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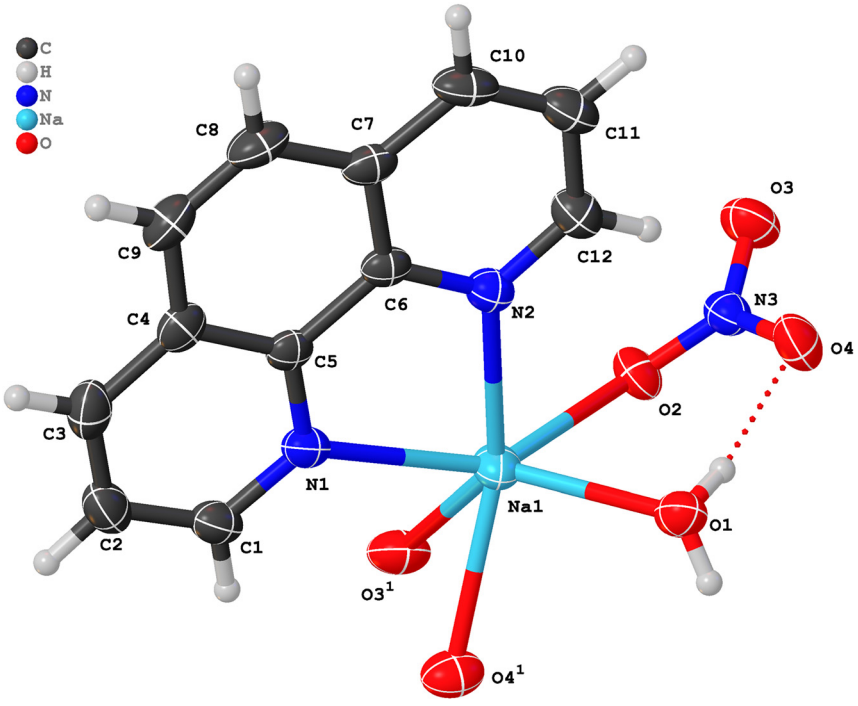
The crystal structure of *catena*-poly[aqua-nitrato-κ^3*O*,*O*:*O*′′-(1,10-phenanthroline-κ^2*N*,*N*′)sodium(I)], $C_{24}H_{18}N_6O_7Na_2$



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Abstract

$C_{24}H_{18}N_6O_7Na_2$, monoclinic, *I*2/*a* (no. 15), *a* = 9.9773(6) Å, *b* = 18.2319(14) Å, *c* = 14.2858(9) Å, *β* = 108.686(7)°, *V* = 2461.7(3) Å^3, *Z* = 4, $R_{gt}(F)$ = 0.0337, w$R_{ref}(F^2)$ = 0.0939, T = 200 K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.13 × 0.11 × 0.09 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.14 mm^{-1}
Diffractometer, scan mode:	SuperNova, *ω*
θ_{max}, completeness:	25.0°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	5264, 2167, 0.020
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 1874
$N(param)_{refined}$:	181
Programs:	Bruker,[1] Olex2,[2] SHELX,[3] Diamond[4]

1 Source of materials

0.1802 g 1,10–Phenanthroline (1.0 mmol) and 0.0850 g sodium nitrate (1.0 mmol) were dissolved to a 20 ml solution of ethanol-water (v:v = 1:1) under stirring. The above

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Na1	0.61706 (6)	0.58577 (4)	0.36254 (4)	0.0346 (2)
O1	0.750000	0.51535 (10)	0.500000	0.0356 (4)
H1	0.711 (2)	0.4884 (13)	0.5309 (15)	0.065 (7)*
O2	0.70264 (11)	0.48418 (7)	0.27690 (8)	0.0372 (3)
O3	0.87687 (13)	0.44111 (7)	0.23416 (8)	0.0441 (3)
O4	0.89169 (12)	0.44347 (7)	0.38784 (8)	0.0406 (3)
N1	0.56556 (13)	0.71707 (8)	0.36252 (9)	0.0292 (3)
N2	0.82901 (13)	0.66105 (8)	0.38474 (9)	0.0302 (3)
N3	0.82237 (14)	0.45644 (7)	0.29864 (10)	0.0310 (3)
C1	0.43948 (17)	0.74537 (11)	0.35256 (11)	0.0352 (4)
H1A	0.365283	0.713191	0.347862	0.042*
C2	0.41112 (19)	0.82017 (11)	0.34868 (12)	0.0398 (4)
H2	0.320437	0.837162	0.341347	0.048*
C3	0.51873 (19)	0.86812 (11)	0.35582 (11)	0.0394 (4)
H3	0.502189	0.918390	0.353535	0.047*
C4	0.65453 (18)	0.84122 (10)	0.36663 (10)	0.0326 (4)
C5	0.67314 (16)	0.76443 (9)	0.36969 (9)	0.0262 (4)
C6	0.81200 (16)	0.73501 (9)	0.38069 (9)	0.0270 (4)
C7	0.92406 (17)	0.78352 (10)	0.38697 (11)	0.0323 (4)
C8	0.89945 (19)	0.86091 (11)	0.38203 (12)	0.0402 (5)
H8	0.973551	0.892775	0.385169	0.048*
C9	0.7715 (2)	0.88813 (10)	0.37298 (12)	0.0404 (4)
H9	0.758450	0.938690	0.370783	0.048*
C10	1.05728 (17)	0.75267 (12)	0.39765 (11)	0.0401 (5)
H10	1.134119	0.782929	0.402102	0.048*
C11	1.07375 (18)	0.67865 (11)	0.40146 (12)	0.0402 (4)
H11	1.161234	0.657535	0.408298	0.048*
C12	0.95628 (17)	0.63518 (11)	0.39486 (11)	0.0361 (4)
H12	0.968423	0.584564	0.397784	0.043*

solution was heated to 85 °C and stirred for 5 h. Then they were cooled to room temperature and filtered. The colorless block crystals were obtained from filtrate after 6 days.

2 Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.93 Å, O–H = 0.83 Å). Their U_{iso} values were set to 1.2 U_{eq} of the parent atoms.

3 Comment

The metal complexes constructed by 1,10-phenanthroline have attracted much attention from coordination chemists for their novel structure,[5] DNA-binding ability and antibacterial activity,[6] fluorescent probe for DNA detection,[7] DNA cleavage study,[8] and enzyme-effector property.[9] In our previous work, metal complexes of 1,10-phenanthroline have been synthesized and structurally characterized, which they also showed excellent performance in photocatalytic CO_2 reduction activity,[10,11] and antitumor activity.[12,13] To further explore the structure and properties of metal complexes with 1,10-phenanthroline ligands, in this work, we synthesized and structural characterized a Na(I) complex using 1,10-phenanthroline and sodium nitrate as materials. The molecular structure of the title complex is shown in the figure. The Na(I) complex is composed of one Na(I) cation, one nitrate anion, one coordinated water molecule, and one 1,10-phenanthroline molecule. The Na(I) ion is six-coordinated with four O atoms (O2, O3^1, O4^1, symmetry code:-1/2 + *x*, 1 – *y*, *z*) of two nitrate, one O atom (O1) of one coordinated H_2O molecules, and two N atoms (N1, N2) of one 1,10-phenanthroline molecule, which forms a distorted NaO_4N_2 octahedral coordination geometry (Figure). The bond angle of N2–Na1–O4^1 is 153.73(5)°, showing that the N2 and O4^1 atoms are at the axial positions, and the N1, O3^1, O1, O2 atoms are at the equatorial plane. The lengths of Na–O bonds and Na–N bonds are in the range of 2.3653(12) to 2.5555(14) Å, and 2.4484(15) to 2.4548(14) Å. The angles around the Na(I) ion range from 79.44(4) to 145.48(5)° in the plane. The nitrate anion adopts tridentate coordination mode. The Na(I) complex molecules form 2D layered structure by the bridge effect of nitrate and coordinated water molecule. The two- dimensional layered structure further formed the three-dimensional network structure through the stacking of 1,10-phenanthroline rings.

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