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Bis(ethylenediammonium) μ-ethylenediaminetetraacetato-1κ^3O,N,O':2κ^3O'',N',O'''-bis[trioxidomolybdate(VI)] tetrahydrate

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Keywords: crystal structure; edta complex; molybdenum oxide; ethylenediaminetetraacetic acid.

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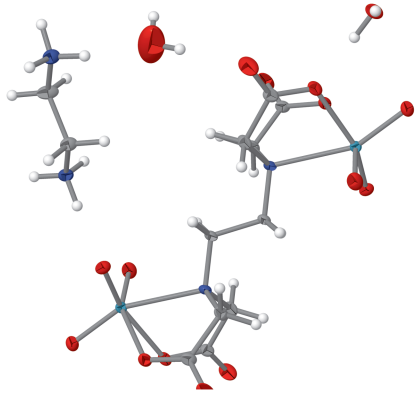
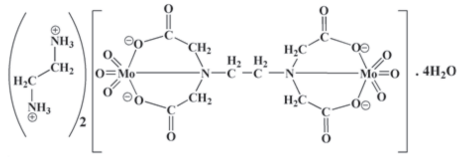
The title compound, $(C_2H_{10}N_2)_2[(C_{10}H_{12}N_2O_8)(MoO_3)_2]\cdot 4H_2O$, which crystallizes in the monoclinic $C2/c$ space group, was obtained by mixing molybdenum oxide, ethylenediamine and ethylenediaminetetraacetic acid (H_4edta) in a 2:4:1 ratio. The complex anion contains two MoO_3 units bridged by an edta^{4-} anion. The midpoint of the central C—C bond of the edta^{4-} anion is located on a crystallographic inversion centre. The independent Mo atom is tridentately coordinated by a nitrogen atom and two carboxylate groups of the edta^{4-} ligand, together with the three oxo ligands, producing a distorted octahedral coordination environment. In the three-dimensional supramolecular crystal structure, the dinuclear anions, the organoammonium counter-ions and the solvent water molecules are linked by N—H$\cdots$O$_w$, N—H$\cdots$O$_{edta}$ and O—H$\cdots$O hydrogen bonds.

3D view



Chemical scheme



Structure description

The advancement of materials science has meant that many well-established materials, such as metals, ceramics or plastics, cannot meet the demand for new applications (photovoltaic cells, field-effect transistors, *etc.*). This desire to design new functional materials demands enormous research effort. In order to overcome this challenge, scientists quickly understood that mixtures of materials could have properties superior to those of their pure counterparts, and thus meet this demand. Hybrid framework materials research is one of the fastest growing research fields.

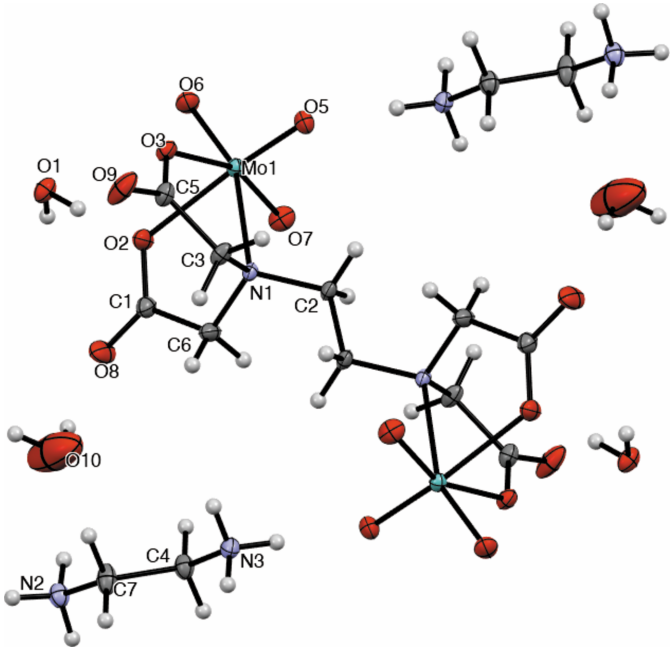


Figure 1
Molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. Unlabelled atoms are generated by inversion symmetry.

Their unique hybrid nature enables the combination of properties from both inorganic and organic materials (Cheetham & Rao, 2007). As organic ligands, polycarboxylates are multidentate chelating agents, widespread in nature and industry, due to their ability to coordinate to various transition metals in different ratios. In this field, the study of molybdenum polycarboxylate complexes has led to thorough investigation over the past three decades. Some well-characterized mono-, bi- and polynuclear molybdenum and tungsten complexes have been reported, for example $[(H_2TEMED)Mo_2O_6(H_2edta)]\cdot H_2O$ (TMED = tetramethylethylenediamine; Kumar *et al.*, 2012), $Mo_2(O_2CCH_2OH)_4$, $M_2[MoO_3(C_2O_4)]$ (M = Na, K, Rb, Cs) and $Na_2[MO_2(C_6H_6O_7)_2]\cdot 3H_2O$ (M = Mo, W; Cotton *et al.*, 2002; Cindrić *et al.*, 2000; Zhou *et al.*, 1999), $Na_2K_2[Mo_2O_6(edta)]\cdot 10H_2O$ and $Na_4[W_2O_6(edta)]\cdot 8H_2O$ (Lin *et al.*, 2006). In our study, the reaction of H_4edta (ethylenediaminetetraacetic acid) with molybdenum oxide has been investigated, and a new binuclear 2:1 Mo–edta complex, $(C_2H_{10}N_2)_2[(C_{10}H_{12}N_2O_8)(MoO_3)_2]\cdot 4H_2O$, including $edta^{4-}$ as ligand has been isolated and structurally characterized.

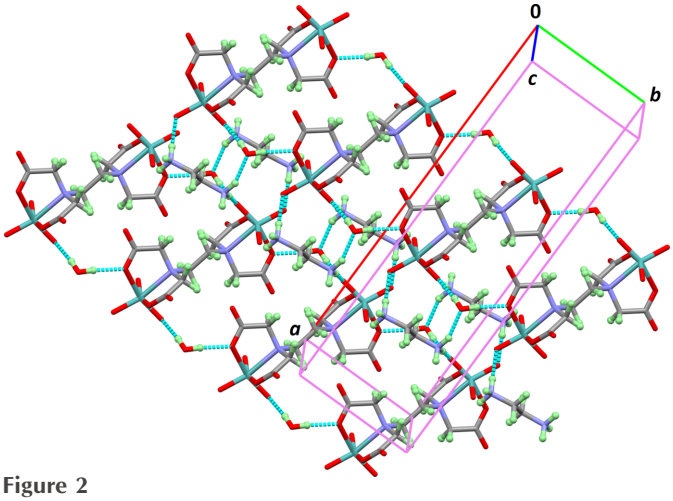


Figure 2
Supramolecular arrangement of the title compound with hydrogen bonds shown as dotted lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2C···O1^{i}	0.91	1.93	2.795 (2)	159
N2—H2D···O10	0.91	2.00	2.715 (4)	134
N2—H2D···O7^{ii}	0.91	2.21	2.786 (2)	121
N2—H2E···O6^{iii}	0.91	1.84	2.748 (2)	172
N3—H3C···O9^{i}	0.91	1.88	2.785 (3)	170
N3—H3D···O1^{iv}	0.91	1.98	2.838 (2)	156
N3—H3E···O5^{v}	0.91	1.84	2.753 (2)	177
O1—H1A···O5^{vi}	0.87	1.83	2.694 (2)	173
O1—H1B···O2	0.87	1.83	2.694 (2)	173
O10—H10A···O8	0.87	1.86	2.692 (4)	160
O10—H10B···O8^{i}	0.87	2.13	2.978 (4)	166

Symmetry codes: (i) $-x+1, y, -z+\frac{1}{2}$; (ii) $-x+1, -y, -z+1$; (iii) $x+\frac{1}{2}, y-\frac{1}{2}, z$; (iv) $x+\frac{1}{2}, y+\frac{1}{2}, z$; (v) $-x+1, -y+1, -z+1$; (vi) $x, y-1, z$.

The single-crystal structure shows that the 2:1 Mo–edta complex anion of the title compound is discrete (Fig. 1). All of the carboxylic groups of H_4edta are deprotonated, coordinating the molybdenum oxide groups by nitrogen and two oxygen atoms. The $edta^{4-}$ ligand itself is a bridge between the two MoO_3 units, and the midpoint of the central C—C bond is situated on an inversion centre. In the 2:1 Mo–edta complex, the $edta^{4-}$ ligand thus chelates a pair of Mo^{VI} centres, in a tridentate fashion, giving a *trans* configuration to the complex. Each Mo^{VI} ion is chelated by the $edta^{4-}$ ligand, simultaneously forming two glycinato rings occupying contiguous vertices that define one face of the coordination polyhedron. The other three vertices of the opposite face are occupied by three terminal oxo atoms of the MoO_3 unit, completing the octahedral geometry. In the complex, the Mo—O bond lengths are in the range 1.7195 (16) to 1.7686 (15) Å for Mo═O_t groups (O_t are terminal oxygen atoms: O5, O6 and O7). The resulting bond angles O_t—Mo—O_t are 107.27 (7), 103.83 (7) and 106.75 (7)°, considerably larger than the expected value of 90° for a regular octahedron, confirming the distortion from octahedral geometry.

The crystal packing can be rationalized in terms of non-bonding interactions between the three tectons: the Mo–edta complex anion, two $(C_2H_{10}N_2)^+$ cations and four lattice water molecules. These units are linked through hydrogen bonds of the type N—H···O_{water}, N—H···O_{edta} and O—H···O (Table 1). This interconnection leads to the supramolecular structure, as shown in Fig. 2.

Synthesis and crystallization

Solid molybdenum oxide (4 mmol) and ethylenediamine (4 mmol) were mixed in 30 ml of distilled water. To this

mixture were slowly added 2 mmol of ethylenediaminetetraacetic acid (H_4edta) under vigorous stirring. The solution was then stirred for 2 h at room temperature. The colourless solution thus obtained was left at room temperature for slow evaporation of water. After a few days, colourless crystals (yield 13.6% based on Mo) were obtained.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$(C_2H_{10}N_2)_2[(C_{10}H_{12}N_2O_8)(MoO_3)_2]\cdot 4H_2O$
M_r	772.40
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	150
a, *b*, *c* (Å)	22.5897 (14), 7.5100 (4), 16.3743 (10)
β (°)	94.716 (2)
V (Å^3)	2768.5 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.00
Crystal size (mm)	0.17 × 0.17 × 0.13
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.691, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24031, 3192, 2946
R_{int}	0.032
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.022, 0.060, 1.06
No. of reflections	3192
No. of parameters	189
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.67, −1.06

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/32* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

Acknowledgements

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full crystallographic data

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Crystal data

$(C_2H_{10}N_2)_2[Mo_2(C_{10}H_{12}N_2O_8)O_6]\cdot 4H_2O$
M_r = 772.40
Monoclinic, $C2/c$
a = 22.5897 (14) Å
b = 7.5100 (4) Å
c = 16.3743 (10) Å
β = 94.716 (2)°
V = 2768.5 (3) Å^3
Z = 4
$F(000)$ = 1576
D_x = 1.853 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9873 reflections
θ = 2.9–27.5°
μ = 1.00 mm^{-1}
T = 150 K
Block, colourless
0.17 × 0.17 × 0.13 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.691, T_{max} = 0.746
24031 measured reflections
3192 independent reflections
2946 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.5°, θ_{min} = 1.8°
h = −29→29
k = −9→9
l = −20→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.060
S = 1.06
3192 reflections
189 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0247P)^2 + 9.3382P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −1.06 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mo1	0.34131 (2)	0.30046 (2)	0.43898 (2)	0.01140 (6)
O2	0.38304 (7)	0.07064 (19)	0.38526 (10)	0.0184 (3)
O3	0.34930 (6)	0.3750 (2)	0.31149 (9)	0.0153 (3)
O5	0.32695 (7)	0.5278 (2)	0.45742 (9)	0.0167 (3)
O6	0.27328 (7)	0.1984 (2)	0.41260 (10)	0.0192 (3)
O7	0.36649 (7)	0.2195 (2)	0.53376 (10)	0.0199 (3)
O8	0.46292 (8)	−0.0988 (2)	0.38094 (12)	0.0305 (4)
O9	0.40393 (8)	0.4592 (3)	0.21238 (10)	0.0313 (4)
N1	0.44444 (7)	0.3699 (2)	0.42662 (10)	0.0110 (3)
N2	0.68095 (9)	−0.1480 (2)	0.31790 (11)	0.0180 (4)
H2C	0.682765	−0.194661	0.266874	0.022*
H2D	0.644495	−0.169814	0.335592	0.022*
H2E	0.709362	−0.199255	0.352923	0.022*
N3	0.68986 (8)	0.3285 (2)	0.39152 (11)	0.0166 (4)
H3C	0.662370	0.374203	0.353458	0.020*
H3D	0.726961	0.352136	0.376498	0.020*
H3E	0.685339	0.379149	0.441115	0.020*
C1	0.43883 (10)	0.0440 (3)	0.39471 (13)	0.0165 (4)
C2	0.46667 (9)	0.4795 (3)	0.49874 (12)	0.0136 (4)
H2A	0.458550	0.415662	0.549512	0.016*
H2B	0.444417	0.593202	0.497625	0.016*
C3	0.44903 (9)	0.4682 (3)	0.34868 (12)	0.0158 (4)
H3A	0.486764	0.435686	0.325738	0.019*
H3B	0.450105	0.597629	0.360192	0.019*
C4	0.68156 (10)	0.1326 (3)	0.39721 (13)	0.0181 (4)
H4A	0.640934	0.106237	0.412324	0.022*
H4B	0.710243	0.083077	0.440266	0.022*
C5	0.39759 (10)	0.4287 (3)	0.28535 (13)	0.0159 (4)
C6	0.47677 (9)	0.1985 (3)	0.42775 (15)	0.0184 (4)
H6A	0.492092	0.171560	0.484797	0.022*
H6B	0.511335	0.210675	0.394705	0.022*
C7	0.69112 (12)	0.0470 (3)	0.31517 (13)	0.0225 (5)
H7A	0.663501	0.100557	0.271922	0.027*
H7B	0.732207	0.070407	0.301180	0.027*
O1	0.30869 (7)	−0.2039 (2)	0.34909 (9)	0.0180 (3)
H1A	0.317459	−0.290614	0.383210	0.027*
H1B	0.333866	−0.120160	0.364109	0.027*
O10	0.56206 (14)	−0.0882 (7)	0.30040 (19)	0.1003 (14)
H10A	0.533675	−0.115649	0.330976	0.151*
H10B	0.549760	−0.103261	0.249098	0.151*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.01159 (9)	0.01140 (9)	0.01128 (9)	−0.00124 (6)	0.00129 (6)	−0.00028 (6)

O2	0.0146 (7)	0.0131 (7)	0.0272 (8)	−0.0018 (6)	−0.0006 (6)	−0.0051 (6)
O3	0.0139 (7)	0.0207 (7)	0.0113 (7)	−0.0022 (6)	−0.0005 (5)	0.0000 (6)
O5	0.0197 (8)	0.0149 (7)	0.0157 (7)	0.0013 (6)	0.0031 (6)	−0.0022 (6)
O6	0.0142 (7)	0.0206 (8)	0.0229 (8)	−0.0029 (6)	0.0024 (6)	−0.0023 (6)
O7	0.0201 (8)	0.0226 (8)	0.0172 (7)	−0.0033 (6)	0.0021 (6)	0.0059 (6)
O8	0.0238 (9)	0.0153 (8)	0.0507 (12)	0.0053 (7)	−0.0067 (8)	−0.0107 (8)
O9	0.0263 (9)	0.0548 (12)	0.0123 (7)	−0.0165 (8)	−0.0016 (7)	0.0047 (8)
N1	0.0129 (8)	0.0100 (7)	0.0097 (7)	−0.0009 (6)	−0.0016 (6)	−0.0013 (6)
N2	0.0225 (9)	0.0163 (9)	0.0152 (8)	0.0008 (7)	0.0019 (7)	0.0001 (7)
N3	0.0183 (9)	0.0176 (9)	0.0137 (8)	0.0017 (7)	−0.0007 (7)	−0.0025 (7)
C1	0.0174 (10)	0.0132 (9)	0.0185 (10)	0.0003 (8)	−0.0018 (8)	−0.0013 (8)
C2	0.0133 (10)	0.0156 (9)	0.0115 (9)	−0.0025 (7)	−0.0017 (7)	−0.0027 (7)
C3	0.0150 (10)	0.0198 (10)	0.0125 (9)	−0.0062 (8)	0.0001 (7)	0.0020 (8)
C4	0.0234 (11)	0.0170 (10)	0.0138 (9)	0.0003 (8)	0.0019 (8)	−0.0002 (8)
C5	0.0190 (10)	0.0160 (10)	0.0125 (9)	−0.0031 (8)	−0.0002 (8)	0.0000 (8)
C6	0.0130 (10)	0.0141 (10)	0.0273 (11)	0.0015 (8)	−0.0038 (8)	−0.0038 (8)
C7	0.0376 (13)	0.0159 (10)	0.0138 (10)	−0.0012 (9)	0.0013 (9)	−0.0001 (8)
O1	0.0207 (8)	0.0152 (7)	0.0175 (7)	−0.0052 (6)	−0.0025 (6)	0.0023 (6)
O10	0.0533 (18)	0.200 (4)	0.0469 (16)	0.015 (2)	0.0000 (14)	0.007 (2)

Geometric parameters (Å, º)

Mo1—O2	2.1858 (15)	N3—C4	1.487 (3)
Mo1—O3	2.1831 (14)	C1—C6	1.516 (3)
Mo1—O5	1.7686 (15)	C2—C2^{i}	1.534 (4)
Mo1—O6	1.7397 (15)	C2—H2A	0.9900
Mo1—O7	1.7195 (16)	C2—H2B	0.9900
Mo1—N1	2.4121 (17)	C3—H3A	0.9900
O2—C1	1.273 (3)	C3—H3B	0.9900
O3—C5	1.270 (3)	C3—C5	1.521 (3)
O8—C1	1.232 (3)	C4—H4A	0.9900
O9—C5	1.236 (3)	C4—H4B	0.9900
N1—C2	1.492 (2)	C4—C7	1.521 (3)
N1—C3	1.485 (3)	C6—H6A	0.9900
N1—C6	1.479 (3)	C6—H6B	0.9900
N2—H2C	0.9100	C7—H7A	0.9900
N2—H2D	0.9100	C7—H7B	0.9900
N2—H2E	0.9100	O1—H1A	0.8703
N2—C7	1.484 (3)	O1—H1B	0.8697
N3—H3C	0.9100	O10—H10A	0.8701
N3—H3D	0.9100	O10—H10B	0.8702
N3—H3E	0.9100		
O2—Mo1—N1	71.68 (6)	O8—C1—C6	119.11 (19)
O3—Mo1—O2	75.25 (6)	N1—C2—C2^{i}	113.4 (2)
O3—Mo1—N1	73.02 (5)	N1—C2—H2A	108.9
O5—Mo1—O2	157.26 (6)	N1—C2—H2B	108.9
O5—Mo1—O3	86.93 (6)	C2^{i}—C2—H2A	108.9

O5—Mo1—N1	89.85 (6)	C2^{i}—C2—H2B	108.9
O6—Mo1—O2	87.34 (6)	H2A—C2—H2B	107.7
O6—Mo1—O3	90.94 (7)	N1—C3—H3A	109.1
O6—Mo1—O5	107.27 (7)	N1—C3—H3B	109.1
O6—Mo1—N1	156.07 (6)	N1—C3—C5	112.68 (16)
O7—Mo1—O2	87.85 (7)	H3A—C3—H3B	107.8
O7—Mo1—O3	155.03 (7)	C5—C3—H3A	109.1
O7—Mo1—O5	103.83 (7)	C5—C3—H3B	109.1
O7—Mo1—O6	106.75 (7)	N3—C4—H4A	109.8
O7—Mo1—N1	84.38 (7)	N3—C4—H4B	109.8
C1—O2—Mo1	122.03 (13)	N3—C4—C7	109.60 (17)
C5—O3—Mo1	123.00 (13)	H4A—C4—H4B	108.2
C2—N1—Mo1	108.51 (11)	C7—C4—H4A	109.8
C3—N1—Mo1	108.40 (12)	C7—C4—H4B	109.8
C3—N1—C2	111.30 (15)	O3—C5—C3	117.47 (18)
C6—N1—Mo1	106.85 (12)	O9—C5—O3	123.7 (2)
C6—N1—C2	109.66 (16)	O9—C5—C3	118.68 (19)
C6—N1—C3	111.95 (16)	N1—C6—C1	113.43 (17)
H2C—N2—H2D	109.5	N1—C6—H6A	108.9
H2C—N2—H2E	109.5	N1—C6—H6B	108.9
H2D—N2—H2E	109.5	C1—C6—H6A	108.9
C7—N2—H2C	109.5	C1—C6—H6B	108.9
C7—N2—H2D	109.5	H6A—C6—H6B	107.7
C7—N2—H2E	109.5	N2—C7—C4	110.94 (18)
H3C—N3—H3D	109.5	N2—C7—H7A	109.5
H3C—N3—H3E	109.5	N2—C7—H7B	109.5
H3D—N3—H3E	109.5	C4—C7—H7A	109.5
C4—N3—H3C	109.5	C4—C7—H7B	109.5
C4—N3—H3D	109.5	H7A—C7—H7B	108.0
C4—N3—H3E	109.5	H1A—O1—H1B	104.5
O2—C1—C6	116.65 (18)	H10A—O10—H10B	109.4
O8—C1—O2	124.2 (2)		

Mo1—O2—C1—O8	164.21 (18)	N1—C3—C5—O3	24.0 (3)
Mo1—O2—C1—C6	−13.7 (3)	N1—C3—C5—O9	−159.7 (2)
Mo1—O3—C5—O9	174.61 (18)	N3—C4—C7—N2	−177.90 (18)
Mo1—O3—C5—C3	−9.3 (3)	C2—N1—C3—C5	−143.96 (17)
Mo1—N1—C2—C2^{i}	175.59 (18)	C2—N1—C6—C1	145.79 (18)
Mo1—N1—C3—C5	−24.7 (2)	C3—N1—C2—C2^{i}	−65.2 (3)
Mo1—N1—C6—C1	28.4 (2)	C3—N1—C6—C1	−90.2 (2)
O2—C1—C6—N1	−13.0 (3)	C6—N1—C2—C2^{i}	59.2 (3)
O8—C1—C6—N1	169.0 (2)	C6—N1—C3—C5	92.9 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*C*···O1^{ii}	0.91	1.93	2.795 (2)	159

N2—H2*D*···O10	0.91	2.00	2.715 (4)	134
N2—H2*D*···O7^{iii}	0.91	2.21	2.786 (2)	121
N2—H2*E*···O6^{iv}	0.91	1.84	2.748 (2)	172
N3—H3*C*···O9^{ii}	0.91	1.88	2.785 (3)	170
N3—H3*D*···O1^{v}	0.91	1.98	2.838 (2)	156
N3—H3*E*···O5^{i}	0.91	1.84	2.753 (2)	177
O1—H1*A*···O5^{vi}	0.87	1.83	2.694 (2)	173
O1—H1*B*···O2	0.87	1.83	2.694 (2)	173
O10—H10*A*···O8	0.87	1.86	2.692 (4)	160
O10—H10*B*···O8^{ii}	0.87	2.13	2.978 (4)	166

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, *y*, −*z*+1/2; (iii) −*x*+1, −*y*, −*z*+1; (iv) *x*+1/2, *y*−1/2, *z*; (v) *x*+1/2, *y*+1/2, *z*; (vi) *x*, *y*−1, *z*.