



Crystal structure of bis(diisopropylammonium) molybdate

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The organic–inorganic title salt, (C₆H₁₆N)₂[MoO₄] or (iPr₂NH₂)₂[MoO₄], was obtained by reacting MoO₃ with diisopropylamine in a 1:2 molar ratio in water. The molybdate anion is located on a twofold rotation axis and exhibits a slightly distorted tetrahedral configuration. In the crystal structure, the diisopropylammonium (iPr₂NH₂)⁺ cations and [MoO₄]²⁻ anions are linked to each other through N—H...O hydrogen bonds, generating rings with R₁₂¹²(36) motifs that give rise to the formation of a three-dimensional network. The structure was refined taking into account inversion twinning (ratio of *ca* 4:1 between the two domains).

1. Chemical context

As a result of the photochromic properties of alkylammonium molybdates (Arnaud-Neu & Schwing-Weill, 1974), molybdenum chemistry is an exciting research area. A large variety of oxidoanions based on molybdenum have been synthesized and characterized with numerous counter-cations. Among these, mononuclear and binuclear anions as well as poly-oxidomolybdates with a much higher nuclearity are known (Gatehouse & Leverett, 1969; Matsumoto *et al.* 1975; Modéc *et al.*, 2004; Müller & Gouzerh, 2012; Pouye *et al.*, 2014; Sarr *et al.*, 2018). Salts containing the tetrahedral molybdate anion [MoO₄]²⁻ combined with cations such as K⁺, Na⁺, (CH₆N₃)⁺, ((C₆H₁₁)₂NH₂)⁺, (NH₃(CH₂)₂NH₃)⁺, (OHRNH₃)⁺ and (CyNH₂)⁺ have been isolated in the past (Gatehouse & Leverett, 1969; Matsumoto *et al.*, 1975; Ozeki *et al.*, 1987; Thiele & Fuchs, 1979; Bensch *et al.*, 1987; Sheikhshoai & Ghazizadeh, 2013; Pouye *et al.*, 2014), but never with the diisopropylammonium cation (iPr₂NH₂)⁺. In a continuation of our work on molybdenum compounds with organic cations, we report here the synthesis and crystal structure of the title compound, (iPr₂NH₂)₂[MoO₄], (I).

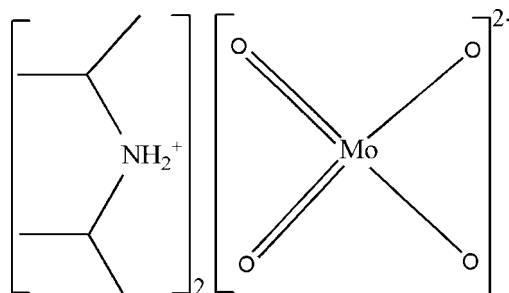
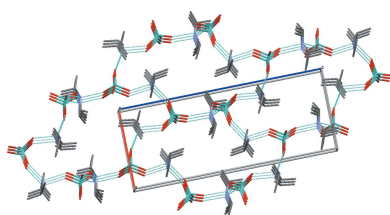


Table 1
Selected bond angles (°).

O1 ⁱ —Mo1—O1	110.33 (12)	O2—Mo1—O1	108.77 (10)
O2—Mo1—O1 ⁱ	109.13 (11)	O2 ⁱ —Mo1—O2	110.7 (2)

Symmetry code: (i) $y, x, -z + 1$.

2. Structural commentary

The asymmetric unit of (I) comprises one (ⁱPr₂NH₂)⁺ cation and an {MoO₂} entity (Fig. 1). The [MoO₄]²⁻ molybdate anion is completed by application of twofold rotation symmetry. The two Mo—O distances are 1.732 (2) and 1.7505 (15) Å and the O—Mo—O angles vary in a narrow range between 108.77 (10) and 110.7 (2)° (Table 1), revealing only slight distortions from ideal values. Similar bond lengths and angles for the molybdate anion were reported in previous studies (Ozeki *et al.*, 1987; Bensch *et al.*, 1987; Sheikhshoae & Ghazizadeh, 2013; Pouye *et al.*, 2014) where the Mo—O distances vary between 1.749 (2) and 1.776 (3) Å, and the O—Mo—O angles between 106.85 (4) and 113.2 (1)°.

In the crystal structure of (CyNH₂)₂MoO₄·2H₂O (Cy = cyclohexyl; Pouye *et al.*, 2014) the four Mo—O bond lengths are equal with 1.7613 (12) Å. Although in this structure similar N—H···O intermolecular interactions between the (CyNH₂)⁺ cation and the molybdate anion are present in comparison with the (ⁱPr₂NH₂)⁺ cation in the title compound, the small differences in the hydrogen-bonding pattern result in slightly different Mo—O bond lengths between the two structures. On one hand this may be related to the presence of additional water molecules in (CyNH₂)₂MoO₄·2H₂O, on the other hand to steric hindrance between the four diisopropylammonium cations that surround each molybdate anion in (I). At least the strengths of the N—H···O hydrogen bonds do not seem to have a noticeable effect on the different Mo—O

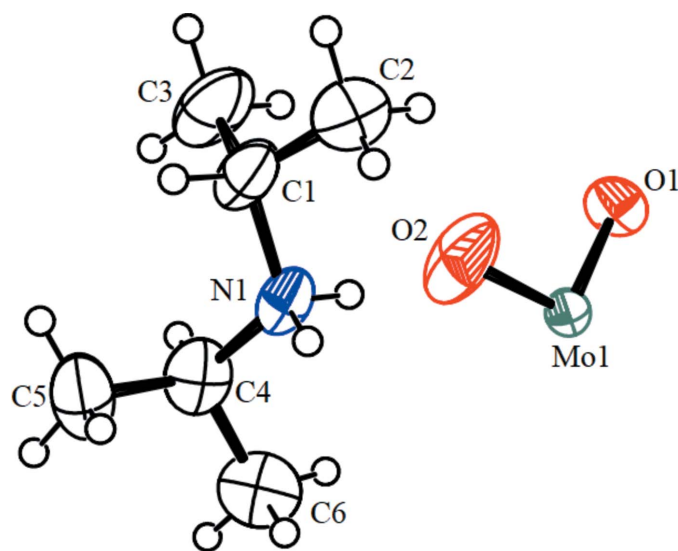


Figure 1
Asymmetric unit view of (I) with displacement ellipsoids drawn at the 50% probability level and hydrogen atoms as spheres of arbitrary radius.

Table 2
Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1A···O2	0.89	1.80	2.684 (3)	170
N1—H1B···O1 ⁱⁱ	0.89	1.81	2.695 (2)	174

Symmetry code: (ii) $y + \frac{1}{2}, -x + \frac{1}{2}, z + \frac{1}{4}$.

distances in (I). Both hydrogen bonds are very similar in terms of N···O distances and N—H···O angles (Table 2).

3. Supramolecular features

In the crystal structure of (I), each [MoO₄]²⁻ anion is linked to two pairs of symmetry-related diisopropylammonium cations through N—H···O hydrogen bonds (Table 2). Contrariwise, each (ⁱPr₂NH₂)⁺ cation is linked to two molybdate [MoO₄]²⁻ anions. The interaction of six molybdate anions with six diisopropylammonium cations leads to [(ⁱPr₂NH₂)₆·MoO₄]₆ ring systems with an *R*₁₂¹²(36) motif (Etter *et al.*, 1990). Each ring is linked to six adjacent rings giving rise to infinite layers extending parallel to (010) (Fig. 2). The connection of the rings into a three-dimensional network structure perpendicular to this plane is shown in Fig. 3.

4. Database survey

A search of the Cambridge Structural Database (Version 5.39 plus 1 update, November 2017; Groom *et al.*, 2016) revealed 226 entries dealing with (ⁱPr₂NH₂)⁺ cations while 32 entries contained the [MoO₄]²⁻ molybdate anion.

5. Synthesis and crystallization

Compound (I) was obtained from a mixture of molybdenum trioxide (3.2 g, 22.23 mmol) and diisopropylamine (4 g, 44.46 mmol) in a 1:2 molar ratio in water. A clear, colourless solution was obtained after stirring for approximately one h. After twenty days of evaporation in an oven at 333 K, some colourless single crystals were obtained.

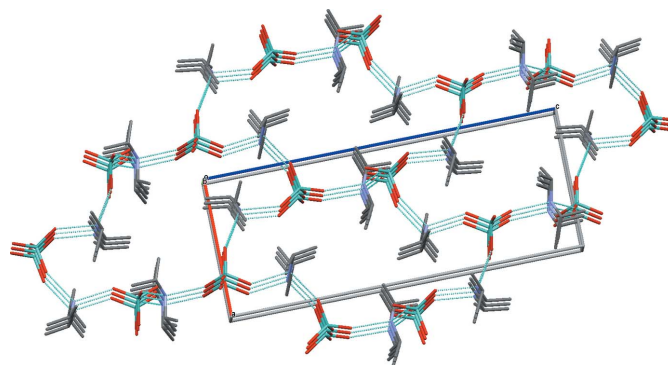


Figure 2
The N—H···O hydrogen-bonding network in (I) (turquoise dashed lines) in a view approximately along [010].

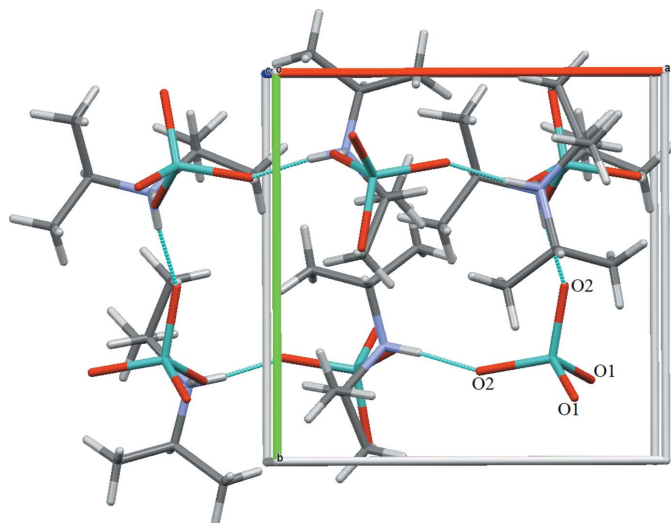


Figure 3
The N—H...O hydrogen-bonding network in (I) (turquoise dashed lines) in a view approximately along [001].

In the IR spectrum of (I) (Fig. 4a), the bands at 899 and 786 cm^{-1} can be attributed to symmetric and asymmetric Mo—O stretching modes, respectively. The diisopropylammonium cation is characterized by a series of vibrational bands in the 3000–2200 cm^{-1} region, which can be attributed to $\nu(\text{N—H})$, $\nu(\text{C—H})$ and combination modes. The $\delta(\text{N—H})$ bending vibrations probably contribute to the signal observed at 1598 cm^{-1} .

In the Raman spectrum of (I) (Fig. 4b), the band at 797 cm^{-1} is attributed to the antisymmetric stretching mode of the $[\text{MoO}_4]^{2-}$ molybdate anion. The symmetric vibration, $\nu_s(\text{Mo—O})$, in the form of a weak shoulder at 839 cm^{-1} in the infrared spectrum, is very intense in the Raman spectrum at 896 cm^{-1} . In the high wavenumber region of the Raman spectrum, the bands between 3000 and 2800 cm^{-1} can be assigned to the $\nu(\text{N—H})$ and $\nu(\text{C—H})$ stretching vibrations of the diisopropylammonium cation.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The structure was refined taking into account twinning by inversion (ratio of *ca* 4:1 between the

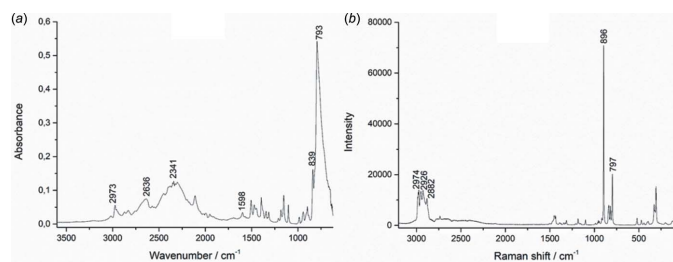


Figure 4
IR (a) and Raman (b) spectra of (I).

Table 3
Experimental details.

Crystal data	
Chemical formula	$(\text{C}_6\text{H}_{16}\text{N})_2[\text{MoO}_4]$
M_r	364.33
Crystal system, space group	Tetragonal, $P4_32_12$
Temperature (K)	293
a, c (\AA)	9.0166 (1), 23.1158 (3)
V (\AA^3)	1879.29 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.71
Crystal size (mm)	$0.38 \times 0.26 \times 0.1$
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, AtlasS2
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2015)
T_{\min} , T_{\max}	0.612, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	111277, 2156, 2109
R_{int}	0.055
$(\sin \theta/\lambda)_{\text{max}}$ (\AA^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.019, 0.049, 1.12
No. of reflections	2156
No. of parameters	92
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e \AA^{-3})	0.21, -0.31
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.19 (7)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

two domains). H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with N—H distances of 0.89 \AA and C—H distances of 0.96 \AA for methyl and of 0.98 \AA for methylene groups, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ or $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$.

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References

- Arnaud-Neu, F. & Schwing-Weill, M. J. (1974). *J. Less-Common Met.* **36**, 71–78.
- Bensch, W., Hug, P., Emmenegger, R., Reller, A. & Oswald, H. R. (1987). *Mater. Res. Bull.* **22**, 447–454.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* **B46**, 256–262.
- Gatehouse, B. M. & Leverett, P. (1969). *J. Chem. Soc. A*, pp. 849–854.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Matsumoto, K. Y., Kobayashi, A. & Sasaki, Y. (1975). *Bull. Chem. Soc. Jpn.*, **48**, 1009–1013.

- Modec, B., Brenčič, J. V. & Koller, J. (2004). *Eur. J. Inorg. Chem.* pp. 1611–1620.
- Müller, A. & Gouzerh, P. (2012). *Chem. Soc. Rev.* **41**, 7431–7463.
- Ozeki, T., Ichida, H. & Sasaki, Y. (1987). *Acta Cryst.* **C43**, 2220–2221.
- Pouye, S. F., Cissé, I., Diop, L., Molloy, K. C. & Kociok-Kohn, G. (2014). *Sci. Study Res.: Chem. Chem. Eng., Biotechnol., Food Ind. (Univ. Bacau)*, **15**, 091–094.
- Rigaku OD (2015). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
- Sarr, B., Diop, C. A. K., Melin, F., Sidibe, M., Hellwig, P., Michaud, F., Maury, F., Senocq, F., Mbaye, A. & Rousselin, Y. (2018). *J. Mol. Struct.* **1170**, 44–50.
- Sheikhshoaie, I. & Ghazizadeh, M. (2013). *Bull. Chem. Soc. Ethiop.* **27**, 69–76.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Thiele, A. & Fuchs, J. (1979). *Z. Naturforsch. Teil B*, **34**, 145–154.

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Acta Cryst. (2018). E74, 1682-1685 [https://doi.org/10.1107/S2056989018014755]

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to solve structure: *SHELXS* (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).

Bis(diisopropylazanium tetraoxomolybdate)

Crystal data

(C₆H₁₆N)₂[MoO₄]
 $M_r = 364.33$
 Tetragonal, $P4_32_12$
 $a = 9.0166$ (1) Å
 $c = 23.1158$ (3) Å
 $V = 1879.29$ (5) Å³
 $Z = 4$
 $F(000) = 768$

$D_x = 1.288$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 49023 reflections
 $\theta = 3.6\text{--}27.7^\circ$
 $\mu = 0.71$ mm⁻¹
 $T = 293$ K
 Prism, clear light colourless
 0.38 × 0.26 × 0.1 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual,
 Cu at zero, AtlasS2
 diffractometer
 Detector resolution: 5.3048 pixels mm⁻¹
 ω scans
 Absorption correction: multi-scan
 (*CrysAlis PRO*; Rigaku OD, 2015)
 $T_{\min} = 0.612$, $T_{\max} = 1.000$

111277 measured reflections
 2156 independent reflections
 2109 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.055$
 $\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.5^\circ$
 $h = -11 \rightarrow 11$
 $k = -11 \rightarrow 11$
 $l = -29 \rightarrow 30$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.019$
 $wR(F^2) = 0.049$
 $S = 1.12$
 2156 reflections
 92 parameters
 0 restraints

Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0245P)^2 + 0.4149P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.21$ e Å⁻³
 $\Delta\rho_{\min} = -0.31$ e Å⁻³
 Absolute structure: Refined as an inversion twin
 Absolute structure parameter: 0.19 (7)

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.

Refinement. Refined as a 2-component inversion twin.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.6950 (2)	0.2985 (3)	0.57328 (7)	0.0451 (5)
H1A	0.607999	0.280281	0.556562	0.054*
H1B	0.681809	0.289840	0.611289	0.054*
C1	0.8015 (3)	0.1790 (4)	0.55462 (12)	0.0603 (7)
H1	0.897057	0.196363	0.573616	0.072*
C2	0.7411 (5)	0.0325 (4)	0.57499 (18)	0.0827 (10)
H2A	0.725309	0.036136	0.616035	0.124*
H2B	0.810811	−0.044698	0.566106	0.124*
H2C	0.648792	0.012618	0.555832	0.124*
C3	0.8245 (4)	0.1852 (5)	0.48930 (13)	0.0872 (11)
H3A	0.731448	0.169286	0.470093	0.131*
H3B	0.893498	0.109574	0.477926	0.131*
H3C	0.863030	0.280735	0.478768	0.131*
C4	0.7349 (4)	0.4560 (3)	0.56091 (11)	0.0590 (7)
H4	0.745520	0.468318	0.518986	0.071*
C5	0.8813 (4)	0.4960 (4)	0.58963 (15)	0.0750 (10)
H5A	0.876969	0.471035	0.629966	0.112*
H5B	0.899069	0.600390	0.585479	0.112*
H5C	0.960302	0.441624	0.571562	0.112*
C6	0.6069 (4)	0.5518 (4)	0.58154 (14)	0.0735 (10)
H6A	0.518209	0.524379	0.561190	0.110*
H6B	0.628992	0.654184	0.574169	0.110*
H6C	0.592529	0.537236	0.622295	0.110*
Mo1	0.26396 (2)	0.26396 (2)	0.500000	0.03021 (9)
O1	0.2086 (2)	0.1625 (2)	0.43916 (6)	0.0510 (5)
O2	0.4506 (2)	0.2317 (4)	0.51236 (10)	0.0959 (9)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0337 (9)	0.0747 (15)	0.0269 (8)	0.0005 (9)	−0.0009 (7)	−0.0005 (9)
C1	0.0350 (13)	0.095 (2)	0.0510 (15)	0.0047 (13)	0.0011 (11)	−0.0167 (15)
C2	0.069 (2)	0.075 (2)	0.104 (3)	0.006 (2)	0.010 (2)	−0.016 (2)
C3	0.070 (2)	0.138 (3)	0.0536 (17)	0.007 (2)	0.0170 (16)	−0.026 (2)
C4	0.0638 (19)	0.0767 (18)	0.0364 (12)	−0.0047 (17)	−0.0013 (14)	0.0133 (12)
C5	0.064 (2)	0.083 (3)	0.078 (2)	−0.0223 (18)	−0.0017 (18)	0.003 (2)
C6	0.086 (2)	0.071 (2)	0.0631 (18)	0.0121 (18)	−0.0156 (17)	0.0083 (17)
Mo1	0.03380 (10)	0.03380 (10)	0.02304 (12)	−0.00356 (9)	−0.00072 (6)	0.00072 (6)

O1	0.0687 (12)	0.0566 (10)	0.0277 (7)	-0.0072 (9)	-0.0063 (7)	-0.0049 (7)
O2	0.0350 (9)	0.178 (3)	0.0751 (14)	0.0026 (14)	-0.0119 (9)	-0.0308 (18)

Geometric parameters (Å, °)

N1—H1A	0.8900	C4—H4	0.9800
N1—H1B	0.8900	C4—C5	1.521 (5)
N1—C1	1.506 (4)	C4—C6	1.518 (5)
N1—C4	1.493 (4)	C5—H5A	0.9600
C1—H1	0.9800	C5—H5B	0.9600
C1—C2	1.504 (5)	C5—H5C	0.9600
C1—C3	1.525 (4)	C6—H6A	0.9600
C2—H2A	0.9600	C6—H6B	0.9600
C2—H2B	0.9600	C6—H6C	0.9600
C2—H2C	0.9600	Mo1—O1	1.7505 (15)
C3—H3A	0.9600	Mo1—O1 ⁱ	1.7504 (15)
C3—H3B	0.9600	Mo1—O2	1.732 (2)
C3—H3C	0.9600	Mo1—O2 ⁱ	1.732 (2)
H1A—N1—H1B	107.1	N1—C4—H4	108.7
C1—N1—H1A	107.8	N1—C4—C5	110.5 (2)
C1—N1—H1B	107.8	N1—C4—C6	107.3 (3)
C4—N1—H1A	107.8	C5—C4—H4	108.7
C4—N1—H1B	107.8	C6—C4—H4	108.7
C4—N1—C1	118.2 (2)	C6—C4—C5	112.9 (3)
N1—C1—H1	108.5	C4—C5—H5A	109.5
N1—C1—C3	110.1 (3)	C4—C5—H5B	109.5
C2—C1—N1	108.0 (3)	C4—C5—H5C	109.5
C2—C1—H1	108.5	H5A—C5—H5B	109.5
C2—C1—C3	113.0 (3)	H5A—C5—H5C	109.5
C3—C1—H1	108.5	H5B—C5—H5C	109.5
C1—C2—H2A	109.5	C4—C6—H6A	109.5
C1—C2—H2B	109.5	C4—C6—H6B	109.5
C1—C2—H2C	109.5	C4—C6—H6C	109.5
H2A—C2—H2B	109.5	H6A—C6—H6B	109.5
H2A—C2—H2C	109.5	H6A—C6—H6C	109.5
H2B—C2—H2C	109.5	H6B—C6—H6C	109.5
C1—C3—H3A	109.5	O1 ⁱ —Mo1—O1	110.33 (12)
C1—C3—H3B	109.5	O2 ⁱ —Mo1—O1	109.13 (11)
C1—C3—H3C	109.5	O2—Mo1—O1 ⁱ	109.13 (11)
H3A—C3—H3B	109.5	O2—Mo1—O1	108.77 (10)
H3A—C3—H3C	109.5	O2 ⁱ —Mo1—O1 ⁱ	108.77 (10)
H3B—C3—H3C	109.5	O2 ⁱ —Mo1—O2	110.7 (2)
C1—N1—C4—C5	-59.1 (3)	C4—N1—C1—C2	176.6 (2)
C1—N1—C4—C6	177.5 (2)	C4—N1—C1—C3	-59.5 (3)

Symmetry code: (i) $y, x, -z+1$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1A···O2	0.89	1.80	2.684 (3)	170
N1—H1B···O1 ⁱⁱ	0.89	1.81	2.695 (2)	174

Symmetry code: (ii) $y+1/2, -x+1/2, z+1/4$.