addenda and errata

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Retraction of articles

This article reports the retraction of articles published in *Acta Crystallographica Section E* between 2005 and 2009.

After further thorough investigation (see Harrison *et al.*, 2010), articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1

Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
Poly[diaquadi-µ ₃ -malonato-µ-pyrazine-dinickel(II)]	Liu et al. (2005)	10.1107/S1600536805026358	GATWAA
catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)samarium(II)]-µ-pyridine-2,6- dicarboxylato] tetrahydrate]	Liu et al. (2006)	10.1107/S1600536806038141	FONCUH03
Poly[[[µ ₄ -4,4'-carbonylbis(benzene-3,4-dicarboxylato)]tetrakis(1,10-phenanthroline)- dipalladium(II)] dihydrate]	Li, Wang, Zhang & Yu (2007e)	10.1107/S1600536807039050	AFELAZ
Poly[diaqua-µ3-malonato-µ-pyrazine-diiron(II)]	Li, Liu et al. (2007)	10.1107/S1600536807038743	AFELON
$Poly[diaqua-di-\mu_3-malonato-\mu-pyrazine-dimanganese(II)]$	Li, Wang, Zhang & Yu (2007f)	10.1107/S1600536807039773	VIJZAQ
$Poly[[aqua(2,2-bipyridine)(\mu_3-pyridine-3,4-dicarboxylato)cobalt(II)]$ monohydrate]	Li, Wang, Zhang & Yu $(2007g)$	10.1107/S1600536807040275	VIKCIC
catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)holmium(III)]-µ-pyridine-2,6- dicarboxylato] tetrahydrate]	Li, Wang, Zhang & Yu (2007a)	10.1107/S1600536807041657	DILGEL
catena-Poly[[(2,2'-bipyridine- $\kappa^2 N, N'$)iron(II)]- μ -5-carboxy-4-carboxylatoimidazol-1-ido- $\kappa^4 N^3. O^4: N^1. O^5$]	Li, Wang, Zhang & Yu (2007 <i>h</i>)	10.1107/S1600536807042122	XIKWAQ
$Poly[[aqua(2,2'-bipyridine)(\mu_3-pyridine-3,4-dicarboxylato)nickel(II)] monohydrate]$	Li, Wang, Zhang & Yu (2007b)	10.1107/S1600536807046466	LEVZAO01
2-(Benzyliminomethyl)-6-methoxyphenol	Li, Wang, Zhang & Yu (2007 <i>i</i>)	10.1107/S1600536807042134	SILDEX
$Poly[aqua(2,2'-bipyridine)(\mu_3-pyridine-2,4-dicarboxylato)palladium(II)]$	Li, Wang, Zhang & Yu (2007c)	10.1107/S1600536807047575	SILXAN
μ -Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]iron(III)} bis(hexafluoridophosphate)	Liu, Dou, Li & Zhang (2007)	10.1107/S1600536807049665	TINRIS
µ-Oxido-bis({4,4'-dibromo-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato]- manganese([II]))	Liu, Dou, Niu & Zhang $(2007a)$	10.1107/S1600536807051008	GIMZAE
Bis[N-(8-quinolyl)pyridine-2-carboxamidato]iron(III) perchlorate monohydrate	(2007 <i>d</i>) Li, Wang, Zhang & Yu (2007 <i>d</i>)	10.1107/S1600536807048556	WIMZIC
µ-Oxido-bis({4,4'-dibromo-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato]- chromium(III))	Liu, Dou, Niu & Zhang (2007b)	10.1107/S1600536807057996	HIQFIX
µ-Oxido-bis[chlorido[tris(2-pyridylmethyl)amine]chromium(III)} bis(hexafluorido- phosphate)	Li, Wang et al. (2008)	10.1107/S1600536807061296	MIRNAD
μ -Oxido-bis({4,4'-dibromo-2,2'-ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- iron(III))	Meng et al. (2008a)	10.1107/S1600536807063143	MIRWUG
$\kappa^{2}O^{1}(O^{4})$	Meng et al. (2008b)	10.1107/S1600536807065051	XISCAE
Oxalatobis(propane-1,3-diamine)manganese(II) chloride monohydrate	Meng et al. (2008e)	10.1107/\$1600536807065361	SISWIB
µ-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]manganese(III)} bis(hexafluorido- phosphate)	Meng et al. (2008c)	10.1107/S1600536807066512	RISRIV
Bis[N-(8-quinolyl)pyridine-2-carboxamidato-κ ³ N,N',N'']manganese(III) perchlorate monohydrate	Meng et al. (2008d)	10.1107/S1600536808000287	GISLEA
Diaquabis(pyridine-2-carboxylato- $\kappa^2 N, O$)cobalt(II)	Huang (2008)	10.1107/S1600536808010507	WIZPOL
Tetra-µ-2,5-difluorobenzoato-bis[(2,2'-bipyridine)(2,5-difluorobenzoato)gadolinium(III)]	Li, Zhang et al. (2008)	10.1107/S1600536808023507	BOFQIX
catena-Poly[[(2,2'-bipyridine- $\kappa^2 N, N'$)nickel(II)]- μ -oxalato- $\kappa^4 O^1 \cdot O^2 \cdot O^{1'} \cdot O^{2'}$]	Li, Yan et al. (2008)	10.1107/S1600536808028389	NOHYUF
catena-Poly[[aqua(2,2'-bipvridyl)cobalt(II)]-u-5-nitroisophthlalato]	Liu <i>et al.</i> (2008)	10.1107/\$1600536808038178	AFIREN
$Diaguabis(pyridine-2-carboxylato-\kappa^2 N.O)iron(II)$	Xia & Sun (2009)	10.1107/\$1600536809005765	RONFEG
catena-Poly[[[diaquathulium(III]]-µ-6-carboxynicotinato-µ-pyridine-2,5-dicarboxylato] dihydrate]	Li et al. (2009)	10.1107/S1600536809008836	NOQNIR
1-Phenyl-3-(2,4,6-trimethoxyphenyl)prop-2-en-1-one	Liu et al. (2009)	10.1107/S1600536809040227	PUGLOT



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metal-organic compounds

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u-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]chromium(III)} bis(hexafluoridophosphate)

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ (C–C) = 0.004 Å; R factor = 0.032; wR factor = 0.089; data-to-parameter ratio = 13.5.

The title compound, [Cr₂Cl₂O(C₁₈H₁₈N₄)₂](PF₆)₂, is isostructural with the V^{III} analogue. Each Cr^{III} atom is chelated by the tetradentate tris(2-pyridylmethyl)amine ligand via four N atoms, and further coordinated by one Cl atom and one bridging O atom, giving a slightly distorted octahedral coordination geometry. The dinuclear complex is centrosym metric, with the bridging O atom lying on a centre of inversion.

Related literature

For the isostructural V^{III} analogue, see: Tajika et al. (2005). For more general related literature, see: Butler & Carrano (1991); Crans et al. (1989); Dey (1974); Chen & Zubieta (1990).



Experimental

Crystal data

[Cr₂Cl₂O(C₁₈H₁₈N₄)₂](PF₆)₂ $\gamma = 91.50 \ (3)^{\circ}$ $M_r = 1061.57$ Triclinic, $P\overline{1}$ a = 8.6107 (17) Åb = 11.302 (2) Å c = 12.798 (3) Å $\alpha = 115.50 \ (3)^{\circ}$ $\beta = 107.45 \ (3)^{\circ}$

Data collection

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Bruker APEXII CCD
  diffractometer
Absorption correction: multi-scan
  (SADABS: Bruker, 2001)
  T_{\min} = 0.804, T_{\max} = 0.867
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Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.033$ $wR(F^2) = 0.089$ S = 1.003877 reflections

V = 1054.8 (4) Å³ Z = 1Mo $K\alpha$ radiation $\mu = 0.81 \text{ mm}^{-1}$ T = 293 (2) K $0.28 \times 0.22 \times 0.18 \text{ mm}$

8686 measured reflections 3877 independent reflections 3594 reflections with $I > 2\sigma(I)$ $R_{\rm int} = 0.021$

87 parameters H-atom parameters constrained $\Delta \rho_{\text{max}} = 0.51 \text{ e } \text{\AA}^ \Delta \rho_{\rm min} = -0.33 \text{ e } \text{\AA}^{-3}$

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2001); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2257).

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supporting information

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µ-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]chromium(III)} bis-(hexafluoridophosphate)

Sheng Li, Shou-Bin Wang, Fu-Li Zhang and Kun Tang

S1. Comment

A classical but nevertheless rapidly developing field of application for related metal-Schiff compounds is their use as catalysts in polymerization, oxidation reactions, and model examples for the interaction of metal ions within the active sites of enzymes (Butler & Carrano, 1991; Crans *et al.*, 1989; Dey, 1974; Chen & Zubieta, 1990). In the dinuclear title compound (Fig. 1), each Cr^{III} atom is chelated by the tetradentate ligand tris(2-pyridylmethyl)amine *via* four N atoms, and further coordinated by one Cl atom and one bridging O atom to give a slightly distorted octahedral coordination geometry.

S2. Experimental

A mixture of chromium(III) trichloride (1 mmol) and tris(2-pyridylmethyl)amine (1 mmol) in 20 ml me thanol was refluxed for two hours. After cooling, the solution was filtered and the filtrate was evaporated naturally at room temperature. Blue blocks of the title compound were obtained after a few days with a yield of 31%. Elemental analysis calculated: C 40.39, H 3.35, N 10.44%; found: C 40.35, H 3.39, N 10.42%.

S3. Refinement

All H atoms were placed in calculated positions with C—H = 0.93 or 0.97 Å and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.



 $\theta = 3.0 - 25.5^{\circ}$

 $\mu = 0.81 \text{ mm}^{-1}$

 $0.28 \times 0.22 \times 0.18 \text{ mm}$

T = 293 K

Block, blue

Figure 1

The molecular structure drawn with 30% probability displacement ellipsoids for the non-H atoms.

 μ -Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]chronium(III)} dihexafluoridophosphate

Crystal data $[Cr_2Cl_2O(C_{18}H_{18}N_4)_2](PF_6)_2$ $M_r = 1061.57$ Triclinic, $P\overline{1}$ Hall symbol: -P 1 a = 8.6107 (17) Åb = 11.302 (2) Å *c* = 12.798 (3) Å $\alpha = 115.50 (3)^{\circ}$ $\beta = 107.45 (3)^{\circ}$ $\gamma = 91.50 (3)^{\circ}$ V = 1054.8 (4) Å³

Data collection

Bruker APEX II CCD	8686 measured reflections
diffractometer	3877 independent reflections
Radiation source: fine-focus sealed tube	3594 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\rm int} = 0.021$
φ and ω scans	$\theta_{\rm max} = 25.5^{\circ}, \ \theta_{\rm min} = 3.0^{\circ}$
Absorption correction: multi-scan	$h = -8 \rightarrow 10$
(SADABS; Bruker, 2001)	$k = -13 \rightarrow 13$
$T_{\min} = 0.804, \ T_{\max} = 0.867$	$l = -15 \rightarrow 15$

Refinement

Refinement on F ² Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H-atom parameters constrained
$WR(F^2) = 0.089$	$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 0.3428P]$
S = 1.00	where $P = (F_o^2 + 2F_c^2)/3$
3877 reflections	$(\Delta/\sigma)_{\rm max} < 0.001$
287 parameters	$\Delta \rho_{\rm max} = 0.51 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta \rho_{\rm min} = -0.33 \text{ e} \text{ Å}^{-3}$
Primary atom site location: structure-invariant	Extinction correction: SHELXL,
direct methods	$Fc^* = kFc[1+0.001xFc^2\lambda^3/sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier	Extinction coefficient: 0.042 (3)
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 vR 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	У	Z	$U_{ m iso}$ */ $U_{ m eq}$
Cr1	1.03745 (3)	0.34679 (3)	0.39271 (2)	0.0408 (4)
C1	0.9871 (3)	0.1897 (2)	0.53070 (18)	0.0447 (4)
H1	1.1018	0.1984	0.5573	0.054*
C2	0.8992 (3)	0.1306 (2)	0.5741 (2)	0.0534 (5)
H2	0.9533	0.0998	0.6296	0.064*
C3	0.7284 (3)	0.1173 (3)	0.5340 (2)	0.0605 (6)
Н3	0.6662	0.0779	0.5626	0.073*
C4	0.6514 (3)	0.1630 (2)	0.4513 (2)	0.0552 (5)
H4	0.5367	0.1537	0.4226	0.066*
C5	0.7464 (2)	0.22306 (19)	0.41135 (18)	0.0425 (4)
C6	0.6721 (2)	0.2874 (2)	0.3310 (2)	0.0490 (5)
H6A	0.5643	0.2353	0.2730	0.059*
H6B	0.6563	0.3757	0.3822	0.059*
C7	0.7467 (3)	0.1753 (2)	0.1450 (2)	0.0573 (6)
H7A	0.7443	0.2004	0.0811	0.069*
H7B	0.6381	0.1253	0.1216	0.069*
C8	0.8712 (2)	0.08565 (19)	0.14924 (17)	0.0414 (4)
C9	0.8351 (3)	-0.0448 (2)	0.0588 (2)	0.0528 (5)
Н9	0.7315	-0.0793	-0.0028	0.063*
C10	0.9546 (3)	-0.1237 (2)	0.0606 (2)	0.0617 (6)
H10	0.9327	-0.2119	0.0003	0.074*
C11	1.1069 (3)	-0.0697 (2)	0.1532 (2)	0.0607 (6)
H11	1.1894	-0.1208	0.1564	0.073*

C12	1.1346 (3	3) 0.0	605 (2)	0.2404 (2)	0.0526 (5)	
H12	1.2374	0.0	964	0.3028	0.063*	
C13	0.7605 (3	3) 0.4	147 (2)	0.23723 (19)	0.0475 (5)	
H13A	0.7430	0.4	881	0.3059	0.057*	
H13B	0.6651	0.3	917	0.1639	0.057*	
C14	0.9146 (3	3) 0.4	574 (2)	0.21891 (17)	0.0471 (5)	
C15	0.9138 (4	1) 0.5	296 (2)	0.1547 (2)	0.0606 (6)	
H15	0.8154	0.5	482	0.1149	0.073*	
C16	1.0629 (4	4) 0.5	734 (3)	0.1512 (2)	0.0728 (8)	
H16	1.0650	0.6	237	0.1100	0.087*	
C17	1.2075 (4	(1) 0.5	435 (3)	0.2077(3)	0.0715 (7)	
H17	1.3076	0.5	721	0.2047	0.086*	
C18	1.2007 (3	3) 0.4	704 (3)	0.2686 (2)	0.0610 (6)	
H18	1.2978	0.4	490	0.3069	0.073*	
Cl1	1 31398	(6) 0.3	5078 (6)	0.48445(5)	0.07507(17)	
F1	0 5115 (2	$\begin{array}{c} (0) \\$	0.0789(16)	0.13882(17)	0.0825 (5)	
F2	0.4878 (2	$\frac{1}{2} \qquad 0.8$	490 (2)	0.13002(17) 0.27945(15)	0.0893(5)	
F3	0.5830 (3	3) 0.6	507 (2)	0.27945(15) 0.1912(2)	0.0099(3) 0.1078(7)	
F4	0.3830 (2	(0.0)	507(2)	0.1912(2) 0.24906(17)	0.1078 (7)	
F5	0.7323 (2	$(2) \qquad 0.3^{\circ}$	2005(10)	0.24900(17) 0.04870(17)	0.0999 (0)	
F5 F6	0.0040 (2	(10) 0.7	1102(16)	0.04870(17) 0.08031(14)	0.0929(0)	
N1	1.0102 (2	(13) 0.7	1102(10)	0.08031(14) 0.23060(15)	0.0720(4)	
ND	1.0192 (2	$(2) \qquad 0.1$	5917(10)	0.23909(13)	0.0430(4)	
INZ NI2	1.0300 (2	(10) 0.4	2040(10)	0.27434(10) 0.45104(15)	0.0462(4)	
IN 3 NI4	0.91312	(19) 0.2	3307(13)	0.43104(13)	0.0400(3)	
N4	0.7776 (2	2) 0.2	9834 (10)	0.26214 (15)	0.0424 (4)	
DI	1.0000	(7) 0.3		0.3000	0.0420(4)	
ГІ	0.34870	(/) 0./	5424 (0)	0.10349 (3)	0.05270(17)	
Atomic	displacement para	umeters (Å ²)				
	U^{11}	U ²²	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.0378 (11)	0.0424 (10)	0.0424 (10)	0.0088 (8)	0.0112 (8)	0.0212 (8)
C1	0.0415 (10)	0.0468 (10)	0.0459 (10)	0.0095 (8)	0.0121 (8)	0.0233 (8)
C2	0.0597 (14)	0.0546 (12)	0.0513 (12)	0.0109 (10)	0.0179 (10)	0.0300 (10)
C3	0.0606 (14)	0.0666 (14)	0.0669 (14)	0.0057 (11)	0.0281 (11)	0.0381 (12)
C4	0.0395 (11)	0.0606 (13)	0.0695 (14)	0.0063 (9)	0.0206 (10)	0.0324 (11)
C5	0.0351 (9)	0.0412 (9)	0.0456 (10)	0.0057 (7)	0.0117 (8)	0.0166 (8)
C6	0.0302 (9)	0.0572 (12)	0.0614 (12)	0.0093 (8)	0.0107 (8)	0.0322 (10)
C7	0.0517 (13)	0.0499 (12)	0.0462 (11)	0.0099 (9)	-0.0011 (9)	0.0127 (9)
C8	0.0424 (10)	0.0438 (10)	0.0403 (9)	0.0052 (8)	0.0153 (8)	0.0207 (8)
C9	0.0562 (13)	0.0484 (11)	0.0497 (11)	0.0027 (9)	0.0185 (10)	0.0189 (9)
C10	0.0769 (17)	0.0441 (11)	0.0634 (14)	0.0138 (11)	0.0334 (13)	0.0178 (10)
C11	0.0653 (15)	0.0551 (13)	0.0714 (15)	0.0256 (11)	0.0342 (12)	0.0297 (11)
C12	0.0460 (12)	0.0572 (12)	0.0570 (12)	0.0167 (9)	0.0199 (10)	0.0265 (10)
C13	0.0504 (11)	0.0490 (11)	0.0410 (10)	0.0162 (9)	0.0097 (8)	0.0224 (9)
C14	0.0599 (13)	0.0426 (10)	0.0358 (9)	0.0112 (9)	0.0152 (9)	0.0162 (8)
C15	0.0864 (18)	0.0503 (12)	0.0451 (12)	0.0140 (11)	0.0197 (11)	0.0237 (10)
C16	0.114 (2)	0.0544 (13)	0.0572 (14)	0.0012 (14)	0.0362 (15)	0.0288 (12)

supporting information

Geome	tric parameters (Å	, ^{<i>o</i>})				
P1	0.0429 (3)	0.0665 (4)	0.0529 (3)	0.0075 (3)	0.0151 (2)	0.0321 (3)
01	0.0384 (10)	0.0430 (10)	0.0424 (10)	0.0081 (8)	0.0119 (8)	0.0190 (8)
N4	0.0376 (8)	0.0442 (8)	0.0411 (8)	0.0101 (7)	0.0077 (6)	0.0195 (7)
N3	0.0348 (8)	0.0421 (8)	0.0447 (8)	0.0082 (6)	0.0125 (7)	0.0205 (7)
N2	0.0526 (10)	0.0497 (9)	0.0451 (9)	0.0087 (8)	0.0187 (8)	0.0231 (8)
N1	0.0425 (9)	0.0456 (9)	0.0444 (9)	0.0116 (7)	0.0164 (7)	0.0210 (7)
F6	0.0571 (9)	0.0710 (9)	0.0731 (9)	-0.0042 (7)	0.0144 (7)	0.0248 (7)
F5	0.0973 (13)	0.0965 (12)	0.0873 (12)	0.0083 (10)	0.0563 (10)	0.0288 (10)
F4	0.0483 (9)	0.1549 (19)	0.0854 (12)	-0.0063 (10)	0.0024 (8)	0.0605 (12)
F3	0.1008 (15)	0.1236 (16)	0.163 (2)	0.0524 (12)	0.0641 (14)	0.1074 (16)
F2	0.0836 (12)	0.1141 (14)	0.0632 (9)	0.0059 (10)	0.0336 (8)	0.0300 (9)
F1	0.0810 (11)	0.0724 (10)	0.0988 (12)	0.0060 (8)	0.0208 (9)	0.0507 (9)
Cl1	0.0334 (3)	0.0609 (3)	0.0596 (3)	0.0131 (2)	0.0101 (2)	0.0215 (2)
C18	0.0612 (14)	0.0666 (14)	0.0615 (14)	0.0042 (11)	0.0280 (11)	0.0307 (12)
C17	0.084 (2)	0.0710 (16)	0.0683 (16)	-0.0005 (14)	0.0357 (14)	0.0343 (13)

Cr1-01	1.7986 (7)	С9—Н9	0.930
Cr1—N3	2.1206 (18)	C10—C11	1.378 (4)
Cr1—N2	2.1238 (18)	С10—Н10	0.930
Cr1—N4	2.2370 (19)	C11—C12	1.370 (3)
Cr1—N1	2.2814 (19)	C11—H11	0.930
Cr1—Cl1	2.3070 (9)	C12—N1	1.351 (3)
O1-Cr1 ⁱ	1.7986 (7)	C12—H12	0.930
C1—N3	1.341 (3)	C13—N4	1.482 (3)
C1—C2	1.369 (3)	C13—C14	1.516 (3)
C1—H1	0.930	C13—H13A	0.970
C2—C3	1.386 (4)	C13—H13B	0.970
C2—H2	0.930	C14—N2	1.345 (3)
C3—C4	1.376 (4)	C14—C15	1.383 (3)
С3—Н3	0.930	C15—C16	1.384 (4)
C4—C5	1,382 (3)	C15—H15	0.930
C4—H4	0.930	C16—C17	1.371 (4)
C5—N3	1.352 (3)	C16—H16	0.930
C5—C6	1.506 (3)	C17—C18	1.369 (4)
C6—N4	1.479 (3)	C17—H17	0.930
С6—Н6А	0.970	C18—N2	1.351 (3)
С6—Н6В	0.970	C18—H18	0.930
C7—N4	1.483 (3)	F1—P1	1.5939 (17)
С7—С8	1.499 (3)	F2—P1	1.5803 (18)
C7—H7A	0.970	F3—P1	1.582 (2)
С7—Н7В	0.970	F4—P1	1.5859 (18)
C8—N1	1.342 (3)	F5—P1	1.5804 (18)
C8—C9	1.379 (3)	F6—P1	1.6129 (17)
C9—C10	1.380 (4)		
01—Cr1—N3	91.01 (5)	N1—C12—H12	118.5

O1—Cr1—N2	92.46 (5)	C11—C12—H12	118.5
N3—Cr1—N2	154.67 (7)	N4—C13—C14	110.48 (16)
O1—Cr1—N4	91.36 (6)	N4—C13—H13A	109.6
N3—Cr1—N4	78.03 (7)	C14—C13—H13A	109.6
N2—Cr1—N4	76.81 (7)	N4—C13—H13B	109.6
01—Cr1—N1	166.58 (5)	C14—C13—H13B	109.6
N3—Cr1—N1	81.87 (7)	H13A—C13—H13B	108.1
N2—Cr1—N1	89.30 (7)	N2-C14-C15	120.7 (2)
N4—Cr1—N1	76.09 (7)	N2-C14-C13	116.67 (18)
01—Cr1—Cl1	103.29 (5)	C15—C14—C13	122.5 (2)
N3—Cr1—Cl1	104.03 (5)	C14—C15—C16	118.4 (3)
N_2 —Cr1—Cl1	99.56 (6)	C14—C15—H15	120.8
N4—Cr1—Cl1	165 11 (5)	C16—C15—H15	120.8
N1-Cr1-Cl1	89 52 (6)	C17 - C16 - C15	120.8(2)
$N_3 - C_1 - C_2$	1221(2)	C17—C16—H16	119.6
N3-C1-H1	118.9	C15—C16—H16	119.6
$C_2 - C_1 - H_1$	119.0	C16-C17-C18	118.2 (3)
$C_2 = C_1$	118.8 (2)	C16_C17_H17	120.9
$C_3 - C_2 - H_2$	120.6	C18_C17_H17	120.9
$C_1 - C_2 - H_2$	120.6	$N_2 - C_{18} - C_{17}$	120.9 121.8(3)
$C_{1} = C_{2} = C_{12}$	119.4(2)	$N_2 - C_{18} - H_{18}$	121.8 (5)
$C_2 = C_3 = C_4$	120.3	C17 $C18$ $H18$	110.1
$C_2 = C_3 = H_3$	120.3	C12 N1 $C8$	117.70 (18)
$C_4 = C_5 = 115$	120.3	C12 - NI - C6	117.79(18) 126.02(15)
$C_3 = C_4 = C_3$	119.3 (2)	C_{12} N1 C_{r1}	120.02(13) 115.61(13)
$C_5 = C_4 = H_4$	120.4	$C_0 = 1 \sqrt{1 - C_1}$	113.01(13) 120.1(2)
$C_{3} - C_{4} - 114$	120.4	C14 = N2 = C16	120.1(2)
$N_{3} = C_{5} = C_{4}$	120.93 (19)	$C_{14} = N_2 = C_{11}$	114.43(14) 124.62(17)
N_{3} C_{3} C_{6}	110.79 (10)	$C_{10} = N_2 = C_1$	124.02(17)
C4 - C5 - C0	122.07(19)	C1 = N3 = C3	119.42(18) 125.22(14)
N4 - C0 - C3	1002	CI-N3-CII	123.22(14)
	109.2	CS—NS—CH	113.07(13)
	109.2	C_{0} N4 C_{12}	112.30 (18)
	109.2	$C_0 - N_4 - C_{13}$	112.03 (10)
	109.2	C = N4 = C13	109.74 (17)
H6A—C6—H6B	107.9	C6—N4—Crl	105.11 (12)
	114.97 (17)	C/-N4-CrI	112.78 (13)
N4 - C - H A	108.5	C13 - N4 - CrI	103.96 (12)
	108.5	CrI—OI—CrI ⁺	180.0
N4—C/—H/B	108.5	F5—P1—F3	90.59 (12)
С8—С/—Н/В	108.5	F5—P1—F2	178.06 (11)
H7A—C7—H7B	107.5	F3—P1—F2	90.59 (13)
NI-C8-C9	122.2 (2)	F_{2} P_{1} F_{4}	90.15 (11)
N1—C8—C7	117.57 (17)	F3—P1—F4	91.62 (13)
C9—C8—C7	120.13 (19)	F2—P1—F4	91.35 (11)
C10—C9—C8	119.3 (2)	F5—P1—F1	89.58 (11)
С10—С9—Н9	120.4	F3—P1—F1	179.22 (11)
С8—С9—Н9	120.4	F2—P1—F1	89.22 (11)
C11—C10—C9	118.9 (2)	F4—P1—F1	89.14 (11)

supporting information

С11—С10—Н10	120.5	F5—P1—F6	90.19 (10)
С9—С10—Н10	120.5	F3—P1—F6	90.39 (12)
C10-C11-C12	118.9 (2)	F2—P1—F6	88.26 (10)
С10—С11—Н11	120.6	F4—P1—F6	177.95 (11)
C12-C11-H11	120.6	F1—P1—F6	88.85 (10)
N1—C12—C11	122.9 (2)		

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

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