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# Synthesis and crystal structure of a new hybrid organic–inorganic material containing neutral molecules, cations and heptamolybdate anions

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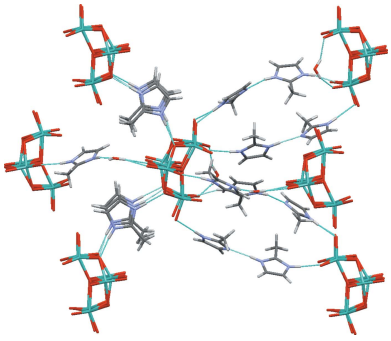
The title compound, hexakis(2-methyl-1*H*-imidazol-3-ium) heptamolybdate 2-methyl-1*H*-imidazole disolvate dihydrate, $(C_4H_7N_2)_6[Mo_7O_{24}]\cdot 2C_4H_6N_2\cdot 2H_2O$, was prepared from 2-methylimidazole and ammonium heptamolybdate tetrahydrate in acid solution. The $[Mo_7O_{24}]^{6-}$ heptamolybdate cluster anion is accompanied by six protonated $(C_4H_7N_2)^+$ 2-methylimidazolium cations, two neutral $C_4H_6N_2$ 2-methylimidazole molecules and two water molecules of crystallization. The cluster consists of seven distorted $MoO_6$ octahedra sharing edges or vertices. In the crystal, the components are linked by N—H···N, N—H···O, O—H···O, N—H···(O,O) and O—H···(O,O) hydrogen bonds, generating a three-dimensional network. Weak C—H···O interactions consolidate the packing.

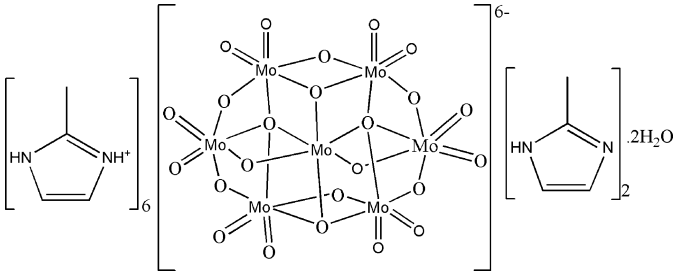
## 1. Chemical context

Polyoxometalates (POMs) are clusters of transition metals (*M* = V, Nb, Ta, Mo, W, ···) and oxygen atoms with a structural and compositional diversity that lead to numerous applications because of their electrochemical, optical, catalytic and photochromic properties as well as their antiviral and antitumor activities (Katsoulis, 1998; Hasenknopf, 2005; Gerth *et al.*, 2005; Coué *et al.*, 2007). In this context, the $[Mo_7O_{24}]^{6-}$ heptamolybdate anion has been isolated with numerous different counter-cations such as 4-aminopyridinium, *N*-pentylammonium, diethylenetriammonium, *N*,*N*,*N*′,*N*′-tetramethylethylenediammonium, tetramethylammonium, guanidinium, hexanediammonium, butan-1-aminium, ammonium, potassium and sodium (Román *et al.*, 1985, 1988, 1990, 1992; Don & Weakly, 1981; Gatehouse & Leverett, 1968; Sjöbom & Hedman, 1973; Niu *et al.*, 1996; Himeno *et al.*, 1997; Reinoso *et al.*, 2008; Ftini, 2015; Khandolkar *et al.*, 2016). As a continuation of our work in this area (Sarr *et al.*, 2018), we now describe the synthesis and structure of the title compound (I), which is notable for the incorporation of both protonated $[C_4H_7N_2]^+$ 2-methylimidazolium cations and neutral $C_4H_6N_2$ 2-methylimidazole molecules in the crystal.



## 2. Structural commentary

The title compound is characterized by the presence of the familiar $[Mo_7O_{24}]^{6-}$ heptamolybdate cluster anion (Fig. 1).




There are four categories of oxygen atoms within the polyanion: $O_t$ (terminal oxygen atoms), $\mu^2$-O (oxygen atoms bridging two molybdenum atoms), $\mu^3$-O (oxygen atoms bridging three molybdenum atoms) and $\mu^4$-O (oxygen atoms bridging four molybdenum atoms). All of the Mo atoms are bound to two terminal oxygen atoms except for Mo7, which is located in the 'core' of the cluster. The geometrical data for the cluster in (I) are consistent with those found in previous studies (Román *et al.*, 1992; Reinoso *et al.*, 2008): the Mo—O bond lengths vary between 1.707 (2) and 1.726 (2) Å for $O_t$, 1.754 (2)—2.453 (2) Å for $\mu^2$-O, 1.8945 (19)–2.3057 (19) Å for $\mu^3$-O and 2.1329 (19)–2.3011 (18) Å for $\mu^4$-O. The variations of Mo—O bond lengths and O—Mo—O angles indicate that all seven octahedra ($MoO_6$) within the cluster are highly distorted. As in the compound $(H_3dien)_2[Mo_7O_{24}]\cdot 4H_2O$ (Román *et al.*, 1988), we note that the longest Mo—O bond length derives from an oxygen atom bridging two molybdenum atoms ($\mu^2$-O). As well as the $[Mo_7O_{24}]^{6-}$ anion, six $(C_4H_7N_2)^+$ cations, two neutral $C_4H_6N_2$ molecules and two water molecules of crystallization are present in the asymmetric unit (Fig. 2).

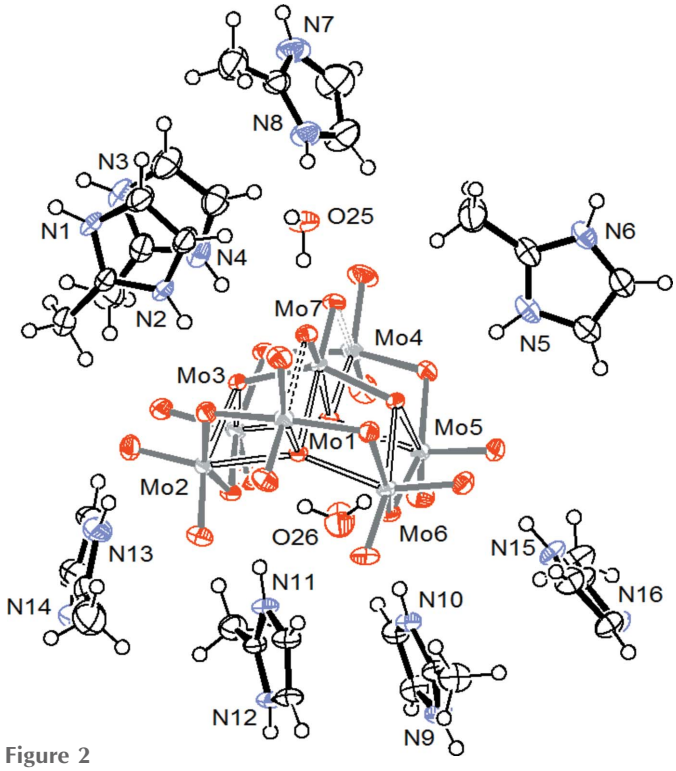



**Figure 2**
The asymmetric unit of (I) with displacement ellipsoids drawn at the 50% probability level.

## 3. Supramolecular features

In the crystal, each heptamolybdate anion interacts with six neighbours *via* the water molecules, $(C_4H_7N_2)^+$ cations and/or neutral 2-methylimidazole molecules (Fig. 3). These interactions occur through simple O—H···O, N—H···O and N—H···N and bifurcated N—H···(O,O) and O—H···(O,O)

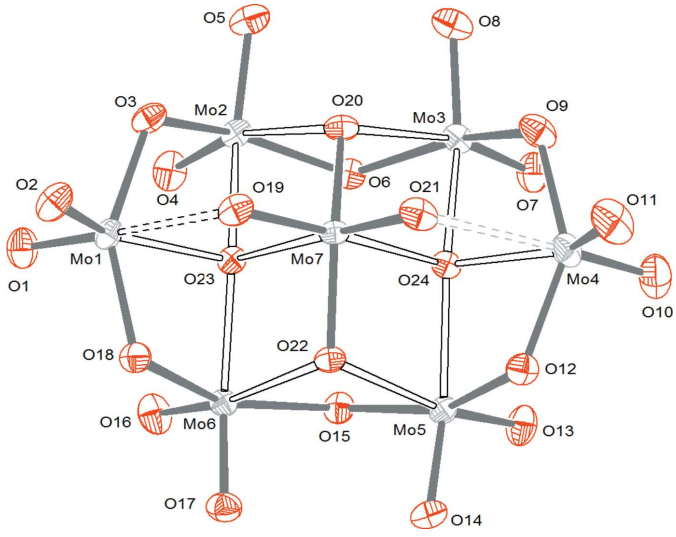



**Figure 1**
Molecular structure of the $[Mo_7O_{24}]^{6-}$ heptamolybdate cluster anion in (I).

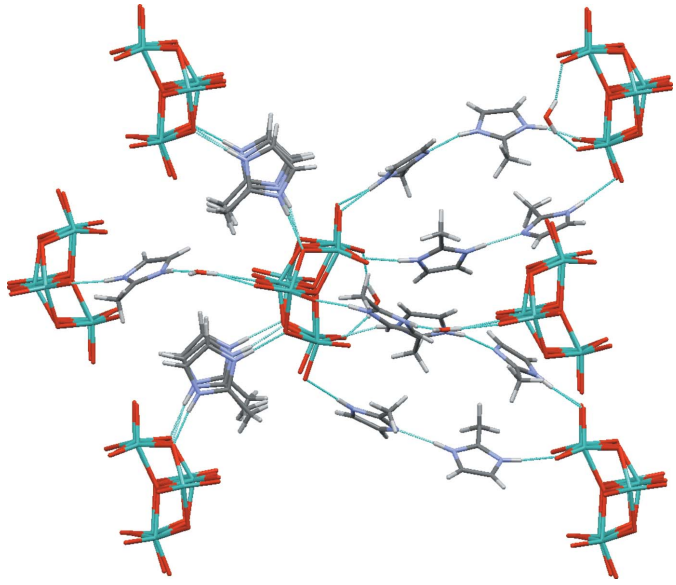


**Figure 3**
Detail of the structure of (I) showing the interconnections of the $[Mo_7O_{24}]^{6-}$ anion with its neighbours.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$N$···O22$^{i}$ | 0.88 (2) | 1.85 (2) | 2.710 (3) | 167 (2) |
| N2—H2$N$···O20 | 0.87 (2) | 1.79 (2) | 2.655 (3) | 172 (2) |
| N3—H3$N$···O18$^{i}$ | 0.88 (2) | 1.87 (2) | 2.743 (4) | 171 (5) |
| N4—H4$N$···O9 | 0.88 (2) | 1.79 (2) | 2.662 (4) | 171 (5) |
| N5—H5$N$···O12 | 0.89 (2) | 1.77 (3) | 2.644 (4) | 168 (4) |
| N6—H6$N$···O3$^{ii}$ | 0.90 (2) | 1.80 (3) | 2.684 (4) | 168 (5) |
| N7—H7$N$···O1$^{iii}$ | 0.89 (3) | 1.83 (3) | 2.697 (4) | 167 (3) |
| N8—H8$N$···O25 | 0.89 (3) | 1.78 (3) | 2.659 (4) | 172 (5) |
| N9—H9$N$···N14$^{iv}$ | 0.89 (2) | 1.81 (2) | 2.698 (4) | 177 (3) |
| N10—H10$N$···O15 | 0.88 (2) | 1.98 (2) | 2.852 (3) | 174 (3) |
| N11—H11$N$···O6 | 0.88 (2) | 1.78 (2) | 2.636 (3) | 166 (3) |
| N12—H12$N$···N16$^{v}$ | 0.88 (2) | 1.87 (2) | 2.725 (4) | 165 (3) |
| N13—H13$N$···O5 | 0.88 (4) | 2.32 (4) | 3.186 (5) | 167 (3) |
| N13—H13$N$···O8 | 0.88 (4) | 2.55 (4) | 3.043 (5) | 116 (2) |
| N15—H15$N$···O14 | 0.87 (3) | 2.22 (3) | 2.953 (4) | 142 (3) |
| N15—H15$N$···O17 | 0.87 (3) | 2.27 (3) | 2.917 (4) | 132 (3) |
| O25—H25$V$···O19 | 0.86 (2) | 2.00 (2) | 2.788 (3) | 154 (5) |
| O25—H25$W$···O26$^{vi}$ | 0.86 (3) | 1.85 (3) | 2.702 (4) | 176 (5) |
| O26—H26$V$···O10 | 0.83 (4) | 2.50 (6) | 2.999 (4) | 119 (5) |
| O26—H26$V$···O13 | 0.83 (4) | 2.25 (5) | 3.009 (4) | 151 (6) |
| O26—H26$W$···O7 | 0.83 (4) | 1.99 (6) | 2.737 (4) | 149 (6) |
| C4—H4$A$···O8 | 0.98 | 2.35 | 3.228 (5) | 149 |
| C8—H8$B$···O2$^{i}$ | 0.98 | 2.54 | 3.517 (6) | 176 |
| C8—H8$C$···O8 | 0.98 | 2.49 | 3.386 (5) | 152 |
| C10—H10···O26$^{vii}$ | 0.95 | 2.45 | 3.318 (5) | 151 |
| C12—H12$A$···O5$^{ii}$ | 0.98 | 2.44 | 3.407 (5) | 167 |
| C13—H13···O4$^{iii}$ | 0.95 | 2.50 | 3.297 (6) | 141 |
| C17—H17···O2$^{viii}$ | 0.95 | 2.46 | 3.154 (4) | 130 |
| C18—H18···O26 | 0.95 | 2.58 | 3.522 (5) | 172 |
| C21—H21···O16 | 0.95 | 2.46 | 3.302 (4) | 147 |
| C22—H22···O11$^{ix}$ | 0.95 | 2.22 | 3.113 (4) | 156 |
| C24—H24$B$···O7 | 0.98 | 2.50 | 3.346 (5) | 145 |
| C25—H25···O8 | 0.95 | 2.59 | 3.055 (5) | 110 |
| C32—H32$B$···O14 | 0.98 | 2.55 | 3.234 (5) | 126 |

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

hydrogen bonds (Table 1) involving three categories of oxygen atoms of the polyanion: $O_t$, $\mu^2$-O and $\mu^3$-O. The N—H···N hydrogen bonds from N9 and N12 link $(C_4H_7N_2)^+$ cations to neutral molecules. The packing is consolidated by weak C—H···O links (Table 1). The overall hydrogen-bonding topology is an infinite three-dimensional network.

## 4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.40, update November 2018; Groom *et al.*, 2016) resulted in 35 hits for the heptamolybdate anion and 90 hits for the 2-methylimidazolium cation.

## 5. Synthesis and crystallization

Sulfuric acid (2.1 g, 21.7 mmol), 2-methylimidazole (3.5 g, 43.4 mmol) and ammonium heptamolybdate tetrahydrate (2.2 g, 1.8 mmol) in a ratio of 1:2:1/12 were dissolved in water (60 ml). The solution was stirred for one h and evaporated in the oven at 333 K to yield a whitish precipitate. The precipitate was recrystallized from methanol solution: after two weeks at room temperature, colourless prisms of (I) were recovered.

The IR spectrum of (I) is included in the supporting information. The absorption bands at 3400 and 3395 cm$^{-1}$ correspond to $\nu$(O—H) stretches and indicate the presence of water molecules and those at 1621 and 1564 cm$^{-1}$ to the deformation vibrations $\delta$(O—H). The bands centered at 3132 and 1431 cm$^{-1}$ with shoulders are respectively attributed to the stretching and deformation vibrations of the N—H bonds of the protonated and/or non-protonated entities of 2-methylimidazole (Jinnah *et al.*, 2004). The bands between 2904–2686 cm$^{-1}$ are attributed to the stretching vibrations of the C—H bonds, while that at 1291 cm$^{-1}$ is a $\delta$(C—H) deformation vibration (Jinnah *et al.*, 2004). The two bands at 929 and 900 cm$^{-1}$ correspond to $\nu$(Mo—Ot) stretching vibrations while the bands between 838 and 650 cm$^{-1}$ are typical for the vibrations of $\nu$(Mo—O—Mo) and $\nu$[Mo—($\mu$-O)] groupings (Dey *et al.*, 2011).

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $(C_4H_7N_2)_6[Mo_7O_{24}]\cdot 2C_4H_6N_2\cdot 2H_2O$ |
| $M_r$ | 1754.52 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 170 |
| $a$, $b$, $c$ (Å) | 16.5325 (2), 17.5842 (2), 19.8873 (2) |
| $\beta$ (°) | 90.653 (1) |
| $V$ (Å$^3$) | 5781.08 (11) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 1.56 |
| Crystal size (mm) | 0.38 × 0.28 × 0.19 |
| | |
| Data collection | |
| Diffractometer | Agilent Xcalibur, Sapphire2 |
| Absorption correction | Multi-scan (*CrysAlis PRO*; Agilent, 2014) |
| $T_{min}$, $T_{max}$ | 0.476, 0.756 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 104921, 27993, 21593 |
| $R_{int}$ | 0.053 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.833 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.046, 0.120, 1.15 |
| No. of reflections | 27993 |
| No. of parameters | 792 |
| No. of restraints | 58 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 1.83, −2.87 |

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SIR92* (Altomare *et al.*, 1992), *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

## 6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms treated by a mixture of independent and constrained refinement were placed in

geometrically idealized positions and constrained to ride on their parent atoms, with N—H distances of 0.87 (2), 0.88 (2) and 0.89 (2) Å, Cmethyl—H = 0.97/0.98 Å and Cmethine—H = 0.94/0.95 Å, and with $U_{iso}$ (H) = 1.2$U_{eq}$(C,N) or 1.5$U_{eq}$(C-methyl).

## Acknowledgements

The authors thank the Université Cheikh Anta Diop Dakar-Sénégal, the Laboratoire de Chimie et de Physique des Matériaux (LCPM) de l'Université Assane Seck de Ziguinchor, Sénégal and the service commun d'analyse par diffraction des rayons *X*, Universitée de Bretagne Occidentale, France for financial support. All measurements were performed in the institutes above quoted.

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# supporting information

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## Synthesis and crystal structure of a new hybrid organic–inorganic material containing neutral molecules, cations and heptamolybdate anions

**Bougar Sarr, Abdou Mbaye, Wally Diallo, Cheikh Abdoul Khadir Diop, Mamadou Sidibe and Francois Michaud**

### Computing details

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO* (Agilent, 2014); data reduction: *CrysAlis PRO* (Agilent, 2014); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1992); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

### Hexakis(2-methyl-1*H*-imidazol-3-ium) heptamolybdate 2-methyl-1*H*-imidazole disolvate dihydrate

*Crystal data*

$(C_4H_7N_2)_6[Mo_7O_{24}]\cdot 2C_4H_6N_2\cdot 2H_2O$
$M_r$ = 1754.52
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 16.5325 (2) Å
$b$ = 17.5842 (2) Å
$c$ = 19.8873 (2) Å
$\beta$ = 90.653 (1)°
$V$ = 5781.08 (11) Å$^3$
$Z$ = 4
$F(000)$ = 3456
$D_x$ = 2.016 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 38522 reflections
$\theta$ = 3.5–37.4°
$\mu$ = 1.56 mm$^{-1}$
$T$ = 170 K
Fragment of prism, colourless
0.38 × 0.28 × 0.19 mm

*Data collection*

Agilent Xcalibur, Sapphire2, large Be window diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 8.3622 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
$T_{min}$ = 0.476, $T_{max}$ = 0.756
104921 measured reflections
27993 independent reflections
21593 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.053
$\theta_{max}$ = 36.3°, $\theta_{min}$ = 3.3°
$h$ = −24→27
$k$ = −29→29
$l$ = −33→33

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.120
$S$ = 1.15
27993 reflections
792 parameters
58 restraints
Primary atom site location: structure-invariant direct methods

| | |
|---|---|
| Secondary atom site location: difference Fourier map | $w = 1/[\sigma^2(F_o^2) + (0.0397P)^2 + 11.2859P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| Hydrogen site location: inferred from neighbouring sites | $(\Delta/\sigma)_{max} = 0.011$ |
| H atoms treated by a mixture of independent and constrained refinement | $\Delta\rho_{max} = 1.83$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -2.87$ e Å$^{-3}$ |

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | −0.04305 (13) | 0.24793 (14) | 0.39565 (12) | 0.0280 (4) |
| O2 | 0.00551 (14) | 0.27946 (14) | 0.26843 (11) | 0.0284 (5) |
| O3 | 0.07596 (13) | 0.15830 (12) | 0.34241 (10) | 0.0230 (4) |
| O4 | 0.07336 (14) | 0.12579 (14) | 0.48407 (11) | 0.0269 (4) |
| O5 | 0.15457 (15) | 0.03530 (13) | 0.39571 (12) | 0.0295 (5) |
| O6 | 0.23807 (12) | 0.13563 (11) | 0.47918 (9) | 0.0185 (3) |
| O7 | 0.40034 (14) | 0.12283 (14) | 0.50582 (12) | 0.0284 (5) |
| O8 | 0.33831 (15) | 0.04054 (13) | 0.40157 (12) | 0.0280 (4) |
| O9 | 0.42573 (14) | 0.16391 (13) | 0.36926 (12) | 0.0268 (4) |
| O10 | 0.52563 (15) | 0.25984 (16) | 0.44633 (15) | 0.0364 (6) |
| O11 | 0.50709 (16) | 0.28585 (17) | 0.31122 (14) | 0.0393 (6) |
| O12 | 0.41549 (13) | 0.37036 (12) | 0.40412 (11) | 0.0223 (4) |
| O13 | 0.39387 (13) | 0.34235 (15) | 0.54308 (11) | 0.0277 (4) |
| O14 | 0.32385 (14) | 0.46326 (12) | 0.47845 (11) | 0.0246 (4) |
| O15 | 0.23109 (12) | 0.33656 (12) | 0.51719 (9) | 0.0197 (3) |
| O16 | 0.06318 (13) | 0.33595 (15) | 0.52098 (11) | 0.0278 (5) |
| O17 | 0.13927 (14) | 0.45859 (13) | 0.46625 (11) | 0.0251 (4) |
| O18 | 0.06704 (13) | 0.36491 (12) | 0.37905 (10) | 0.0213 (4) |
| O19 | 0.16800 (13) | 0.28094 (12) | 0.28601 (10) | 0.0227 (4) |
| O20 | 0.24914 (12) | 0.16416 (11) | 0.35550 (9) | 0.0191 (3) |
| O21 | 0.33322 (14) | 0.28445 (13) | 0.29412 (11) | 0.0253 (4) |
| O22 | 0.24226 (12) | 0.36427 (11) | 0.39099 (9) | 0.0171 (3) |
| O23 | 0.14447 (11) | 0.25197 (11) | 0.41666 (9) | 0.0164 (3) |
| O24 | 0.33781 (11) | 0.25392 (11) | 0.42940 (9) | 0.0172 (3) |
| Mo1 | 0.042356 (14) | 0.264056 (14) | 0.348758 (11) | 0.01907 (5) |
| Mo2 | 0.142420 (14) | 0.128403 (13) | 0.420960 (11) | 0.01805 (4) |
| Mo3 | 0.342279 (14) | 0.130828 (14) | 0.434127 (12) | 0.01888 (4) |
| Mo4 | 0.454713 (15) | 0.269540 (15) | 0.383726 (13) | 0.02328 (5) |
| Mo5 | 0.333156 (14) | 0.365314 (13) | 0.475739 (11) | 0.01745 (4) |

| | | | | |
|---|---|---|---|---|
| Mo6 | 0.134696 (14) | 0.360541 (13) | 0.463691 (11) | 0.01669 (4) |
| Mo7 | 0.248954 (14) | 0.271359 (12) | 0.343147 (10) | 0.01554 (4) |
| C1 | 0.2405 (3) | 0.0776 (2) | 0.1309 (2) | 0.0436 (9) |
| H1 | 0.235 | 0.0891 | 0.0844 | 0.052* |
| C2 | 0.2374 (3) | 0.1281 (2) | 0.18283 (19) | 0.0366 (8) |
| H2 | 0.2294 | 0.1814 | 0.1794 | 0.044* |
| C3 | 0.25571 (18) | 0.01393 (18) | 0.22512 (16) | 0.0243 (5) |
| C4 | 0.2682 (3) | −0.0505 (2) | 0.2726 (2) | 0.0466 (10) |
| H4A | 0.2705 | −0.031 | 0.3188 | 0.07* |
| H4B | 0.3192 | −0.0763 | 0.2623 | 0.07* |
| H4C | 0.2233 | −0.0865 | 0.2681 | 0.07* |
| N1 | 0.25288 (17) | 0.00771 (16) | 0.15858 (13) | 0.0265 (5) |
| N2 | 0.24786 (16) | 0.08720 (15) | 0.24065 (13) | 0.0236 (5) |
| H1N | 0.255 (2) | −0.0354 (12) | 0.1362 (13) | 0.028* |
| H2N | 0.248 (2) | 0.1084 (15) | 0.2801 (10) | 0.028* |
| C5 | 0.4466 (3) | 0.0710 (3) | 0.1457 (2) | 0.0472 (10) |
| H5 | 0.4409 | 0.0769 | 0.0984 | 0.057* |
| C6 | 0.4432 (3) | 0.1273 (3) | 0.1927 (2) | 0.0429 (9) |
| H6 | 0.4352 | 0.1801 | 0.1847 | 0.051* |
| C7 | 0.46291 (19) | 0.0184 (2) | 0.2452 (2) | 0.0338 (7) |
| C8 | 0.4797 (3) | −0.0370 (3) | 0.3006 (2) | 0.0458 (10) |
| H8A | 0.5322 | −0.0253 | 0.3215 | 0.069* |
| H8B | 0.4807 | −0.0887 | 0.2822 | 0.069* |
| H8C | 0.4372 | −0.0333 | 0.3344 | 0.069* |
| N3 | 0.45995 (18) | 0.00367 (19) | 0.18011 (18) | 0.0356 (7) |
| N4 | 0.45352 (17) | 0.09260 (18) | 0.25376 (18) | 0.0343 (6) |
| H3N | 0.457 (3) | −0.0409 (12) | 0.1597 (14) | 0.041* |
| H4N | 0.450 (3) | 0.1166 (16) | 0.2926 (10) | 0.041* |
| C9 | 0.4628 (3) | 0.5730 (2) | 0.3839 (2) | 0.0417 (9) |
| H9 | 0.4661 | 0.5816 | 0.431 | 0.05* |
| C10 | 0.4672 (2) | 0.6261 (2) | 0.3346 (2) | 0.0389 (8) |
| H10 | 0.4739 | 0.6794 | 0.3407 | 0.047* |
| C11 | 0.45236 (19) | 0.5147 (2) | 0.28609 (19) | 0.0308 (7) |
| C12 | 0.4469 (3) | 0.4532 (3) | 0.2355 (2) | 0.0536 (12) |
| H12A | 0.4124 | 0.4697 | 0.1979 | 0.08* |
| H12B | 0.4235 | 0.4077 | 0.2561 | 0.08* |
| H12C | 0.5011 | 0.4413 | 0.219 | 0.08* |
| N5 | 0.45244 (17) | 0.50405 (18) | 0.35196 (16) | 0.0316 (6) |
| N6 | 0.46028 (17) | 0.58857 (17) | 0.27414 (16) | 0.0316 (6) |
| H5N | 0.446 (3) | 0.4604 (12) | 0.3735 (13) | 0.038* |
| H6N | 0.456 (3) | 0.6126 (15) | 0.2346 (10) | 0.038* |
| C13 | 0.4092 (3) | 0.3119 (4) | 0.0588 (3) | 0.0606 (14) |
| H13 | 0.4644 | 0.327 | 0.0599 | 0.073* |
| C14 | 0.3540 (3) | 0.3234 (3) | 0.1070 (3) | 0.0549 (12) |
| H14 | 0.363 | 0.3476 | 0.1492 | 0.066* |
| C15 | 0.2921 (3) | 0.2642 (2) | 0.02298 (19) | 0.0364 (8) |
| C16 | 0.2296 (4) | 0.2267 (3) | −0.0190 (3) | 0.0564 (12) |
| H16A | 0.2271 | 0.1726 | −0.0075 | 0.085* |

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|---|---|---|---|---|
| H16B | 0.2433 | 0.2323 | −0.0666 | 0.085* |
| H16C | 0.177 | 0.2503 | −0.0108 | 0.085* |
| N7 | 0.3698 (2) | 0.2740 (2) | 0.00784 (19) | 0.0475 (9) |
| N8 | 0.2818 (2) | 0.2935 (2) | 0.08359 (17) | 0.0398 (7) |
| H7N | 0.3920 (18) | 0.263 (3) | −0.0313 (13) | 0.048* |
| H8N | 0.2341 (13) | 0.301 (3) | 0.1029 (17) | 0.048* |
| C17 | 0.3403 (2) | 0.3084 (2) | 0.75070 (18) | 0.0319 (7) |
| H17 | 0.3787 | 0.2916 | 0.7834 | 0.038* |
| C18 | 0.34305 (19) | 0.2954 (2) | 0.68388 (18) | 0.0300 (6) |
| H18 | 0.3836 | 0.2681 | 0.6606 | 0.036* |
| C19 | 0.23323 (18) | 0.36274 (19) | 0.70469 (15) | 0.0251 (5) |
| C20 | 0.1568 (2) | 0.4053 (3) | 0.6948 (2) | 0.0404 (9) |
| H20A | 0.119 | 0.392 | 0.7305 | 0.061* |
| H20B | 0.1328 | 0.392 | 0.651 | 0.061* |
| H20C | 0.1679 | 0.46 | 0.6962 | 0.061* |
| N9 | 0.27156 (17) | 0.35055 (18) | 0.76280 (14) | 0.0292 (5) |
| N10 | 0.27544 (16) | 0.32947 (17) | 0.65606 (13) | 0.0260 (5) |
| H9N | 0.2597 (19) | 0.369 (2) | 0.8029 (10) | 0.031* |
| H10N | 0.2612 (19) | 0.328 (2) | 0.6133 (9) | 0.031* |
| C21 | 0.1295 (2) | 0.2036 (2) | 0.62572 (16) | 0.0294 (6) |
| H21 | 0.0909 | 0.2298 | 0.5985 | 0.035* |
| C22 | 0.12795 (19) | 0.1954 (2) | 0.69351 (15) | 0.0289 (6) |
| H22 | 0.0878 | 0.2144 | 0.7228 | 0.035* |
| C23 | 0.23697 (19) | 0.13713 (18) | 0.65689 (14) | 0.0241 (5) |
| C24 | 0.3139 (2) | 0.0943 (2) | 0.6550 (2) | 0.0356 (7) |
| H24A | 0.3575 | 0.1257 | 0.6739 | 0.053* |
| H24B | 0.3264 | 0.0813 | 0.6083 | 0.053* |
| H24C | 0.3088 | 0.0476 | 0.6815 | 0.053* |
| N11 | 0.19766 (16) | 0.16674 (17) | 0.60401 (12) | 0.0262 (5) |
| N12 | 0.19571 (16) | 0.15416 (17) | 0.71190 (12) | 0.0257 (5) |
| H11N | 0.2134 (19) | 0.164 (2) | 0.5621 (9) | 0.031* |
| H12N | 0.2122 (19) | 0.145 (2) | 0.7531 (9) | 0.031* |
| C25 | 0.3331 (3) | −0.0694 (3) | 0.5204 (2) | 0.0543 (12) |
| H25 | 0.3753 | −0.0638 | 0.4888 | 0.065* |
| C26 | 0.3380 (3) | −0.1023 (3) | 0.5821 (2) | 0.0498 (11) |
| H26 | 0.3853 | −0.1248 | 0.6009 | 0.06* |
| C27 | 0.2140 (3) | −0.0632 (2) | 0.5699 (2) | 0.0439 (10) |
| C28 | 0.1286 (4) | −0.0448 (3) | 0.5815 (3) | 0.0625 (14) |
| H28A | 0.0994 | −0.0912 | 0.5938 | 0.094* |
| H28B | 0.1046 | −0.0234 | 0.5404 | 0.094* |
| H28C | 0.1248 | −0.0077 | 0.618 | 0.094* |
| N13 | 0.2543 (3) | −0.0461 (2) | 0.51329 (18) | 0.0523 (10) |
| N14 | 0.2641 (2) | −0.0981 (2) | 0.61320 (16) | 0.0421 (8) |
| H13N | 0.2347 (18) | −0.022 (3) | 0.4779 (15) | 0.05* |
| C29 | 0.1459 (2) | 0.5736 (2) | 0.59154 (18) | 0.0331 (7) |
| H29 | 0.0966 | 0.5697 | 0.5669 | 0.04* |
| C30 | 0.1591 (2) | 0.6127 (2) | 0.64964 (18) | 0.0325 (7) |
| H30 | 0.1195 | 0.6411 | 0.673 | 0.039* |

| | | | | |
|---|---|---|---|---|
| C31 | 0.2732 (2) | 0.5611 (2) | 0.62385 (16) | 0.0289 (6) |
| C32 | 0.3600 (2) | 0.5372 (3) | 0.6246 (2) | 0.0472 (11) |
| H32A | 0.3916 | 0.5723 | 0.6526 | 0.071* |
| H32B | 0.3807 | 0.5378 | 0.5786 | 0.071* |
| H32C | 0.3645 | 0.4856 | 0.643 | 0.071* |
| N15 | 0.21866 (17) | 0.54082 (17) | 0.57597 (14) | 0.0287 (5) |
| N16 | 0.23894 (17) | 0.60467 (18) | 0.66955 (14) | 0.0302 (6) |
| H15N | 0.2266 (18) | 0.511 (2) | 0.5419 (15) | 0.036* |
| O25 | 0.14267 (16) | 0.30433 (19) | 0.14871 (12) | 0.0369 (6) |
| H25V | 0.134 (3) | 0.300 (3) | 0.1909 (10) | 0.055* |
| H25W | 0.0957 (17) | 0.302 (3) | 0.130 (2) | 0.055* |
| O26 | 0.4963 (2) | 0.2100 (2) | 0.58818 (17) | 0.0519 (8) |
| H26V | 0.482 (4) | 0.248 (2) | 0.566 (3) | 0.078* |
| H26W | 0.482 (4) | 0.172 (2) | 0.566 (3) | 0.078* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0214 (9) | 0.0333 (12) | 0.0294 (11) | −0.0021 (8) | 0.0030 (8) | 0.0072 (9) |
| O2 | 0.0330 (11) | 0.0339 (12) | 0.0182 (9) | −0.0065 (9) | −0.0104 (8) | 0.0047 (8) |
| O3 | 0.0288 (10) | 0.0217 (9) | 0.0183 (9) | −0.0051 (8) | −0.0051 (7) | 0.0004 (7) |
| O4 | 0.0258 (10) | 0.0345 (12) | 0.0206 (9) | −0.0030 (9) | 0.0017 (8) | 0.0070 (8) |
| O5 | 0.0382 (12) | 0.0218 (10) | 0.0285 (11) | −0.0060 (9) | −0.0035 (9) | −0.0020 (8) |
| O6 | 0.0218 (8) | 0.0208 (9) | 0.0129 (7) | −0.0003 (7) | 0.0016 (6) | 0.0024 (6) |
| O7 | 0.0255 (10) | 0.0328 (12) | 0.0268 (11) | 0.0018 (9) | −0.0034 (8) | 0.0067 (9) |
| O8 | 0.0375 (12) | 0.0221 (10) | 0.0247 (10) | 0.0050 (9) | 0.0080 (9) | 0.0008 (8) |
| O9 | 0.0295 (10) | 0.0258 (10) | 0.0253 (10) | 0.0044 (8) | 0.0119 (8) | 0.0025 (8) |
| O10 | 0.0240 (11) | 0.0398 (14) | 0.0452 (15) | 0.0009 (10) | −0.0018 (10) | 0.0059 (12) |
| O11 | 0.0371 (13) | 0.0433 (15) | 0.0379 (14) | 0.0011 (11) | 0.0227 (11) | 0.0077 (11) |
| O12 | 0.0239 (9) | 0.0206 (9) | 0.0223 (9) | −0.0029 (7) | 0.0041 (7) | 0.0025 (7) |
| O13 | 0.0233 (10) | 0.0389 (13) | 0.0206 (9) | −0.0016 (9) | −0.0060 (8) | 0.0031 (9) |
| O14 | 0.0312 (10) | 0.0204 (9) | 0.0222 (9) | −0.0040 (8) | −0.0020 (8) | −0.0034 (7) |
| O15 | 0.0219 (9) | 0.0257 (9) | 0.0116 (7) | −0.0001 (7) | −0.0011 (6) | 0.0004 (7) |
| O16 | 0.0256 (10) | 0.0402 (13) | 0.0177 (9) | 0.0037 (9) | 0.0059 (8) | 0.0036 (8) |
| O17 | 0.0310 (11) | 0.0228 (10) | 0.0215 (9) | 0.0033 (8) | −0.0038 (8) | −0.0032 (7) |
| O18 | 0.0242 (9) | 0.0206 (9) | 0.0189 (9) | 0.0013 (7) | −0.0031 (7) | 0.0008 (7) |
| O19 | 0.0306 (10) | 0.0237 (9) | 0.0137 (8) | −0.0029 (8) | −0.0038 (7) | 0.0018 (7) |
| O20 | 0.0283 (9) | 0.0160 (8) | 0.0129 (7) | −0.0013 (7) | 0.0032 (7) | −0.0007 (6) |
| O21 | 0.0321 (11) | 0.0255 (10) | 0.0186 (9) | 0.0004 (8) | 0.0110 (8) | 0.0020 (7) |
| O22 | 0.0229 (8) | 0.0167 (8) | 0.0117 (7) | −0.0007 (6) | 0.0003 (6) | −0.0007 (6) |
| O23 | 0.0187 (8) | 0.0189 (8) | 0.0117 (7) | −0.0014 (6) | 0.0007 (6) | 0.0008 (6) |
| O24 | 0.0198 (8) | 0.0175 (8) | 0.0143 (7) | 0.0004 (6) | 0.0029 (6) | 0.0014 (6) |
| Mo1 | 0.01912 (9) | 0.02215 (10) | 0.01584 (9) | −0.00268 (8) | −0.00351 (7) | 0.00174 (7) |
| Mo2 | 0.02159 (10) | 0.01762 (9) | 0.01494 (9) | −0.00348 (7) | −0.00019 (7) | 0.00209 (7) |
| Mo3 | 0.02075 (10) | 0.01832 (10) | 0.01763 (9) | 0.00146 (8) | 0.00352 (7) | 0.00293 (7) |
| Mo4 | 0.01970 (10) | 0.02472 (11) | 0.02561 (11) | 0.00006 (8) | 0.00868 (8) | 0.00360 (9) |
| Mo5 | 0.01950 (9) | 0.01916 (10) | 0.01367 (9) | −0.00115 (7) | −0.00133 (7) | −0.00076 (7) |
| Mo6 | 0.01876 (9) | 0.01945 (10) | 0.01188 (8) | 0.00120 (7) | 0.00054 (7) | −0.00103 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| Mo7 | 0.02116 (9) | 0.01513 (9) | 0.01035 (8) | −0.00110 (7) | 0.00168 (7) | −0.00035 (6) |
| C1 | 0.069 (3) | 0.0360 (19) | 0.0254 (16) | 0.0063 (19) | −0.0037 (17) | −0.0048 (14) |
| C2 | 0.054 (2) | 0.0268 (15) | 0.0291 (16) | 0.0069 (15) | −0.0016 (15) | −0.0060 (12) |
| C3 | 0.0225 (12) | 0.0242 (13) | 0.0263 (13) | 0.0004 (10) | 0.0014 (10) | −0.0075 (10) |
| C4 | 0.076 (3) | 0.0280 (17) | 0.036 (2) | −0.0038 (18) | 0.002 (2) | −0.0050 (15) |
| N1 | 0.0293 (12) | 0.0281 (12) | 0.0222 (11) | 0.0017 (10) | 0.0000 (9) | −0.0128 (9) |
| N2 | 0.0248 (11) | 0.0248 (11) | 0.0211 (11) | 0.0002 (9) | 0.0014 (9) | −0.0092 (9) |
| C5 | 0.052 (2) | 0.051 (3) | 0.038 (2) | 0.000 (2) | −0.0123 (18) | −0.0113 (18) |
| C6 | 0.047 (2) | 0.041 (2) | 0.041 (2) | 0.0030 (17) | −0.0089 (17) | −0.0061 (17) |
| C7 | 0.0215 (13) | 0.0335 (17) | 0.047 (2) | −0.0041 (12) | 0.0096 (13) | −0.0113 (14) |
| C8 | 0.045 (2) | 0.046 (2) | 0.046 (2) | 0.0079 (18) | 0.0100 (18) | −0.0030 (18) |
| N3 | 0.0256 (13) | 0.0373 (16) | 0.0439 (17) | −0.0015 (11) | 0.0025 (12) | −0.0179 (13) |
| N4 | 0.0231 (12) | 0.0330 (15) | 0.0469 (18) | −0.0027 (11) | 0.0027 (11) | −0.0127 (13) |
| C9 | 0.050 (2) | 0.037 (2) | 0.038 (2) | −0.0067 (17) | 0.0036 (17) | 0.0054 (15) |
| C10 | 0.043 (2) | 0.0313 (17) | 0.043 (2) | −0.0031 (15) | 0.0023 (16) | 0.0063 (15) |
| C11 | 0.0230 (13) | 0.0311 (15) | 0.0380 (17) | −0.0034 (11) | −0.0103 (12) | 0.0118 (13) |
| C12 | 0.073 (3) | 0.040 (2) | 0.047 (2) | −0.004 (2) | −0.020 (2) | 0.0017 (19) |
| N5 | 0.0250 (12) | 0.0308 (14) | 0.0389 (16) | −0.0056 (10) | −0.0032 (11) | 0.0133 (12) |
| N6 | 0.0261 (12) | 0.0306 (14) | 0.0380 (15) | −0.0036 (10) | −0.0054 (11) | 0.0120 (12) |
| C13 | 0.037 (2) | 0.077 (4) | 0.068 (3) | 0.002 (2) | 0.012 (2) | −0.008 (3) |
| C14 | 0.045 (2) | 0.070 (3) | 0.050 (3) | −0.003 (2) | 0.005 (2) | −0.020 (2) |
| C15 | 0.047 (2) | 0.0326 (17) | 0.0296 (16) | 0.0093 (15) | 0.0081 (14) | 0.0016 (13) |
| C16 | 0.077 (4) | 0.044 (3) | 0.047 (3) | 0.002 (2) | −0.011 (2) | −0.005 (2) |
| N7 | 0.053 (2) | 0.052 (2) | 0.0381 (18) | 0.0154 (17) | 0.0202 (16) | 0.0027 (16) |
| N8 | 0.0393 (16) | 0.0454 (19) | 0.0350 (16) | 0.0044 (14) | 0.0116 (13) | −0.0041 (14) |
| C17 | 0.0242 (13) | 0.0393 (18) | 0.0321 (16) | 0.0027 (12) | −0.0053 (12) | 0.0007 (13) |
| C18 | 0.0220 (13) | 0.0359 (17) | 0.0322 (16) | 0.0035 (12) | 0.0030 (11) | −0.0006 (13) |
| C19 | 0.0228 (12) | 0.0309 (15) | 0.0215 (12) | 0.0022 (11) | 0.0018 (10) | −0.0001 (10) |
| C20 | 0.0333 (17) | 0.048 (2) | 0.040 (2) | 0.0146 (16) | −0.0022 (14) | 0.0057 (17) |
| N9 | 0.0293 (13) | 0.0380 (15) | 0.0203 (11) | 0.0040 (11) | −0.0012 (9) | −0.0007 (10) |
| N10 | 0.0266 (12) | 0.0338 (13) | 0.0177 (10) | −0.0006 (10) | 0.0024 (9) | −0.0001 (9) |
| C21 | 0.0277 (14) | 0.0417 (18) | 0.0190 (12) | 0.0009 (13) | 0.0000 (10) | 0.0026 (12) |
| C22 | 0.0268 (13) | 0.0415 (18) | 0.0187 (12) | −0.0004 (12) | 0.0069 (10) | 0.0002 (11) |
| C23 | 0.0288 (13) | 0.0282 (14) | 0.0155 (11) | −0.0015 (11) | 0.0017 (10) | −0.0007 (9) |
| C24 | 0.0362 (17) | 0.0365 (18) | 0.0343 (17) | 0.0089 (14) | 0.0056 (14) | 0.0012 (14) |
| N11 | 0.0289 (12) | 0.0374 (14) | 0.0124 (9) | −0.0002 (10) | 0.0027 (8) | 0.0008 (9) |
| N12 | 0.0293 (12) | 0.0347 (14) | 0.0132 (9) | −0.0017 (10) | 0.0013 (8) | 0.0037 (9) |
| C25 | 0.081 (3) | 0.039 (2) | 0.043 (2) | 0.008 (2) | 0.026 (2) | 0.0121 (18) |
| C26 | 0.066 (3) | 0.042 (2) | 0.042 (2) | 0.003 (2) | 0.013 (2) | 0.0089 (18) |
| C27 | 0.074 (3) | 0.0266 (16) | 0.0306 (17) | −0.0031 (18) | 0.0014 (18) | 0.0015 (13) |
| C28 | 0.075 (4) | 0.054 (3) | 0.058 (3) | −0.001 (3) | −0.006 (3) | 0.005 (2) |
| N13 | 0.095 (3) | 0.0330 (17) | 0.0288 (16) | 0.0064 (19) | 0.0075 (18) | 0.0112 (13) |
| N14 | 0.065 (2) | 0.0348 (16) | 0.0260 (14) | −0.0038 (15) | 0.0053 (14) | 0.0052 (12) |
| C29 | 0.0285 (15) | 0.0419 (19) | 0.0286 (15) | 0.0052 (13) | −0.0094 (12) | −0.0013 (13) |
| C30 | 0.0307 (15) | 0.0369 (17) | 0.0298 (15) | 0.0115 (13) | −0.0028 (12) | −0.0057 (13) |
| C31 | 0.0290 (14) | 0.0355 (16) | 0.0222 (13) | 0.0043 (12) | −0.0059 (11) | −0.0094 (12) |
| C32 | 0.0322 (18) | 0.068 (3) | 0.041 (2) | 0.0155 (19) | −0.0086 (15) | −0.019 (2) |
| N15 | 0.0315 (13) | 0.0327 (14) | 0.0217 (11) | 0.0048 (11) | −0.0046 (10) | −0.0109 (10) |

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|---|---|---|---|---|---|---|
| N16 | 0.0302 (13) | 0.0364 (15) | 0.0240 (12) | 0.0088 (11) | −0.0057 (10) | −0.0092 (11) |
| O25 | 0.0344 (12) | 0.0563 (17) | 0.0199 (10) | 0.0001 (12) | 0.0025 (9) | 0.0003 (11) |
| O26 | 0.066 (2) | 0.0466 (18) | 0.0422 (17) | −0.0038 (16) | −0.0272 (15) | 0.0040 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—Mo1 | 1.724 (2) | C11—N6 | 1.328 (4) |
| O2—Mo1 | 1.725 (2) | C11—C12 | 1.479 (6) |
| O3—Mo1 | 1.945 (2) | C12—H12A | 0.98 |
| O3—Mo2 | 1.971 (2) | C12—H12B | 0.98 |
| O4—Mo2 | 1.707 (2) | C12—H12C | 0.98 |
| O5—Mo2 | 1.725 (2) | N5—H5N | 0.886 (17) |
| O6—Mo3 | 1.9528 (19) | N6—H6N | 0.895 (17) |
| O6—Mo2 | 1.953 (2) | C13—C14 | 1.347 (7) |
| O7—Mo3 | 1.715 (2) | C13—N7 | 1.372 (7) |
| O8—Mo3 | 1.716 (2) | C13—H13 | 0.95 |
| O9—Mo4 | 1.939 (2) | C14—N8 | 1.379 (6) |
| O9—Mo3 | 1.987 (2) | C14—H14 | 0.95 |
| O10—Mo4 | 1.709 (3) | C15—N8 | 1.324 (5) |
| O11—Mo4 | 1.715 (2) | C15—N7 | 1.333 (5) |
| O12—Mo4 | 1.932 (2) | C15—C16 | 1.476 (6) |
| O12—Mo5 | 1.983 (2) | C16—H16A | 0.98 |
| O13—Mo5 | 1.713 (2) | C16—H16B | 0.98 |
| O14—Mo5 | 1.730 (2) | C16—H16C | 0.98 |
| O15—Mo6 | 1.9521 (19) | N7—H7N | 0.887 (17) |
| O15—Mo5 | 1.953 (2) | N8—H8N | 0.893 (17) |
| O16—Mo6 | 1.707 (2) | C17—C18 | 1.350 (5) |
| O17—Mo6 | 1.726 (2) | C17—N9 | 1.380 (4) |
| O18—Mo1 | 1.916 (2) | C17—H17 | 0.95 |
| O18—Mo6 | 2.012 (2) | C18—N10 | 1.379 (4) |
| O19—Mo7 | 1.754 (2) | C18—H18 | 0.95 |
| O19—Mo1 | 2.453 (2) | C19—N9 | 1.329 (4) |
| O20—Mo7 | 1.901 (2) | C19—N10 | 1.334 (4) |
| O20—Mo3 | 2.259 (2) | C19—C20 | 1.480 (5) |
| O20—Mo2 | 2.292 (2) | C20—H20A | 0.98 |
| O21—Mo7 | 1.725 (2) | C20—H20B | 0.98 |
| O22—Mo7 | 1.8945 (19) | C20—H20C | 0.98 |
| O22—Mo5 | 2.2453 (19) | N9—H9N | 0.886 (17) |
| O22—Mo6 | 2.3057 (19) | N10—H10N | 0.880 (17) |
| O23—Mo6 | 2.1329 (19) | C21—C22 | 1.356 (4) |
| O23—Mo1 | 2.1604 (19) | C21—N11 | 1.374 (4) |
| O23—Mo2 | 2.1748 (19) | C21—H21 | 0.95 |
| O23—Mo7 | 2.3011 (18) | C22—N12 | 1.380 (4) |
| O24—Mo4 | 2.1624 (19) | C22—H22 | 0.95 |
| O24—Mo5 | 2.1665 (19) | C23—N12 | 1.330 (4) |
| O24—Mo3 | 2.1677 (19) | C23—N11 | 1.336 (4) |
| O24—Mo7 | 2.2665 (19) | C23—C24 | 1.479 (5) |
| Mo1—Mo6 | 3.2178 (3) | C24—H24A | 0.98 |

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|---|---|---|---|
| Mo4—Mo5 | 3.2105 (3) | C24—H24B | 0.98 |
| C1—C2 | 1.362 (5) | C24—H24C | 0.98 |
| C1—N1 | 1.362 (5) | N11—H11N | 0.877 (17) |
| C1—H1 | 0.95 | N12—H12N | 0.876 (17) |
| C2—N2 | 1.365 (5) | C25—C26 | 1.357 (6) |
| C2—H2 | 0.95 | C25—N13 | 1.371 (7) |
| C3—N1 | 1.328 (4) | C25—H25 | 0.95 |
| C3—N2 | 1.332 (4) | C26—N14 | 1.377 (6) |
| C3—C4 | 1.488 (5) | C26—H26 | 0.95 |
| C4—H4A | 0.98 | C27—N14 | 1.338 (6) |
| C4—H4B | 0.98 | C27—N13 | 1.348 (6) |
| C4—H4C | 0.98 | C27—C28 | 1.470 (8) |
| N1—H1N | 0.881 (17) | C28—H28A | 0.98 |
| N2—H2N | 0.868 (17) | C28—H28B | 0.98 |
| C5—C6 | 1.363 (6) | C28—H28C | 0.98 |
| C5—N3 | 1.384 (6) | N13—H13N | 0.880 (19) |
| C5—H5 | 0.95 | C29—C30 | 1.360 (5) |
| C6—N4 | 1.367 (6) | C29—N15 | 1.372 (4) |
| C6—H6 | 0.95 | C29—H29 | 0.95 |
| C7—N3 | 1.321 (5) | C30—N16 | 1.380 (4) |
| C7—N4 | 1.325 (5) | C30—H30 | 0.95 |
| C7—C8 | 1.493 (6) | C31—N16 | 1.321 (4) |
| C8—H8A | 0.98 | C31—N15 | 1.352 (4) |
| C8—H8B | 0.98 | C31—C32 | 1.495 (5) |
| C8—H8C | 0.98 | C32—H32A | 0.98 |
| N3—H3N | 0.884 (17) | C32—H32B | 0.98 |
| N4—H4N | 0.884 (17) | C32—H32C | 0.98 |
| C9—C10 | 1.357 (6) | N15—H15N | 0.867 (19) |
| C9—N5 | 1.378 (5) | O25—H25V | 0.857 (19) |
| C9—H9 | 0.95 | O25—H25W | 0.856 (18) |
| C10—N6 | 1.375 (5) | O26—H26V | 0.842 (19) |
| C10—H10 | 0.95 | O26—H26W | 0.843 (19) |
| C11—N5 | 1.323 (5) | | |

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| Mo1—O3—Mo2 | 111.13 (10) | C3—C4—H4A | 109.5 |
| Mo3—O6—Mo2 | 115.96 (9) | C3—C4—H4B | 109.5 |
| Mo4—O9—Mo3 | 110.89 (11) | H4A—C4—H4B | 109.5 |
| Mo4—O12—Mo5 | 110.14 (10) | C3—C4—H4C | 109.5 |
| Mo6—O15—Mo5 | 114.70 (9) | H4A—C4—H4C | 109.5 |
| Mo1—O18—Mo6 | 110.01 (10) | H4B—C4—H4C | 109.5 |
| Mo7—O19—Mo1 | 107.64 (9) | C3—N1—C1 | 109.4 (3) |
| Mo7—O20—Mo3 | 110.29 (9) | C3—N1—H1N | 125.1 (19) |
| Mo7—O20—Mo2 | 110.20 (9) | C1—N1—H1N | 125.4 (19) |
| Mo3—O20—Mo2 | 93.36 (7) | C3—N2—C2 | 109.0 (3) |
| Mo7—O22—Mo5 | 109.98 (9) | C3—N2—H2N | 128.7 (19) |
| Mo7—O22—Mo6 | 109.89 (9) | C2—N2—H2N | 122.3 (19) |
| Mo5—O22—Mo6 | 92.51 (7) | C6—C5—N3 | 106.9 (4) |
| Mo6—O23—Mo1 | 97.09 (8) | C6—C5—H5 | 126.6 |

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| Mo6—O23—Mo2 | 151.14 (9) | N3—C5—H5 | 126.6 |
| Mo1—O23—Mo2 | 96.34 (7) | C5—C6—N4 | 106.2 (4) |
| Mo6—O23—Mo7 | 101.96 (8) | C5—C6—H6 | 126.9 |
| Mo1—O23—Mo7 | 100.09 (7) | N4—C6—H6 | 126.9 |
| Mo2—O23—Mo7 | 100.67 (7) | N3—C7—N4 | 108.4 (4) |
| Mo4—O24—Mo5 | 95.74 (8) | N3—C7—C8 | 126.8 (4) |
| Mo4—O24—Mo3 | 96.60 (8) | N4—C7—C8 | 124.7 (4) |
| Mo5—O24—Mo3 | 152.34 (9) | C7—C8—H8A | 109.5 |
| Mo4—O24—Mo7 | 103.86 (7) | C7—C8—H8B | 109.5 |
| Mo5—O24—Mo7 | 100.00 (8) | H8A—C8—H8B | 109.5 |
| Mo3—O24—Mo7 | 100.92 (8) | C7—C8—H8C | 109.5 |
| O1—Mo1—O2 | 104.12 (11) | H8A—C8—H8C | 109.5 |
| O1—Mo1—O18 | 98.92 (11) | H8B—C8—H8C | 109.5 |
| O2—Mo1—O18 | 102.57 (10) | C7—N3—C5 | 108.7 (3) |
| O1—Mo1—O3 | 96.55 (11) | C7—N3—H3N | 129 (2) |
| O2—Mo1—O3 | 100.84 (10) | C5—N3—H3N | 122 (2) |
| O18—Mo1—O3 | 147.73 (9) | C7—N4—C6 | 109.9 (3) |
| O1—Mo1—O23 | 106.54 (9) | C7—N4—H4N | 126 (2) |
| O2—Mo1—O23 | 149.29 (10) | C6—N4—H4N | 124 (2) |
| O18—Mo1—O23 | 74.47 (8) | C10—C9—N5 | 106.3 (4) |
| O3—Mo1—O23 | 74.03 (8) | C10—C9—H9 | 126.9 |
| O1—Mo1—O19 | 176.53 (9) | N5—C9—H9 | 126.9 |
| O2—Mo1—O19 | 78.58 (10) | C9—C10—N6 | 107.2 (4) |
| O18—Mo1—O19 | 82.49 (8) | C9—C10—H10 | 126.4 |
| O3—Mo1—O19 | 80.71 (8) | N6—C10—H10 | 126.4 |
| O23—Mo1—O19 | 70.72 (7) | N5—C11—N6 | 108.4 (3) |
| O1—Mo1—Mo6 | 95.01 (8) | N5—C11—C12 | 124.7 (3) |
| O2—Mo1—Mo6 | 137.30 (8) | N6—C11—C12 | 126.8 (4) |
| O18—Mo1—Mo6 | 35.98 (6) | C11—C12—H12A | 109.5 |
| O3—Mo1—Mo6 | 114.62 (6) | C11—C12—H12B | 109.5 |
| O23—Mo1—Mo6 | 41.13 (5) | H12A—C12—H12B | 109.5 |
| O19—Mo1—Mo6 | 84.26 (5) | C11—C12—H12C | 109.5 |
| O4—Mo2—O5 | 105.64 (12) | H12A—C12—H12C | 109.5 |
| O4—Mo2—O6 | 96.30 (9) | H12B—C12—H12C | 109.5 |
| O5—Mo2—O6 | 97.94 (10) | C11—N5—C9 | 109.3 (3) |
| O4—Mo2—O3 | 102.62 (10) | C11—N5—H5N | 127.0 (19) |
| O5—Mo2—O3 | 95.05 (10) | C9—N5—H5N | 123.7 (19) |
| O6—Mo2—O3 | 153.21 (8) | C11—N6—C10 | 108.7 (3) |
| O4—Mo2—O23 | 93.82 (10) | C11—N6—H6N | 127.8 (19) |
| O5—Mo2—O23 | 159.22 (10) | C10—N6—H6N | 123.1 (19) |
| O6—Mo2—O23 | 86.87 (8) | C14—C13—N7 | 106.2 (4) |
| O3—Mo2—O23 | 73.22 (8) | C14—C13—H13 | 126.9 |
| O4—Mo2—O20 | 161.90 (10) | N7—C13—H13 | 126.9 |
| O5—Mo2—O20 | 90.12 (10) | C13—C14—N8 | 107.0 (4) |
| O6—Mo2—O20 | 72.28 (7) | C13—C14—H14 | 126.5 |
| O3—Mo2—O20 | 84.40 (8) | N8—C14—H14 | 126.5 |
| O23—Mo2—O20 | 72.01 (7) | N8—C15—N7 | 106.8 (4) |
| O8—Mo3—O7 | 104.86 (12) | N8—C15—C16 | 126.4 (4) |

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| O8—Mo3—O6 | 100.55 (10) | N7—C15—C16 | 126.8 (4) |
| O7—Mo3—O6 | 96.34 (10) | C15—C16—H16A | 109.5 |
| O8—Mo3—O9 | 92.85 (10) | C15—C16—H16B | 109.5 |
| O7—Mo3—O9 | 100.23 (11) | H16A—C16—H16B | 109.5 |
| O6—Mo3—O9 | 155.25 (9) | C15—C16—H16C | 109.5 |
| O8—Mo3—O24 | 155.03 (9) | H16A—C16—H16C | 109.5 |
| O7—Mo3—O24 | 97.84 (10) | H16B—C16—H16C | 109.5 |
| O6—Mo3—O24 | 86.96 (8) | C15—N7—C13 | 110.3 (4) |
| O9—Mo3—O24 | 72.72 (8) | C15—N7—H7N | 125 (2) |
| O8—Mo3—O20 | 87.48 (10) | C13—N7—H7N | 124 (2) |
| O7—Mo3—O20 | 165.23 (10) | C15—N8—C14 | 109.7 (4) |
| O6—Mo3—O20 | 73.05 (7) | C15—N8—H8N | 125 (2) |
| O9—Mo3—O20 | 86.99 (9) | C14—N8—H8N | 124 (2) |
| O24—Mo3—O20 | 71.84 (7) | C18—C17—N9 | 107.4 (3) |
| O10—Mo4—O11 | 106.30 (14) | C18—C17—H17 | 126.3 |
| O10—Mo4—O12 | 99.66 (12) | N9—C17—H17 | 126.3 |
| O11—Mo4—O12 | 101.36 (12) | C17—C18—N10 | 106.6 (3) |
| O10—Mo4—O9 | 100.30 (12) | C17—C18—H18 | 126.7 |
| O11—Mo4—O9 | 99.31 (12) | N10—C18—H18 | 126.7 |
| O12—Mo4—O9 | 145.80 (9) | N9—C19—N10 | 108.1 (3) |
| O10—Mo4—O24 | 106.87 (10) | N9—C19—C20 | 126.5 (3) |
| O11—Mo4—O24 | 146.81 (11) | N10—C19—C20 | 125.3 (3) |
| O12—Mo4—O24 | 74.02 (8) | C19—C20—H20A | 109.5 |
| O9—Mo4—O24 | 73.74 (8) | C19—C20—H20B | 109.5 |
| O10—Mo4—Mo5 | 93.77 (10) | H20A—C20—H20B | 109.5 |
| O11—Mo4—Mo5 | 135.81 (10) | C19—C20—H20C | 109.5 |
| O12—Mo4—Mo5 | 35.45 (6) | H20A—C20—H20C | 109.5 |
| O9—Mo4—Mo5 | 115.58 (6) | H20B—C20—H20C | 109.5 |
| O24—Mo4—Mo5 | 42.18 (5) | C19—N9—C17 | 108.7 (3) |
| O13—Mo5—O14 | 105.18 (11) | C19—N9—H9N | 128.0 (19) |
| O13—Mo5—O15 | 96.34 (10) | C17—N9—H9N | 123.0 (19) |
| O14—Mo5—O15 | 99.61 (10) | C19—N10—C18 | 109.2 (3) |
| O13—Mo5—O12 | 99.85 (10) | C19—N10—H10N | 125.4 (19) |
| O14—Mo5—O12 | 92.28 (10) | C18—N10—H10N | 125.4 (19) |
| O15—Mo5—O12 | 156.65 (9) | C22—C21—N11 | 106.6 (3) |
| O13—Mo5—O24 | 95.51 (10) | C22—C21—H21 | 126.7 |
| O14—Mo5—O24 | 156.48 (9) | N11—C21—H21 | 126.7 |
| O15—Mo5—O24 | 88.88 (8) | C21—C22—N12 | 107.2 (3) |
| O12—Mo5—O24 | 72.96 (8) | C21—C22—H22 | 126.4 |
| O13—Mo5—O22 | 165.08 (10) | N12—C22—H22 | 126.4 |
| O14—Mo5—O22 | 88.42 (9) | N12—C23—N11 | 108.1 (3) |
| O15—Mo5—O22 | 74.97 (7) | N12—C23—C24 | 125.8 (3) |
| O12—Mo5—O22 | 85.42 (8) | N11—C23—C24 | 126.1 (3) |
| O24—Mo5—O22 | 72.54 (7) | C23—C24—H24A | 109.5 |
| O13—Mo5—Mo4 | 87.53 (8) | C23—C24—H24B | 109.5 |
| O14—Mo5—Mo4 | 126.61 (8) | H24A—C24—H24B | 109.5 |
| O15—Mo5—Mo4 | 130.86 (6) | C23—C24—H24C | 109.5 |
| O12—Mo5—Mo4 | 34.41 (6) | H24A—C24—H24C | 109.5 |

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| O24—Mo5—Mo4 | 42.08 (5) | H24B—C24—H24C | 109.5 |
| O22—Mo5—Mo4 | 89.18 (5) | C23—N11—C21 | 109.3 (2) |
| O16—Mo6—O17 | 105.29 (12) | C23—N11—H11N | 125.3 (18) |
| O16—Mo6—O15 | 98.56 (10) | C21—N11—H11N | 125.4 (18) |
| O17—Mo6—O15 | 99.46 (10) | C23—N12—C22 | 108.8 (2) |
| O16—Mo6—O18 | 100.69 (10) | C23—N12—H12N | 124.9 (19) |
| O17—Mo6—O18 | 90.59 (9) | C22—N12—H12N | 125.9 (19) |
| O15—Mo6—O18 | 155.08 (8) | C26—C25—N13 | 105.5 (4) |
| O16—Mo6—O23 | 97.03 (10) | C26—C25—H25 | 127.2 |
| O17—Mo6—O23 | 154.60 (9) | N13—C25—H25 | 127.2 |
| O15—Mo6—O23 | 88.86 (8) | C25—C26—N14 | 109.8 (5) |
| O18—Mo6—O23 | 73.23 (8) | C25—C26—H26 | 125.1 |
| O16—Mo6—O22 | 166.13 (10) | N14—C26—H26 | 125.1 |
| O17—Mo6—O22 | 87.49 (9) | N14—C27—N13 | 109.4 (4) |
| O15—Mo6—O22 | 73.58 (7) | N14—C27—C28 | 126.1 (4) |
| O18—Mo6—O22 | 84.24 (8) | N13—C27—C28 | 124.5 (4) |
| O23—Mo6—O22 | 71.80 (7) | C27—C28—H28A | 109.5 |
| O16—Mo6—Mo1 | 90.80 (8) | C27—C28—H28B | 109.5 |
| O17—Mo6—Mo1 | 124.59 (7) | H28A—C28—H28B | 109.5 |
| O15—Mo6—Mo1 | 130.62 (6) | C27—C28—H28C | 109.5 |
| O18—Mo6—Mo1 | 34.01 (6) | H28A—C28—H28C | 109.5 |
| O23—Mo6—Mo1 | 41.78 (5) | H28B—C28—H28C | 109.5 |
| O22—Mo6—Mo1 | 86.14 (5) | C27—N13—C25 | 108.9 (4) |
| O21—Mo7—O19 | 103.66 (11) | C27—N13—H13N | 126 (2) |
| O21—Mo7—O22 | 102.76 (10) | C25—N13—H13N | 125 (2) |
| O19—Mo7—O22 | 101.19 (9) | C27—N14—C26 | 106.3 (4) |
| O21—Mo7—O20 | 101.84 (10) | C30—C29—N15 | 105.7 (3) |
| O19—Mo7—O20 | 100.32 (9) | C30—C29—H29 | 127.1 |
| O22—Mo7—O20 | 142.21 (8) | N15—C29—H29 | 127.1 |
| O21—Mo7—O24 | 85.71 (9) | C29—C30—N16 | 109.6 (3) |
| O19—Mo7—O24 | 170.59 (8) | C29—C30—H30 | 125.2 |
| O22—Mo7—O24 | 77.15 (8) | N16—C30—H30 | 125.2 |
| O20—Mo7—O24 | 76.58 (8) | N16—C31—N15 | 110.4 (3) |
| O21—Mo7—O23 | 174.78 (9) | N16—C31—C32 | 125.2 (3) |
| O19—Mo7—O23 | 81.55 (8) | N15—C31—C32 | 124.4 (3) |
| O22—Mo7—O23 | 76.12 (8) | C31—C32—H32A | 109.5 |
| O20—Mo7—O23 | 76.77 (8) | C31—C32—H32B | 109.5 |
| O24—Mo7—O23 | 89.07 (6) | H32A—C32—H32B | 109.5 |
| C2—C1—N1 | 106.8 (3) | C31—C32—H32C | 109.5 |
| C2—C1—H1 | 126.6 | H32A—C32—H32C | 109.5 |
| N1—C1—H1 | 126.6 | H32B—C32—H32C | 109.5 |
| C1—C2—N2 | 106.9 (3) | C31—N15—C29 | 108.1 (3) |
| C1—C2—H2 | 126.6 | C31—N15—H15N | 127.1 (19) |
| N2—C2—H2 | 126.6 | C29—N15—H15N | 124.8 (19) |
| N1—C3—N2 | 108.0 (3) | C31—N16—C30 | 106.1 (3) |
| N1—C3—C4 | 125.0 (3) | H25V—O25—H25W | 105 (3) |
| N2—C3—C4 | 127.0 (3) | H26V—O26—H26W | 107 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*N*···O22$^{i}$ | 0.88 (2) | 1.85 (2) | 2.710 (3) | 167 (2) |
| N2—H2*N*···O20 | 0.87 (2) | 1.79 (2) | 2.655 (3) | 172 (2) |
| N3—H3*N*···O18$^{i}$ | 0.88 (2) | 1.87 (2) | 2.743 (4) | 171 (5) |
| N4—H4*N*···O9 | 0.88 (2) | 1.79 (2) | 2.662 (4) | 171 (5) |
| N5—H5*N*···O12 | 0.89 (2) | 1.77 (3) | 2.644 (4) | 168 (4) |
| N6—H6*N*···O3$^{ii}$ | 0.90 (2) | 1.80 (3) | 2.684 (4) | 168 (5) |
| N7—H7*N*···O1$^{iii}$ | 0.89 (3) | 1.83 (3) | 2.697 (4) | 167 (3) |
| N8—H8*N*···O25 | 0.89 (3) | 1.78 (3) | 2.659 (4) | 172 (5) |
| N9—H9*N*···N14$^{iv}$ | 0.89 (2) | 1.81 (2) | 2.698 (4) | 177 (3) |
| N10—H10*N*···O15 | 0.88 (2) | 1.98 (2) | 2.852 (3) | 174 (3) |
| N11—H11*N*···O6 | 0.88 (2) | 1.78 (2) | 2.636 (3) | 166 (3) |
| N12—H12*N*···N16$^{v}$ | 0.88 (2) | 1.87 (2) | 2.725 (4) | 165 (3) |
| N13—H13*N*···O5 | 0.88 (4) | 2.32 (4) | 3.186 (5) | 167 (3) |
| N13—H13*N*···O8 | 0.88 (4) | 2.55 (4) | 3.043 (5) | 116 (2) |
| N15—H15*N*···O14 | 0.87 (3) | 2.22 (3) | 2.953 (4) | 142 (3) |
| N15—H15*N*···O17 | 0.87 (3) | 2.27 (3) | 2.917 (4) | 132 (3) |
| O25—H25*V*···O19 | 0.86 (2) | 2.00 (2) | 2.788 (3) | 154 (5) |
| O25—H25*W*···O26$^{vi}$ | 0.86 (3) | 1.85 (3) | 2.702 (4) | 176 (5) |
| O26—H26*V*···O10 | 0.83 (4) | 2.50 (6) | 2.999 (4) | 119 (5) |
| O26—H26*V*···O13 | 0.83 (4) | 2.25 (5) | 3.009 (4) | 151 (6) |
| O26—H26*W*···O7 | 0.83 (4) | 1.99 (6) | 2.737 (4) | 149 (6) |
| C4—H4*A*···O8 | 0.98 | 2.35 | 3.228 (5) | 149 |
| C8—H8*B*···O2$^{i}$ | 0.98 | 2.54 | 3.517 (6) | 176 |
| C8—H8*C*···O8 | 0.98 | 2.49 | 3.386 (5) | 152 |
| C10—H10···O26$^{vii}$ | 0.95 | 2.45 | 3.318 (5) | 151 |
| C12—H12*A*···O5$^{ii}$ | 0.98 | 2.44 | 3.407 (5) | 167 |
| C13—H13···O4$^{iii}$ | 0.95 | 2.50 | 3.297 (6) | 141 |
| C17—H17···O2$^{viii}$ | 0.95 | 2.46 | 3.154 (4) | 130 |
| C18—H18···O26 | 0.95 | 2.58 | 3.522 (5) | 172 |
| C21—H21···O16 | 0.95 | 2.46 | 3.302 (4) | 147 |
| C22—H22···O11$^{ix}$ | 0.95 | 2.22 | 3.113 (4) | 156 |
| C24—H24*B*···O7 | 0.98 | 2.50 | 3.346 (5) | 145 |
| C25—H25···O8 | 0.95 | 2.59 | 3.055 (5) | 110 |
| C32—H32*B*···O14 | 0.98 | 2.55 | 3.234 (5) | 126 |

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+1/2; (ii) −*x*+1/2, *y*+1/2, −*z*+1/2; (iii) *x*+1/2, −*y*+1/2, *z*−1/2; (iv) −*x*+1/2, *y*+1/2, −*z*+3/2; (v) −*x*+1/2, *y*−1/2, −*z*+3/2; (vi) *x*−1/2, −*y*+1/2, *z*−1/2; (vii) −*x*+1, −*y*+1, −*z*+1; (viii) *x*+1/2, −*y*+1/2, *z*+1/2; (ix) *x*−1/2, −*y*+1/2, *z*+1/2.