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 Aqua(2,2'-bipyridine)trifluorido-
chromium(III) dihydrate

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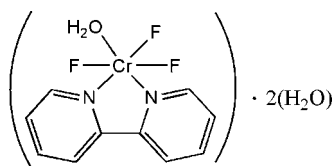
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.040; wR factor = 0.129; data-to-parameter ratio = 12.9.

The title compound, $[\text{CrF}_3(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]\cdot 2\text{H}_2\text{O}$, was prepared by the reaction of CrF_3 and 2,2'-bipyridine under hydrous conditions. The metal centre is coordinated in a distorted octahedral mode by two N atoms from the organic ligand, three F atoms and one O atom of a water molecule. The crystal packing is stabilized by $\text{O}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{F}$ hydrogen-bonding contacts, which form a one-dimensional belt extending parallel to (100).

Related literature

For anion structures, see: Kumar *et al.* (2007); Krishnan *et al.* (2007); Wu *et al.* (2007); Dong *et al.* (2005). For related structures, see: Timco *et al.* (2005); Larsen *et al.* (2003); Ochsenbein *et al.* (2008).



Experimental

Crystal data

$[\text{CrF}_3(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]\cdot 2\text{H}_2\text{O}$
 $M_r = 319.23$
 Monoclinic, $P2_1/c$
 $a = 9.0100$ (18) Å
 $b = 7.4170$ (15) Å
 $c = 20.759$ (6) Å
 $\beta = 112.35$ (3)°

$V = 1283.1$ (5) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.93$ mm⁻¹
 $T = 293$ K
 $0.24 \times 0.18 \times 0.17$ mm

Data collection

Bruker SMART CCD area-detector
 diffractometer
 Absorption correction: none
 6478 measured reflections
 2257 independent reflections
 1916 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.129$
 $S = 1.12$
 2257 reflections
 175 parameters
 3 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.52$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.56$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|-------|-------------|-------------|---------------|
| $\text{O1W}-\text{H2W1}\cdots\text{F1}$ | 0.85 | 2.22 | 2.699 (3) | 116 |
| $\text{O1W}-\text{H2W1}\cdots\text{F2}^{\text{i}}$ | 0.85 | 2.02 | 2.567 (3) | 121 |
| $\text{O1W}-\text{H2W1}\cdots\text{F2}^{\text{j}}$ | 0.85 | 2.02 | 2.567 (3) | 121 |
| $\text{O1W}-\text{H1W1}\cdots\text{F1}^{\text{ii}}$ | 0.85 | 1.97 | 2.550 (3) | 125 |
| $\text{O2W}-\text{H1W2}\cdots\text{F3}^{\text{ii}}$ | 0.85 | 2.10 | 2.664 (4) | 124 |
| $\text{O2W}-\text{H2W2}\cdots\text{O3W}^{\text{iii}}$ | 0.85 | 2.33 | 2.730 (5) | 110 |
| $\text{O3W}-\text{H2W3}\cdots\text{F2}^{\text{iv}}$ | 0.80 | 1.98 | 2.767 (3) | 171 |
| $\text{O3W}-\text{H1W3}\cdots\text{O3W}^{\text{v}}$ | 0.84 | 2.18 | 2.748 (7) | 125 |

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2114).

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supplementary materials

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Aqua(2,2'-bipyridine)trifluoridochromium(III) dihydrate

H.-X. Liu

Comment

In recent, the aspect of anion attracts much research interesting in coordination chemistry, like X^- , NO_3^- (Kumar *et al.*, 2007), BF_4^- , ClO_4^- (Krishnan *et al.*, 2007), SO_3^{2-} (Wu *et al.*, 2007). The anion components facily either coordinate to metal atoms or fill the vacancy of Metal-organic frameworks, and intensively influence the supramolecular framework by hydrogen bonding and electrostatic interactions. But the study of F^- anion is still deficient. Because the HF strong acid easily attacks the glass surface and creates SiF_6^{2-} in the synthetical progress. Here we describe the synthesis and structure of the title Cr compound coordinating with F atom.

The title structure (Fig. 1) was build up of one Cr atom, one 2,2'-bipyridine ligand, three coordination F atoms, one coordination water molecule and two free water molecules. Cr atom is coordinated with two N atoms from 2,2'-bipyridine ligand, three F atoms, one water molecule, presenting a distorted octahedron geometry. The mean Cr—N, Cr—O and Cr—F bond lengths are similar to the reported (Timco *et al.*, 2005, Larsen *et al.*, 2003 & Ochsenbein *et al.*, 2008). The torsion angles of C1—N1—Cr1—O1w, C10—N2—Cr1—F3 are 4.13 (2) and -4.25 (2)°, respectively.

The free water molecules link each other by intermolecular O—H \cdots O hydrogen bonds. And F atoms contact with water molecules *via* intermolecular O—H \cdots F hydrogen bonds (Table 2). The hydrogen-bonding interactions display as the one-dimensional belt linking the the crystal packing as shown in Fig. 2.

Experimental

All commercially obtained reagent-grade chemicals were used without further purification. The novelty $\text{Cr}(\text{OH})_3$ was prepared by mixture $\text{CrCl}_3 \cdot 6\text{H}_2\text{O}$ (5.33 g, 20 mmol) with NaOH (2.40 g, 60 mmol) in water solution. After filtered and washed with water, $\text{Cr}(\text{OH})_3$ was added to hydrofluoric acid (1.20 g, 60 mmol). The stirring did not stop until the solid dissolved completely. The CrF_3 solution was obtained after increasing the pH value from 5 to 7. Ten drops of prepared CrF_3 solution were added in the solution of 2,2'-bipyridine (0.48 g, 3 mmol) in water and methanol (3:1 v/v, 40 ml). The resulting solution was refluxed for 2 h and filtered. The brown prism crystals were collected, after cooling and filtering (yield 1.10 g).

Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C-H and O-H distances of 0.93–0.96 and 0.85 Å, respectively, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$ of the parent atoms.

Figures

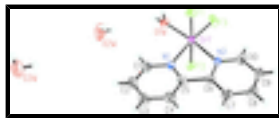


Fig. 1. The molecular structure of the title compound with the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

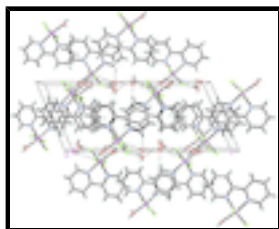


Fig. 2. The packing view of the molecules of (I) along the crystallographic b direction.

Aqua(2,2'-bipyridine)trifluoridochromium(III) dihydrate

Crystal data

[CrF₃(C₁₀H₈N₂)(H₂O)]·2H₂O

M_r = 319.23

Monoclinic, *P*2₁/*c*

Hall symbol: -*P* 2ybc

a = 9.0100 (18) Å

b = 7.4170 (15) Å

c = 20.759 (6) Å

β = 112.35 (3)°

V = 1283.1 (5) Å³

Z = 4

*F*₀₀₀ = 652

D_x = 1.653 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 1024 reflections

θ = 2.4–25.0°

μ = 0.93 mm⁻¹

T = 293 K

Prism, brown

0.24 × 0.18 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 293 K

φ and ω scans

Absorption correction: none

6478 measured reflections

2257 independent reflections

1916 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.023

θ_{max} = 25.0°

θ_{min} = 2.4°

h = -10→10

k = -8→8

l = -21→24

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.040

wR (*F*²) = 0.129

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

w = 1/[σ²(*F*_o²) + (0.0755*P*)² + 0.6391*P*]

| | |
|--|--|
| $S = 1.12$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 2257 reflections | $(\Delta/\sigma)_{\max} < 0.001$ |
| 175 parameters | $\Delta\rho_{\max} = 0.52 \text{ e } \text{\AA}^{-3}$ |
| 3 restraints | $\Delta\rho_{\min} = -0.56 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|-------------|-------------|--------------|----------------------------------|
| Cr1 | 0.15638 (5) | 0.28271 (7) | 0.32953 (2) | 0.0283 (2) |
| F1 | 0.2014 (2) | 0.0442 (2) | 0.31271 (9) | 0.0393 (5) |
| F2 | 0.1128 (2) | 0.5267 (2) | 0.34286 (9) | 0.0436 (5) |
| F3 | -0.0083 (2) | 0.2083 (3) | 0.35635 (12) | 0.0521 (6) |
| N1 | 0.3615 (3) | 0.3591 (4) | 0.31451 (13) | 0.0331 (6) |
| N2 | 0.3252 (3) | 0.2663 (3) | 0.42877 (13) | 0.0318 (6) |
| C1 | 0.3689 (4) | 0.4133 (5) | 0.25417 (18) | 0.0453 (8) |
| H1A | 0.2741 | 0.4299 | 0.2157 | 0.054* |
| C2 | 0.5145 (5) | 0.4453 (5) | 0.2477 (2) | 0.0540 (10) |
| H2A | 0.5168 | 0.4829 | 0.2054 | 0.065* |
| C3 | 0.6529 (5) | 0.4212 (6) | 0.3035 (2) | 0.0579 (10) |
| H3A | 0.7513 | 0.4406 | 0.2997 | 0.069* |
| C4 | 0.6469 (4) | 0.3678 (6) | 0.3661 (2) | 0.0533 (10) |
| H4A | 0.7410 | 0.3513 | 0.4050 | 0.064* |
| C5 | 0.4997 (4) | 0.3393 (4) | 0.37029 (17) | 0.0358 (7) |
| C6 | 0.4791 (4) | 0.2890 (4) | 0.43569 (17) | 0.0353 (7) |
| C7 | 0.6048 (5) | 0.2693 (5) | 0.4996 (2) | 0.0506 (10) |
| H7A | 0.7105 | 0.2842 | 0.5037 | 0.061* |
| C8 | 0.5698 (6) | 0.2272 (6) | 0.5569 (2) | 0.0613 (12) |
| H8A | 0.6521 | 0.2127 | 0.6003 | 0.074* |
| C9 | 0.4128 (5) | 0.2068 (5) | 0.54970 (18) | 0.0559 (11) |
| H9A | 0.3875 | 0.1802 | 0.5881 | 0.067* |
| C10 | 0.2933 (5) | 0.2264 (5) | 0.48461 (18) | 0.0432 (8) |
| H10A | 0.1870 | 0.2113 | 0.4796 | 0.052* |
| O1W | 0.0184 (3) | 0.3056 (3) | 0.22962 (11) | 0.0363 (5) |

supplementary materials

| | | | | |
|------|------------|------------|--------------|-------------|
| H1W1 | -0.0536 | 0.3443 | 0.1923 | 0.044* |
| H2W1 | 0.0476 | 0.2023 | 0.2211 | 0.044* |
| O2W | 0.0891 (5) | 0.4622 (5) | 0.06932 (16) | 0.0883 (11) |
| H1W2 | 0.0245 | 0.4742 | 0.0901 | 0.106* |
| H2W2 | 0.1487 | 0.3719 | 0.0871 | 0.106* |
| O3W | 0.9992 (4) | 0.1082 (5) | 0.05359 (17) | 0.0790 (10) |
| H2W3 | 0.9750 | 0.0764 | 0.0850 | 0.095* |
| H1W3 | 1.0333 | 0.0066 | 0.0477 | 0.095* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Cr1 | 0.0252 (3) | 0.0273 (3) | 0.0288 (3) | 0.00016 (18) | 0.0059 (2) | 0.00170 (18) |
| F1 | 0.0344 (10) | 0.0296 (10) | 0.0462 (10) | 0.0000 (8) | 0.0068 (8) | -0.0007 (8) |
| F2 | 0.0530 (12) | 0.0329 (10) | 0.0371 (10) | 0.0091 (9) | 0.0084 (9) | -0.0017 (8) |
| F3 | 0.0343 (11) | 0.0647 (15) | 0.0608 (13) | -0.0003 (10) | 0.0221 (10) | 0.0137 (10) |
| N1 | 0.0326 (14) | 0.0322 (14) | 0.0334 (14) | -0.0042 (11) | 0.0113 (11) | 0.0016 (11) |
| N2 | 0.0322 (14) | 0.0298 (14) | 0.0288 (14) | -0.0015 (11) | 0.0063 (11) | 0.0028 (10) |
| C1 | 0.048 (2) | 0.046 (2) | 0.0418 (19) | -0.0066 (17) | 0.0172 (16) | 0.0051 (15) |
| C2 | 0.068 (3) | 0.050 (2) | 0.059 (2) | -0.0085 (19) | 0.042 (2) | 0.0035 (18) |
| C3 | 0.043 (2) | 0.066 (3) | 0.072 (3) | -0.0106 (19) | 0.030 (2) | -0.001 (2) |
| C4 | 0.0329 (18) | 0.063 (2) | 0.062 (2) | -0.0048 (18) | 0.0159 (17) | 0.000 (2) |
| C5 | 0.0315 (16) | 0.0313 (16) | 0.0425 (18) | -0.0038 (13) | 0.0116 (14) | -0.0021 (14) |
| C6 | 0.0303 (17) | 0.0296 (17) | 0.0384 (18) | -0.0028 (13) | 0.0046 (14) | -0.0014 (13) |
| C7 | 0.0354 (19) | 0.052 (2) | 0.046 (2) | -0.0042 (16) | -0.0048 (17) | 0.0025 (16) |
| C8 | 0.062 (3) | 0.062 (3) | 0.037 (2) | -0.003 (2) | -0.0079 (19) | 0.0087 (17) |
| C9 | 0.072 (3) | 0.057 (3) | 0.0294 (19) | -0.006 (2) | 0.0090 (18) | 0.0086 (16) |
| C10 | 0.045 (2) | 0.045 (2) | 0.0367 (19) | -0.0040 (16) | 0.0128 (16) | 0.0048 (15) |
| O1W | 0.0351 (12) | 0.0310 (11) | 0.0305 (11) | 0.0072 (9) | -0.0013 (9) | -0.0002 (9) |
| O2W | 0.124 (3) | 0.079 (2) | 0.081 (2) | 0.037 (2) | 0.060 (2) | 0.0043 (18) |
| O3W | 0.096 (2) | 0.083 (2) | 0.079 (2) | -0.002 (2) | 0.0559 (19) | 0.0067 (19) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|---------|-------------|----------|-----------|
| Cr1—F3 | 1.856 (2) | C4—H4A | 0.9300 |
| Cr1—F1 | 1.8769 (18) | C5—C6 | 1.486 (5) |
| Cr1—F2 | 1.8942 (19) | C6—C7 | 1.386 (5) |
| Cr1—O1W | 1.979 (2) | C7—C8 | 1.379 (6) |
| Cr1—N2 | 2.047 (3) | C7—H7A | 0.9300 |
| Cr1—N1 | 2.067 (3) | C8—C9 | 1.373 (6) |
| N1—C1 | 1.341 (4) | C8—H8A | 0.9300 |
| N1—C5 | 1.348 (4) | C9—C10 | 1.378 (5) |
| N2—C10 | 1.329 (4) | C9—H9A | 0.9300 |
| N2—C6 | 1.350 (4) | C10—H10A | 0.9300 |
| C1—C2 | 1.388 (5) | O1W—H1W1 | 0.8498 |
| C1—H1A | 0.9300 | O1W—H2W1 | 0.8500 |
| C2—C3 | 1.353 (6) | O2W—H1W2 | 0.8500 |
| C2—H2A | 0.9300 | O2W—H2W2 | 0.8500 |
| C3—C4 | 1.378 (6) | O3W—H2W3 | 0.7978 |

| | | | |
|------------|-------------|---------------|------------|
| C3—H3A | 0.9300 | O3W—H1W3 | 0.840 (10) |
| C4—C5 | 1.378 (5) | | |
| F3—Cr1—F1 | 91.69 (9) | C2—C3—H3A | 120.3 |
| F3—Cr1—F2 | 90.37 (10) | C4—C3—H3A | 120.3 |
| F1—Cr1—F2 | 177.37 (8) | C3—C4—C5 | 119.1 (4) |
| F3—Cr1—O1W | 94.86 (10) | C3—C4—H4A | 120.4 |
| F1—Cr1—O1W | 88.84 (8) | C5—C4—H4A | 120.4 |
| F2—Cr1—O1W | 89.35 (8) | N1—C5—C4 | 121.7 (3) |
| F3—Cr1—N2 | 93.05 (10) | N1—C5—C6 | 114.7 (3) |
| F1—Cr1—N2 | 90.05 (9) | C4—C5—C6 | 123.6 (3) |
| F2—Cr1—N2 | 91.48 (9) | N2—C6—C7 | 121.4 (3) |
| O1W—Cr1—N2 | 172.04 (10) | N2—C6—C5 | 114.5 (3) |
| F3—Cr1—N1 | 171.69 (10) | C7—C6—C5 | 124.1 (3) |
| F1—Cr1—N1 | 87.80 (9) | C8—C7—C6 | 118.6 (4) |
| F2—Cr1—N1 | 90.39 (10) | C8—C7—H7A | 120.7 |
| O1W—Cr1—N1 | 93.42 (10) | C6—C7—H7A | 120.7 |
| N2—Cr1—N1 | 78.66 (11) | C9—C8—C7 | 119.7 (4) |
| C1—N1—C5 | 118.5 (3) | C9—C8—H8A | 120.2 |
| C1—N1—Cr1 | 126.0 (2) | C7—C8—H8A | 120.2 |
| C5—N1—Cr1 | 115.3 (2) | C8—C9—C10 | 118.9 (4) |
| C10—N2—C6 | 119.3 (3) | C8—C9—H9A | 120.5 |
| C10—N2—Cr1 | 124.5 (2) | C10—C9—H9A | 120.5 |
| C6—N2—Cr1 | 116.1 (2) | N2—C10—C9 | 122.1 (4) |
| N1—C1—C2 | 121.7 (3) | N2—C10—H10A | 119.0 |
| N1—C1—H1A | 119.1 | C9—C10—H10A | 119.0 |
| C2—C1—H1A | 119.1 | Cr1—O1W—H1W1 | 160.5 |
| C3—C2—C1 | 119.5 (3) | Cr1—O1W—H2W1 | 91.2 |
| C3—C2—H2A | 120.3 | H1W1—O1W—H2W1 | 107.7 |
| C1—C2—H2A | 120.3 | H1W2—O2W—H2W2 | 107.7 |
| C2—C3—C4 | 119.4 (4) | H2W3—O3W—H1W3 | 94.7 |

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> |
|-------------------------------|-------------|---------------|-----------------------|-------------------------|
| O1W—H2W1...F1 | 0.85 | 2.22 | 2.699 (3) | 116 |
| O1W—H2W1...F2 ⁱ | 0.85 | 2.02 | 2.567 (3) | 121 |
| O1W—H2W1...F2 ⁱ | 0.85 | 2.02 | 2.567 (3) | 121 |
| O1W—H1W1...F1 ⁱⁱ | 0.85 | 1.97 | 2.550 (3) | 125 |
| O2W—H1W2...F3 ⁱⁱ | 0.85 | 2.10 | 2.664 (4) | 124 |
| O2W—H2W2...O3W ⁱⁱⁱ | 0.85 | 2.33 | 2.730 (5) | 110 |
| O3W—H2W3...F2 ^{iv} | 0.80 | 1.98 | 2.767 (3) | 171 |
| O3W—H2W3...F3 ^{iv} | 0.80 | 2.96 | 3.490 (4) | 126 |
| O3W—H1W3...O3W ^v | 0.84 | 2.18 | 2.748 | 125 |

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

Fig. 1

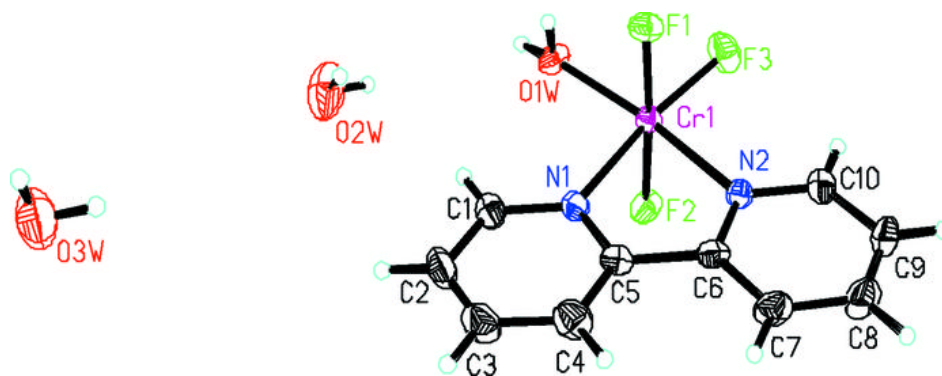


Fig. 2

