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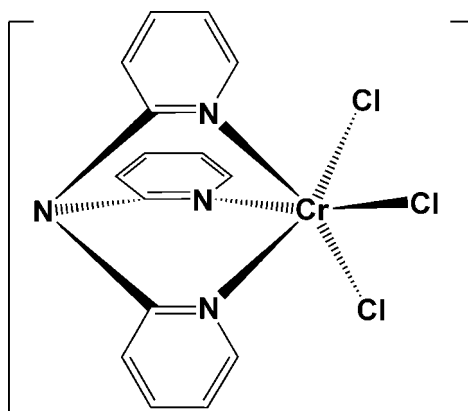
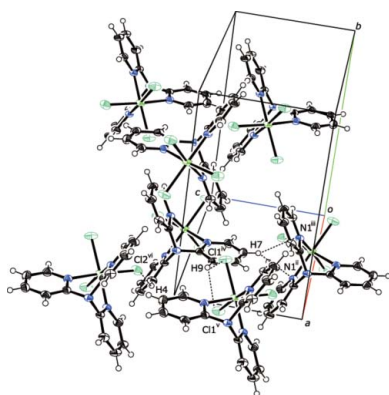
Crystal structure of *fac*-trichlorido[tris(pyridin-2-yl-*N*)amine]chromium(III)

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In the neutral complex molecule of the title compound, *fac*-[CrCl₃(tpa)] [tpa is tris(pyridin-2-yl)amine; C₁₅H₁₂N₄], 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*-[CrCl₃(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

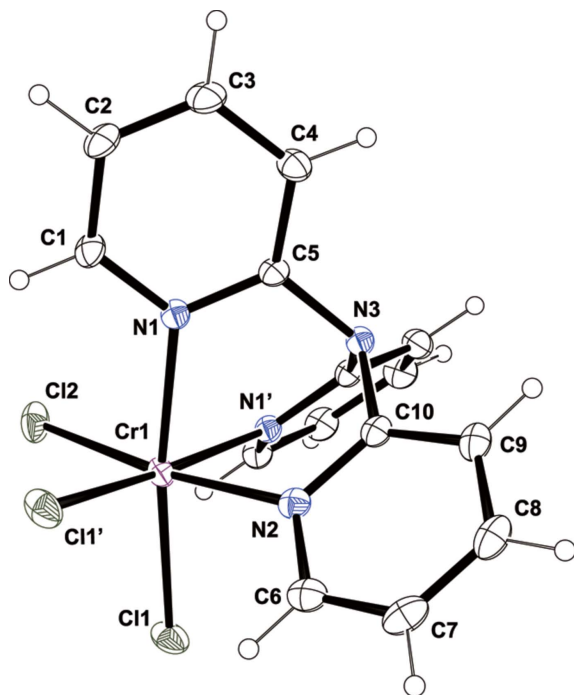


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (') $x, -y + \frac{1}{2}, z$.]

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 $fac\text{-}[\text{Cr}(\text{tpa})(\text{H}_2\text{O})_3]^{3+}$ [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*-[CrCl₃(terpy)] [terpy is 2,2',2''-terpyridine; C₁₅H₁₁N₃; 2.292 (1) Å] (Cloete *et al.*, 2007); *mer*-[CrCl₃py₃] [py is pyridine, C₅H₅N; 2.320 (7) Å] (Howard & Hardcastle, 1985) or *mer*-[CrCl₃(Etpy)₃] [Etpy is 4-ethylpyridine, C₇H₉N₃; 2.320 (7) Å] (Modéc *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

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

| <i>D</i> –H··· <i>A</i> | <i>D</i> –H | H··· <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> –H··· <i>A</i> |
|----------------------------|-------------|---------------|-----------------------|-------------------------|
| 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) $x + \frac{1}{2}, -y + \frac{1}{2}, -z + \frac{5}{2}$.

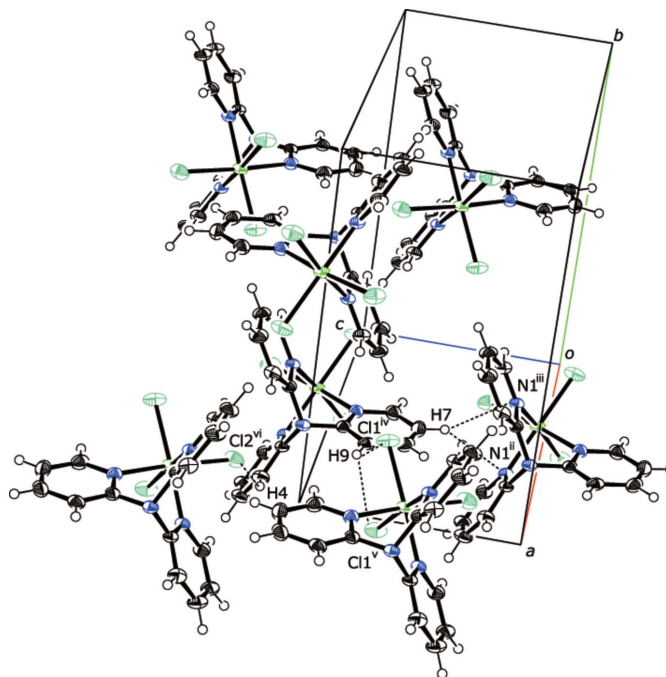


Figure 2
Hydrogen-bonding interactions in the crystal structure of (I), shown as black dashed lines. [Symmetry codes: (ii) $x, -y + \frac{1}{2}, z - 1$; (iii) $x, y, z - 1$; (iv) $x + \frac{1}{2}, y, -z + \frac{3}{2}$; (v) $x + \frac{1}{2}, -y + \frac{1}{2}, -z + \frac{3}{2}$; (vi) $x + \frac{1}{2},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

atoms (Fig. 2, Table 1). In addition, C–H···N hydrogen-bonding interactions are also present, consolidating the molecules into a three-dimensional network.

Table 2
Experimental details.

| | |
|--|---|
| Crystal data | [CrCl ₃ (C ₁₅ H ₁₂ N ₄)] |
| Chemical formula | 406.64 |
| <i>M_r</i> | Orthorhombic, <i>Pnma</i> |
| Crystal system, space group | 150 |
| Temperature (K) | 15.152 (13), 13.704 (12), 8.014 (7) |
| <i>a, b, c</i> (Å) | 1664 (2) |
| <i>V</i> (Å ³) | 4 |
| <i>Z</i> | Mo <i>Kα</i> |
| Radiation type | 1.17 |
| μ (mm ⁻¹) | 0.06 × 0.05 × 0.04 |
| Crystal size (mm) | |
| Data collection | |
| Diffractometer | Bruker APEXII CCD area detector |
| Absorption correction | Multi-scan (<i>SADABS</i> ; Bruker, 2014) |
| No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections | 15895, 1779, 1401 |
| <i>R</i> _{int} | 0.061 |
| (sin θ/λ) _{max} (Å ⁻¹) | 0.625 |
| Refinement | |
| <i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i> | 0.038, 0.113, 1.20 |
| No. of reflections | 1779 |
| No. of parameters | 118 |
| H-atom treatment | H-atom parameters constrained |
| Δρ _{max} , Δρ _{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-[CrCl₃(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): $\lambda_{\max}(\epsilon) = 720$ (16), 645 (37), 464 (59) nm (L mol⁻¹ cm⁻¹). Elemental analysis, calculated for C₁₅H₁₂C₁₃CrN₄: 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 $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$.

Acknowledgements

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References

- Bruker (2014). *APEX2, SADABS, SAINT and XPREP*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Cloete, N., Visser, H. G. & Roodt, A. (2007). *Acta Cryst.* **E63**, m45–m47.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Howard, S. A. & Hardcastle, K. I. (1985). *J. Crystallogr. Spectrosc. Res.* **15**, 643–649.
- Kaizaki, S. (1996). *Trends Inorg. Chem.* **6**, 105–136.
- Kaizaki, S. & Legg, J. I. (1994). *Inorg. Chim. Acta*, **218**, 179–184.
- Kaizaki, S. & Takemoto, H. (1990). *Inorg. Chem.* **29**, 4960–4964.
- Modec, B., Brenčič, J. V. & Giester, G. (2000). *J. Chem. Crystallogr.* **30**, 345–349.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Terasaki, Y., Fujihara, T., Nagasawa, A. & Kaizaki, S. (2004). *Acta Cryst.* **E60**, m854–m856.
- Terasaki, Y., Fujihara, T., Schönherr, T. & Kaizaki, S. (1999). *Inorg. Chim. Acta*, **295**, 84–90.
- Terasaki, Y. & Kaizaki, S. (1995). *J. Chem. Soc. Dalton Trans.* pp. 2837–2841.
- Yamaguchi-Terasaki, Y., Fujihara, A. & Kaizaki, S. (2007b). *Eur. J. Inorg. Chem.* **21**, 3394–3399.
- Yamaguchi-Terasaki, Y., Fujihara, A. & Kaizaki, S. (2007c). *Eur. J. Inorg. Chem.* **21**, 3400–3404.
- Yamaguchi-Terasaki, Y., Fujihara, T., Nagasawa, A. & Kaizaki, S. (2007a). *Acta Cryst.* **E63**, m593–m595.

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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

[CrCl₃(C₁₅H₁₂N₄)]

$M_r = 406.64$

Orthorhombic, *Pnma*

$a = 15.152$ (13) Å

$b = 13.704$ (12) Å

$c = 8.014$ (7) Å

$V = 1664$ (2) Å³

$Z = 4$

$F(000) = 820$

$D_x = 1.623$ 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

$0.06 \times 0.05 \times 0.04$ 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

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2014)

$T_{\min} = ?$, $T_{\max} = ?$

15895 measured reflections

1779 independent reflections

1401 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.061$

$\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 2.7^\circ$

$h = -18 \rightarrow 18$

$k = -17 \rightarrow 17$

$l = -10 \rightarrow 10$

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| 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* |
| C11 | 0.75326 (4) | 0.37578 (5) | 0.89695 (10) | 0.0388 (2) |
| C12 | 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 (\AA^2)

| | 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 (\AA , $^\circ$)

| | | | |
|----------|-----------|--------------------------|-------------|
| 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 ($\text{\AA}, ^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|-------|-------------|-------------|---------------|
| C7—H7 ⁱⁱ ···N1 ⁱⁱ | 0.95 | 2.75 | 3.578 (5) | 146 |
| C7—H7 ⁱⁱⁱ ···N1 ⁱⁱⁱ | 0.95 | 2.75 | 3.578 (5) | 146 |
| C9—H9 ^{iv} ···Cl1 ^{iv} | 0.95 | 2.82 | 3.447 (4) | 124 |
| C9—H9 ^v ···Cl1 ^v | 0.95 | 2.82 | 3.447 (4) | 124 |
| C4—H4 ^{vi} ···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) $x+1/2, -y+1/2, -z+5/2$.