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Bis[2-(pyrimidin-2-ylamino)pyrimidinium] hexamolybdate

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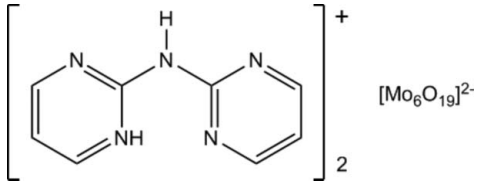
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.018 Å; R factor = 0.057; wR factor = 0.146; data-to-parameter ratio = 11.5.

The title compound, $(C_8H_8N_5)_2[Mo_6O_{19}]$, was prepared by reaction of $Mo(CO)_6$ and dipyrimidylamine in refluxing toluene. The hexanuclear polyoxomolybdate anions lie on centres of inversion. Each 2-(pyrimidin-2-ylamino)pyrimidinium cation forms an intramolecular N—H···N hydrogen bond and the cations are linked through self-complementary pairs of N—H···N hydrogen bonds into dimers across centres of inversion. The cations and anions are interlinked through C—H···O contacts.

Related literature

For related literature, see: Shivaiah (2006); Bridgeman & Cavigliasso (2002); Shi *et al.* (2006); Wang *et al.* (2004); Guo *et al.* (2004); Burkholder & Zubieta (2004); Hagrman *et al.* (1999).



Experimental

Crystal data

$(C_8H_8N_5)_2[Mo_6O_{19}]$
M_r = 1228.03
Monoclinic, $P2_1/n$
a = 10.4338 (19) Å
b = 13.7437 (19) Å
c = 11.0792 (17) Å
β = 105.471 (13)°
V = 1531.2 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.48 mm^{-1}
T = 295 (2) K
0.40 × 0.20 × 0.05 mm

Data collection

Bruker $P4$ diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.578, T_{max} = 0.883
3399 measured reflections
2660 independent reflections
1833 reflections with $I > 2\sigma(I)$
R_{int} = 0.082
3 standard reflections
every 97 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.146
S = 1.02
2660 reflections
232 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$\Delta\rho_{min}$ = −1.78 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3N···N4	0.86	1.95	2.605 (12)	132
N1—H1N···N5^{i}	0.86	2.07	2.924 (13)	180
C2—H2···O8^{ii}	0.93	2.65	3.444 (14)	144
C4—H4···O2^{iii}	0.93	2.69	3.391 (14)	133
C6—H6···O6^{iv}	0.93	2.38	3.250 (15)	157
C7—H7···O1^{v}	0.93	2.51	3.196 (14)	131

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (iv) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (v) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS* program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2259).

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supporting information

Acta Cryst. (2008). E**64**, m41 [https://doi.org/10.1107/S1600536807062897]

Bis[2-(pyrimidin-2-ylamino)pyrimidinium] hexamolybdate

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S1. Comment

Polyoxomolybdates are an important class of metal-oxygen cluster compounds (Shivaiah, 2006; Bridgeman & Cavigliasso, 2002) which show interesting chemical and physical properties (Shi, *et al.*, 2006; Wang, *et al.*, 2004; Guo, *et al.*, 2004; Burkholder & Zubieta, 2004; Hagrman, *et al.*, 1999). Since the anions contain many oxygen atoms which are good hydrogen-bond acceptors, cocrystallization with organic cations should result in interesting supramolecular chemistry. In the title complex (Fig. 1), the protonated dipyrimidylamine molecules (Hdipm) are linked into dimers by N—H···N hydrogen bonds. The cations and anions are interlinked through C—H···O contacts (Fig. 2).

S2. Experimental

$Mo(CO)_6$ (0.52 g, 2.00 mmol) was added to a solution of dipyrimidylamine (dipm) (0.34 g, 2.00 mmol) in 20 ml toluene. The mixture was refluxed for 18 h to yield an orange solution. The solvent was reduced and *n*-hexanes added to induce precipitation. The precipitate was filtered and washed by ether (3 × 10 ml) and then dried under reduced pressure to give an orange powder. The green plate crystals were obtained by slow diffusion of ether into a CH_2Cl_2 solution of the orange powder. The crystals were filtered and washed by ether (3 × 10 ml) and then dried under reduced pressure. Overall crystal yield: 0.207 g (8.43%, based on Mo). Elemental analysis calculated: C, 15.16%; H, 1.31%; N, 11.41%; found: C, 15.02%; H, 1.34%; N, 11.03%.

S3. Refinement

H atoms were placed geometrically with C—H = 0.93 Å and N—H = 0.86 Å, and refined as riding with U_{iso}(H) = U_{eq}(C/N).

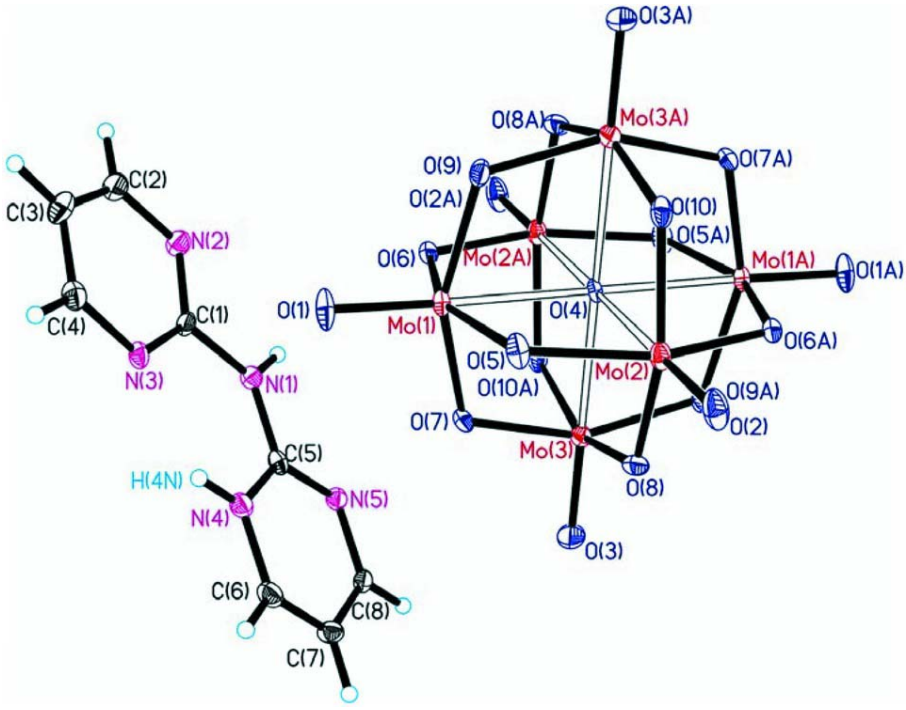

Figure 1

The molecular structure of the title compound showing displacement ellipsoids at the 30% probability level for non-H atoms.

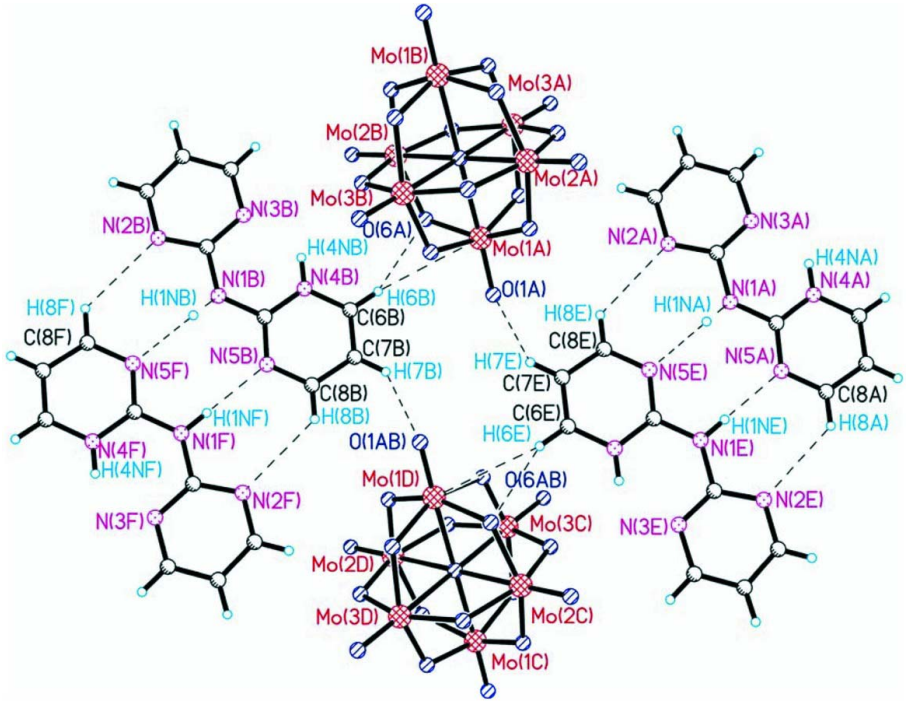

Figure 2

Partial packing diagram showing N—H···N hydrogen bonding between Hdipm molecules and C—H···O contacts to the polyoxometalate.

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$(C_8H_8N_5)_2[Mo_6O_{19}]$
$M_r = 1228.03$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.4338\ (19)$ Å
$b = 13.7437\ (19)$ Å
$c = 11.0792\ (17)$ Å
$\beta = 105.471\ (13)°$
$V = 1531.2\ (4)$ Å^3
$Z = 2$
$F(000) = 1172$
$D_x = 2.664$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 31 reflections
$\theta = 4.8–12.5°$
$\mu = 2.48$ mm^{-1}
$T = 295$ K
Plate, green
0.40 × 0.20 × 0.05 mm

Data collection

Bruker P4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.578$, $T_{max} = 0.883$
3399 measured reflections
2660 independent reflections
1833 reflections with $I > 2\sigma(I)$
$R_{int} = 0.082$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -1 \rightarrow 12$
$k = -1 \rightarrow 16$
$l = -13 \rightarrow 12$
3 standard reflections every 97 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.146$
$S = 1.02$
2660 reflections
232 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0858P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.91$ e Å^{-3}
$\Delta\rho_{min} = -1.78$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
Mo1	0.06601 (9)	0.95848 (7)	0.32376 (8)	0.0380 (3)
Mo2	−0.15184 (9)	0.87281 (7)	0.46013 (9)	0.0418 (3)
Mo3	0.16049 (9)	0.89727 (7)	0.61876 (9)	0.0434 (3)

N1	0.4384 (8)	0.9695 (6)	0.3239 (8)	0.040 (2)
H1N	0.4607	1.0166	0.3764	0.048*
N2	0.4053 (10)	1.0908 (7)	0.1792 (9)	0.052 (2)
N3	0.3659 (9)	0.9281 (7)	0.1128 (8)	0.043 (2)
H3N	0.3676	0.8676	0.1331	0.052*
N4	0.4025 (9)	0.8036 (6)	0.2961 (9)	0.046 (2)
N5	0.4845 (8)	0.8709 (6)	0.4968 (9)	0.040 (2)
O1	0.1142 (7)	0.9318 (7)	0.1952 (7)	0.065 (2)
O2	−0.2622 (8)	0.7811 (6)	0.4336 (9)	0.072 (3)
O3	0.2743 (9)	0.8222 (7)	0.7019 (9)	0.076 (3)
O4	0.0000	1.0000	0.5000	0.0286 (19)
O5	−0.0732 (7)	0.8658 (5)	0.3211 (7)	0.052 (2)
O6	0.1775 (7)	1.0683 (5)	0.3902 (7)	0.0414 (17)
O7	0.1797 (7)	0.8825 (5)	0.4514 (7)	0.0446 (18)
O8	0.0033 (7)	0.8138 (5)	0.5623 (8)	0.056 (2)
O9	−0.0736 (7)	1.0520 (6)	0.2626 (6)	0.052 (2)
O10	−0.2525 (6)	0.9816 (6)	0.3719 (6)	0.0465 (19)
C1	0.4034 (10)	0.9955 (8)	0.1993 (9)	0.041 (3)
C2	0.3673 (12)	1.1171 (10)	0.0578 (12)	0.060 (3)
H2	0.3699	1.1827	0.0376	0.072*
C3	0.3249 (13)	1.0509 (11)	−0.0372 (12)	0.064 (4)
H3	0.2968	1.0711	−0.1202	0.077*
C4	0.3252 (12)	0.9553 (10)	−0.0069 (11)	0.055 (3)
H4	0.2971	0.9089	−0.0694	0.066*
C5	0.4425 (9)	0.8789 (7)	0.3750 (10)	0.037 (2)
C6	0.4060 (12)	0.7135 (9)	0.3495 (12)	0.054 (3)
H6	0.3774	0.6596	0.2987	0.064*
C7	0.4491 (11)	0.7019 (8)	0.4714 (11)	0.048 (3)
H7	0.4537	0.6402	0.5068	0.057*
C8	0.4876 (10)	0.7831 (8)	0.5462 (10)	0.046 (3)
H8	0.5161	0.7758	0.6327	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.0374 (5)	0.0496 (6)	0.0324 (5)	−0.0021 (4)	0.0188 (4)	−0.0061 (4)
Mo2	0.0393 (5)	0.0414 (5)	0.0508 (6)	−0.0114 (4)	0.0228 (4)	−0.0095 (4)
Mo3	0.0400 (5)	0.0502 (6)	0.0424 (6)	0.0122 (4)	0.0151 (4)	0.0098 (5)
N1	0.043 (5)	0.041 (5)	0.035 (5)	−0.002 (4)	0.009 (4)	−0.005 (4)
N2	0.059 (6)	0.049 (6)	0.048 (6)	−0.006 (5)	0.016 (5)	0.000 (5)
N3	0.053 (5)	0.046 (5)	0.034 (5)	0.004 (4)	0.016 (4)	−0.005 (4)
N4	0.047 (5)	0.042 (5)	0.051 (6)	0.003 (4)	0.018 (4)	−0.007 (5)
N5	0.036 (5)	0.045 (5)	0.038 (5)	0.004 (4)	0.009 (4)	0.001 (4)
O1	0.046 (4)	0.120 (7)	0.036 (4)	−0.014 (5)	0.023 (4)	−0.025 (5)
O2	0.069 (6)	0.067 (6)	0.100 (7)	−0.029 (5)	0.054 (5)	−0.034 (5)
O3	0.067 (6)	0.088 (7)	0.075 (6)	0.035 (5)	0.026 (5)	0.038 (5)
O4	0.024 (4)	0.037 (5)	0.029 (5)	−0.002 (4)	0.014 (4)	−0.009 (4)
O5	0.047 (4)	0.055 (5)	0.061 (5)	−0.024 (4)	0.029 (4)	−0.029 (4)

O6	0.040 (4)	0.042 (4)	0.049 (4)	0.004 (3)	0.025 (3)	0.003 (3)
O7	0.042 (4)	0.042 (4)	0.058 (5)	0.012 (3)	0.028 (4)	0.003 (4)
O8	0.062 (5)	0.032 (4)	0.085 (6)	0.012 (4)	0.037 (5)	0.014 (4)
O9	0.042 (4)	0.083 (6)	0.034 (4)	0.013 (4)	0.017 (3)	0.016 (4)
O10	0.028 (3)	0.077 (5)	0.035 (4)	−0.003 (4)	0.009 (3)	−0.002 (4)
C1	0.046 (6)	0.047 (7)	0.034 (6)	−0.002 (5)	0.018 (5)	0.004 (5)
C2	0.063 (8)	0.066 (8)	0.053 (8)	0.001 (7)	0.021 (7)	0.007 (7)
C3	0.067 (8)	0.085 (10)	0.039 (7)	−0.007 (7)	0.011 (6)	0.010 (7)
C4	0.055 (7)	0.066 (8)	0.046 (8)	0.004 (6)	0.017 (6)	−0.005 (6)
C5	0.025 (5)	0.047 (6)	0.038 (6)	−0.001 (4)	0.008 (4)	−0.012 (5)
C6	0.061 (7)	0.044 (7)	0.060 (9)	0.002 (6)	0.023 (6)	−0.012 (6)
C7	0.058 (7)	0.035 (6)	0.048 (8)	0.000 (5)	0.011 (6)	−0.002 (5)
C8	0.051 (7)	0.052 (7)	0.041 (7)	0.007 (5)	0.023 (5)	0.008 (6)

Geometric parameters (Å, º)

Mo1—O1	1.673 (7)	N3—C1	1.315 (13)
Mo1—O7	1.897 (7)	N3—C4	1.333 (14)
Mo1—O9	1.926 (7)	N3—H3N	0.860
Mo1—O5	1.926 (7)	N4—C5	1.347 (13)
Mo1—O6	1.927 (7)	N4—C6	1.369 (15)
Mo1—O4	2.3087 (9)	N5—C5	1.308 (13)
Mo2—O2	1.680 (8)	N5—C8	1.321 (13)
Mo2—O8	1.892 (8)	O4—Mo1^{i}	2.3087 (9)
Mo2—O6^{i}	1.927 (7)	O4—Mo3^{i}	2.3137 (9)
Mo2—O5	1.931 (8)	O4—Mo2^{i}	2.3210 (9)
Mo2—O10	1.935 (7)	O6—Mo2^{i}	1.927 (7)
Mo2—O4	2.3210 (9)	O9—Mo3^{i}	1.916 (7)
Mo3—O3	1.655 (8)	O10—Mo3^{i}	1.911 (8)
Mo3—O10^{i}	1.911 (8)	C2—C3	1.372 (18)
Mo3—O9^{i}	1.916 (7)	C2—H2	0.930
Mo3—O7	1.928 (8)	C3—C4	1.356 (19)
Mo3—O8	1.963 (8)	C3—H3	0.930
Mo3—O4	2.3137 (9)	C4—H4	0.930
N1—C5	1.364 (13)	C6—C7	1.314 (16)
N1—C1	1.378 (13)	C6—H6	0.930
N1—H1N	0.860	C7—C8	1.384 (15)
N2—C1	1.329 (14)	C7—H7	0.930
N2—C2	1.347 (15)	C8—H8	0.930
O1—Mo1—O7	104.1 (4)	C1—N3—H3N	120.6
O1—Mo1—O9	102.6 (4)	C4—N3—H3N	120.6
O7—Mo1—O9	153.3 (3)	C5—N4—C6	116.5 (10)
O1—Mo1—O5	103.8 (4)	C5—N5—C8	117.9 (9)
O7—Mo1—O5	88.1 (3)	Mo1^{i}—O4—Mo1	180.0
O9—Mo1—O5	86.5 (4)	Mo1^{i}—O4—Mo3	90.22 (4)
O1—Mo1—O6	102.0 (4)	Mo1—O4—Mo3	89.78 (4)
O7—Mo1—O6	87.3 (3)	Mo1^{i}—O4—Mo3^{i}	89.78 (4)

O9—Mo1—O6	86.2 (3)	Mo1—O4—Mo3^{i}	90.22 (4)
O5—Mo1—O6	154.1 (3)	Mo3—O4—Mo3^{i}	180.0
O1—Mo1—O4	178.3 (4)	Mo1^{i}—O4—Mo2	90.27 (3)
O7—Mo1—O4	76.9 (2)	Mo1—O4—Mo2	89.73 (3)
O9—Mo1—O4	76.4 (2)	Mo3—O4—Mo2	90.14 (4)
O5—Mo1—O4	77.4 (2)	Mo3^{i}—O4—Mo2	89.86 (4)
O6—Mo1—O4	76.7 (2)	Mo1^{i}—O4—Mo2^{i}	89.73 (3)
O2—Mo2—O8	102.7 (4)	Mo1—O4—Mo2^{i}	90.27 (3)
O2—Mo2—O6^{i}	102.7 (4)	Mo3—O4—Mo2^{i}	89.86 (4)
O8—Mo2—O6^{i}	87.6 (3)	Mo3^{i}—O4—Mo2^{i}	90.14 (4)
O2—Mo2—O5	103.9 (3)	Mo2—O4—Mo2^{i}	180.0
O8—Mo2—O5	88.8 (4)	Mo1—O5—Mo2	115.7 (3)
O6^{i}—Mo2—O5	153.3 (3)	Mo2^{i}—O6—Mo1	116.7 (3)
O2—Mo2—O10	103.7 (4)	Mo1—O7—Mo3	117.0 (3)
O8—Mo2—O10	153.6 (3)	Mo2—O8—Mo3	116.7 (3)
O6^{i}—Mo2—O10	85.9 (3)	Mo3^{i}—O9—Mo1	116.9 (3)
O5—Mo2—O10	85.6 (3)	Mo3^{i}—O10—Mo2	116.6 (3)
O2—Mo2—O4	179.1 (3)	N3—C1—N2	125.9 (10)
O8—Mo2—O4	77.2 (2)	N3—C1—N1	119.6 (10)
O6^{i}—Mo2—O4	76.4 (2)	N2—C1—N1	114.3 (10)
O5—Mo2—O4	77.0 (2)	N2—C2—C3	122.4 (13)
O10—Mo2—O4	76.4 (2)	N2—C2—H2	118.8
O3—Mo3—O10^{i}	103.7 (4)	C3—C2—H2	118.8
O3—Mo3—O9^{i}	104.2 (4)	C4—C3—C2	118.3 (12)
O10^{i}—Mo3—O9^{i}	88.2 (3)	C4—C3—H3	120.9
O3—Mo3—O7	103.1 (4)	C2—C3—H3	120.9
O10^{i}—Mo3—O7	88.0 (3)	N3—C4—C3	119.8 (12)
O9^{i}—Mo3—O7	152.6 (3)	N3—C4—H4	120.1
O3—Mo3—O8	103.1 (4)	C3—C4—H4	120.1
O10^{i}—Mo3—O8	153.1 (3)	N5—C5—N4	124.5 (10)
O9^{i}—Mo3—O8	85.6 (3)	N5—C5—N1	118.0 (9)
O7—Mo3—O8	85.7 (3)	N4—C5—N1	117.5 (9)
O3—Mo3—O4	179.0 (4)	C7—C6—N4	121.1 (11)
O10^{i}—Mo3—O4	77.1 (2)	C7—C6—H6	119.5
O9^{i}—Mo3—O4	76.4 (2)	N4—C6—H6	119.5
O7—Mo3—O4	76.2 (2)	C6—C7—C8	118.8 (11)
O8—Mo3—O4	76.0 (2)	C6—C7—H7	120.6
C5—N1—C1	128.6 (9)	C8—C7—H7	120.6
C5—N1—H1N	115.7	N5—C8—C7	121.2 (10)
C1—N1—H1N	115.7	N5—C8—H8	119.4
C1—N2—C2	114.8 (10)	C7—C8—H8	119.4
C1—N3—C4	118.7 (10)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*N*···N4	0.86	1.95	2.605 (12)	132

N1—H1*N*···N5^{ii}	0.86	2.07	2.924 (13)	180
C2—H2···O8^{iii}	0.93	2.65	3.444 (14)	144
C4—H4···O2^{iv}	0.93	2.69	3.391 (14)	133
C6—H6···O6^{v}	0.93	2.38	3.250 (15)	157
C7—H7···O1^{vi}	0.93	2.51	3.196 (14)	131

Symmetry codes: (ii) $-x+1, -y+2, -z+1$; (iii) $-x+1/2, y+1/2, -z+1/2$; (iv) $x+1/2, -y+3/2, z-1/2$; (v) $-x+1/2, y-1/2, -z+1/2$; (vi) $x+1/2, -y+3/2, z+1/2$.