 2.086 (5) and 2.296 (4) Å, respectively. The complex molecule is located on a mirror plane. In the crystal, a combination of C—H···N and C—H···Cl hydrogen-bonding interactions connect the molecules into a three-dimensional network.

## 1. Chemical context

One aspect of solvatochromism is the dependence of ligand-field parameters on the solvent coordination sphere. This has been demonstrated by measuring the ligand-field absorption spectra and/or multinuclear NMR spectra for several types of $Cr^{III}$ complexes in previous studies (Kaizaki, 1996; Kaizaki & Takemoto, 1990; Terasaki & Kaizaki, 1995; Terasaki *et al.*, 1999; Yamaguchi-Terasaki *et al.*, 2007*a*,*b*,*c*). As a part of the above-mentioned systematic investigations, we report here the crystal structure of the title compound, *fac*-[$CrCl_3$(tpa)], (I), where tpa is tris(pyridin-2-yl)amine.






## 2. Structural commentary

The molecular structure of (I) is illustrated in Fig. 1. The $Cr^{III}$ ion is coordinated by three N atoms that are constrained to a *facial* arrangement by the tpa ligand and three chloride ligands in a slightly distorted octahedral geometry. The entire complex

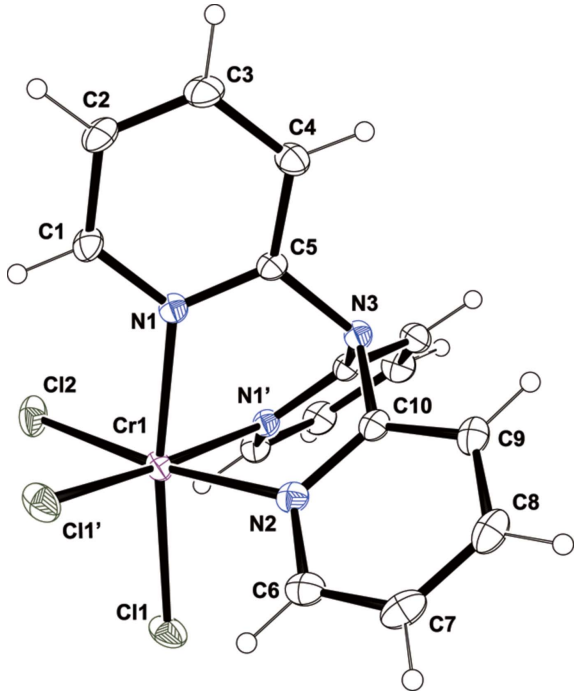



**Figure 1**
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (′) $x, -y+\frac{1}{2}, z$.]

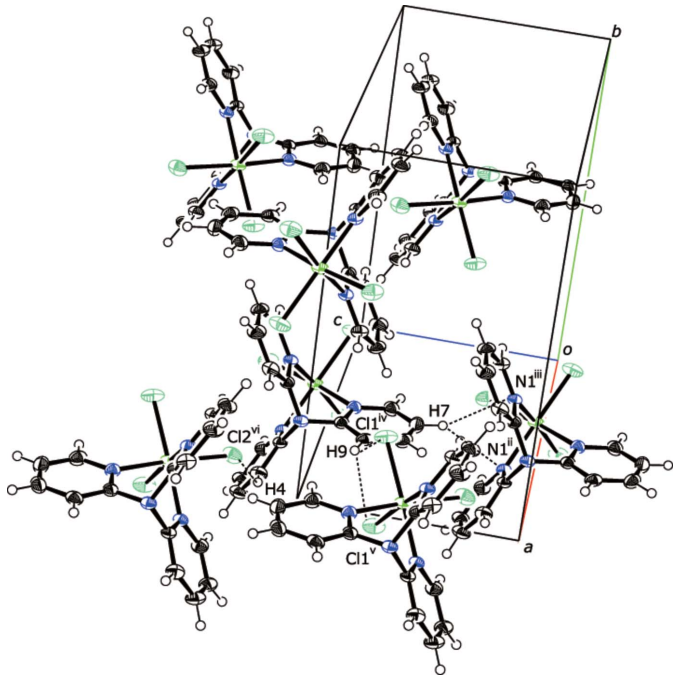



**Figure 2**
Hydrogen-bonding interactions in the crystal structure of (I), shown as black dashed lines. [Symmetry codes: (ii) $x, -y+\frac{1}{2}, z-1$; (iii) $x, y, z-1$; (iv) $x+\frac{1}{2}, y, -z+\frac{3}{2}$; (v) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{3}{2}$; (vi) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{5}{2}$.]

molecule is located on a mirror plane. The average Cr—N bond length of 2.086 (5) Å is comparable to that in the related tpa complex cation *fac*-$[Cr(tpa)(H_2O)_3]^{3+}$ [2.040 (1) Å; Terasaki *et al.*, 2004]. In addition, the average Cr—Cl bond length of the coordinating chlorine atoms being in *trans* positions to the N atoms [2.296 (4) Å] is similar to those found for other pyridine-chromium(III) complexes, such as *mer*-$[CrCl_3(terpy)]$ [terpy is 2,2′,2″-terpyridine; $C_{15}H_{11}N_3$; 2.292 (1) Å] (Cloete *et al.*, 2007); *mer*-$[CrCl_3py_3]$ [py is pyridine, $C_5H_5N$; 2.320 (7) Å] (Howard & Hardcastle, 1985) or *mer*-$[CrCl_3(Etpy)_3]$ [Etpy is 4-ethylpyridine, $C_7H_9N_3$; 2.320 (7) Å] (Modec *et al.*, 2000). All bond lengths and angles within the pyridine rings are within normal ranges. The dihedral angles between the least-squares planes of the pyridine rings are 58.33 (6) and 63.37 (8)°.

## 3. Supramolecular features

The chlorine atoms act as hydrogen-bond acceptors, forming intermolecular C—H···Cl hydrogen bonds with the pyridine rings (Fig. 2, Table 1). In addition, C—H···N hydrogen-bonding interactions are also present, consolidating the molecules into a three-dimensional network.

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C7—H7···N1$^{i}$ | 0.95 | 2.75 | 3.578 (5) | 146 |
| C7—H7···N1$^{ii}$ | 0.95 | 2.75 | 3.578 (5) | 146 |
| C9—H9···Cl1$^{iii}$ | 0.95 | 2.82 | 3.447 (4) | 124 |
| C9—H9···Cl1$^{iv}$ | 0.95 | 2.82 | 3.447 (4) | 124 |
| C4—H4···Cl2$^{v}$ | 0.95 | 2.77 | 3.534 (4) | 138 |

Symmetry codes: (i) $x, -y+\frac{1}{2}, z-1$; (ii) $x, y, z-1$; (iii) $x+\frac{1}{2}, y, -z+\frac{3}{2}$; (iv) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{3}{2}$; (v) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{5}{2}$.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[CrCl_3(C_{15}H_{12}N_4)]$ |
| $M_r$ | 406.64 |
| Crystal system, space group | Orthorhombic, *Pnma* |
| Temperature (K) | 150 |
| $a, b, c$ (Å) | 15.152 (13), 13.704 (12), 8.014 (7) |
| $V$ (Å$^3$) | 1664 (2) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 1.17 |
| Crystal size (mm) | 0.06 × 0.05 × 0.04 |
| | |
| Data collection | |
| Diffractometer | Bruker APEXII CCD area detector |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2014) |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 15895, 1779, 1401 |
| $R_{int}$ | 0.061 |
| $(\sin\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.625 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.038, 0.113, 1.20 |
| No. of reflections | 1779 |
| No. of parameters | 118 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.66, −0.51 |

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2014), *SHELXS2014*, *SHELXL2014* and *XCIF* (Sheldrick, 2008) and *ORTEP-3 for Windows* (Farrugia, 2012).

## 4. Synthesis and crystallization

*fac*-[$CrCl_3$(tpa)] was synthesized according to a previously reported procedure (Kaizaki & Legg, 1994). Green crystals of (I) suitable for X-ray analysis were obtained by slow cooling from the reaction solution. UV–vis(DMSO): $\lambda_{max}(\varepsilon)$ = 720 (16), 645 (37), 464 (59) nm (L $mol^{-1}$ $cm^{-1}$). Elemental analysis, calculated for $C_{15}H_{12}C_{l3}CrN_4$: C, 44.31, H, 2.97, N, 13.78%; found: C, 44.29; H, 2.99; N, 13.76%.

## 5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H atoms were placed in calculated positions, with C—H = 0.95 Å, and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}$.

## Acknowledgements

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# supporting information

*Acta Cryst.* (2015). E**71**, 73-75 [https://doi.org/10.1107/S2056989014027066]

## Crystal structure of *fac*-trichlorido[tris(pyridin-2-yl-*N*)amine]chromium(III)

**Yukiko Yamaguchi-Terasaki, Takashi Fujihara, Akira Nagasawa and Sumio Kaizaki**

### Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* and *XPREP* (Bruker, 2014); program(s) used to solve structure: *SHELXS2014* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *XCIF* (Sheldrick, 2008).

### *fac*-trichlorido[tris(pyridin-2-yl-*N*)amine]chromium(III)

*Crystal data*

$[CrCl_3(C_{15}H_{12}N_4)]$
$M_r = 406.64$
Orthorhombic, *Pnma*
$a = 15.152$ (13) Å
$b = 13.704$ (12) Å
$c = 8.014$ (7) Å
$V = 1664$ (2) Å$^3$
$Z = 4$
$F(000) = 820$
$D_x = 1.623$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3388 reflections
$\theta = 2.7$–$26.4°$
$\mu = 1.17$ mm$^{-1}$
$T = 150$ K
Needle, green
0.06 × 0.05 × 0.04 mm

*Data collection*

Bruker APEXII CCD area-detector diffractometer
Radiation source: Bruker TXS fine-focus rotating anode
Bruker Helios multilayer confocal mirror monochromator
Detector resolution: 8.333 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
15895 measured reflections
1779 independent reflections
1401 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.7°$
$h = -18 \rightarrow 18$
$k = -17 \rightarrow 17$
$l = -10 \rightarrow 10$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.113$
$S = 1.20$
1779 reflections
118 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 0.050P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.66$ e Å$^{-3}$
$\Delta\rho_{min} = -0.51$ 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.
Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)
- 0.0000 (0.0001) x + 13.7040 (0.0118) y - 0.0000 (0.0000) z = 3.4260 (0.0030)
* 0.0000 (0.0000) N2 * 0.0000 (0.0000) C6 * 0.0000 (0.0000) C7 * 0.0000 (0.0000) C8 * 0.0000 (0.0000) C9 * 0.0000 (0.0000) C10
Rms deviation of fitted atoms = 0.0000
- 0.2014 (0.0170) x - 7.1958 (0.0145) y + 6.8195 (0.0076) z = 4.9979 (0.0213)
Angle to previous plane (with approximate esd) = 58.326 ( 0.080 )
* -0.0024 (0.0017) N1_$6 * -0.0057 (0.0019) C1_$6 * 0.0081 (0.0020) C2_$6 * -0.0029 (0.0020) C3_$6 * -0.0049 (0.0019) C4_$6 * 0.0078 (0.0018) C5_$6
Rms deviation of fitted atoms = 0.0057
0.2014 (0.0171) x + 7.1958 (0.0145) y + 6.8195 (0.0076) z = 8.8847 (0.0184)
Angle to previous plane (with approximate esd) = 63.371 ( 0.081 )
* -0.0024 (0.0017) N1 * -0.0057 (0.0019) C1 * 0.0081 (0.0020) C2 * -0.0029 (0.0020) C3 * -0.0049 (0.0019) C4 * 0.0078 (0.0018) C5
Rms deviation of fitted atoms = 0.0057

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.89047 (17) | 0.06834 (18) | 1.2036 (3) | 0.0287 (6) |
| H1 | 0.8290 | 0.0568 | 1.2158 | 0.034* |
| C2 | 0.94935 (19) | 0.0033 (2) | 1.2726 (4) | 0.0336 (7) |
| H2 | 0.9287 | −0.0516 | 1.3336 | 0.040* |
| C3 | 1.0382 (2) | 0.0186 (2) | 1.2521 (4) | 0.0355 (7) |
| H3 | 1.0796 | −0.0262 | 1.2972 | 0.043* |
| C4 | 1.06674 (17) | 0.0997 (2) | 1.1654 (4) | 0.0309 (6) |
| H4 | 1.1279 | 0.1117 | 1.1495 | 0.037* |
| C5 | 1.00429 (16) | 0.16273 (18) | 1.1026 (3) | 0.0224 (6) |
| C10 | 1.0039 (2) | 0.2500 | 0.8449 (5) | 0.0239 (8) |
| C6 | 0.8905 (3) | 0.2500 | 0.6541 (5) | 0.0328 (9) |
| H6 | 0.8292 | 0.2500 | 0.6295 | 0.039* |
| C7 | 0.9499 (3) | 0.2500 | 0.5256 (5) | 0.0378 (10) |
| H7 | 0.9295 | 0.2500 | 0.4136 | 0.045* |
| C8 | 1.0383 (3) | 0.2500 | 0.5577 (5) | 0.0358 (10) |
| H8 | 1.0797 | 0.2500 | 0.4688 | 0.043* |
| C9 | 1.0667 (2) | 0.2500 | 0.7224 (5) | 0.0293 (9) |
| H9 | 1.1277 | 0.2500 | 0.7490 | 0.035* |
| Cl1 | 0.75326 (4) | 0.37578 (5) | 0.89695 (10) | 0.0388 (2) |
| Cl2 | 0.75220 (6) | 0.2500 | 1.26071 (14) | 0.0379 (3) |
| Cr1 | 0.83104 (4) | 0.2500 | 1.01679 (7) | 0.0239 (2) |
| N1 | 0.91747 (13) | 0.14774 (15) | 1.1195 (3) | 0.0225 (5) |
| N2 | 0.91684 (19) | 0.2500 | 0.8144 (4) | 0.0256 (7) |
| N3 | 1.03099 (19) | 0.2500 | 1.0163 (4) | 0.0227 (7) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0299 (13) | 0.0202 (13) | 0.0360 (16) | −0.0023 (11) | 0.0030 (12) | 0.0013 (12) |
| C2 | 0.0433 (16) | 0.0167 (13) | 0.0407 (17) | 0.0001 (12) | 0.0019 (13) | 0.0046 (12) |
| C3 | 0.0413 (16) | 0.0190 (14) | 0.0462 (18) | 0.0045 (12) | −0.0051 (13) | 0.0039 (13) |
| C4 | 0.0268 (13) | 0.0264 (14) | 0.0394 (16) | 0.0011 (11) | −0.0038 (12) | −0.0018 (13) |
| C5 | 0.0259 (13) | 0.0145 (13) | 0.0267 (14) | 0.0022 (10) | −0.0001 (10) | −0.0007 (10) |
| C10 | 0.0296 (19) | 0.0151 (17) | 0.027 (2) | 0.000 | 0.0023 (16) | 0.000 |
| C6 | 0.039 (2) | 0.024 (2) | 0.035 (2) | 0.000 | −0.0078 (19) | 0.000 |
| C7 | 0.061 (3) | 0.027 (2) | 0.026 (2) | 0.000 | 0.000 (2) | 0.000 |
| C8 | 0.052 (3) | 0.022 (2) | 0.034 (2) | 0.000 | 0.015 (2) | 0.000 |
| C9 | 0.034 (2) | 0.0163 (18) | 0.038 (2) | 0.000 | 0.0086 (18) | 0.000 |
| Cl1 | 0.0309 (4) | 0.0240 (4) | 0.0615 (5) | 0.0046 (3) | −0.0127 (3) | 0.0036 (3) |
| Cl2 | 0.0295 (5) | 0.0309 (6) | 0.0534 (7) | 0.000 | 0.0160 (4) | 0.000 |
| Cr1 | 0.0191 (3) | 0.0170 (3) | 0.0356 (4) | 0.000 | −0.0005 (2) | 0.000 |
| N1 | 0.0240 (11) | 0.0161 (10) | 0.0276 (12) | −0.0001 (8) | 0.0011 (9) | −0.0018 (9) |
| N2 | 0.0288 (16) | 0.0196 (16) | 0.0285 (17) | 0.000 | −0.0012 (13) | 0.000 |
| N3 | 0.0225 (15) | 0.0162 (15) | 0.0295 (17) | 0.000 | 0.0011 (12) | 0.000 |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.344 (3) | C6—C7 | 1.367 (6) |
| C1—C2 | 1.377 (4) | C6—H6 | 0.9500 |
| C1—H1 | 0.9500 | C7—C8 | 1.363 (7) |
| C2—C3 | 1.372 (4) | C7—H7 | 0.9500 |
| C2—H2 | 0.9500 | C8—C9 | 1.388 (6) |
| C3—C4 | 1.380 (4) | C8—H8 | 0.9500 |
| C3—H3 | 0.9500 | C9—H9 | 0.9500 |
| C4—C5 | 1.376 (4) | Cl1—Cr1 | 2.2983 (15) |
| C4—H4 | 0.9500 | Cl2—Cr1 | 2.2909 (19) |
| C5—N1 | 1.338 (3) | Cr1—N2 | 2.079 (3) |
| C5—N3 | 1.440 (3) | Cr1—N1$^{i}$ | 2.087 (2) |
| C10—N2 | 1.342 (4) | Cr1—N1 | 2.087 (2) |
| C10—C9 | 1.366 (5) | Cr1—Cl1$^{i}$ | 2.2983 (15) |
| C10—N3 | 1.434 (5) | N3—C5$^{i}$ | 1.440 (3) |
| C6—N2 | 1.345 (5) | | |
| | | | |
| N1—C1—C2 | 121.9 (3) | C10—C9—C8 | 117.9 (4) |
| N1—C1—H1 | 119.1 | C10—C9—H9 | 121.1 |
| C2—C1—H1 | 119.1 | C8—C9—H9 | 121.1 |
| C3—C2—C1 | 119.2 (3) | N2—Cr1—N1$^{i}$ | 85.14 (10) |
| C3—C2—H2 | 120.4 | N2—Cr1—N1 | 85.14 (10) |
| C1—C2—H2 | 120.4 | N1$^{i}$—Cr1—N1 | 84.35 (13) |
| C2—C3—C4 | 119.4 (3) | N2—Cr1—Cl2 | 172.72 (9) |
| C2—C3—H3 | 120.3 | N1$^{i}$—Cr1—Cl2 | 89.46 (8) |
| C4—C3—H3 | 120.3 | N1—Cr1—Cl2 | 89.46 (8) |
| C5—C4—C3 | 118.3 (3) | N2—Cr1—Cl1$^{i}$ | 89.69 (8) |

| | | | |
|---|---|---|---|
| C5—C4—H4 | 120.9 | N1$^{i}$—Cr1—Cl1$^{i}$ | 171.91 (6) |
| C3—C4—H4 | 120.9 | N1—Cr1—Cl1$^{i}$ | 89.03 (8) |
| N1—C5—C4 | 122.9 (2) | Cl2—Cr1—Cl1$^{i}$ | 95.12 (5) |
| N1—C5—N3 | 116.9 (2) | N2—Cr1—Cl1 | 89.69 (8) |
| C4—C5—N3 | 120.2 (2) | N1$^{i}$—Cr1—Cl1 | 89.03 (8) |
| N2—C10—C9 | 123.6 (4) | N1—Cr1—Cl1 | 171.91 (6) |
| N2—C10—N3 | 117.1 (3) | Cl2—Cr1—Cl1 | 95.12 (5) |
| C9—C10—N3 | 119.3 (3) | Cl1$^{i}$—Cr1—Cl1 | 97.18 (7) |
| N2—C6—C7 | 121.6 (4) | C5—N1—C1 | 118.3 (2) |
| N2—C6—H6 | 119.2 | C5—N1—Cr1 | 118.28 (17) |
| C7—C6—H6 | 119.2 | C1—N1—Cr1 | 123.39 (18) |
| C8—C7—C6 | 120.3 (4) | C10—N2—C6 | 117.7 (3) |
| C8—C7—H7 | 119.8 | C10—N2—Cr1 | 118.2 (2) |
| C6—C7—H7 | 119.8 | C6—N2—Cr1 | 124.0 (3) |
| C7—C8—C9 | 118.9 (4) | C10—N3—C5 | 112.33 (18) |
| C7—C8—H8 | 120.5 | C10—N3—C5$^{i}$ | 112.33 (18) |
| C9—C8—H8 | 120.5 | C5—N3—C5$^{i}$ | 112.4 (3) |
| | | | |
| N1—C1—C2—C3 | −1.4 (4) | C2—C1—N1—Cr1 | −178.7 (2) |
| C1—C2—C3—C4 | 1.1 (4) | C9—C10—N2—C6 | 0.000 (1) |
| C2—C3—C4—C5 | 0.2 (4) | N3—C10—N2—C6 | 180.000 (1) |
| C3—C4—C5—N1 | −1.2 (4) | C9—C10—N2—Cr1 | 180.000 (1) |
| C3—C4—C5—N3 | 177.9 (2) | N3—C10—N2—Cr1 | 0.000 (1) |
| N2—C6—C7—C8 | 0.000 (1) | C7—C6—N2—C10 | 0.000 (1) |
| C6—C7—C8—C9 | 0.000 (1) | C7—C6—N2—Cr1 | 180.000 (1) |
| N2—C10—C9—C8 | 0.000 (1) | N2—C10—N3—C5 | 63.9 (2) |
| N3—C10—C9—C8 | 180.000 (1) | C9—C10—N3—C5 | −116.1 (2) |
| C7—C8—C9—C10 | 0.000 (1) | N2—C10—N3—C5$^{i}$ | −63.9 (2) |
| C4—C5—N1—C1 | 1.0 (4) | C9—C10—N3—C5$^{i}$ | 116.1 (2) |
| N3—C5—N1—C1 | −178.1 (2) | N1—C5—N3—C10 | −64.4 (3) |
| C4—C5—N1—Cr1 | −179.9 (2) | C4—C5—N3—C10 | 116.4 (3) |
| N3—C5—N1—Cr1 | 1.0 (3) | N1—C5—N3—C5$^{i}$ | 63.4 (4) |
| C2—C1—N1—C5 | 0.3 (4) | C4—C5—N3—C5$^{i}$ | −115.8 (3) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7—H7···N1$^{ii}$ | 0.95 | 2.75 | 3.578 (5) | 146 |
| C7—H7···N1$^{iii}$ | 0.95 | 2.75 | 3.578 (5) | 146 |
| C9—H9···Cl1$^{iv}$ | 0.95 | 2.82 | 3.447 (4) | 124 |
| C9—H9···Cl1$^{v}$ | 0.95 | 2.82 | 3.447 (4) | 124 |
| C4—H4···Cl2$^{vi}$ | 0.95 | 2.77 | 3.534 (4) | 138 |

Symmetry codes: (ii) $x$, $-y+1/2$, $z-1$; (iii) $x$, $y$, $z-1$; (iv) $x+1/2$, $y$, $-z+3/2$; (v) $x+1/2$, $-y+1/2$, $-z+3/2$; (vi) $x+1/2$, $-y+1/2$, $-z+5/2$.