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Synthesis and structure of 9-(dimethylamino)-1,10-phenanthrolin-1-ium nitrate

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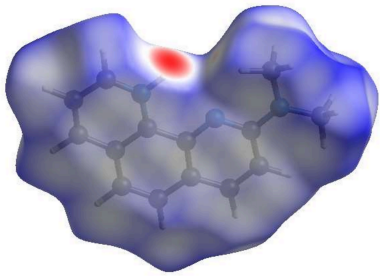
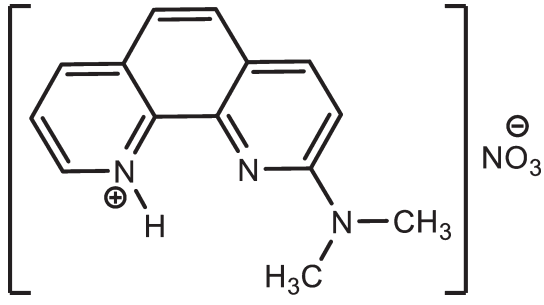
In the title salt, $C_{14}H_{14}N_3^+\cdot NO_3^-$, the cation is almost planar (r.m.s. deviation = 0.015 Å), implying significant conjugation of the lone pair of the tertiary amino group N atom with the aromatic ring system. In the extended structure, N—H···O and C—H···O hydrogen bonds link the components into infinite chains of alternating cations and anions propagating along the *b*-axis direction. Aromatic π–π stacking interactions with centroid–centroid distances of 3.5773 (12) and 3.5889 (12) Å may help to consolidate the packing. Hirshfeld surface analysis revealed that the most important contributions for the crystal packing are from H···H (39.2%), H···O/O···H (31.6%), H···C/C···H (10.3%) and C···C (9.1%) interactions.

1. Chemical context

1,10-Phenanthroline and its derivatives are widely used in medicinal, catalysis, materials and coordination chemistry (*e.g.*, Queffelec *et al.*, 2024; Krawiec *et al.*, 2005; Kumar *et al.*, 2022). Polyaromatic rings in this class of organic compounds possess rigidity and robustness, which may be significant in the design of functional materials such as catalysts, luminescent coordination scaffolds, supramolecular aggregates, sensors and theranostics. 1,10-Phenanthroline derivatives are popular ligands in coordination chemistry due to their strong affinities for a wide range of metals with various oxidation states (Naithani *et al.*, 2023). Substitution of the aromatic ring of 1,10-phenanthroline can be used as an important synthetic strategy towards new materials (Figueiredo *et al.*, 2022; Tsvetkov *et al.*, 2025).





As part of our studies in this area, we now report the synthesis and structure of the title salt, $C_{14}H_{14}N_3^+\cdot NO_3^-$ (**I**).

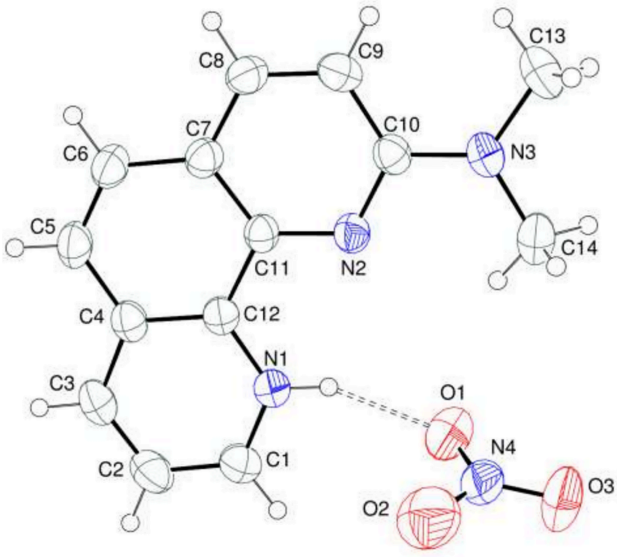


Figure 1
The molecular structure of (**I**) with 50% probability ellipsoids. The N—H···O hydrogen bond is shown as a dashed line.

2. Structural commentary

The asymmetric unit of (**I**), which crystallizes in space group $P2_1/n$, consists of one dimethylaminophenanthroline cation and one nitrate counter ion (Fig. 1). The phenanthroline ring system is almost planar with an r.m.s. deviation of 0.0125 Å. Atoms N3, C13 and C14 are displaced by −0.035 (2), −0.001 (3) and −0.011 (3) Å, respectively, away from the best least-squares plane of the phenanthroline ring system. Evidence of their near co-planarity with the ring system is further supported by the C13—N3—C10—N2 [–178.5 (2)°] and C14—N3—C10—N2 [–2.6 (3)°] torsion angles. The C1—N1—C12 [123.41 (18)°] bond angle at the protonated N1 atom of the ring system is significantly enlarged compared to the unprotonated C10—N2—C11 [117.80 (17)°] bond angle, which is consistent with previous studies, e.g., Hensen *et al.* (2000) and Büyükekşi *et al.* (2019). The N1—C1 [1.322 (3) Å] and N1—C12 [1.353 (2) Å] bond lengths of the protonated N1 atom are similar to the N2—C10 [1.336 (2) Å] and N2—C11 [1.345 (2) Å] bonds of the non-protonated N2 atom. In the pendant dimethylamino group, the N3—C10 [1.357 (3) Å] bond length is significantly shorter than N3—C13 [1.453 (3) Å] and N3—C14 [1.444 (3) Å] bonds, presumably because of resonance-assisted π-conjugation, where the N atom of the dimethylamino group acts as a strong electron donor to the aromatic ring system. On the other hand, the C10—N3—C13 [123.3 (2)°] and C14—N3—C13 [115.69 (19)°] bond angles are significantly enlarged and narrowed according to the bond angle of C10—N3—C14 [120.86 (18)°], respectively. In the nitrate counter-ion, the N4—O3 [1.204 (3) Å] bond is significantly shorter than N4—O1 [1.251 (3) Å] and N4—O2 [1.245 (3) Å], possibly due to hydrogen bonding and crystal packing effects, where O1 acts as hydrogen-bond acceptor interacting with the protonated N1 atom of the phenanthroline ring system. The O2—N4—O1 [117.5 (2)°] bond angle is significantly narrower than O3—N4—O1 [120.6 (3)°] and O3—N4—O2 [121.8 (3)°].

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.86 (1)	2.04 (2)	2.819 (3)	150 (3)
C5—H5···O3^{i}	0.93	2.55	3.407 (3)	154

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

3. Supramolecular features

In the extended structure, the N1—H1···O1 hydrogen bond (Table 1) links the cation to the anion (Fig. 2) and a C5—H5···O3 hydrogen bond (Table 2) links the ion pairs into infinite chains propagating along the *b*-axis direction (Fig. 2). Further, π–π stacking interactions between the *A* (N1/C1–C4/C12) and *B* (N2/C7–C11) rings and also between the *B* and *C* (C4–C12) rings of the phenanthroline ring system with centroid–to–centroid distances of 3.5773 (12) Å [α = 1.34 (10)° and slippage = 1.212 Å] and 3.5889 (12) Å [α = 0.84 (9)° and slippage = 1.198 Å], respectively, help to consolidate the packing. No C—H···π(ring) interactions are observed.

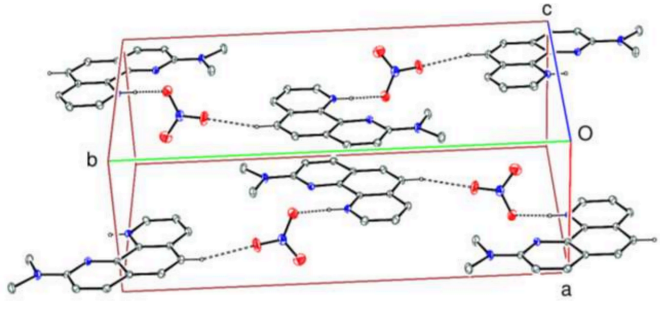


Figure 2
Packing diagram of (**I**) showing N—H···O and C—H···O hydrogen bonds as dashed lines with the infinite chains propagating along the *b*-axis direction.

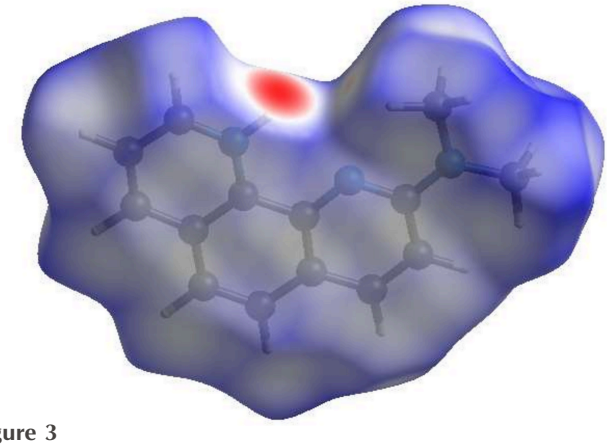


Figure 3
View of the three-dimensional Hirshfeld surface for (**I**) plotted over d_{norm} in the range −0.54 to 1.08 a.u.

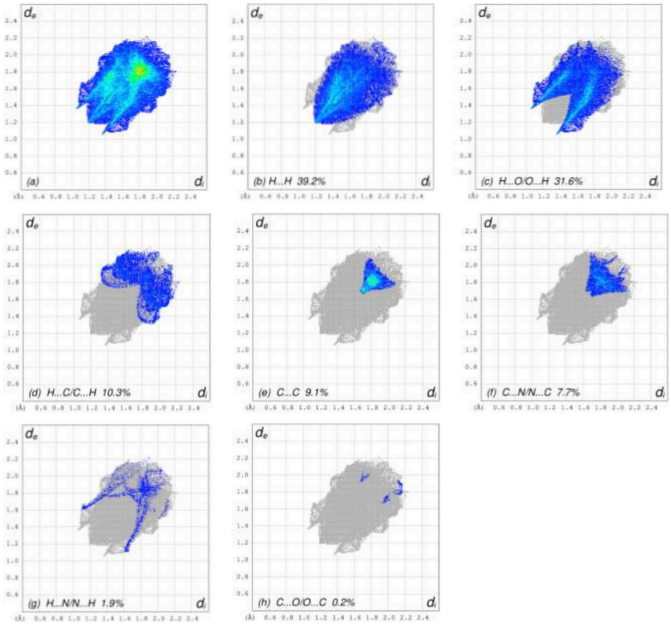


Figure 4
Two-dimensional fingerprint plots for (**I**), showing (*a*) all interactions, and delineated (*b*)–(*f*) into different contact types. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

The intermolecular interactions in the crystal were visualized by carrying out the Hirshfeld surface (HS) analysis using *CrystalExplorer* 17.5 (Spackman *et al.*, 2021). Fig. 3 shows the Hirshfeld surface with the red spots corresponding to the hydrogen-bond donors and acceptors noted above. The overall two-dimensional fingerprint plot is shown in Fig. 4*a* and those delineated into the different contact types are illustrated in Fig. 4 (*b*)–(*h*), respectively. According to the two-dimensional fingerprint plots the H···H, H···O/O···H, H···C/C···H and C···C contacts make the most significant contributions to the HS, at 39.2%, 31.6%, 10.3% and 9.1%, respectively.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.45, updated September 2024; Groom *et al.*, 2016) identified eight compounds with close structural similarity to (**I**). These include: 1,10-phenanthrolin-1-ium-6-sulfonate hydrogen peroxide, $C_{12}H_8N_2O_3S{\cdot}H_2O_2$ (CSD refcode BIPZUZ; Bezzubov *et al.*, 2023), 1,10-phenanthrolin-1-ium chloride, $C_{12}H_9N_2^+{\cdot}Cl^-$ (CUZDIK; Hensen *et al.*, 2000), 2,9-dimethyl-1,10-phenanthrolin-1-ium picrate, $C_6H_2N_3O_7^-{\cdot}C_{14}H_{13}N_2^+$ (CIYPIL; Chan *et al.*, 2014), 6-ethynyl-1,10-phenanthrolin-1-ium trifluoromethanesulfonate, $CF_3O_3S^-{\cdot}C_{14}H_9N_2^+$ (DILPIA; Doistau *et al.*, 2018), 2-amino-1,10-phenanthrolin-1-ium chloride, $C_{12}H_{10}N_3^+{\cdot}Cl^-$ (LUZZAL; Büyükekşi *et al.*, 2019), 9-phenyl-1,10-phenanthrolin-1-ium trifluoromethanesulfonate, $C_{18}H_{13}N_2^+{\cdot}CF_3SO_3^-$ (NIYSUL; Krause *et al.*, 2014), 9-phenyl-1,10-phenanthrolin-1-ium tetrachlorogold(III), $C_{18}H_{13}N_2{\cdot}AuCl_4$ (NIYTAS; Krause *et al.*, 2014) and 1,10-phenanthrolin-1-ium tetrafluoroborate, $C_{12}H_9N_2^+{\cdot}BF_4^-$ (WUJWUX; Ghorai *et al.*, 2024).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{14}N_3^+{\cdot}NO_3^-$
M_r	286.29
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	6.7438 (3), 19.8224 (7), 9.8185 (4)
β (°)	94.762 (3)
V (Å^3)	1307.99 (9)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.88
Crystal size (mm)	0.2 × 0.16 × 0.14
Data collection	
Diffractometer	XtaLAB Synergy, Single source at home/near, HyPix-Bantam
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2026)
T_{min}, T_{max}	0.243, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12223, 2527, 1881
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.059, 0.184, 1.07
No. of reflections	2527
No. of parameters	196
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, −0.20

Computer programs: *CrysAlis PRO* (Rigaku OD, 2026), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

5. Synthesis and crystallization

2-Bromo-1,10-phenanthroline (2.59 g, 10 mmol) and Cs_2CO_3 (3.25 g, 10 mmol) were dissolved in *N*,*N*-dimethylformide (DMF) (75 ml), and the resulting mixture was heated with stirring at 413 K for 6 h (Fig. 5). After completion of the reaction, the solvent was removed under reduced pressure. The residue was washed with ethyl acetate and water. The neutral molecule was isolated from the ethyl acetate fraction after concentration, giving a yield of 60%. An equimolar amount of 1 *M* aqueous HNO_3 was added dropwise, with stirring, to an ethanolic solution and the resulting solution was left to crystallize at room temperature. Colorless crystals of (**I**) were obtained after 6 days. Yield: 65%. Analysis (%) for $C_{14}H_{14}N_4O_3$, calculated (obtained): C 58.74 (58.70), H 4.93 (4.89), N 19.57 (19.52). ^{1}H NMR (400 MHz, DMSO-d_6, ppm): δ 3.19 (6H, NMe_2), 7.57–9.20 (7H). $^{13}C\{^1H\}$ NMR (100 MHz,

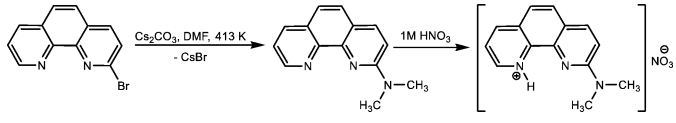


Figure 5
Synthesis of (**I**).

DMSO-d_6, ppm): δ 42.3, 111.7, 122.7, 123.8, 125.5, 126.9, 128.4, 138.2, 143.5, 144.9, 146.1, 150.4, 157.3.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The N-bound H atom was located from a difference-Fourier map and refined isotropically. The C-bound H-atom positions were calculated geometrically at distances of 0.93–0.96 Å and refined using a riding model by applying the constraint $U_{iso}(H) = k \times U_{eq}$ (C), where k = 1.2 for aromatic CH hydrogen atoms and k = 1.5 for methyl hydrogen atoms.

Acknowledgements

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supporting information

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Computing details

9-(Dimethylamino)-1,10-phenanthrolin-1-ium nitrate

Crystal data

$C_{14}H_{14}N_3^+·NO_3^-$
M_r = 286.29
Monoclinic, $P2_1/n$
a = 6.7438 (3) Å
b = 19.8224 (7) Å
c = 9.8185 (4) Å
β = 94.762 (3)°
V = 1307.99 (9) Å^3
Z = 4
$F(000)$ = 600
D_x = 1.454 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 4514 reflections
θ = 4.5–71.4°
μ = 0.88 mm^{-1}
T = 293 K
Block, colorless
0.2 × 0.16 × 0.14 mm

Data collection

XtaLAB Synergy, Single source at home/near, HyPix-Bantam diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2026)
T_{min} = 0.243, T_{max} = 1.000
12223 measured reflections
2527 independent reflections
1881 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 71.6°, θ_{min} = 4.5°
h = −8→8
k = −22→24
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.184
S = 1.07
2527 reflections
196 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1045P)^2 + 0.2504P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.5907 (4)	0.61057 (11)	0.1377 (2)	0.0922 (7)
O2	0.8825 (4)	0.60068 (15)	0.0709 (3)	0.1135 (8)
O3	0.7228 (5)	0.69350 (10)	0.0406 (3)	0.1222 (10)
N4	0.7340 (4)	0.63673 (11)	0.0841 (2)	0.0707 (6)
N1	0.7044 (3)	0.48753 (9)	0.26544 (17)	0.0469 (4)
N2	0.7379 (2)	0.57058 (8)	0.48756 (17)	0.0441 (4)
N3	0.7401 (3)	0.67846 (9)	0.5727 (2)	0.0595 (5)
C1	0.6868 (4)	0.45120 (12)	0.1522 (2)	0.0575 (6)
H1A	0.668242	0.472441	0.067649	0.069*
C2	0.6959 (4)	0.38109 (12)	0.1595 (3)	0.0637 (6)
H2	0.683511	0.355146	0.080373	0.076*
C3	0.7233 (3)	0.35116 (11)	0.2844 (3)	0.0574 (6)
H3	0.729509	0.304362	0.289935	0.069*
C4	0.7424 (3)	0.38943 (10)	0.4051 (2)	0.0469 (5)
C5	0.7720 (3)	0.36087 (11)	0.5380 (3)	0.0556 (6)
H5	0.778823	0.314270	0.548464	0.067*
C6	0.7903 (3)	0.40108 (11)	0.6490 (2)	0.0553 (6)
H6	0.809475	0.381530	0.735149	0.066*
C7	0.7810 (3)	0.47261 (10)	0.6381 (2)	0.0459 (5)
C8	0.8034 (3)	0.51706 (11)	0.7505 (2)	0.0509 (5)
H8	0.826659	0.499836	0.838442	0.061*
C9	0.7912 (3)	0.58476 (11)	0.7312 (2)	0.0518 (5)
H9	0.805535	0.613818	0.805706	0.062*
C10	0.7564 (3)	0.61119 (10)	0.5964 (2)	0.0444 (5)
C11	0.7504 (3)	0.50365 (9)	0.50939 (19)	0.0395 (4)
C12	0.7314 (3)	0.46029 (9)	0.39193 (19)	0.0423 (5)
C13	0.7615 (5)	0.72889 (12)	0.6803 (3)	0.0765 (8)
H13A	0.758735	0.707236	0.767585	0.115*
H13B	0.654123	0.760685	0.668229	0.115*
H13C	0.885878	0.752077	0.676224	0.115*
C14	0.7127 (4)	0.70437 (12)	0.4350 (3)	0.0714 (7)
H14A	0.838078	0.719632	0.406935	0.107*
H14B	0.620567	0.741374	0.431959	0.107*
H14C	0.661062	0.669325	0.374545	0.107*
H1	0.693 (4)	0.5304 (6)	0.254 (3)	0.074 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1127 (17)	0.0782 (13)	0.0871 (14)	0.0041 (12)	0.0165 (13)	0.0218 (11)
O2	0.1078 (18)	0.129 (2)	0.1037 (18)	0.0283 (16)	0.0054 (14)	0.0172 (15)
O3	0.195 (3)	0.0546 (12)	0.1178 (19)	−0.0092 (14)	0.0194 (18)	0.0274 (12)
N4	0.1038 (18)	0.0568 (12)	0.0496 (11)	0.0007 (12)	−0.0039 (11)	0.0033 (9)
N1	0.0551 (10)	0.0411 (9)	0.0444 (9)	0.0024 (8)	0.0039 (7)	−0.0003 (7)
N2	0.0478 (9)	0.0373 (9)	0.0474 (9)	−0.0018 (7)	0.0061 (7)	0.0013 (7)
N3	0.0833 (14)	0.0369 (9)	0.0583 (11)	−0.0038 (9)	0.0051 (9)	−0.0057 (8)
C1	0.0674 (14)	0.0557 (13)	0.0488 (12)	0.0032 (11)	0.0023 (10)	−0.0064 (9)
C2	0.0729 (16)	0.0556 (13)	0.0621 (14)	0.0023 (11)	0.0029 (11)	−0.0181 (11)
C3	0.0615 (14)	0.0402 (11)	0.0711 (15)	0.0010 (9)	0.0082 (11)	−0.0092 (10)
C4	0.0445 (11)	0.0392 (10)	0.0581 (12)	−0.0008 (8)	0.0101 (9)	−0.0009 (9)
C5	0.0624 (13)	0.0371 (10)	0.0684 (14)	0.0015 (9)	0.0120 (11)	0.0092 (10)
C6	0.0651 (14)	0.0461 (11)	0.0553 (12)	0.0026 (10)	0.0094 (10)	0.0135 (10)
C7	0.0466 (11)	0.0448 (11)	0.0472 (11)	0.0005 (8)	0.0099 (8)	0.0060 (8)
C8	0.0570 (12)	0.0553 (12)	0.0408 (10)	0.0021 (10)	0.0074 (8)	0.0055 (9)
C9	0.0561 (13)	0.0545 (12)	0.0454 (11)	−0.0035 (10)	0.0082 (9)	−0.0097 (9)
C10	0.0439 (10)	0.0402 (10)	0.0495 (11)	−0.0039 (8)	0.0068 (8)	−0.0029 (8)
C11	0.0378 (10)	0.0360 (9)	0.0451 (10)	−0.0011 (7)	0.0063 (7)	0.0020 (8)
C12	0.0399 (10)	0.0399 (11)	0.0477 (11)	0.0000 (8)	0.0073 (8)	0.0007 (8)
C13	0.102 (2)	0.0454 (13)	0.0827 (18)	−0.0057 (13)	0.0089 (15)	−0.0187 (12)
C14	0.0960 (19)	0.0424 (12)	0.0753 (16)	0.0012 (12)	0.0042 (14)	0.0082 (11)

Geometric parameters (Å, º)

O1—N4	1.251 (3)	C4—C12	1.412 (3)
O2—N4	1.245 (3)	C5—H5	0.9300
O3—N4	1.204 (3)	C5—C6	1.347 (3)
N1—C1	1.322 (3)	C6—H6	0.9300
N1—C12	1.353 (2)	C6—C7	1.423 (3)
N1—H1	0.861 (10)	C7—C8	1.410 (3)
N2—C10	1.336 (2)	C7—C11	1.405 (3)
N2—C11	1.345 (2)	C8—H8	0.9300
N3—C10	1.357 (3)	C8—C9	1.357 (3)
N3—C13	1.453 (3)	C9—H9	0.9300
N3—C14	1.444 (3)	C9—C10	1.424 (3)
C1—H1A	0.9300	C11—C12	1.435 (3)
C1—C2	1.393 (3)	C13—H13A	0.9600
C2—H2	0.9300	C13—H13B	0.9600
C2—C3	1.361 (4)	C13—H13C	0.9600
C3—H3	0.9300	C14—H14A	0.9600
C3—C4	1.404 (3)	C14—H14B	0.9600
C4—C5	1.421 (3)	C14—H14C	0.9600
O2—N4—O1	117.5 (2)	C11—C7—C6	120.40 (19)
O3—N4—O1	120.6 (3)	C11—C7—C8	115.35 (18)

O3—N4—O2	121.8 (3)	C7—C8—H8	119.8
C1—N1—C12	123.41 (18)	C9—C8—C7	120.49 (19)
C1—N1—H1	115.1 (19)	C9—C8—H8	119.8
C12—N1—H1	121.4 (19)	C8—C9—H9	120.1
C10—N2—C11	117.80 (17)	C8—C9—C10	119.80 (19)
C10—N3—C13	123.3 (2)	C10—C9—H9	120.1
C10—N3—C14	120.86 (18)	N2—C10—N3	117.00 (18)
C14—N3—C13	115.69 (19)	N2—C10—C9	121.26 (18)
N1—C1—H1A	120.0	N3—C10—C9	121.74 (18)
N1—C1—C2	120.0 (2)	N2—C11—C7	125.28 (17)
C2—C1—H1A	120.0	N2—C11—C12	117.53 (16)
C1—C2—H2	120.5	C7—C11—C12	117.19 (17)
C3—C2—C1	118.9 (2)	N1—C12—C4	118.91 (17)
C3—C2—H2	120.5	N1—C12—C11	119.66 (17)
C2—C3—H3	119.3	C4—C12—C11	121.42 (17)
C2—C3—C4	121.4 (2)	N3—C13—H13A	109.5
C4—C3—H3	119.3	N3—C13—H13B	109.5
C3—C4—C5	123.77 (19)	N3—C13—H13C	109.5
C3—C4—C12	117.35 (19)	H13A—C13—H13B	109.5
C12—C4—C5	118.88 (19)	H13A—C13—H13C	109.5
C4—C5—H5	119.9	H13B—C13—H13C	109.5
C6—C5—C4	120.20 (19)	N3—C14—H14A	109.5
C6—C5—H5	119.9	N3—C14—H14B	109.5
C5—C6—H6	119.0	N3—C14—H14C	109.5
C5—C6—C7	121.9 (2)	H14A—C14—H14B	109.5
C7—C6—H6	119.0	H14A—C14—H14C	109.5
C8—C7—C6	124.24 (19)	H14B—C14—H14C	109.5

N1—C1—C2—C3	−0.1 (4)	C7—C8—C9—C10	−0.3 (3)
N2—C11—C12—N1	0.7 (3)	C7—C11—C12—N1	−179.14 (17)
N2—C11—C12—C4	−179.94 (17)	C7—C11—C12—C4	0.2 (3)
C1—N1—C12—C4	0.2 (3)	C8—C7—C11—N2	−1.2 (3)
C1—N1—C12—C11	179.61 (19)	C8—C7—C11—C12	178.60 (17)
C1—C2—C3—C4	0.0 (4)	C8—C9—C10—N2	−0.9 (3)
C2—C3—C4—C5	−179.7 (2)	C8—C9—C10—N3	179.0 (2)
C2—C3—C4—C12	0.2 (3)	C10—N2—C11—C7	0.1 (3)
C3—C4—C5—C6	179.6 (2)	C10—N2—C11—C12	−179.69 (16)
C3—C4—C12—N1	−0.3 (3)	C11—N2—C10—N3	−178.92 (18)
C3—C4—C12—C11	−179.66 (18)	C11—N2—C10—C9	1.0 (3)
C4—C5—C6—C7	0.0 (3)	C11—C7—C8—C9	1.2 (3)
C5—C4—C12—N1	179.62 (18)	C12—N1—C1—C2	−0.1 (3)
C5—C4—C12—C11	0.3 (3)	C12—C4—C5—C6	−0.4 (3)
C5—C6—C7—C8	−178.6 (2)	C13—N3—C10—N2	−178.5 (2)
C5—C6—C7—C11	0.5 (3)	C13—N3—C10—C9	1.6 (3)
C6—C7—C8—C9	−179.6 (2)	C14—N3—C10—N2	−2.6 (3)
C6—C7—C11—N2	179.55 (18)	C14—N3—C10—C9	177.5 (2)
C6—C7—C11—C12	−0.6 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.86 (1)	2.04 (2)	2.819 (3)	150 (3)
C5—H5···O3^{i}	0.93	2.55	3.407 (3)	154

Symmetry code: (i) −*x*+3/2, *y*−1/2, −*z*+1/2.