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A molecular substitutional disorder case study suitable for instruction: $L_2Cr^{II}(THF)/L_2[(trimethylsilyl)methyl]Cr^{III}$ (L is 2,5-bis{[(2,6-diisopropylphenyl)imino]methyl}pyrrol-1-ide)

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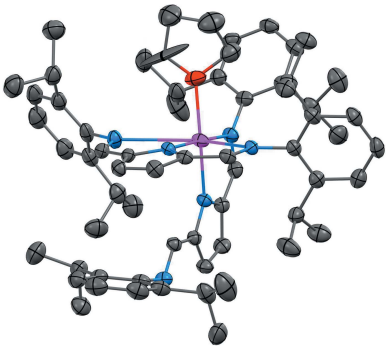
A solution of Cr^{II} and Cr^{III} complexes, bis(2,5-bis{[(2,6-diisopropylphenyl)imino]methyl}pyrrol-1-ido)(tetrahydrofuran)chromium(II)–bis(2,5-bis{[(2,6-diisopropylphenyl)imino]methyl}pyrrol-1-ido)[(trimethylsilyl)methyl]chromium(III) (0.88/0.12), $[Cr(C_{30}H_{38}N_3)_2(C_4H_8O)]_{0.88}[Cr(C_{30}H_{38}N_3)_2(C_4H_{11}Si)]_{0.12}$ or $L_2Cr^{II}(THF)/L_2[(trimethylsilyl)methyl]Cr^{III}$ (L = 2,5-bis{[(2,6-diisopropylphenyl)imino]methyl}pyrrol-1-ide and THF is tetrahydrofuran), in pentane crystallizes in the monoclinic space group $P2_1/c$. The structure obtained shows most of the atoms coincident but with THF disordered with the (trimethylsilyl)methyl ligand. Structures with this disorder, involving more than two or three atoms, seem to appear rarely in the literature; however, in this case, the data set is ideal for the crystallographic instruction of molecular substitution disorder.

1. Introduction

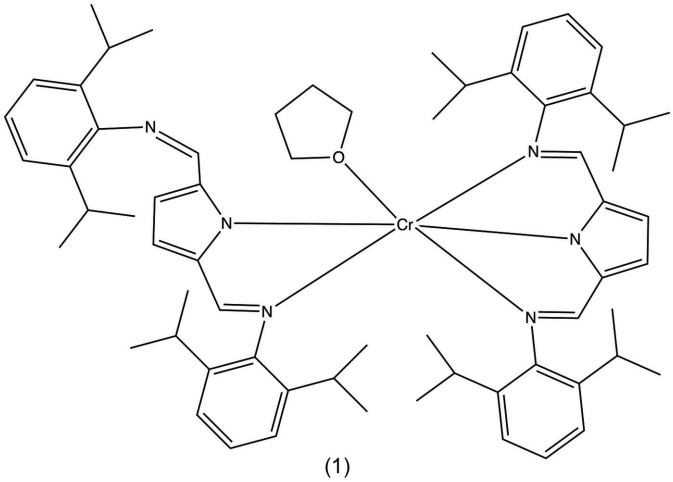
It can be difficult finding data sets that are both relatively easy to solve while presenting a challenging specific crystallographic problem (Chang *et al.*, 2022). While atomic substitutionally disordered examples are readily available, especially in mineral samples (Fitzgerald *et al.*, 2016), examples of molecular disorder are more challenging to find. A search of the Cambridge Structural Database (CSD, Version 5.42; Groom *et al.*, 2016) using the keyword 'disordered' yielded 302314 hits. However, perusing this list revealed many structures not displaying substitutional disorder. Perhaps substitutionally disordered structures might not be published often as they are structures from chemically impure, albeit crystalline, materials (Clegg, 2020). Using broader query terms such as 'solid solution', 'cocrystal', or 'mixed crystal' may lead to hits that do not specifically involve molecular substitutional disorder (Bredikhin *et al.*, 2014). A narrower search for the keywords 'disorder' and 'substitution' yielded 71 hits. In some cases, the disorder is mentioned but not modeled. Several display substitution of atoms, of small ligands such as OH^- for OCN^-, of solvent molecules with similar connectivity, such as diethyl ether for tetrahydrofuran (THF), or of atoms in mixed metal clusters. In a structure displaying a Br^- disordered with a *m*-terphenylimido ligand, there should be a space when Br^- is present. No occupying moieties were modeled together with the Br^- and it was unclear if the space is empty (Powers *et al.*, 2020). Upon reflection, we recall a preliminary data set that was abandoned in favor of repeating the data collection on a chemically pure crystal obtained from an alternative synthetic route (Salisbury *et al.*, 2007).



2. Experimental

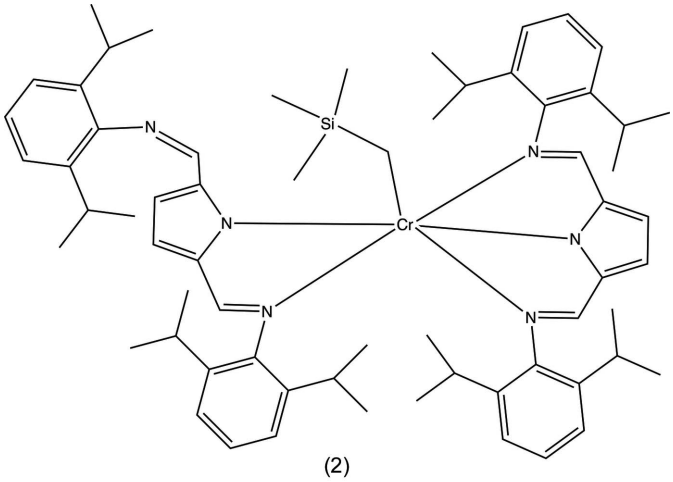
2.1. Synthesis and crystallization

The data crystal was obtained from the attempted alkylation of $L\mathrm{Cr^{III}Cl_2(THF)}$ (where L is 2,5-bis{[(2,6-diisopropylphenyl)imino]methyl}pyrrol-1-ide) with [(trimethylsilyl)methyl]lithium, which predominantly yields $L_2\mathrm{Cr^{II}(THF)}$, (1) (Scheme 1), occasionally in association with L_2[(trimethylsilyl)methyl]$\mathrm{Cr^{III}}$, (2) (Scheme 2), as an impurity. The synthesis



(1)
Scheme 1

and spectral characterization of (1) were reported previously by us (Salisbury *et al.*, 2007). Despite varying the stoichiometric ratios of the reagents, compound (2) is consistently produced only as a minor side product. Isolation of pure (2) from the crude mix was not successful because of the similarity in solubilities in common laboratory solvents and no further characterization of (2) was attempted. A concentrated solution of the crude product residue in pentane cooled to −30 °C afforded X-ray-quality crystals upon standing.



(2)
Scheme 2

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The atoms of the (trimethylsilyl)methyl group were treated with similar U^{ij} components. Methyl C-to-Si distances were restrained to be similar. H atoms were placed in calculated positions, with U_{iso}(H) values equal to 1.2–1.5U_{eq} of the attached atom.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Cr(C_{30}H_{38}N_3)_2(C_4H_8O)]_{0.88}$-$[Cr(C_{30}H_{38}N_3)_2(C_4H_{11}Si)]_{0.12}$
M_r	1007.22
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, b, c (Å)	22.028 (4), 13.487 (2), 19.587 (3)
β (°)	90.809 (3)
V (Å^3)	5818.3 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.24
Crystal size (mm)	0.3 × 0.15 × 0.15
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 1997)
T_{min}, T_{max}	0.918, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	35989, 13521, 9166
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.130, 1.03
No. of reflections	13521
No. of parameters	695
No. of restraints	27
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.48, −0.38

Computer programs: *SMART* (Bruker, 1997), *SAINT* (Bruker, 1997), *SHELXS1997* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2020).

3. Results and discussion

The data set was originally refined in 2007 with *SHEXL97* (Sheldrick, 2008) and the structure obtained (Fig. 1) showed the predominant chemical species (1) but a cursory inspection of the ellipsoid for atom C64 in contrast to neighboring atoms clearly indicates more modelling is required. *checkCIF* (Spek, 2020) reports THF atom C64 causing a 'level A' alert, having a prolate 6.1 max/min atomic displacement parameter ratio, and two 'level B' alerts, failing the Hirshfeld test and having a large U_{eq} value compared to neighboring atoms. The *checkCIF* report also includes an alert for a solvent-accessible void of 35 Å^3. Treating atom C64 with an isotropic restraint removes level A and B alerts but introduces new level B alerts regarding a large residual density, roughly located in the center of the THF ring, 1.18 Å from C63. Repeating the refinement with *SHELXL2018* (Sheldrick, 2015) without any restraints does not yield the prolate C64, but instead shows a large residual peak located roughly in the center of the THF ligand. In any case, at this stage, the largest peak can be identified as a partially occupied Si atom, whose occupancy is tied to the THF ligand, surrounded by four peaks in a tetrahedral orientation that could be assigned as C atoms, completing the (trimethylsilyl)methyl ligand. Treating the

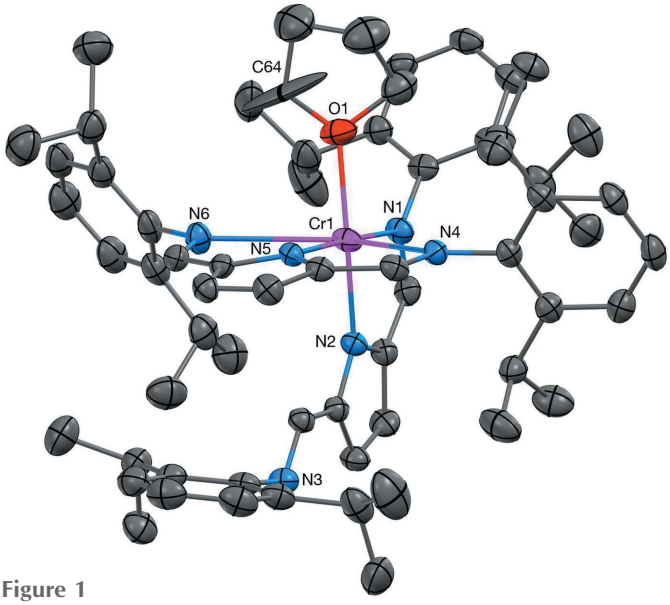


Figure 1
Molecular diagram of the presumed compound (1), drawn with 50% probability ellipsoids and with H atoms omitted, as refined with *SHEXTL97* (Sheldrick, 2008) without restraints. Note the prolate atom C64.

(trimethylsilyl)methyl ligand with similar U^{ij} restraints, adding calculated H atoms, and refining to convergence completes the structure (Fig. 2). The mechanism for (2) starting from $L\mathrm{Cr^{III}Cl_2(THF)}$ and [(trimethylsilyl)methyl]lithium is unclear. Perhaps alkylation followed by reductive elimination and comproportionation of a putative unobserved $\mathrm{Cr^{I}}$ species with the starting $\mathrm{Cr^{III}}$ species could yield (2).

In both compounds, one imino ligand is tridentate and meridional, while the other is bidentate (Fig. 3). A weak interaction between C18—H18 and N5, with a donor–acceptor contact distance of 3.232 (2) Å, may help stabilize the bidentate coordinated ligand. In (1), the Cr—O distance falls within the range observed in the CSD (267 hits, 1.982–2.579 Å). Searching for Cr complexes with a monodentate terminal (trimethylsilyl)methyl ligand yielded 38 hits with Cr—C distances in the range 1.953–2.152 Å and Cr—C—Si angles in the range 111.057–138.459°, consistent with the structure observed for (2). The compound in the literature with the closest Cr—C—Si angle to (2), a value of 131.89 (9)° for [*N*,*N*′-bis(mesityl)pentane-2,4-diiminato](cyclopentadienyl)[(trimethylsilyl)methyl]chromium(III) (Heintz *et al.*, 1998), (3), has a substantially crowded coordination sphere similar to (2). While the major disordered contribution (1) is Cr in the +2 oxidation state, compound (2) has Cr in the +3 oxidation state. The Cr—C distance is longer in (3) [2.1031 (17) Å] than in (2), but perhaps this is because of the pseudotetrahedral coordination, counting the six-electron donor cyclopentadienyl ligand as a coordination apex, as opposed to the octahedral environment in (2), which may allow the closer approach of the C atom to Cr while bringing the isopropyl groups close to and crowding the trimethylsilyl group (Heintz *et al.*, 1998).

An alternative interpretation of the trimethylsilyl-bearing moiety as part of a neutral amide ligand was also considered based on the crystallographic refinement alone. Indeed, replacement of the C1*A* atom as an N atom gives a slight improvement of refinement indicators. For example, the *R* factor drops from 5.03 to 5.02%. In addition, the resulting Cr—N distance would also be in the range of reported similar compounds. However, under the conditions of the synthesis, there doesn't seem to be a plausible pathway to convert the

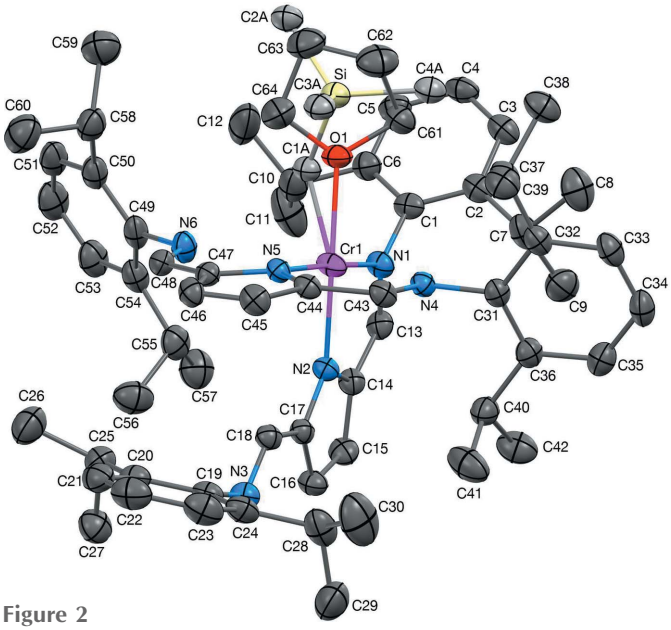


Figure 2
Molecular diagram of the disordered title complexes, drawn with 50% probability ellipsoids and with H atoms omitted for clarity.

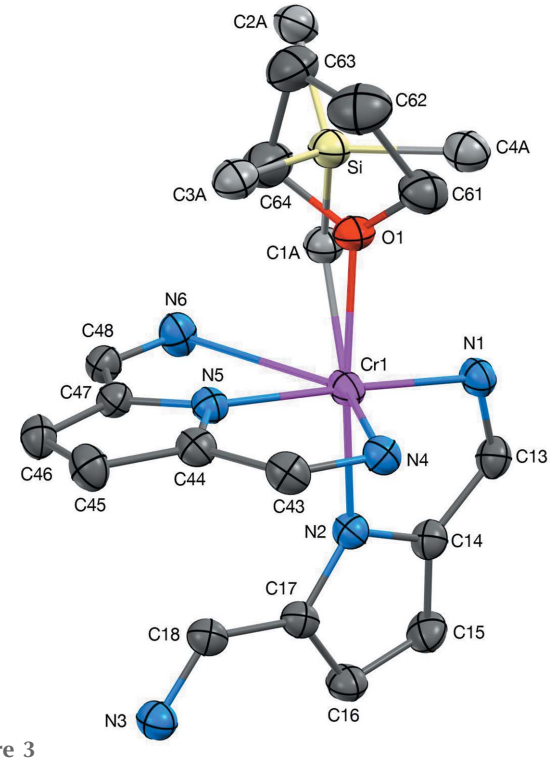


Figure 3
Molecular diagram with the aryl groups omitted, showing the meridional tridentate coordination and the bidentate coordination of the two imido ligands. Displacement ellipsoids are drawn at the 50% probability level.

trimethylsilylmethyl reagent to trimethylsilylamide. As a further test, the atom in question could be assigned a fluorine identity which is even more implausible and yet results in an even better *R* value of 5.01%.

The crystal data is in an unambiguous space group, $P2_1/c$, and the absence of any crystallographic issues other than molecular substitutional disorder affords a focused case study suitable for instruction. (Other educational crystallographic data sets can be found at https://xray.chem.wisc.edu/crystallographic-problems/.)

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Acta Cryst. (2022). C**78** [https://doi.org/10.1107/S2053229622003825]

A molecular substitutional disorder case study suitable for instruction: $L_2Cr^{II}(THF)/L_2[(trimethylsilyl)methyl]Cr^{III}$ (*L* is 2,5-bis{[(2,6-diisopropylphenyl)-imino]methyl}pyrrol-1-ide)

Brian A. Salisbury, John F. Young, Klaus H. Theopold and Glenn P. A. Yap

Computing details

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART* (Bruker, 1997); data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS1997* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2020).

Bis(2,5-bis{[(2,6-diisopropylphenyl)imino]methyl}pyrrol-1-ido)(tetrahydrofuran)chromium(II)–bis(2,5-bis{[(2,6-diisopropylphenyl)imino]methyl}pyrrol-1-ido)[(trimethylsilyl)methyl]chromium(III) (0.88/0.12)

Crystal data

$[Cr(C_{30}H_{38}N_3)_2(C_4H_8O)]_{0.88}[Cr(C_{30}H_{38}N_3)_2(C_4H_{11}Si)]_{0.12}$
M_r = 1007.22
Monoclinic, $P2_1/c$
a = 22.028 (4) Å
b = 13.487 (2) Å
c = 19.587 (3) Å
β = 90.809 (3)°
V = 5818.3 (16) Å^3
Z = 4
$F(000)$ = 2172
D_x = 1.150 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 956 reflections
θ = 2.6–22.3°
μ = 0.24 mm^{-1}
T = 150 K
Blade, red
0.3 × 0.15 × 0.15 mm

Data collection

Bruker SMART APEX CCD diffractometer
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 1997)
T_{min} = 0.918, T_{max} = 1.000
35989 measured reflections
13521 independent reflections
9166 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 28.3°, θ_{min} = 2.1°
h = −28→29
k = −17→17
l = −14→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.130
S = 1.03
13521 reflections
695 parameters
27 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0586P)^2 + 0.8162P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 0.48 e Å^{-3} $\Delta\rho_{min}$ = −0.38 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cr1	0.74664 (2)	0.70388 (2)	0.81646 (2)	0.02747 (9)	
N1	0.75178 (7)	0.76400 (11)	0.71758 (8)	0.0279 (3)	
N2	0.77644 (7)	0.58078 (11)	0.76381 (7)	0.0242 (3)	
N3	0.80391 (7)	0.34464 (11)	0.84828 (8)	0.0292 (4)	
N4	0.85178 (6)	0.72469 (11)	0.88930 (8)	0.0244 (3)	
N5	0.73883 (6)	0.63613 (11)	0.90853 (7)	0.0229 (3)	
N6	0.62809 (7)	0.61742 (12)	0.83578 (8)	0.0318 (4)	
C1	0.73822 (9)	0.86494 (14)	0.69691 (9)	0.0281 (4)	
C2	0.78498 (9)	0.93566 (14)	0.70023 (9)	0.0304 (4)	
C3	0.77051 (10)	1.03391 (15)	0.68397 (10)	0.0346 (5)	
H3	0.801518	1.082865	0.684965	0.042*	
C4	0.71168 (10)	1.06091 (15)	0.66646 (10)	0.0362 (5)	
H4	0.702496	1.128013	0.655775	0.043*	
C5	0.66652 (10)	0.99035 (15)	0.66454 (11)	0.0372 (5)	
H5	0.626225	1.009677	0.652841	0.045*	
C6	0.67864 (9)	0.89107 (15)	0.67941 (10)	0.0332 (5)	
C7	0.84976 (10)	0.90758 (16)	0.71893 (11)	0.0384 (5)	
H7	0.848280	0.846507	0.747810	0.046*	
C8	0.88342 (11)	0.98794 (18)	0.76001 (12)	0.0522 (6)	
H8A	0.924832	0.965511	0.770486	0.078*	
H8B	0.884960	1.049149	0.733126	0.078*	
H8C	0.861970	1.000468	0.802645	0.078*	
C9	0.88554 (10)	0.88274 (18)	0.65505 (13)	0.0482 (6)	
H9A	0.927222	0.864800	0.668099	0.072*	
H9B	0.866220	0.826893	0.631230	0.072*	
H9C	0.886158	0.940576	0.624773	0.072*	
C10	0.62724 (10)	0.81617 (16)	0.67327 (13)	0.0447 (6)	
H10	0.641577	0.752374	0.693921	0.054*	
C11	0.61223 (14)	0.7972 (2)	0.59824 (15)	0.0721 (9)	
H11A	0.579097	0.748955	0.594576	0.108*	
H11B	0.599747	0.859503	0.576398	0.108*	
H11C	0.648184	0.771090	0.575483	0.108*	
C12	0.57048 (11)	0.8495 (2)	0.71158 (18)	0.0738 (9)	
H12A	0.538617	0.799236	0.706298	0.111*	
H12B	0.580546	0.857777	0.760141	0.111*	
H12C	0.556032	0.912681	0.692770	0.111*	
C13	0.76714 (8)	0.69774 (14)	0.67287 (9)	0.0284 (4)	
H13	0.769456	0.714785	0.625924	0.034*	

Version of record at: https://doi.org/10.1107/S2053229622003825

C14	0.78042 (8)	0.59975 (14)	0.69473 (9)	0.0267 (4)
C15	0.79756 (9)	0.51364 (14)	0.65984 (10)	0.0329 (5)
H15	0.803019	0.506959	0.612040	0.039*
C16	0.80498 (9)	0.44035 (14)	0.70862 (10)	0.0307 (4)
H16	0.816908	0.373685	0.700729	0.037*
C17	0.79156 (8)	0.48302 (13)	0.77193 (9)	0.0249 (4)
C18	0.79068 (8)	0.43649 (13)	0.83909 (10)	0.0262 (4)
H18	0.779935	0.475511	0.877444	0.031*
C19	0.79648 (9)	0.30639 (13)	0.91613 (10)	0.0291 (4)
C20	0.73872 (9)	0.27080 (14)	0.93465 (10)	0.0323 (4)
C21	0.73250 (10)	0.23067 (16)	0.99966 (11)	0.0408 (5)
H21	0.693993	0.206521	1.013241	0.049*
C22	0.78098 (11)	0.22523 (16)	1.04474 (11)	0.0457 (6)
H22	0.775760	0.197640	1.088900	0.055*
C23	0.83737 (11)	0.26014 (16)	1.02547 (11)	0.0428 (5)
H23	0.870587	0.256407	1.056831	0.051*
C24	0.84620 (9)	0.30044 (14)	0.96118 (11)	0.0348 (5)
C25	0.68595 (9)	0.27782 (16)	0.88385 (11)	0.0376 (5)
H25	0.687009	0.346165	0.864095	0.045*
C26	0.62345 (10)	0.2649 (2)	0.91544 (14)	0.0563 (7)
H26A	0.592036	0.270322	0.879706	0.084*
H26B	0.620996	0.199475	0.937047	0.084*
H26C	0.617204	0.316494	0.949848	0.084*
C27	0.69412 (11)	0.20545 (17)	0.82425 (12)	0.0447 (5)
H27A	0.659605	0.211484	0.792398	0.067*
H27B	0.731758	0.221161	0.800464	0.067*
H27C	0.696204	0.137482	0.841821	0.067*
C28	0.90767 (10)	0.33824 (17)	0.93854 (12)	0.0444 (6)
H28	0.900297	0.401650	0.913297	0.053*
C29	0.93605 (11)	0.2663 (2)	0.88851 (15)	0.0601 (7)
H29A	0.975619	0.291802	0.874438	0.090*
H29B	0.941428	0.201598	0.910497	0.090*
H29C	0.909405	0.259234	0.848312	0.090*
C30	0.95196 (13)	0.3617 (2)	0.99724 (16)	0.0751 (9)
H30A	0.990371	0.385523	0.978653	0.113*
H30B	0.934504	0.412974	1.026465	0.113*
H30C	0.959381	0.301552	1.024185	0.113*
C31	0.91060 (8)	0.76809 (13)	0.88007 (9)	0.0258 (4)
C32	0.92817 (9)	0.85244 (14)	0.91739 (10)	0.0294 (4)
C33	0.98460 (9)	0.89489 (15)	0.90391 (11)	0.0360 (5)
H33	0.997196	0.951778	0.928958	0.043*
C34	1.02238 (9)	0.85639 (16)	0.85529 (11)	0.0385 (5)
H34	1.060510	0.886618	0.846893	0.046*
C35	1.00459 (9)	0.77362 (16)	0.81881 (11)	0.0364 (5)
H35	1.030843	0.747205	0.785314	0.044*
C36	0.94875 (8)	0.72789 (14)	0.83012 (10)	0.0300 (4)
C37	0.88923 (9)	0.89559 (14)	0.97359 (10)	0.0326 (5)
H37	0.847587	0.866794	0.968435	0.039*

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C38	0.88334 (10)	1.00887 (15)	0.96946 (11)	0.0421 (5)
H38A	0.857886	1.032500	1.006733	0.063*
H38B	0.923698	1.039061	0.973452	0.063*
H38C	0.864665	1.027343	0.925570	0.063*
C39	0.91437 (10)	0.86467 (16)	1.04366 (11)	0.0401 (5)
H39A	0.888971	0.892841	1.079475	0.060*
H39B	0.914196	0.792190	1.047195	0.060*
H39C	0.956028	0.889193	1.049186	0.060*
C40	0.93144 (9)	0.63250 (15)	0.79360 (11)	0.0362 (5)
H40	0.886170	0.627039	0.794025	0.043*
C41	0.95708 (13)	0.54456 (17)	0.83274 (12)	0.0565 (7)
H41A	0.944282	0.548086	0.880397	0.085*
H41B	0.942017	0.482925	0.812126	0.085*
H41C	1.001515	0.545859	0.830996	0.085*
C42	0.95105 (11)	0.62756 (17)	0.71982 (11)	0.0482 (6)
H42A	0.934379	0.684492	0.694759	0.072*
H42B	0.995475	0.628956	0.717938	0.072*
H42C	0.935976	0.566022	0.699068	0.072*
C43	0.84278 (8)	0.67144 (13)	0.94247 (9)	0.0268 (4)
H43	0.875064	0.662551	0.974562	0.032*
C44	0.78519 (8)	0.62471 (13)	0.95496 (9)	0.0252 (4)
C45	0.76840 (9)	0.55868 (14)	1.00646 (9)	0.0307 (4)
H45	0.792408	0.538865	1.044754	0.037*
C46	0.70986 (9)	0.52788 (14)	0.99062 (9)	0.0292 (4)
H46	0.685979	0.482494	1.015833	0.035*
C47	0.69278 (8)	0.57650 (13)	0.93041 (9)	0.0248 (4)
C48	0.63737 (8)	0.56820 (14)	0.89097 (10)	0.0278 (4)
H48	0.606558	0.524657	0.906387	0.033*
C49	0.57042 (8)	0.61089 (15)	0.80135 (11)	0.0338 (5)
C50	0.51780 (9)	0.65000 (15)	0.83105 (11)	0.0366 (5)
C51	0.46404 (9)	0.64825 (16)	0.79208 (13)	0.0436 (6)
H51	0.427935	0.674224	0.811113	0.052*
C52	0.46207 (10)	0.61015 (17)	0.72734 (13)	0.0478 (6)
H52	0.425079	0.610546	0.701820	0.057*
C53	0.51397 (9)	0.57115 (17)	0.69920 (12)	0.0436 (5)
H53	0.512030	0.544125	0.654432	0.052*
C54	0.56899 (9)	0.57047 (15)	0.73479 (11)	0.0360 (5)
C55	0.62495 (9)	0.52083 (16)	0.70660 (11)	0.0403 (5)
H55	0.661226	0.557479	0.724643	0.048*
C56	0.62863 (11)	0.41434 (17)	0.73359 (13)	0.0519 (6)
H56A	0.664795	0.381863	0.715476	0.078*
H56B	0.631138	0.415377	0.783576	0.078*
H56C	0.592301	0.377662	0.718976	0.078*
C57	0.62847 (11)	0.52038 (19)	0.62861 (12)	0.0532 (6)
H57A	0.665847	0.487052	0.614725	0.080*
H57B	0.593292	0.485030	0.609441	0.080*
H57C	0.628511	0.588790	0.611730	0.080*
C58	0.51648 (10)	0.69035 (16)	0.90325 (12)	0.0418 (5)

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H58	0.559478	0.696689	0.919734	0.050*	
C59	0.48719 (12)	0.79329 (18)	0.90770 (15)	0.0586 (7)	
H59A	0.487589	0.815553	0.955331	0.088*	
H59B	0.510095	0.840271	0.879890	0.088*	
H59C	0.445184	0.789817	0.890722	0.088*	
C60	0.48440 (11)	0.6183 (2)	0.95087 (14)	0.0581 (7)	
H60A	0.484086	0.645831	0.997162	0.087*	
H60B	0.442565	0.608062	0.934703	0.087*	
H60C	0.505975	0.554735	0.951299	0.087*	
O1	0.70954 (8)	0.83552 (12)	0.85469 (8)	0.0313 (4)	0.876 (2)
C61	0.74640 (11)	0.92255 (19)	0.87079 (13)	0.0387 (6)	0.876 (2)
H61A	0.742780	0.972730	0.834074	0.046*	0.876 (2)
H61B	0.789666	0.904059	0.876558	0.046*	0.876 (2)
C62	0.72137 (13)	0.9621 (2)	0.93677 (14)	0.0528 (8)	0.876 (2)
H62A	0.727881	1.034464	0.940931	0.063*	0.876 (2)
H62B	0.739954	0.928389	0.976823	0.063*	0.876 (2)
C63	0.65438 (13)	0.9373 (2)	0.92942 (15)	0.0501 (7)	0.876 (2)
H63A	0.634448	0.935141	0.974387	0.060*	0.876 (2)
H63B	0.632983	0.985641	0.899648	0.060*	0.876 (2)
C64	0.65631 (13)	0.8375 (2)	0.89744 (17)	0.0560 (8)	0.876 (2)
H64A	0.659208	0.785428	0.932960	0.067*	0.876 (2)
H64B	0.619140	0.825818	0.869594	0.067*	0.876 (2)
Si	0.6947 (2)	0.8988 (3)	0.9045 (2)	0.0300 (16)	0.124 (2)
C1A	0.6894 (9)	0.8005 (14)	0.8463 (10)	0.0282 (19)	0.124 (2)
H1AA	0.674727	0.832082	0.803530	0.034*	0.124 (2)
H1AB	0.654836	0.760630	0.862818	0.034*	0.124 (2)
C2A	0.6197 (6)	0.9612 (12)	0.9090 (9)	0.034 (2)	0.124 (2)
H2AA	0.622170	1.016355	0.941495	0.051*	0.124 (2)
H2AB	0.608193	0.986516	0.863772	0.051*	0.124 (2)
H2AC	0.589109	0.913531	0.924211	0.051*	0.124 (2)
C3A	0.7174 (7)	0.8500 (11)	0.9897 (6)	0.033 (3)	0.124 (2)
H3AA	0.720365	0.904858	1.022349	0.050*	0.124 (2)
H3AB	0.686907	0.802344	1.005150	0.050*	0.124 (2)
H3AC	0.756855	0.816890	0.986554	0.050*	0.124 (2)
C4A	0.7544 (6)	0.9811 (12)	0.8698 (8)	0.033 (2)	0.124 (2)
H4AA	0.759922	1.038371	0.900031	0.050*	0.124 (2)
H4AB	0.792640	0.944318	0.866962	0.050*	0.124 (2)
H4AC	0.742084	1.003881	0.824188	0.050*	0.124 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.04094 (19)	0.02119 (16)	0.02033 (16)	0.00349 (13)	0.00230 (13)	0.00162 (12)
N1	0.0347 (9)	0.0252 (8)	0.0238 (8)	0.0007 (7)	0.0007 (7)	0.0036 (7)
N2	0.0275 (8)	0.0235 (8)	0.0216 (8)	0.0001 (6)	−0.0011 (6)	−0.0008 (6)
N3	0.0330 (9)	0.0275 (9)	0.0272 (9)	0.0023 (7)	−0.0006 (7)	−0.0004 (7)
N4	0.0245 (8)	0.0235 (8)	0.0250 (8)	−0.0016 (6)	−0.0017 (6)	−0.0011 (6)
N5	0.0254 (8)	0.0213 (8)	0.0222 (8)	−0.0013 (6)	−0.0005 (6)	−0.0014 (6)

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N6	0.0258 (8)	0.0334 (9)	0.0359 (9)	−0.0040 (7)	−0.0044 (7)	0.0062 (8)
C1	0.0402 (11)	0.0271 (10)	0.0171 (9)	0.0041 (8)	0.0031 (8)	0.0037 (8)
C2	0.0417 (11)	0.0292 (10)	0.0203 (9)	−0.0010 (9)	−0.0008 (8)	0.0012 (8)
C3	0.0486 (12)	0.0274 (10)	0.0278 (10)	−0.0039 (9)	−0.0022 (9)	0.0004 (8)
C4	0.0524 (13)	0.0254 (10)	0.0309 (11)	0.0062 (10)	0.0053 (10)	0.0042 (9)
C5	0.0402 (12)	0.0333 (11)	0.0381 (12)	0.0097 (9)	0.0055 (10)	0.0063 (9)
C6	0.0395 (11)	0.0310 (11)	0.0292 (10)	0.0019 (9)	0.0052 (9)	0.0065 (9)
C7	0.0432 (12)	0.0345 (11)	0.0370 (12)	−0.0058 (9)	−0.0105 (10)	0.0115 (9)
C8	0.0539 (15)	0.0581 (16)	0.0442 (14)	−0.0150 (12)	−0.0162 (12)	0.0055 (12)
C9	0.0389 (12)	0.0473 (14)	0.0583 (15)	0.0043 (10)	−0.0062 (11)	−0.0005 (12)
C10	0.0356 (12)	0.0369 (12)	0.0616 (15)	0.0006 (9)	0.0000 (11)	0.0175 (11)
C11	0.0743 (19)	0.0620 (18)	0.079 (2)	−0.0274 (15)	−0.0283 (16)	0.0156 (15)
C12	0.0445 (15)	0.0574 (17)	0.120 (3)	0.0043 (13)	0.0232 (16)	0.0329 (18)
C13	0.0317 (10)	0.0328 (10)	0.0207 (9)	−0.0023 (8)	0.0015 (8)	0.0015 (8)
C14	0.0285 (10)	0.0289 (10)	0.0226 (9)	−0.0021 (8)	−0.0004 (8)	−0.0012 (8)
C15	0.0403 (11)	0.0337 (11)	0.0247 (10)	−0.0015 (9)	0.0051 (9)	−0.0045 (9)
C16	0.0374 (11)	0.0259 (10)	0.0290 (10)	0.0023 (8)	0.0022 (9)	−0.0031 (8)
C17	0.0240 (9)	0.0234 (9)	0.0271 (10)	−0.0010 (7)	−0.0022 (8)	−0.0022 (8)
C18	0.0262 (9)	0.0249 (10)	0.0273 (10)	0.0004 (8)	−0.0025 (8)	−0.0023 (8)
C19	0.0381 (11)	0.0203 (9)	0.0288 (10)	0.0042 (8)	−0.0001 (9)	−0.0012 (8)
C20	0.0399 (11)	0.0261 (10)	0.0310 (11)	0.0063 (8)	0.0033 (9)	−0.0012 (8)
C21	0.0471 (13)	0.0345 (12)	0.0411 (13)	0.0042 (10)	0.0131 (11)	0.0026 (10)
C22	0.0663 (16)	0.0400 (13)	0.0311 (11)	0.0111 (11)	0.0038 (11)	0.0094 (10)
C23	0.0556 (14)	0.0371 (12)	0.0354 (12)	0.0067 (11)	−0.0116 (11)	0.0055 (10)
C24	0.0416 (12)	0.0251 (10)	0.0375 (11)	0.0049 (9)	−0.0052 (9)	0.0025 (9)
C25	0.0344 (11)	0.0364 (12)	0.0421 (12)	0.0013 (9)	0.0022 (10)	0.0001 (10)
C26	0.0379 (13)	0.0677 (17)	0.0635 (17)	0.0006 (12)	0.0066 (12)	−0.0021 (14)
C27	0.0448 (13)	0.0440 (13)	0.0452 (13)	−0.0047 (10)	−0.0042 (11)	−0.0044 (11)
C28	0.0421 (12)	0.0381 (12)	0.0526 (14)	−0.0048 (10)	−0.0148 (11)	0.0130 (11)
C29	0.0410 (13)	0.0634 (17)	0.0763 (19)	0.0025 (12)	0.0113 (13)	0.0083 (15)
C30	0.0637 (17)	0.077 (2)	0.084 (2)	−0.0191 (16)	−0.0348 (16)	0.0128 (17)
C31	0.0247 (9)	0.0261 (9)	0.0264 (10)	−0.0013 (8)	−0.0062 (8)	0.0040 (8)
C32	0.0320 (10)	0.0258 (10)	0.0299 (10)	−0.0026 (8)	−0.0088 (8)	0.0035 (8)
C33	0.0359 (11)	0.0320 (11)	0.0400 (12)	−0.0098 (9)	−0.0100 (10)	0.0012 (9)
C34	0.0293 (10)	0.0408 (12)	0.0452 (13)	−0.0109 (9)	−0.0044 (10)	0.0087 (10)
C35	0.0292 (10)	0.0447 (12)	0.0353 (11)	−0.0007 (9)	0.0012 (9)	0.0036 (10)
C36	0.0281 (10)	0.0319 (11)	0.0299 (10)	−0.0013 (8)	−0.0050 (8)	0.0010 (8)
C37	0.0342 (11)	0.0299 (11)	0.0335 (11)	−0.0033 (8)	−0.0064 (9)	−0.0046 (9)
C38	0.0537 (14)	0.0330 (12)	0.0394 (12)	−0.0013 (10)	−0.0098 (11)	−0.0032 (10)
C39	0.0469 (13)	0.0398 (12)	0.0335 (11)	−0.0003 (10)	−0.0012 (10)	−0.0019 (10)
C40	0.0294 (10)	0.0377 (12)	0.0416 (12)	−0.0018 (9)	0.0020 (9)	−0.0083 (10)
C41	0.091 (2)	0.0351 (13)	0.0431 (14)	−0.0052 (13)	0.0083 (14)	0.0044 (11)
C42	0.0650 (16)	0.0426 (13)	0.0366 (12)	0.0047 (12)	−0.0067 (11)	−0.0039 (10)
C43	0.0291 (10)	0.0264 (10)	0.0248 (10)	−0.0010 (8)	−0.0073 (8)	−0.0021 (8)
C44	0.0303 (10)	0.0241 (9)	0.0212 (9)	−0.0009 (8)	−0.0025 (8)	−0.0024 (7)
C45	0.0378 (11)	0.0323 (11)	0.0218 (9)	−0.0011 (9)	−0.0042 (8)	0.0038 (8)
C46	0.0339 (10)	0.0294 (10)	0.0243 (10)	−0.0043 (8)	0.0036 (8)	0.0026 (8)
C47	0.0273 (9)	0.0239 (9)	0.0232 (9)	0.0002 (8)	0.0032 (8)	−0.0001 (7)

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C48	0.0256 (9)	0.0263 (10)	0.0318 (10)	−0.0007 (8)	0.0048 (8)	−0.0003 (8)
C49	0.0253 (10)	0.0321 (11)	0.0439 (12)	−0.0055 (8)	−0.0068 (9)	0.0139 (9)
C50	0.0290 (10)	0.0334 (11)	0.0474 (13)	−0.0040 (9)	−0.0030 (9)	0.0121 (10)
C51	0.0276 (11)	0.0394 (13)	0.0635 (16)	−0.0001 (9)	−0.0045 (11)	0.0148 (11)
C52	0.0332 (12)	0.0504 (14)	0.0593 (16)	−0.0047 (10)	−0.0173 (11)	0.0099 (12)
C53	0.0363 (12)	0.0443 (13)	0.0496 (14)	−0.0065 (10)	−0.0138 (10)	0.0050 (11)
C54	0.0333 (11)	0.0318 (11)	0.0425 (12)	−0.0071 (9)	−0.0082 (9)	0.0080 (9)
C55	0.0318 (11)	0.0446 (13)	0.0441 (13)	−0.0055 (9)	−0.0095 (10)	−0.0019 (10)
C56	0.0546 (15)	0.0472 (14)	0.0535 (15)	0.0100 (12)	−0.0090 (12)	−0.0012 (12)
C57	0.0522 (15)	0.0593 (16)	0.0482 (14)	−0.0070 (12)	−0.0030 (12)	0.0012 (12)
C58	0.0299 (11)	0.0456 (13)	0.0500 (14)	0.0008 (10)	0.0025 (10)	0.0059 (11)
C59	0.0539 (15)	0.0514 (15)	0.0706 (18)	0.0076 (12)	−0.0002 (14)	−0.0003 (14)
C60	0.0517 (15)	0.0646 (17)	0.0585 (16)	0.0043 (13)	0.0141 (13)	0.0122 (14)
O1	0.0392 (10)	0.0247 (9)	0.0301 (9)	0.0057 (7)	0.0073 (8)	−0.0032 (7)
C61	0.0399 (14)	0.0306 (14)	0.0455 (15)	−0.0019 (11)	−0.0004 (12)	−0.0073 (12)
C62	0.0597 (18)	0.0543 (18)	0.0443 (16)	0.0076 (15)	−0.0040 (14)	−0.0145 (14)
C63	0.0565 (19)	0.0498 (17)	0.0443 (16)	0.0117 (15)	0.0137 (14)	−0.0028 (13)
C64	0.0497 (17)	0.0451 (17)	0.074 (2)	0.0007 (14)	0.0209 (15)	−0.0079 (15)
Si	0.034 (3)	0.027 (3)	0.029 (2)	0.0034 (19)	0.0016 (18)	−0.0015 (18)
C1A	0.033 (3)	0.025 (3)	0.027 (3)	0.002 (3)	0.002 (3)	−0.002 (3)
C2A	0.038 (4)	0.028 (4)	0.036 (4)	0.005 (4)	0.000 (4)	0.001 (4)
C3A	0.039 (4)	0.032 (4)	0.030 (4)	0.002 (4)	0.003 (4)	−0.006 (4)
C4A	0.038 (4)	0.031 (4)	0.030 (4)	0.003 (4)	−0.002 (4)	−0.002 (4)

Geometric parameters (Å, º)

Cr1—N1	2.1042 (16)	C33—C34	1.375 (3)
Cr1—N2	2.0663 (15)	C34—H34	0.9500
Cr1—N4	2.7175 (15)	C34—C35	1.379 (3)
Cr1—N5	2.0311 (15)	C35—H35	0.9500
Cr1—N6	2.8897 (16)	C35—C36	1.396 (3)
Cr1—O1	2.0971 (16)	C36—C40	1.518 (3)
Cr1—C1A	1.911 (18)	C37—H37	1.0000
N1—C1	1.450 (2)	C37—C38	1.535 (3)
N1—C13	1.299 (2)	C37—C39	1.531 (3)
N2—C14	1.381 (2)	C38—H38A	0.9800
N2—C17	1.369 (2)	C38—H38B	0.9800
N3—C18	1.285 (2)	C38—H38C	0.9800
N3—C19	1.437 (2)	C39—H39A	0.9800
N4—C31	1.435 (2)	C39—H39B	0.9800
N4—C43	1.283 (2)	C39—H39C	0.9800
N5—C44	1.367 (2)	C40—H40	1.0000
N5—C47	1.368 (2)	C40—C41	1.517 (3)
N6—C48	1.283 (2)	C40—C42	1.516 (3)
N6—C49	1.433 (2)	C41—H41A	0.9800
C1—C2	1.405 (3)	C41—H41B	0.9800
C1—C6	1.397 (3)	C41—H41C	0.9800
C2—C3	1.398 (3)	C42—H42A	0.9800

C2—C7	1.516 (3)	C42—H42B	0.9800
C3—H3	0.9500	C42—H42C	0.9800
C3—C4	1.385 (3)	C43—H43	0.9500
C4—H4	0.9500	C43—C44	1.441 (3)
C4—C5	1.377 (3)	C44—C45	1.399 (3)
C5—H5	0.9500	C45—H45	0.9500
C5—C6	1.395 (3)	C45—C46	1.386 (3)
C6—C10	1.521 (3)	C46—H46	0.9500
C7—H7	1.0000	C46—C47	1.396 (3)
C7—C8	1.535 (3)	C47—C48	1.440 (3)
C7—C9	1.525 (3)	C48—H48	0.9500
C8—H8A	0.9800	C49—C50	1.407 (3)
C8—H8B	0.9800	C49—C54	1.413 (3)
C8—H8C	0.9800	C50—C51	1.400 (3)
C9—H9A	0.9800	C50—C58	1.516 (3)
C9—H9B	0.9800	C51—H51	0.9500
C9—H9C	0.9800	C51—C52	1.368 (3)
C10—H10	1.0000	C52—H52	0.9500
C10—C11	1.523 (4)	C52—C53	1.380 (3)
C10—C12	1.534 (3)	C53—H53	0.9500
C11—H11A	0.9800	C53—C54	1.389 (3)
C11—H11B	0.9800	C54—C55	1.514 (3)
C11—H11C	0.9800	C55—H55	1.0000
C12—H12A	0.9800	C55—C56	1.532 (3)
C12—H12B	0.9800	C55—C57	1.531 (3)
C12—H12C	0.9800	C56—H56A	0.9800
C13—H13	0.9500	C56—H56B	0.9800
C13—C14	1.418 (3)	C56—H56C	0.9800
C14—C15	1.402 (3)	C57—H57A	0.9800
C15—H15	0.9500	C57—H57B	0.9800
C15—C16	1.383 (3)	C57—H57C	0.9800
C16—H16	0.9500	C58—H58	1.0000
C16—C17	1.402 (3)	C58—C59	1.534 (3)
C17—C18	1.458 (3)	C58—C60	1.527 (3)
C18—H18	0.9500	C59—H59A	0.9800
C19—C20	1.412 (3)	C59—H59B	0.9800
C19—C24	1.399 (3)	C59—H59C	0.9800
C20—C21	1.392 (3)	C60—H60A	0.9800
C20—C25	1.522 (3)	C60—H60B	0.9800
C21—H21	0.9500	C60—H60C	0.9800
C21—C22	1.378 (3)	O1—C61	1.459 (3)
C22—H22	0.9500	O1—C64	1.451 (3)
C22—C23	1.386 (3)	C61—H61A	0.9900
C23—H23	0.9500	C61—H61B	0.9900
C23—C24	1.388 (3)	C61—C62	1.509 (4)
C24—C28	1.519 (3)	C62—H62A	0.9900
C25—H25	1.0000	C62—H62B	0.9900
C25—C26	1.527 (3)	C62—C63	1.518 (4)

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C25—C27	1.534 (3)	C63—H63A	0.9900
C26—H26A	0.9800	C63—H63B	0.9900
C26—H26B	0.9800	C63—C64	1.485 (4)
C26—H26C	0.9800	C64—H64A	0.9900
C27—H27A	0.9800	C64—H64B	0.9900
C27—H27B	0.9800	Si—C1A	1.751 (19)
C27—H27C	0.9800	Si—C2A	1.857 (10)
C28—H28	1.0000	Si—C3A	1.856 (10)
C28—C29	1.520 (3)	Si—C4A	1.856 (10)
C28—C30	1.530 (3)	C1A—H1AA	0.9900
C29—H29A	0.9800	C1A—H1AB	0.9900
C29—H29B	0.9800	C2A—H2AA	0.9800
C29—H29C	0.9800	C2A—H2AB	0.9800
C30—H30A	0.9800	C2A—H2AC	0.9800
C30—H30B	0.9800	C3A—H3AA	0.9800
C30—H30C	0.9800	C3A—H3AB	0.9800
C31—C32	1.404 (3)	C3A—H3AC	0.9800
C31—C36	1.407 (3)	C4A—H4AA	0.9800
C32—C33	1.397 (3)	C4A—H4AB	0.9800
C32—C37	1.521 (3)	C4A—H4AC	0.9800
C33—H33	0.9500		

N1—Cr1—N4	112.77 (5)	C35—C34—H34	120.2
N1—Cr1—N6	109.66 (6)	C34—C35—H35	119.3
N2—Cr1—N1	80.13 (6)	C34—C35—C36	121.3 (2)
N2—Cr1—N4	94.05 (5)	C36—C35—H35	119.3
N2—Cr1—N6	92.01 (5)	C31—C36—C40	120.36 (17)
N2—Cr1—O1	170.58 (6)	C35—C36—C31	118.43 (18)
N4—Cr1—N6	137.56 (5)	C35—C36—C40	121.04 (18)
N5—Cr1—N1	175.51 (6)	C32—C37—H37	107.7
N5—Cr1—N2	96.50 (6)	C32—C37—C38	113.01 (17)
N5—Cr1—N4	70.28 (5)	C32—C37—C39	110.13 (16)
N5—Cr1—N6	67.31 (5)	C38—C37—H37	107.7
N5—Cr1—O1	91.46 (6)	C39—C37—H37	107.7
O1—Cr1—N1	91.64 (6)	C39—C37—C38	110.34 (17)
O1—Cr1—N4	93.37 (6)	C37—C38—H38A	109.5
O1—Cr1—N6	86.41 (6)	C37—C38—H38B	109.5
C1A—Cr1—N1	93.6 (6)	C37—C38—H38C	109.5
C1A—Cr1—N2	156.4 (6)	H38A—C38—H38B	109.5
C1A—Cr1—N4	109.3 (6)	H38A—C38—H38C	109.5
C1A—Cr1—N5	88.3 (6)	H38B—C38—H38C	109.5
C1A—Cr1—N6	68.5 (6)	C37—C39—H39A	109.5
C1—N1—Cr1	127.25 (12)	C37—C39—H39B	109.5
C13—N1—Cr1	111.91 (12)	C37—C39—H39C	109.5
C13—N1—C1	120.80 (15)	H39A—C39—H39B	109.5
C14—N2—Cr1	111.42 (12)	H39A—C39—H39C	109.5
C17—N2—Cr1	142.61 (13)	H39B—C39—H39C	109.5
C17—N2—C14	105.88 (15)	C36—C40—H40	107.6

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C18—N3—C19	116.57 (16)	C41—C40—C36	109.58 (18)
C31—N4—Cr1	137.73 (11)	C41—C40—H40	107.6
C43—N4—Cr1	103.19 (11)	C42—C40—C36	114.42 (18)
C43—N4—C31	118.73 (16)	C42—C40—H40	107.6
C44—N5—Cr1	124.73 (12)	C42—C40—C41	109.78 (18)
C44—N5—C47	106.01 (15)	C40—C41—H41A	109.5
C47—N5—Cr1	127.95 (12)	C40—C41—H41B	109.5
C48—N6—Cr1	100.69 (12)	C40—C41—H41C	109.5
C48—N6—C49	119.66 (16)	H41A—C41—H41B	109.5
C49—N6—Cr1	139.48 (12)	H41A—C41—H41C	109.5
C2—C1—N1	118.46 (17)	H41B—C41—H41C	109.5
C6—C1—N1	119.64 (17)	C40—C42—H42A	109.5
C6—C1—C2	121.72 (17)	C40—C42—H42B	109.5
C1—C2—C7	121.91 (17)	C40—C42—H42C	109.5
C3—C2—C1	117.91 (18)	H42A—C42—H42B	109.5
C3—C2—C7	120.16 (18)	H42A—C42—H42C	109.5
C2—C3—H3	119.5	H42B—C42—H42C	109.5
C4—C3—C2	121.01 (19)	N4—C43—H43	119.0
C4—C3—H3	119.5	N4—C43—C44	121.97 (17)
C3—C4—H4	120.1	C44—C43—H43	119.0
C5—C4—C3	119.89 (19)	N5—C44—C43	119.29 (16)
C5—C4—H4	120.1	N5—C44—C45	110.41 (16)
C4—C5—H5	119.3	C45—C44—C43	130.04 (17)
C4—C5—C6	121.4 (2)	C44—C45—H45	126.7
C6—C5—H5	119.3	C46—C45—C44	106.50 (16)
C1—C6—C10	123.20 (18)	C46—C45—H45	126.7
C5—C6—C1	118.02 (19)	C45—C46—H46	126.7
C5—C6—C10	118.73 (19)	C45—C46—C47	106.68 (17)
C2—C7—H7	107.7	C47—C46—H46	126.7
C2—C7—C8	113.36 (18)	N5—C47—C46	110.39 (16)
C2—C7—C9	110.61 (17)	N5—C47—C48	120.29 (16)
C8—C7—H7	107.7	C46—C47—C48	129.27 (17)
C9—C7—H7	107.7	N6—C48—C47	122.41 (17)
C9—C7—C8	109.49 (19)	N6—C48—H48	118.8
C7—C8—H8A	109.5	C47—C48—H48	118.8
C7—C8—H8B	109.5	C50—C49—N6	120.83 (19)
C7—C8—H8C	109.5	C50—C49—C54	121.22 (18)
H8A—C8—H8B	109.5	C54—C49—N6	117.79 (18)
H8A—C8—H8C	109.5	C49—C50—C58	123.17 (18)
H8B—C8—H8C	109.5	C51—C50—C49	117.6 (2)
C7—C9—H9A	109.5	C51—C50—C58	119.17 (19)
C7—C9—H9B	109.5	C50—C51—H51	119.1
C7—C9—H9C	109.5	C52—C51—C50	121.8 (2)
H9A—C9—H9B	109.5	C52—C51—H51	119.1
H9A—C9—H9C	109.5	C51—C52—H52	120.1
H9B—C9—H9C	109.5	C51—C52—C53	119.8 (2)
C6—C10—H10	108.0	C53—C52—H52	120.1
C6—C10—C11	109.80 (19)	C52—C53—H53	119.2

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C6—C10—C12	112.2 (2)	C52—C53—C54	121.6 (2)
C11—C10—H10	108.0	C54—C53—H53	119.2
C11—C10—C12	110.7 (2)	C49—C54—C55	119.96 (18)
C12—C10—H10	108.0	C53—C54—C49	117.9 (2)
C10—C11—H11A	109.5	C53—C54—C55	121.9 (2)
C10—C11—H11B	109.5	C54—C55—H55	107.7
C10—C11—H11C	109.5	C54—C55—C56	109.15 (18)
H11A—C11—H11B	109.5	C54—C55—C57	114.75 (19)
H11A—C11—H11C	109.5	C56—C55—H55	107.7
H11B—C11—H11C	109.5	C57—C55—H55	107.7
C10—C12—H12A	109.5	C57—C55—C56	109.7 (2)
C10—C12—H12B	109.5	C55—C56—H56A	109.5
C10—C12—H12C	109.5	C55—C56—H56B	109.5
H12A—C12—H12B	109.5	C55—C56—H56C	109.5
H12A—C12—H12C	109.5	H56A—C56—H56B	109.5
H12B—C12—H12C	109.5	H56A—C56—H56C	109.5
N1—C13—H13	120.3	H56B—C56—H56C	109.5
N1—C13—C14	119.47 (17)	C55—C57—H57A	109.5
C14—C13—H13	120.3	C55—C57—H57B	109.5
N2—C14—C13	116.92 (16)	C55—C57—H57C	109.5
N2—C14—C15	110.20 (16)	H57A—C57—H57B	109.5
C15—C14—C13	132.88 (17)	H57A—C57—H57C	109.5
C14—C15—H15	126.7	H57B—C57—H57C	109.5
C16—C15—C14	106.58 (17)	C50—C58—H58	107.5
C16—C15—H15	126.7	C50—C58—C59	113.1 (2)
C15—C16—H16	126.5	C50—C58—C60	110.89 (19)
C15—C16—C17	107.06 (17)	C59—C58—H58	107.5
C17—C16—H16	126.5	C60—C58—H58	107.5
N2—C17—C16	110.27 (16)	C60—C58—C59	110.04 (19)
N2—C17—C18	120.88 (16)	C58—C59—H59A	109.5
C16—C17—C18	128.82 (17)	C58—C59—H59B	109.5
N3—C18—C17	122.39 (17)	C58—C59—H59C	109.5
N3—C18—H18	118.8	H59A—C59—H59B	109.5
C17—C18—H18	118.8	H59A—C59—H59C	109.5
C20—C19—N3	118.32 (17)	H59B—C59—H59C	109.5
C24—C19—N3	120.36 (18)	C58—C60—H60A	109.5
C24—C19—C20	121.25 (18)	C58—C60—H60B	109.5
C19—C20—C25	119.57 (18)	C58—C60—H60C	109.5
C21—C20—C19	117.90 (19)	H60A—C60—H60B	109.5
C21—C20—C25	122.53 (19)	H60A—C60—H60C	109.5
C20—C21—H21	119.3	H60B—C60—H60C	109.5
C22—C21—C20	121.4 (2)	C61—O1—Cr1	122.66 (14)
C22—C21—H21	119.3	C64—O1—Cr1	122.95 (16)
C21—C22—H22	120.1	C64—O1—C61	108.20 (19)
C21—C22—C23	119.8 (2)	O1—C61—H61A	110.7
C23—C22—H22	120.1	O1—C61—H61B	110.7
C22—C23—H23	119.4	O1—C61—C62	105.1 (2)
C22—C23—C24	121.2 (2)	H61A—C61—H61B	108.8

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C24—C23—H23	119.4	C62—C61—H61A	110.7
C19—C24—C28	119.33 (18)	C62—C61—H61B	110.7
C23—C24—C19	118.4 (2)	C61—C62—H62A	111.4
C23—C24—C28	122.2 (2)	C61—C62—H62B	111.4
C20—C25—H25	106.8	C61—C62—C63	102.0 (2)
C20—C25—C26	114.36 (19)	H62A—C62—H62B	109.2
C20—C25—C27	111.16 (17)	C63—C62—H62A	111.4
C26—C25—H25	106.8	C63—C62—H62B	111.4
C26—C25—C27	110.58 (19)	C62—C63—H63A	111.4
C27—C25—H25	106.8	C62—C63—H63B	111.4
C25—C26—H26A	109.5	H63A—C63—H63B	109.3
C25—C26—H26B	109.5	C64—C63—C62	101.9 (2)
C25—C26—H26C	109.5	C64—C63—H63A	111.4
H26A—C26—H26B	109.5	C64—C63—H63B	111.4
H26A—C26—H26C	109.5	O1—C64—C63	106.8 (2)
H26B—C26—H26C	109.5	O1—C64—H64A	110.4
C25—C27—H27A	109.5	O1—C64—H64B	110.4
C25—C27—H27B	109.5	C63—C64—H64A	110.4
C25—C27—H27C	109.5	C63—C64—H64B	110.4
H27A—C27—H27B	109.5	H64A—C64—H64B	108.6
H27A—C27—H27C	109.5	C1A—Si—C2A	108.8 (9)
H27B—C27—H27C	109.5	C1A—Si—C3A	109.3 (8)
C24—C28—H28	107.0	C1A—Si—C4A	104.8 (9)
C24—C28—C29	110.53 (19)	C3A—Si—C2A	110.3 (8)
C24—C28—C30	114.3 (2)	C3A—Si—C4A	111.0 (8)
C29—C28—H28	107.0	C4A—Si—C2A	112.5 (8)
C29—C28—C30	110.6 (2)	Cr1—C1A—H1AA	104.1
C30—C28—H28	107.0	Cr1—C1A—H1AB	104.1
C28—C29—H29A	109.5	Si—C1A—Cr1	132.6 (11)
C28—C29—H29B	109.5	Si—C1A—H1AA	104.1
C28—C29—H29C	109.5	Si—C1A—H1AB	104.1
H29A—C29—H29B	109.5	H1AA—C1A—H1AB	105.5
H29A—C29—H29C	109.5	Si—C2A—H2AA	109.5
H29B—C29—H29C	109.5	Si—C2A—H2AB	109.5
C28—C30—H30A	109.5	Si—C2A—H2AC	109.5
C28—C30—H30B	109.5	H2AA—C2A—H2AB	109.5
C28—C30—H30C	109.5	H2AA—C2A—H2AC	109.5
H30A—C30—H30B	109.5	H2AB—C2A—H2AC	109.5
H30A—C30—H30C	109.5	Si—C3A—H3AA	109.5
H30B—C30—H30C	109.5	Si—C3A—H3AB	109.5
C32—C31—N4	120.51 (16)	Si—C3A—H3AC	109.5
C32—C31—C36	120.74 (17)	H3AA—C3A—H3AB	109.5
C36—C31—N4	118.64 (16)	H3AA—C3A—H3AC	109.5
C31—C32—C37	122.20 (17)	H3AB—C3A—H3AC	109.5
C33—C32—C31	118.25 (18)	Si—C4A—H4AA	109.5
C33—C32—C37	119.50 (17)	Si—C4A—H4AB	109.5
C32—C33—H33	119.2	Si—C4A—H4AC	109.5
C34—C33—C32	121.66 (19)	H4AA—C4A—H4AB	109.5

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C34—C33—H33	119.2	H4AA—C4A—H4AC	109.5
C33—C34—H34	120.2	H4AB—C4A—H4AC	109.5
C33—C34—C35	119.60 (19)		

Cr1—N1—C1—C2	88.33 (19)	C19—C20—C25—C26	−163.59 (19)
Cr1—N1—C1—C6	−86.8 (2)	C19—C20—C25—C27	70.3 (2)
Cr1—N1—C13—C14	−2.6 (2)	C19—C24—C28—C29	−74.6 (2)
Cr1—N2—C14—C13	3.2 (2)	C19—C24—C28—C30	159.8 (2)
Cr1—N2—C14—C15	−176.85 (12)	C20—C19—C24—C23	−1.1 (3)
Cr1—N2—C17—C16	175.81 (15)	C20—C19—C24—C28	179.04 (18)
Cr1—N2—C17—C18	−2.6 (3)	C20—C21—C22—C23	−0.1 (3)
Cr1—N4—C31—C32	111.05 (18)	C21—C20—C25—C26	16.1 (3)
Cr1—N4—C31—C36	−65.3 (2)	C21—C20—C25—C27	−110.0 (2)
Cr1—N4—C43—C44	−5.1 (2)	C21—C22—C23—C24	−0.2 (3)
Cr1—N5—C44—C43	6.5 (2)	C22—C23—C24—C19	0.8 (3)
Cr1—N5—C44—C45	−168.30 (12)	C22—C23—C24—C28	−179.4 (2)
Cr1—N5—C47—C46	167.53 (13)	C23—C24—C28—C29	105.6 (2)
Cr1—N5—C47—C48	−10.3 (2)	C23—C24—C28—C30	−20.1 (3)
Cr1—N6—C48—C47	8.0 (2)	C24—C19—C20—C21	0.9 (3)
Cr1—N6—C49—C50	−118.3 (2)	C24—C19—C20—C25	−179.43 (18)
Cr1—N6—C49—C54	57.2 (3)	C25—C20—C21—C22	−179.94 (19)
Cr1—O1—C61—C62	−138.96 (17)	C31—N4—C43—C44	−179.43 (16)
Cr1—O1—C64—C63	164.54 (18)	C31—C32—C33—C34	0.4 (3)
N1—C1—C2—C3	−176.35 (16)	C31—C32—C37—C38	−134.74 (19)
N1—C1—C2—C7	5.2 (3)	C31—C32—C37—C39	101.4 (2)
N1—C1—C6—C5	175.47 (17)	C31—C36—C40—C41	−90.2 (2)
N1—C1—C6—C10	−6.9 (3)	C31—C36—C40—C42	146.07 (19)
N1—C13—C14—N2	−0.4 (3)	C32—C31—C36—C35	0.3 (3)
N1—C13—C14—C15	179.6 (2)	C32—C31—C36—C40	175.61 (17)
N2—C14—C15—C16	−0.7 (2)	C32—C33—C34—C35	−0.2 (3)
N2—C17—C18—N3	179.13 (17)	C33—C32—C37—C38	48.1 (2)
N3—C19—C20—C21	177.78 (17)	C33—C32—C37—C39	−75.8 (2)
N3—C19—C20—C25	−2.5 (3)	C33—C34—C35—C36	0.1 (3)
N3—C19—C24—C23	−178.00 (18)	C34—C35—C36—C31	−0.1 (3)
N3—C19—C24—C28	2.2 (3)	C34—C35—C36—C40	−175.42 (19)
N4—C31—C32—C33	−176.68 (17)	C35—C36—C40—C41	85.0 (2)
N4—C31—C32—C37	6.1 (3)	C35—C36—C40—C42	−38.7 (3)
N4—C31—C36—C35	176.64 (17)	C36—C31—C32—C33	−0.4 (3)
N4—C31—C36—C40	−8.0 (3)	C36—C31—C32—C37	−177.63 (17)
N4—C43—C44—N5	0.9 (3)	C37—C32—C33—C34	177.65 (18)
N4—C43—C44—C45	174.45 (19)	C43—N4—C31—C32	−77.1 (2)
N5—C44—C45—C46	0.6 (2)	C43—N4—C31—C36	106.5 (2)
N5—C47—C48—N6	−2.1 (3)	C43—C44—C45—C46	−173.46 (19)
N6—C49—C50—C51	174.85 (17)	C44—N5—C47—C46	0.3 (2)
N6—C49—C50—C58	−7.1 (3)	C44—N5—C47—C48	−177.55 (16)
N6—C49—C54—C53	−175.06 (18)	C44—C45—C46—C47	−0.4 (2)
N6—C49—C54—C55	9.8 (3)	C45—C46—C47—N5	0.1 (2)
C1—N1—C13—C14	179.69 (17)	C45—C46—C47—C48	177.64 (18)

C1—C2—C3—C4	1.2 (3)	C46—C47—C48—N6	−179.41 (19)
C1—C2—C7—C8	−145.58 (19)	C47—N5—C44—C43	174.26 (16)
C1—C2—C7—C9	91.0 (2)	C47—N5—C44—C45	−0.5 (2)
C1—C6—C10—C11	−104.7 (2)	C48—N6—C49—C50	67.5 (3)
C1—C6—C10—C12	131.8 (2)	C48—N6—C49—C54	−117.0 (2)
C2—C1—C6—C5	0.5 (3)	C49—N6—C48—C47	−175.83 (17)
C2—C1—C6—C10	178.15 (19)	C49—C50—C51—C52	0.0 (3)
C2—C3—C4—C5	−0.3 (3)	C49—C50—C58—C59	130.3 (2)
C3—C2—C7—C8	36.0 (3)	C49—C50—C58—C60	−105.6 (2)
C3—C2—C7—C9	−87.4 (2)	C49—C54—C55—C56	81.5 (2)
C3—C4—C5—C6	−0.5 (3)	C49—C54—C55—C57	−154.9 (2)
C4—C5—C6—C1	0.4 (3)	C50—C49—C54—C53	0.5 (3)
C4—C5—C6—C10	−177.3 (2)	C50—C49—C54—C55	−174.62 (18)
C5—C6—C10—C11	73.0 (3)	C50—C51—C52—C53	0.7 (3)
C5—C6—C10—C12	−50.6 (3)	C51—C50—C58—C59	−51.7 (3)
C6—C1—C2—C3	−1.3 (3)	C51—C50—C58—C60	72.4 (2)
C6—C1—C2—C7	−179.75 (18)	C51—C52—C53—C54	−0.8 (3)
C7—C2—C3—C4	179.69 (18)	C52—C53—C54—C49	0.2 (3)
C13—N1—C1—C2	−94.3 (2)	C52—C53—C54—C55	175.2 (2)
C13—N1—C1—C6	90.6 (2)	C53—C54—C55—C56	−93.4 (2)
C13—C14—C15—C16	179.3 (2)	C53—C54—C55—C57	30.2 (3)
C14—N2—C17—C16	0.0 (2)	C54—C49—C50—C51	−0.5 (3)
C14—N2—C17—C18	−178.46 (16)	C54—C49—C50—C58	177.45 (19)
C14—C15—C16—C17	0.6 (2)	C58—C50—C51—C52	−178.1 (2)
C15—C16—C17—N2	−0.4 (2)	O1—C61—C62—C63	−33.4 (3)
C15—C16—C17—C18	177.88 (18)	C61—O1—C64—C63	11.7 (3)
C16—C17—C18—N3	1.0 (3)	C61—C62—C63—C64	39.7 (3)
C17—N2—C14—C13	−179.55 (16)	C62—C63—C64—O1	−32.2 (3)
C17—N2—C14—C15	0.4 (2)	C64—O1—C61—C62	14.0 (3)
C18—N3—C19—C20	86.2 (2)	C2A—Si—C1A—Cr1	−179.1 (13)
C18—N3—C19—C24	−96.8 (2)	C3A—Si—C1A—Cr1	−58.6 (16)
C19—N3—C18—C17	−175.12 (16)	C4A—Si—C1A—Cr1	60.4 (16)
C19—C20—C21—C22	−0.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18···N5	0.95	2.43	3.232 (2)	142
C1*A*—H1*AB*···N6	0.99	2.09	2.820 (19)	130