Acta Cryst E
CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

An unsymmetrical dinuclear scandium complex comprising salophen ligands [H_2salophen = *N*,*N*′-bis(salicylidene)-1,2-phenylenediamine]

Volker Lorenz, Phil Liebing, Liane Hilfert, Sabine Busse and Frank T. Edelmann*

Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany. *Correspondence e-mail: frank.edelmann@ovgu.de

Received 2 January 2019
Accepted 3 January 2019

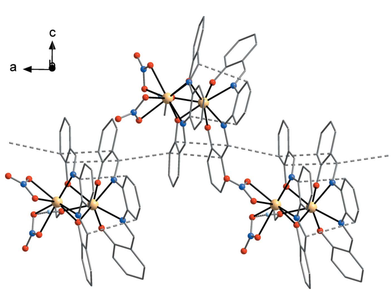
Edited by M. Zeller, Purdue University, USA

Keywords: scandium; salophen ligand; Schiff base; dinuclear scandium complex; crystal structure; π–π stacking.

CCDC reference: 1880860

Supporting information: this article has supporting information at journals.iucr.org/e

Treatment of scandium nitrate tetrahydrate with the tetradentate ligand H_2salophen [*N*,*N*′-bis(salicylidene)-1,2-phenylenediamine] afforded the yellow dinuclear complex $Sc(NO_3)_2(\mu$-salophen)Sc(salophen)(EtOH) or $[Sc_2(C_{20}H_{14}N_2O_2)_2(NO_3)_2(C_2H_6O)]$ (systematic name: (ethanol-κO)bis(nitrato-$\kappa^2 O,O'$){μ-2,2′-[1,2-phenylenebis(nitrilomethanylylidene)]diphenolato-$\kappa^4 N,N',O,O':\kappa^2 O,O'$}{2,2′-[1,2-phenylenebis(nitrilomethanylylidene)]diphenolato-$\kappa^4 O,N,N',O'$}discandium). In this compound, one salophen ligand displays a bridging coordination *via* the two oxygen atoms, while the other salophen ligand is attached to only one Sc center. This arrangement is stabilized by a hydrogen-bonded EtOH co-ligand, and by π–π stacking interactions between the two salophen ligands.



1. Chemical context

In the coordination chemistry of lanthanides, salen-type Schiff-base ligands such as H_2salen [*N*,*N*′-bis(salicylidene)-ethylenediamine] and H_2salophen [*N*,*N*′-bis(salicylidene)-1,2-phenylenediamine] are among the best known multidentate ligands. Lanthanide complexes comprising salen-type ligands are of significant interest due to their variety of molecular structures (Akine & Nabeshima, 2009) and their promising magnetic properties (Costes *et al.*, 1998; Yao *et al.*, 2012; Pajerowski *et al.*, 2014) and luminescence properties (Bi *et al.*, 2009; Li *et al.*, 2013; Mikhalyova *et al.*, 2014; Yang *et al.*, 2014). They also have potential applications in electronic devices (Magadur *et al.*, 2012) and homogeneous catalysis (Wu *et al.*, 2017). The first lanthanide–salen and salophen complexes were reported fifty years ago (Dutt & Nag, 1968). Since then, a variety of interesting structures have been reported for such complexes, including mononuclear complexes (Evans *et al.*, 1999; Yao *et al.*, 2012), sandwich-like di- and trinuclear species (Chen & Archer, 1994; Costes *et al.*, 1998; Camp *et al.*, 2012; Li *et al.*, 2012, 2013; Mikhalyova *et al.*, 2014), clusters (Zhao *et al.*, 2012; Pajerowski *et al.*, 2014) and 3*d*–4*f* heterobimetallic complexes (Condorelli *et al.*, 1975; Winpenny, 1998; Sakamoto *et al.*, 2001; Camp *et al.*, 2017).

Scandium complexes comprising salen-type Schiff-base ligands are fairly rare, with the majority of such compounds having been reported by Anwander and co-workers (Meermann *et al.*, 2006, 2009). Access to these complexes was achieved *via* treatment of the scandium silylamide precursor $Sc[N(SiHMe_2)_3]_3(THF)$ with substituted H_2salen precursors under anaerobic conditions. We report here the straightforward formation and structural characterization of a dinuclear scandium complex comprising salophen ligands using scan-

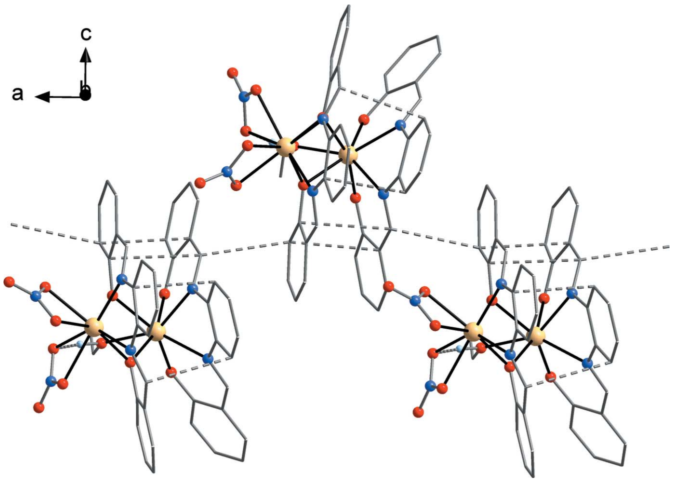
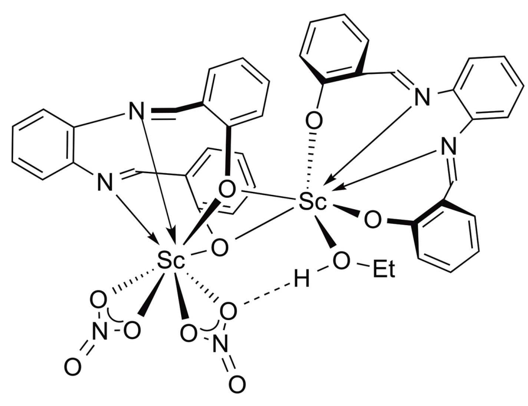


Figure 2
Illustration of intra- and intermolecular π–π stacking interactions. The association of the complex molecules results in a supramolecular chain structure, which extends along the *a*-axis direction.

dium nitrate tetrahydrate as the starting material. Treatment of a diluted solution of $Sc(NO_3)_3{\cdot}4H_2O$ in ethanol with an ethanolic solution of the protonated ligand H_2salophen (Bonnaire *et al.*, 1981) resulted in the rapid formation of a yellow precipitate which was identified as the title complex $Sc(NO_3)_2$(μ-salophen)Sc(salophen)(EtOH). The analytically pure material could be isolated in 70% yield. The title compound was fully characterized through the usual set of elemental analysis and spectroscopic methods (IR, NMR, MS). The NMR spectra in DMSO-d_6 solution showed only one set of salophen ^{1}H and ^{13}C signals, and only one ^{45}Sc signal, and consequently the dimeric structure seems to be split into a monomeric species in DMSO. The mass spectrum did not display the molecular ion, but other high-molecular-mass peaks attributable to dimeric species, *e.g.* $[M - CH_3]^+$ at *m*/*z* 863, $[M - EtOH]^+$ at *m*/*z* 843, and $[M - EtOH - NO_3]^+$ at *m*/*z* 780.



2. Structural commentary

The asymmetric unit of the title compound recrystallized from ethanol contains two scandium atoms, two nitrate moieties, two salophen ligands, and one EtOH molecule (Fig. 1). Both Sc atoms are situated in the tetradentate coordination pocket of a salophen ligand. Sc1 is coordinatively saturated by two chelating nitrate anions, resulting in a somewhat square-anti-prismatic coordination. Sc2 is connected to the two oxygen atoms of the other Sc(salophen) unit, thus connecting the two parts of the molecule. An irregular seven-coordination of Sc2 is completed by an EtOH ligand. This asymmetrical structure is stabilized by an intramolecular O—H$\cdots$O hydrogen bond between EtOH and a nitrate ligand [O6$\cdots$O11 2.787 (3) Å, O6$\cdots$H approx. 2.01 Å; Table 1].

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

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D$$\cdots$$A$	D—H$\cdots$$A$
O11—H29$\cdots$O6	0.83 (2)	2.01 (2)	2.787 (3)	156 (3)

The Sc—O bond lengths within the central Sc_2O_2 ring (including O1, O2) are significantly different, and surprisingly the bonds at the seven-coordinated Sc2 [2.214 (2) and 2.342 (2) Å] are longer than those at the octa-coordinated Sc1 [2.062 (2) and 2.110 (2) Å]. The bonds of Sc2 to the terminally coordinated salophene oxygen atoms (O3, O4) are 2.006 (2) and 1.995 (2) Å, respectively. The Sc—N bonds are also slightly longer for Sc2 [2.286 (2) and 2.341 (2) Å] than for Sc1 [2.270 (2) and 2.278 (2) Å]. These values of Sc—N distances are larger than in related scandium–salen complexes (Meermann *et al.*, 2006, 2009), reflecting the higher coordination numbers of scandium in the title compound. However, the terminal Sc—O(salicylidene) bonds are similar or only marginally elongated as compared to the reference compounds. The Sc—O(nitrate) separations are in the range 2.263 (2)–2.323 (2) Å, resembling the values observed for other scandium–nitrate complexes (*e.g.* Arif *et al.*, 1984, Cotton *et al.*, 2008).

The octa-coordinated Sc1 is displaced from the salophene's N_2O_2 coordination plane by 1.091 (1) Å, while the corresponding value for the seven-coordinated Sc2 is only

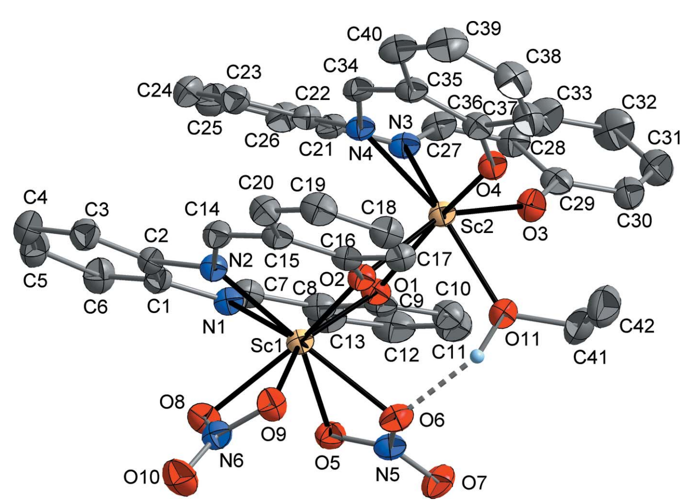


Figure 1
Molecular structure of the title compound in the crystalline state, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms attached to C atoms are omitted for clarity.

1.014 (1) Å. Both values are considerably larger than those observed in related complexes (Meermann *et al.*, 2006, 2009), which can again be traced back to the higher coordination numbers of scandium. Both salophen ligands deviate markedly from planarity, as the two salicylidene arms are twisted out of the particular phenylene-diamine plane around the C—N single-bonds. The (phenylene)C═C—N═C(imide) torsion angles (which would be 0° in the case of perfect planarity) are 15.7 (4) and 24.6 (4)° for the salophen ligand at Sc1, and 30.0 (4) and 34.7 (4)° for the salophen ligand at Sc2. The corresponding angles between the salicylidene C_6 rings are 12.9 (2)° for Sc1 and 53.5 (1)° for Sc2, being in the same range as in the reference compounds (Meermann *et al.*, 2006, 2009). Intramolecular π–π stacking interactions between the two salophen ligands may contribute to the stabilization of the dimeric structure. The two phenylene-diamine moieties are oriented almost parallel to each other with an angle of 11.8 (1)° between the C_6 rings, and the closest interatomic contact between the rings is 3.401 (4) Å (C2···C23). The same is true for the two salicylidene moieties, with an angle of 14.4 (1)° and the closest contact being 3.247 (4) Å (C17···C35). The remaining two salicylidene moieties are not in a proper orientation for efficient π–π stacking [angle between C_6 rings = 37.1 (2)°].

3. Supramolecular features

The molecules seem to be primarily associated by π–π stacking interactions (Fig. 2). The closest intermolecular contact is 3.369 (4) Å [C17···C34($\frac{1}{2}+x, y, \frac{1}{2}-z$)] between two salicylidene moieties [angle between C_6 rings of 13.0 (1)°].

4. Database survey

For review articles on rare-earth complexes with salen-type Schiff-base ligands, see: Akine & Nabeshima (2009); Yang *et al.* (2014). For review articles on 3*d*–4*f* heteronuclear complexes with polydentate Schiff-base ligands, see: Winpenny (1998); Sakamoto *et al.* (2001). For related Sc complexes comprising salen-type Schiff-base ligands, see: Meermann *et al.* (2006, 2009).

5. Synthesis and crystallization

0.50 g (1.58 mmol) of H_2salophen dissolved in *ca* 150 ml of ethanol were added to a solution of 0.63 g (2.08 mmol) $Sc(NO_3)_3 \cdot 4H_2O$ in 100 ml ethanol at 323 K. After a few minutes the solution became turbid and $Sc(NO_3)_2$(μ-salophen)Sc(salophen)(EtOH) precipitated as a microcrystalline yellow solid. Yield: 0.5 g (70%). Recrystallization from hot ethanol afforded yellow, plate-like single crystals. Decomp. 443 K. Analysis calculated for $C_{42}H_{34}N_6O_{11}Sc_2$ (M = 888.68 g mol^{-1}): C 56.77, H 3.86, N 9.46; found: C 56.36, H 3.95, N 9.81%.

^{1}H NMR (400.1 MHz, DMSO-d_6, 294 K): δ = 8.74 (*s*, 4H, *H*C═N), 7.71–7.68 (*m*, 4H, *m*-C_6H_4N), 7.57 (*d*, 4H, *o*-C_6H_4C), 7.46–7.43 (*m*, 4H, *o*-C_6H_4N), 7.38 (*t*, 4H, *m*-C_6H_4C), 6.73 (*d*, 4H, *o*-C_6H_4O), 6.71 (*t*, 4H, *m*-C_6H_4O) ppm; CH_3CH_2OH not observed. **^{13}C NMR** (100.6 MHz, DMSO-d_6, 294 K): δ = 166.1 (O—C_6H$_4$), 161.9 (H*C*═N), 144.2 (N—C_6H$_4$), 135.1 (*o*-C_6H$_4$C, *m*-C_6H$_4$C), 128.0 (*o*-C_6H$_4$N), 122.5 (C-C_6H$_4$), 120.3 (*o*-C_6H$_4$O), 118.3 (*m*-C_6H$_4$N), 115.5 (*m*-C_6H$_4$O) ppm; CH_3CH_2OH not observed. **^{45}Sc NMR** (97.2 MHz, DMSO-d_6, 294 KC): δ = 49.8 ppm.

IR (ATR): ν = 3426*w*, 3058*w*, 3026*w*, 2973*w*, 1609*vs*, 1580*m*, 1540*m*, 1526*s*, 1472*s*, 1443*m*, 1380*m*, 1348*w*, 1300*s*, 1276*s*, 1236*m*, 1193*m*, 1150*m*, 1123*m*, 1032*w*, 1021*w*, 984*w*, 946*w*, 920*m*, 864*w*, 851*w*, 802*m*, 747*vs*, 729*s*, 699*w*, 667*w*, 641*w*, 606*m*, 583*w*, 564*m*, 531*s*, 513*w*, 486*m*, 470*w*, 450*m*, 400*m*, 378*vs*, 353*m*, 306*vs*, 281*vs*, 231*m*, 169*w*, 157*w*, 137*w*, 118w, 107*w*, 91*w*, 77*w*, 68w, 61*w*, 54*w* cm^{-1}.

MS (70 eV): m/z = 863 (1%) [M − CH$_3$]$^+$, 843 (<1%) [M − EtOH]$^+$, 780 (2%) [M − EtOH − NO$_3$]$^+$, 733 (4%), 705 (1%), 662 (65%) [M − EtOH − NO$_3$ − NC$_6$H$_4$O]$^+$, 647 (70%), 580 (5%), 568 (27%), 555 (8%), 506 (100%), 480 (42%).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms attached to C atoms were fixed geometrically and refined using a riding model. All C—H distances within the salophen ligands were constrained to 0.95 Å. For the EtOH ligand, the C—H distances within the CH$_2$ group were constrained to 0.99 Å, the C—H distances within the CH$_3$ group were constrained to 0.98 Å, and the CH$_3$

Table 2
Experimental details.

Crystal data	
Chemical formula	[Sc$_2$(C$_{42}$H$_{34}$N$_6$O$_{11}$)]
M_r	888.67
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	153
a, b, c (Å)	13.6092 (3), 21.5880 (7), 26.5297 (7)
V (Å^3)	7794.3 (4)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.42
Crystal size (mm)	0.32 × 0.13 × 0.09
Data collection	
Diffractometer	STOE IPDS 2T
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25118, 6849, 5105
R_{int}	0.064
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.098, 1.04
No. of reflections	6849
No. of parameters	555
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.34

Computer programs: *X-AREA* and *X-RED32* (Stoe & Cie, 2002), *SIR97* (Altomare *et al.*, 1999), *SHELXL2018/3* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 1999) and *publCIF* (Westrip, 2010).

group was allowed to rotate freely around the C–C vector. The oxygen-bound EtOH hydrogen atom was located in the difference-Fourier map and refined freely, the corresponding O—H distance was restrained to 0.84 (2) Å. The U_{iso}(H) values were set at $1.2U_{eq}(X)$ (X = C, O). The reflections 020 and 021 disagreed strongly with the structural model and were therefore omitted from the refinement.

Acknowledgements

General financial support by the Otto-von-Guericke-Universität Magdeburg is gratefully acknowledged.

References

Akine, S. & Nabeshima, T. (2009). *Dalton Trans.* pp. 10395–10408.
Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Arif, A. M., Hart, F. A., Hursthouse, M. B., Thornton-Pett, M. & Zhu, W. (1984). *J. Chem. Soc. Dalton Trans.* pp. 2449–2454.
Bi, W., Wei, T., Lü, X., Hui, Y., Song, J., Zhao, S., Wong, W.-K. & Jones, R. A. (2009). *New J. Chem.* **33**, 2326–2334.
Bonnaire, R., Manoli, J. M., Potvin, C., Platzer, N. & Goasdoue, N. (1981). *Inorg. Chem.* **20**, 2691–2696.
Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Camp, C., Guidal, V., Biswas, B., Pécaut, J., Dubois, L. & Mazzanti, M. (2012). *Chem. Sci.* **3**, 2433–2448.
Camp, C., Toniolo, D., Andrez, J., Pécaut, J. & Mazzanti, M. (2017). *Dalton Trans.* **46**, 11145–11148.
Chen, H. & Archer, R. D. (1994). *Inorg. Chem.* **33**, 5195–5202.
Condorelli, G., Fragalà, I., Giuffrida, S. & Cassol, A. (1975). *Z. Anorg. Allg. Chem.* **412**, 251–257.
Costes, J.-P., Dupuis, A. & Laurent, J.-P. (1998). *Inorg. Chim. Acta*, **268**, 125–130.
Cotton, S. A., Fisher, V. M. A., Raithby, P. R., Schiffers, S. & Teat, S. J. (2008). *Inorg. Chem. Commun.* **11**, 822–824.
Dutt, N. K. & Nag, K. (1968). *J. Inorg. Nucl. Chem.* **30**, 2493–2499.
Evans, W. J., Fujimoto, C. H. & Ziller, J. W. (1999). *Chem. Commun.* pp. 311–312.
Li, Q., Chen, S., Yan, P., Chen, P., Hou, G. & Li, G. (2013). *J. Coord. Chem.* **66**, 1084–1093.
Li, Q., Yan, P., Chen, P., Hou, G. & Li, G. (2012). *J. Inorg. Organomet. Polym. Mater.* **22**, 1174–1181.
Magadur, G., Bouanis, F., Norman, E., Guillot, R., Lauret, J.-S., Huc, V., Cojocaru, C.-S. & Mallah, T. (2012). *Chem. Commun.* **48**, 9071–9073.
Meermann, C., Sirsch, P., Törnroos, K. W. & Anwander, R. (2006). *Dalton Trans.* pp. 1041–1050.
Meermann, C., Törnroos, K. W. & Anwander, R. (2009). *Inorg. Chem.* **48**, 2561–2570.
Mikhalyova, E. A., Yakovenko, A. V., Zeller, M., Gavrilenko, K. S., Lofland, S. E., Addison, A. W. & Pavlishchuk, V. V. (2014). *Inorg. Chim. Acta*, **414**, 97–104.
Pajerowski, D. M., Li, Q., Hyun, J., Dennis, C. L., Phelan, D., Yan, P., Chen, P. & Li, G. (2014). *Dalton Trans.* **43**, 11973–11980.
Sakamoto, M., Manseki, K. & Okawa, H. (2001). *Coord. Chem. Rev.* **219–221**, 379–414.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Stoe & Cie (2002). *X-AREA* and *X-RED32*. Stoe & Cie, Darmstadt, Germany.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Winpenny, R. E. P. (1998). *Chem. Soc. Rev.* **27**, 447–452.
Wu, T., Wang, T., Sun, L., Deng, K., Deng, W. & Lu, R. (2017). *ChemistrySelect* **2**, 4533–4537.
Yang, X., Jones, R. A. & Huang, S. (2014). *Coord. Chem. Rev.* **273–274**, 63–75.
Yao, M.-X., Zheng, Q., Gao, F., Li, Y.-Z., Song, Y. & Zuo, J.-L. (2012). *Dalton Trans.* **41**, 13682–13690.
Zhao, L., Xue, S. & Tang, J. (2012). *Inorg. Chem.* **51**, 5994–5996.

supporting information

Acta Cryst. (2019). E**75**, 175-178 [https://doi.org/10.1107/S2056989019000094]

An unsymmetrical dinuclear scandium complex comprising salophen ligands [H_2salophen = *N*,*N′*-bis(salicylidene)-1,2-phenylenediamine]

Volker Lorenz, Phil Liebing, Liane Hilfert, Sabine Busse and Frank T. Edelmann

Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-AREA* and *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2010).

(Ethanol-*κO*)bis(nitrato-κ^2O,O'){*μ*-2,2′-[1,2-phenylenebis(nitrilomethanylylidene)]diphenolato-κ^4N,N',O,O':κ^2O,O'}{2,2′-[1,2-phenylenebis(nitrilomethanylylidene)]diphenolato-κ^4O,N,N',O'}discandium

Crystal data

$[Sc_2(C_{20}H_{14}N_2O_2)_2(NO_3)_2(C_2H_6O)]$
M_r = 888.67
Orthorhombic, *Pbca*
a = 13.6092 (3) Å
b = 21.5880 (7) Å
c = 26.5297 (7) Å
V = 7794.3 (4) Å^3
Z = 8
F(000) = 3664
D_x = 1.515 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 25274 reflections
θ = 1.9–25.1°
μ = 0.42 mm^{-1}
T = 153 K
Plate, yellow
0.32 × 0.13 × 0.09 mm

Data collection

STOE IPDS 2T diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 6.67 pixels mm^{-1}
area detector scans
25118 measured reflections
6849 independent reflections
5105 reflections with $I > 2\sigma(I)$
R_{int} = 0.064
θ_{max} = 25.0°, θ_{min} = 1.9°
h = −16→13
k = −25→25
l = −27→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.098
S = 1.04
6849 reflections
555 parameters
1 restraint
Primary atom site location: heavy-atom method
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 1.8222P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Extinction correction: *SHELXL2018/3* (Sheldrick, 2015), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00110 (14)

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}
C1	0.4169 (2)	0.37468 (12)	0.37720 (10)	0.0288 (6)
C2	0.4285 (2)	0.36467 (12)	0.32549 (10)	0.0286 (6)
C3	0.4074 (2)	0.41236 (13)	0.29195 (11)	0.0374 (7)
H1	0.415046	0.405955	0.256739	0.045*
C4	0.3755 (2)	0.46863 (14)	0.30958 (12)	0.0417 (7)
H2	0.359832	0.500726	0.286441	0.050*
C5	0.3661 (3)	0.47893 (13)	0.36070 (12)	0.0440 (8)
H3	0.343986	0.518025	0.372627	0.053*
C6	0.3887 (2)	0.43240 (13)	0.39456 (12)	0.0395 (7)
H4	0.384852	0.440072	0.429763	0.047*
C7	0.3910 (2)	0.31818 (13)	0.45144 (10)	0.0311 (6)
H5	0.354354	0.353106	0.462447	0.037*
C8	0.3950 (2)	0.26510 (13)	0.48419 (10)	0.0305 (6)
C9	0.4137 (2)	0.20494 (13)	0.46694 (10)	0.0293 (6)
C10	0.4117 (2)	0.15587 (14)	0.50090 (10)	0.0362 (7)
H6	0.426733	0.115071	0.489928	0.043*
C11	0.3876 (3)	0.16692 (16)	0.55097 (11)	0.0462 (8)
H7	0.384366	0.133093	0.573820	0.055*
C12	0.3682 (3)	0.22552 (17)	0.56815 (10)	0.0454 (8)
H8	0.352461	0.232186	0.602605	0.054*
C13	0.3718 (2)	0.27431 (15)	0.53541 (10)	0.0384 (7)
H9	0.358442	0.314954	0.547320	0.046*
C14	0.4470 (2)	0.28648 (13)	0.26559 (10)	0.0310 (6)
H10	0.418676	0.315312	0.242784	0.037*
C15	0.4732 (2)	0.22675 (12)	0.24603 (10)	0.0291 (6)
C16	0.4917 (2)	0.17455 (12)	0.27593 (9)	0.0254 (6)
C17	0.5164 (2)	0.11931 (13)	0.25251 (10)	0.0305 (6)
H11	0.531690	0.083924	0.272314	0.037*
C18	0.5190 (2)	0.11538 (13)	0.20037 (11)	0.0351 (7)
H12	0.535121	0.077002	0.184917	0.042*
C19	0.4988 (2)	0.16611 (14)	0.17044 (10)	0.0369 (7)
H13	0.500778	0.162894	0.134746	0.044*
C20	0.4758 (2)	0.22097 (13)	0.19312 (10)	0.0348 (7)
H14	0.461175	0.256021	0.172809	0.042*
C21	0.2072 (2)	0.22444 (12)	0.38836 (10)	0.0292 (6)

C22	0.2308 (2)	0.22964 (12)	0.33720 (10)	0.0278 (6)
C23	0.2145 (2)	0.28503 (13)	0.31215 (11)	0.0347 (6)
H15	0.229900	0.288685	0.277355	0.042*
C24	0.1756 (2)	0.33495 (14)	0.33805 (12)	0.0414 (7)
H16	0.165563	0.373207	0.321119	0.050*
C25	0.1513 (2)	0.32942 (15)	0.38855 (12)	0.0439 (8)
H17	0.123577	0.363688	0.405934	0.053*
C26	0.1671 (2)	0.27442 (13)	0.41373 (11)	0.0368 (7)
H18	0.150594	0.270862	0.448400	0.044*
C27	0.1757 (2)	0.14652 (14)	0.44698 (10)	0.0347 (7)
H19	0.123756	0.172725	0.457844	0.042*
C28	0.1883 (2)	0.08875 (14)	0.47336 (10)	0.0358 (7)
C29	0.2627 (2)	0.04610 (13)	0.45997 (10)	0.0318 (6)
C30	0.2688 (2)	−0.00922 (13)	0.48758 (10)	0.0371 (7)
H20	0.318190	−0.038658	0.479358	0.044*
C31	0.2046 (3)	−0.02153 (15)	0.52636 (11)	0.0448 (8)
H21	0.210072	−0.059403	0.544379	0.054*
C32	0.1325 (3)	0.02028 (18)	0.53944 (12)	0.0558 (9)
H22	0.088460	0.011353	0.566272	0.067*
C33	0.1248 (3)	0.07493 (17)	0.51331 (12)	0.0503 (9)
H23	0.075452	0.103930	0.522519	0.060*
C34	0.2507 (2)	0.16197 (13)	0.26938 (10)	0.0302 (6)
H24	0.213717	0.191577	0.250913	0.036*
C35	0.2793 (2)	0.10654 (12)	0.24355 (10)	0.0299 (6)
C36	0.3223 (2)	0.05556 (12)	0.26821 (10)	0.0300 (6)
C37	0.3414 (2)	0.00209 (13)	0.24052 (11)	0.0375 (7)
H25	0.368266	−0.033093	0.257046	0.045*
C38	0.3221 (3)	−0.00068 (15)	0.18940 (11)	0.0453 (8)
H26	0.337343	−0.037128	0.170926	0.054*
C39	0.2804 (3)	0.04985 (16)	0.16510 (11)	0.0466 (8)
H27	0.266941	0.047973	0.129993	0.056*
C40	0.2586 (2)	0.10217 (15)	0.19168 (10)	0.0400 (7)
H28	0.229035	0.136271	0.174894	0.048*
C41	0.5291 (3)	0.00620 (14)	0.39612 (13)	0.0490 (8)
H31	0.474832	−0.011480	0.416354	0.059*
H30	0.590119	0.003390	0.416346	0.059*
C42	0.5411 (3)	−0.03072 (16)	0.34884 (16)	0.0658 (12)
H32	0.552749	−0.074255	0.357452	0.079*
H34	0.597145	−0.014731	0.329630	0.079*
H33	0.481301	−0.027384	0.328455	0.079*
N1	0.43390 (17)	0.32154 (10)	0.40802 (8)	0.0285 (5)
N2	0.45891 (17)	0.30419 (9)	0.31149 (8)	0.0267 (5)
N3	0.22859 (17)	0.16566 (10)	0.41003 (8)	0.0291 (5)
N4	0.27121 (16)	0.17499 (10)	0.31579 (8)	0.0266 (5)
N5	0.64150 (17)	0.19007 (10)	0.44454 (8)	0.0306 (5)
N6	0.68564 (18)	0.30939 (11)	0.33592 (8)	0.0318 (5)
O1	0.43324 (14)	0.19366 (8)	0.41759 (6)	0.0270 (4)
O2	0.48202 (14)	0.17742 (8)	0.32666 (6)	0.0258 (4)

O3	0.32397 (15)	0.05685 (8)	0.42285 (7)	0.0329 (4)
O4	0.34377 (15)	0.05783 (8)	0.31673 (7)	0.0311 (4)
O5	0.61104 (15)	0.24485 (8)	0.45084 (7)	0.0337 (4)
O6	0.63584 (15)	0.16986 (9)	0.39927 (6)	0.0326 (4)
O7	0.67244 (17)	0.15794 (10)	0.47845 (7)	0.0424 (5)
O8	0.63219 (15)	0.33161 (8)	0.37050 (7)	0.0346 (4)
O9	0.66019 (15)	0.25579 (9)	0.32055 (7)	0.0348 (5)
O10	0.75629 (17)	0.33665 (10)	0.31869 (9)	0.0485 (6)
O11	0.50835 (16)	0.07027 (9)	0.38540 (8)	0.0379 (5)
H29	0.5584 (18)	0.0918 (14)	0.3877 (13)	0.046*
Sc1	0.53071 (4)	0.24711 (2)	0.37359 (2)	0.02440 (13)
Sc2	0.36511 (4)	0.11983 (2)	0.37139 (2)	0.02536 (13)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0250 (15)	0.0306 (13)	0.0307 (14)	0.0029 (11)	0.0024 (11)	0.0012 (11)
C2	0.0274 (15)	0.0263 (13)	0.0320 (15)	0.0003 (11)	−0.0023 (12)	0.0002 (11)
C3	0.0428 (19)	0.0350 (15)	0.0345 (15)	−0.0001 (13)	−0.0032 (13)	0.0028 (12)
C4	0.045 (2)	0.0323 (15)	0.0482 (18)	0.0057 (14)	−0.0044 (15)	0.0063 (13)
C5	0.048 (2)	0.0310 (15)	0.054 (2)	0.0089 (14)	0.0088 (16)	0.0004 (13)
C6	0.0418 (19)	0.0371 (16)	0.0396 (16)	0.0052 (14)	0.0095 (14)	−0.0028 (13)
C7	0.0298 (16)	0.0362 (15)	0.0272 (14)	−0.0008 (12)	0.0019 (11)	−0.0057 (11)
C8	0.0276 (15)	0.0431 (16)	0.0209 (13)	−0.0002 (12)	0.0021 (11)	−0.0012 (11)
C9	0.0239 (15)	0.0417 (15)	0.0222 (13)	−0.0042 (12)	−0.0010 (11)	0.0007 (11)
C10	0.0417 (18)	0.0431 (16)	0.0238 (14)	−0.0059 (14)	−0.0053 (12)	0.0049 (12)
C11	0.051 (2)	0.060 (2)	0.0274 (15)	−0.0099 (17)	−0.0071 (14)	0.0116 (14)
C12	0.044 (2)	0.074 (2)	0.0184 (14)	−0.0079 (17)	−0.0006 (13)	0.0010 (14)
C13	0.0328 (17)	0.0550 (18)	0.0273 (14)	0.0013 (14)	0.0007 (13)	−0.0050 (13)
C14	0.0321 (17)	0.0355 (15)	0.0254 (14)	−0.0013 (12)	−0.0019 (12)	0.0051 (11)
C15	0.0291 (15)	0.0360 (14)	0.0220 (13)	−0.0022 (12)	−0.0014 (11)	−0.0017 (11)
C16	0.0219 (14)	0.0339 (14)	0.0204 (12)	−0.0026 (11)	0.0012 (10)	−0.0022 (10)
C17	0.0294 (16)	0.0335 (14)	0.0287 (14)	0.0018 (12)	0.0000 (12)	−0.0017 (11)
C18	0.0356 (17)	0.0401 (15)	0.0294 (15)	0.0012 (13)	0.0057 (13)	−0.0074 (12)
C19	0.0436 (19)	0.0505 (17)	0.0165 (13)	−0.0041 (14)	0.0035 (12)	−0.0044 (12)
C20	0.0418 (18)	0.0396 (15)	0.0230 (14)	−0.0052 (14)	−0.0024 (12)	0.0022 (12)
C21	0.0272 (15)	0.0340 (14)	0.0265 (13)	0.0028 (12)	−0.0053 (11)	−0.0017 (11)
C22	0.0225 (14)	0.0316 (14)	0.0292 (14)	−0.0002 (11)	−0.0025 (11)	−0.0013 (11)
C23	0.0320 (16)	0.0375 (15)	0.0345 (15)	−0.0009 (13)	−0.0021 (13)	0.0064 (12)
C24	0.0364 (18)	0.0344 (16)	0.0536 (19)	0.0055 (14)	−0.0031 (15)	0.0023 (14)
C25	0.041 (2)	0.0436 (17)	0.0474 (18)	0.0086 (15)	−0.0021 (15)	−0.0104 (14)
C26	0.0377 (18)	0.0438 (16)	0.0289 (14)	0.0060 (14)	−0.0027 (13)	−0.0073 (12)
C27	0.0330 (17)	0.0464 (16)	0.0247 (14)	0.0037 (13)	0.0002 (12)	−0.0007 (12)
C28	0.0364 (18)	0.0461 (16)	0.0249 (14)	−0.0017 (14)	0.0008 (12)	0.0031 (12)
C29	0.0363 (17)	0.0399 (15)	0.0194 (12)	−0.0061 (13)	−0.0051 (12)	−0.0013 (11)
C30	0.049 (2)	0.0366 (15)	0.0257 (14)	−0.0030 (14)	−0.0060 (13)	0.0014 (12)
C31	0.056 (2)	0.0489 (18)	0.0290 (16)	−0.0093 (17)	−0.0032 (15)	0.0075 (13)
C32	0.056 (2)	0.076 (2)	0.0347 (17)	−0.003 (2)	0.0145 (17)	0.0181 (16)

C33	0.046 (2)	0.071 (2)	0.0337 (17)	0.0087 (18)	0.0116 (15)	0.0118 (16)
C34	0.0252 (15)	0.0388 (15)	0.0264 (14)	−0.0005 (12)	−0.0041 (11)	0.0041 (11)
C35	0.0274 (15)	0.0403 (15)	0.0220 (13)	−0.0012 (12)	−0.0025 (11)	−0.0004 (11)
C36	0.0339 (16)	0.0360 (15)	0.0202 (13)	−0.0057 (12)	−0.0014 (11)	−0.0005 (11)
C37	0.047 (2)	0.0350 (15)	0.0306 (15)	−0.0037 (14)	0.0006 (13)	−0.0029 (12)
C38	0.058 (2)	0.0470 (18)	0.0312 (16)	−0.0045 (16)	0.0019 (15)	−0.0129 (14)
C39	0.053 (2)	0.062 (2)	0.0243 (15)	0.0008 (17)	−0.0046 (14)	−0.0096 (14)
C40	0.0403 (19)	0.0549 (18)	0.0248 (14)	0.0022 (15)	−0.0063 (13)	−0.0018 (13)
C41	0.047 (2)	0.0432 (17)	0.057 (2)	0.0106 (16)	0.0011 (17)	0.0158 (16)
C42	0.085 (3)	0.0386 (19)	0.074 (3)	0.0079 (19)	−0.026 (2)	−0.0036 (18)
N1	0.0287 (13)	0.0332 (12)	0.0237 (11)	0.0005 (10)	0.0010 (9)	−0.0003 (9)
N2	0.0301 (13)	0.0277 (11)	0.0223 (11)	0.0005 (10)	−0.0004 (9)	−0.0009 (9)
N3	0.0296 (13)	0.0379 (12)	0.0197 (11)	−0.0004 (10)	−0.0032 (10)	−0.0008 (9)
N4	0.0245 (12)	0.0326 (11)	0.0227 (11)	0.0000 (10)	−0.0007 (9)	0.0003 (9)
N5	0.0277 (13)	0.0382 (13)	0.0258 (12)	0.0006 (11)	−0.0012 (10)	−0.0020 (10)
N6	0.0302 (14)	0.0364 (13)	0.0288 (12)	0.0012 (11)	0.0008 (10)	0.0029 (10)
O1	0.0303 (10)	0.0331 (10)	0.0175 (8)	−0.0032 (8)	0.0000 (7)	−0.0019 (7)
O2	0.0297 (11)	0.0306 (9)	0.0172 (8)	−0.0004 (8)	−0.0009 (7)	0.0004 (7)
O3	0.0383 (12)	0.0361 (10)	0.0241 (9)	0.0006 (9)	0.0052 (9)	0.0038 (8)
O4	0.0381 (12)	0.0320 (10)	0.0232 (9)	−0.0017 (8)	−0.0046 (8)	0.0004 (7)
O5	0.0335 (11)	0.0336 (10)	0.0342 (10)	0.0013 (9)	−0.0062 (9)	−0.0044 (8)
O6	0.0329 (11)	0.0433 (11)	0.0217 (9)	0.0056 (9)	−0.0023 (8)	−0.0028 (8)
O7	0.0509 (14)	0.0479 (12)	0.0283 (10)	0.0061 (10)	−0.0109 (10)	0.0092 (9)
O8	0.0333 (11)	0.0379 (10)	0.0327 (10)	−0.0032 (9)	0.0057 (9)	−0.0067 (9)
O9	0.0372 (12)	0.0314 (10)	0.0358 (11)	0.0003 (9)	0.0089 (9)	−0.0044 (8)
O10	0.0415 (14)	0.0516 (13)	0.0524 (13)	−0.0117 (11)	0.0150 (11)	0.0058 (10)
O11	0.0334 (12)	0.0318 (10)	0.0486 (12)	0.0013 (9)	−0.0052 (10)	0.0062 (9)
Sc1	0.0253 (3)	0.0282 (2)	0.0197 (2)	0.0010 (2)	−0.0002 (2)	−0.0008 (2)
Sc2	0.0274 (3)	0.0291 (2)	0.0197 (2)	0.0004 (2)	−0.0019 (2)	0.0002 (2)

Geometric parameters (Å, º)

C1—C6	1.383 (4)	C28—C29	1.414 (4)
C1—C2	1.398 (4)	C29—O3	1.311 (3)
C1—N1	1.428 (3)	C29—C30	1.404 (4)
C2—C3	1.391 (4)	C30—C31	1.376 (4)
C2—N2	1.419 (3)	C30—H20	0.9500
C3—C4	1.372 (4)	C31—C32	1.378 (5)
C3—H1	0.9500	C31—H21	0.9500
C4—C5	1.380 (4)	C32—C33	1.372 (5)
C4—H2	0.9500	C32—H22	0.9500
C5—C6	1.382 (4)	C33—H23	0.9500
C5—H3	0.9500	C34—N4	1.293 (3)
C6—H4	0.9500	C34—C35	1.433 (4)
C7—N1	1.293 (3)	C34—H24	0.9500
C7—C8	1.439 (4)	C35—C40	1.408 (4)
C7—H5	0.9500	C35—C36	1.408 (4)
C8—C9	1.400 (4)	C36—O4	1.321 (3)

C8—C13	1.409 (4)	C36—C37	1.393 (4)
C9—O1	1.358 (3)	C37—C38	1.383 (4)
C9—C10	1.391 (4)	C37—H25	0.9500
C10—C11	1.389 (4)	C38—C39	1.389 (5)
C10—H6	0.9500	C38—H26	0.9500
C11—C12	1.370 (5)	C39—C40	1.364 (4)
C11—H7	0.9500	C39—H27	0.9500
C12—C13	1.366 (4)	C40—H28	0.9500
C12—H8	0.9500	C41—O11	1.440 (3)
C13—H9	0.9500	C41—C42	1.495 (5)
C14—N2	1.287 (3)	C41—H31	0.9900
C14—C15	1.435 (4)	C41—H30	0.9900
C14—H10	0.9500	C42—H32	0.9800
C15—C16	1.401 (4)	C42—H34	0.9800
C15—C20	1.410 (4)	C42—H33	0.9800
C16—O2	1.354 (3)	N1—Sc1	2.270 (2)
C16—C17	1.386 (4)	N2—Sc1	2.278 (2)
C17—C18	1.386 (4)	N3—Sc2	2.341 (2)
C17—H11	0.9500	N4—Sc2	2.286 (2)
C18—C19	1.380 (4)	N5—O7	1.212 (3)
C18—H12	0.9500	N5—O5	1.264 (3)
C19—C20	1.365 (4)	N5—O6	1.280 (3)
C19—H13	0.9500	N5—Sc1	2.708 (2)
C20—H14	0.9500	N6—O10	1.216 (3)
C21—C26	1.384 (4)	N6—O8	1.265 (3)
C21—C22	1.399 (4)	N6—O9	1.275 (3)
C21—N3	1.423 (3)	N6—Sc1	2.693 (2)
C22—C23	1.386 (4)	O1—Sc1	2.1103 (18)
C22—N4	1.420 (3)	O1—Sc2	2.2139 (18)
C23—C24	1.383 (4)	O2—Sc1	2.0622 (18)
C23—H15	0.9500	O2—Sc2	2.3420 (18)
C24—C25	1.385 (5)	O3—Sc2	2.0065 (18)
C24—H16	0.9500	O4—Sc2	1.9949 (18)
C25—C26	1.379 (4)	O5—Sc1	2.3233 (19)
C25—H17	0.9500	O6—Sc1	2.300 (2)
C26—H18	0.9500	O8—Sc1	2.289 (2)
C27—N3	1.285 (4)	O9—Sc1	2.263 (2)
C27—C28	1.440 (4)	O11—Sc2	2.255 (2)
C27—H19	0.9500	O11—H29	0.827 (18)
C28—C33	1.400 (4)	Sc1—Sc2	3.5541 (7)

C6—C1—C2	119.8 (3)	C41—C42—H34	109.5
C6—C1—N1	125.3 (2)	H32—C42—H34	109.5
C2—C1—N1	114.8 (2)	C41—C42—H33	109.5
C3—C2—C1	119.3 (2)	H32—C42—H33	109.5
C3—C2—N2	125.0 (2)	H34—C42—H33	109.5
C1—C2—N2	115.6 (2)	C7—N1—C1	118.8 (2)
C4—C3—C2	120.2 (3)	C7—N1—Sc1	125.50 (19)

C4—C3—H1	119.9	C1—N1—Sc1	115.62 (16)
C2—C3—H1	119.9	C14—N2—C2	119.0 (2)
C3—C4—C5	120.5 (3)	C14—N2—Sc1	125.29 (18)
C3—C4—H2	119.8	C2—N2—Sc1	115.69 (16)
C5—C4—H2	119.8	C27—N3—C21	118.7 (2)
C4—C5—C6	120.0 (3)	C27—N3—Sc2	130.0 (2)
C4—C5—H3	120.0	C21—N3—Sc2	111.25 (17)
C6—C5—H3	120.0	C34—N4—C22	118.6 (2)
C5—C6—C1	120.0 (3)	C34—N4—Sc2	128.43 (19)
C5—C6—H4	120.0	C22—N4—Sc2	113.00 (15)
C1—C6—H4	120.0	O7—N5—O5	123.5 (2)
N1—C7—C8	124.4 (3)	O7—N5—O6	121.5 (2)
N1—C7—H5	117.8	O5—N5—O6	115.0 (2)
C8—C7—H5	117.8	O7—N5—Sc1	165.9 (2)
C9—C8—C13	119.1 (3)	O5—N5—Sc1	58.94 (12)
C9—C8—C7	123.2 (2)	O6—N5—Sc1	57.95 (12)
C13—C8—C7	117.5 (3)	O10—N6—O8	122.9 (2)
O1—C9—C10	119.5 (2)	O10—N6—O9	122.2 (2)
O1—C9—C8	121.1 (2)	O8—N6—O9	114.8 (2)
C10—C9—C8	119.4 (2)	O10—N6—Sc1	179.0 (2)
C11—C10—C9	119.6 (3)	O8—N6—Sc1	58.00 (13)
C11—C10—H6	120.2	O9—N6—Sc1	56.83 (12)
C9—C10—H6	120.2	C9—O1—Sc1	123.94 (16)
C12—C11—C10	121.5 (3)	C9—O1—Sc2	125.50 (16)
C12—C11—H7	119.3	Sc1—O1—Sc2	110.53 (7)
C10—C11—H7	119.3	C16—O2—Sc1	127.04 (16)
C13—C12—C11	119.6 (3)	C16—O2—Sc2	123.06 (15)
C13—C12—H8	120.2	Sc1—O2—Sc2	107.44 (7)
C11—C12—H8	120.2	C29—O3—Sc2	143.93 (18)
C12—C13—C8	120.8 (3)	C36—O4—Sc2	139.96 (17)
C12—C13—H9	119.6	N5—O5—Sc1	93.28 (14)
C8—C13—H9	119.6	N5—O6—Sc1	93.91 (14)
N2—C14—C15	125.3 (3)	N6—O8—Sc1	94.06 (15)
N2—C14—H10	117.3	N6—O9—Sc1	95.04 (14)
C15—C14—H10	117.3	C41—O11—Sc2	131.2 (2)
C16—C15—C20	119.2 (2)	C41—O11—H29	111 (2)
C16—C15—C14	124.2 (2)	Sc2—O11—H29	117 (2)
C20—C15—C14	116.5 (2)	O2—Sc1—O1	74.52 (7)
O2—C16—C17	120.6 (2)	O2—Sc1—O9	86.29 (7)
O2—C16—C15	120.6 (2)	O1—Sc1—O9	151.49 (7)
C17—C16—C15	118.8 (2)	O2—Sc1—N1	124.95 (8)
C16—C17—C18	120.4 (3)	O1—Sc1—N1	78.44 (8)
C16—C17—H11	119.8	O9—Sc1—N1	130.06 (8)
C18—C17—H11	119.8	O2—Sc1—N2	79.64 (7)
C19—C18—C17	121.4 (3)	O1—Sc1—N2	115.23 (8)
C19—C18—H12	119.3	O9—Sc1—N2	80.76 (8)
C17—C18—H12	119.3	N1—Sc1—N2	70.06 (8)
C20—C19—C18	118.7 (3)	O2—Sc1—O8	138.89 (7)

C20—C19—H13	120.6	O1—Sc1—O8	146.58 (7)
C18—C19—H13	120.6	O9—Sc1—O8	56.08 (7)
C19—C20—C15	121.4 (3)	N1—Sc1—O8	78.49 (8)
C19—C20—H14	119.3	N2—Sc1—O8	78.57 (8)
C15—C20—H14	119.3	O2—Sc1—O6	81.36 (7)
C26—C21—C22	120.0 (3)	O1—Sc1—O6	80.26 (7)
C26—C21—N3	125.4 (2)	O9—Sc1—O6	76.10 (7)
C22—C21—N3	114.6 (2)	N1—Sc1—O6	139.03 (7)
C23—C22—C21	119.8 (3)	N2—Sc1—O6	150.84 (7)
C23—C22—N4	125.9 (2)	O8—Sc1—O6	102.30 (7)
C21—C22—N4	114.2 (2)	O2—Sc1—O5	131.95 (7)
C24—C23—C22	119.7 (3)	O1—Sc1—O5	78.25 (7)
C24—C23—H15	120.1	O9—Sc1—O5	100.59 (8)
C22—C23—H15	120.1	N1—Sc1—O5	86.16 (7)
C23—C24—C25	120.3 (3)	N2—Sc1—O5	148.35 (7)
C23—C24—H16	119.9	O8—Sc1—O5	76.38 (7)
C25—C24—H16	119.9	O6—Sc1—O5	55.31 (6)
C26—C25—C24	120.4 (3)	O2—Sc1—N6	113.07 (7)
C26—C25—H17	119.8	O1—Sc1—N6	166.03 (7)
C24—C25—H17	119.8	O9—Sc1—N6	28.14 (7)
C25—C26—C21	119.8 (3)	N1—Sc1—N6	104.50 (8)
C25—C26—H18	120.1	N2—Sc1—N6	78.31 (8)
C21—C26—H18	120.1	O8—Sc1—N6	27.94 (7)
N3—C27—C28	125.6 (3)	O6—Sc1—N6	89.13 (7)
N3—C27—H19	117.2	O5—Sc1—N6	88.25 (7)
C28—C27—H19	117.2	O2—Sc1—N5	105.47 (7)
C33—C28—C29	119.6 (3)	O1—Sc1—N5	73.55 (7)
C33—C28—C27	118.6 (3)	O9—Sc1—N5	92.08 (7)
C29—C28—C27	121.8 (3)	N1—Sc1—N5	111.43 (7)
O3—C29—C30	120.3 (3)	N2—Sc1—N5	171.01 (8)
O3—C29—C28	121.9 (2)	O8—Sc1—N5	92.95 (7)
C30—C29—C28	117.8 (3)	O6—Sc1—N5	28.14 (6)
C31—C30—C29	121.1 (3)	O5—Sc1—N5	27.78 (6)
C31—C30—H20	119.4	N6—Sc1—N5	92.81 (7)
C29—C30—H20	119.4	O2—Sc1—Sc2	38.95 (5)
C30—C31—C32	121.0 (3)	O1—Sc1—Sc2	35.69 (5)
C30—C31—H21	119.5	O9—Sc1—Sc2	123.21 (5)
C32—C31—H21	119.5	N1—Sc1—Sc2	100.71 (6)
C33—C32—C31	119.3 (3)	N2—Sc1—Sc2	97.72 (6)
C33—C32—H22	120.3	O8—Sc1—Sc2	176.27 (6)
C31—C32—H22	120.3	O6—Sc1—Sc2	80.73 (5)
C32—C33—C28	121.3 (3)	O5—Sc1—Sc2	107.26 (5)
C32—C33—H23	119.4	N6—Sc1—Sc2	151.21 (5)
C28—C33—H23	119.4	N5—Sc1—Sc2	90.74 (5)
N4—C34—C35	125.3 (3)	O4—Sc2—O3	89.96 (8)
N4—C34—H24	117.3	O4—Sc2—O1	161.16 (8)
C35—C34—H24	117.3	O3—Sc2—O1	103.19 (7)
C40—C35—C36	119.0 (3)	O4—Sc2—O11	85.82 (8)

C40—C35—C34	118.0 (3)	O3—Sc2—O11	78.90 (8)
C36—C35—C34	122.9 (2)	O1—Sc2—O11	83.59 (7)
O4—C36—C37	120.2 (3)	O4—Sc2—N4	78.40 (8)
O4—C36—C35	121.1 (2)	O3—Sc2—N4	129.49 (8)
C37—C36—C35	118.7 (2)	O1—Sc2—N4	102.50 (7)
C38—C37—C36	121.2 (3)	O11—Sc2—N4	146.80 (8)
C38—C37—H25	119.4	O4—Sc2—N3	119.10 (8)
C36—C37—H25	119.4	O3—Sc2—N3	76.53 (8)
C37—C38—C39	120.0 (3)	O1—Sc2—N3	77.63 (7)
C37—C38—H26	120.0	O11—Sc2—N3	144.55 (8)
C39—C38—H26	120.0	N4—Sc2—N3	67.60 (8)
C40—C39—C38	119.9 (3)	O4—Sc2—O2	94.97 (7)
C40—C39—H27	120.0	O3—Sc2—O2	153.38 (8)
C38—C39—H27	120.0	O1—Sc2—O2	67.28 (6)
C39—C40—C35	121.2 (3)	O11—Sc2—O2	75.40 (7)
C39—C40—H28	119.4	N4—Sc2—O2	77.07 (7)
C35—C40—H28	119.4	N3—Sc2—O2	122.46 (7)
O11—C41—C42	111.6 (3)	O4—Sc2—Sc1	128.53 (6)
O11—C41—H31	109.3	O3—Sc2—Sc1	133.60 (6)
C42—C41—H31	109.3	O1—Sc2—Sc1	33.78 (5)
O11—C41—H30	109.3	O11—Sc2—Sc1	79.39 (5)
C42—C41—H30	109.3	N4—Sc2—Sc1	87.84 (6)
H31—C41—H30	108.0	N3—Sc2—Sc1	99.75 (6)
C41—C42—H32	109.5	O2—Sc2—Sc1	33.61 (4)

C6—C1—C2—C3	−2.7 (4)	C27—C28—C33—C32	179.2 (3)
N1—C1—C2—C3	175.8 (3)	N4—C34—C35—C40	−174.3 (3)
C6—C1—C2—N2	179.2 (3)	N4—C34—C35—C36	8.9 (5)
N1—C1—C2—N2	−2.3 (4)	C40—C35—C36—O4	179.4 (3)
C1—C2—C3—C4	0.0 (5)	C34—C35—C36—O4	−3.9 (4)
N2—C2—C3—C4	177.9 (3)	C40—C35—C36—C37	−1.0 (4)
C2—C3—C4—C5	1.4 (5)	C34—C35—C36—C37	175.7 (3)
C3—C4—C5—C6	0.0 (5)	O4—C36—C37—C38	−178.2 (3)
C4—C5—C6—C1	−2.7 (5)	C35—C36—C37—C38	2.2 (5)
C2—C1—C6—C5	4.1 (5)	C36—C37—C38—C39	−1.8 (5)
N1—C1—C6—C5	−174.3 (3)	C37—C38—C39—C40	0.1 (5)
N1—C7—C8—C9	−23.9 (5)	C38—C39—C40—C35	1.1 (5)
N1—C7—C8—C13	160.8 (3)	C36—C35—C40—C39	−0.6 (5)
C13—C8—C9—O1	177.9 (3)	C34—C35—C40—C39	−177.5 (3)
C7—C8—C9—O1	2.7 (4)	C8—C7—N1—C1	174.4 (3)
C13—C8—C9—C10	−1.8 (4)	C8—C7—N1—Sc1	−2.5 (4)
C7—C8—C9—C10	−177.0 (3)	C6—C1—N1—C7	24.5 (4)
O1—C9—C10—C11	−177.2 (3)	C2—C1—N1—C7	−153.9 (3)
C8—C9—C10—C11	2.4 (4)	C6—C1—N1—Sc1	−158.2 (2)
C9—C10—C11—C12	−1.9 (5)	C2—C1—N1—Sc1	23.3 (3)
C10—C11—C12—C13	0.6 (5)	C15—C14—N2—C2	−179.4 (3)
C11—C12—C13—C8	0.1 (5)	C15—C14—N2—Sc1	2.8 (4)
C9—C8—C13—C12	0.6 (5)	C3—C2—N2—C14	−15.7 (4)

C7—C8—C13—C12	176.0 (3)	C1—C2—N2—C14	162.3 (3)
N2—C14—C15—C16	17.0 (5)	C3—C2—N2—Sc1	162.3 (2)
N2—C14—C15—C20	−165.8 (3)	C1—C2—N2—Sc1	−19.7 (3)
C20—C15—C16—O2	−174.7 (3)	C28—C27—N3—C21	−179.3 (3)
C14—C15—C16—O2	2.5 (4)	C28—C27—N3—Sc2	−1.6 (4)
C20—C15—C16—C17	2.9 (4)	C26—C21—N3—C27	30.0 (4)
C14—C15—C16—C17	−179.9 (3)	C22—C21—N3—C27	−150.6 (3)
O2—C16—C17—C18	175.1 (3)	C26—C21—N3—Sc2	−148.1 (2)
C15—C16—C17—C18	−2.4 (4)	C22—C21—N3—Sc2	31.3 (3)
C16—C17—C18—C19	1.0 (5)	C35—C34—N4—C22	−175.0 (3)
C17—C18—C19—C20	0.0 (5)	C35—C34—N4—Sc2	3.9 (4)
C18—C19—C20—C15	0.5 (5)	C23—C22—N4—C34	−34.8 (4)
C16—C15—C20—C19	−2.0 (5)	C21—C22—N4—C34	145.5 (3)
C14—C15—C20—C19	−179.4 (3)	C23—C22—N4—Sc2	146.2 (2)
C26—C21—C22—C23	0.3 (4)	C21—C22—N4—Sc2	−33.6 (3)
N3—C21—C22—C23	−179.2 (3)	C10—C9—O1—Sc1	−135.2 (2)
C26—C21—C22—N4	−179.9 (3)	C8—C9—O1—Sc1	45.2 (3)
N3—C21—C22—N4	0.6 (3)	C10—C9—O1—Sc2	47.0 (3)
C21—C22—C23—C24	0.5 (4)	C8—C9—O1—Sc2	−132.7 (2)
N4—C22—C23—C24	−179.2 (3)	C17—C16—O2—Sc1	138.4 (2)
C22—C23—C24—C25	−1.2 (5)	C15—C16—O2—Sc1	−44.1 (3)
C23—C24—C25—C26	1.1 (5)	C17—C16—O2—Sc2	−61.7 (3)
C24—C25—C26—C21	−0.2 (5)	C15—C16—O2—Sc2	115.8 (2)
C22—C21—C26—C25	−0.5 (4)	C30—C29—O3—Sc2	−176.3 (2)
N3—C21—C26—C25	178.9 (3)	C28—C29—O3—Sc2	4.2 (5)
N3—C27—C28—C33	179.4 (3)	C37—C36—O4—Sc2	161.4 (2)
N3—C27—C28—C29	−0.6 (5)	C35—C36—O4—Sc2	−19.0 (5)
C33—C28—C29—O3	180.0 (3)	O7—N5—O5—Sc1	−163.6 (2)
C27—C28—C29—O3	−0.1 (4)	O6—N5—O5—Sc1	15.2 (2)
C33—C28—C29—C30	0.5 (4)	O7—N5—O6—Sc1	163.5 (2)
C27—C28—C29—C30	−179.5 (3)	O5—N5—O6—Sc1	−15.4 (2)
O3—C29—C30—C31	−179.4 (3)	O10—N6—O8—Sc1	−179.5 (2)
C28—C29—C30—C31	0.0 (4)	O9—N6—O8—Sc1	0.1 (2)
C29—C30—C31—C32	−0.3 (5)	O10—N6—O9—Sc1	179.5 (2)
C30—C31—C32—C33	0.0 (5)	O8—N6—O9—Sc1	−0.1 (2)
C31—C32—C33—C28	0.6 (6)	C42—C41—O11—Sc2	87.3 (4)
C29—C28—C33—C32	−0.9 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O11—H29···O6	0.83 (2)	2.01 (2)	2.787 (3)	156 (3)