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# [Mn(bpb)(DMAP)(NO)], an {Mn–NO}$^6$ nitrosyl with $Z'$ = 8

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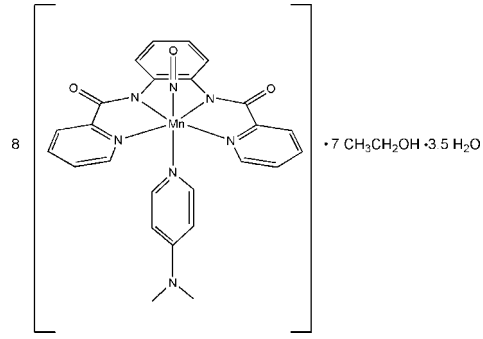
Key indicators: single-crystal X-ray study; $T$ = 90 K; mean $\sigma$(C–C) = 0.024 Å; H-atom completeness 97%; disorder in solvent or counterion; $R$ factor = 0.068; $wR$ factor = 0.151; data-to-parameter ratio = 15.0.

The structure of the title compound octakis{[4-(dimethylamino)pyridine](nitrosyl)[*N*,*N*′-(*o*-phenylene)bis(pyridine-2-carboxamidato)]manganese(II)} ethanol heptasolvate 3.5-hydrate, $[Mn(C_{18}H_{12}N_4O_2)(C_7H_{10}N_2)(NO)]_8\cdot7C_2H_5OH\cdot3.5H_2O$, or 8[Mn(bpb)(DMAP)(NO)]·7EtOH·3.5$H_2O$, is an unusual example of a structure with $Z'$ = 8. The tetradentate bpb ligand, together with the nitrosyl and dimethylaminopyridine ligands, gives rise to a distorted octahedral coordination environment for the Mn(II) ion. The average Mn—$N_{(N=O)}$ bond length is 1.631 (13) Å. The eight molecules in the asymmetric unit differ mainly in the rotation of the DMAP pyridine plane with respect to a reference plane of the Mn and three N atoms, one of which is the N atom of the NO group. The dihedral angles between the normals to these planes range from a minimum of 28.0 (2)° to a maximum of 64.2 (2)°. There are also some differences in O—H···O hydrogen bonding interactions. For example, of the sixteen C=O acceptors, there are seven different interactions with EtOH donors and two interactions with $H_2O$ donors. The crystal studied was found to be a two-component twin, with a 179.9° rotation about the real axis [−0.535, 0.004, 1.000]. Due to the presence of a superlattice and, consequently, the large number of weak reflections, the refinement utilized rigid solvate groups and isotropic displacement parameters for all except the Mn atoms. H atoms were not located for hydrate molecules.

## Related literature

For related structures, see: Eroy-Reveles *et al.* (2008); Feng & Liao (2008); Ghosh *et al.* (2004); Hoffman-Luca *et al.* (2009); Liang *et al.* (2007). For {M—NO}$^x$ formalism, see: Enemark & Feltham (1974).




## Experimental

### Crystal data

$[Mn(C_{18}H_{12}N_4O_2)(C_7H_{10}N_2)(NO)]_8\cdot7C_2H_6O\cdot3.5H_2O$
$M_r$ = 571.63
Monoclinic, *Pc*
$a$ = 24.943 (3) Å
$b$ = 14.4343 (18) Å
$c$ = 29.688 (4) Å
$\beta$ = 101.190 (3)°
$V$ = 10486 (2) Å$^3$
$Z$ = 16
Mo $K\alpha$ radiation
$\mu$ = 0.55 mm$^{-1}$
$T$ = 90 K
0.28 × 0.04 × 0.03 mm

### Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2005)
$T_{min}$ = 0.861, $T_{max}$ = 0.984
158363 measured reflections
94844 independent reflections
26534 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.164

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.151
$S$ = 0.64
19177 reflections
1275 parameters
3166 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.04 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.55 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O25—H20*D*···O22$^{i}$ | 0.96 | 1.88 | 2.751 (15) | 149 |
| O26—H20*J*···O8$^{ii}$ | 0.85 | 1.84 | 2.686 (17) | 178 |
| O27—H20*P*···O16$^{iii}$ | 0.84 | 1.93 | 2.739 (18) | 161 |
| O28—H20*V*···O23 | 0.85 | 1.89 | 2.747 (19) | 179 |
| O29—H21*C*···O20 | 0.84 | 1.93 | 2.709 (17) | 154 |
| O30—H21*J*···O7$^{iv}$ | 0.85 | 1.90 | 2.75 (2) | 178 |
| O31—H21*P*···O13 | 0.85 | 2.04 | 2.887 (17) | 179 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2529).

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# supporting information

*Acta Cryst.* (2011). E**67**, m1451–m1452 [https://doi.org/10.1107/S1600536811038669]

## [Mn(bpb)(DMAP)(NO)], an {Mn–NO}$^6$ nitrosyl with $Z'$ = 8

**Marilyn M. Olmstead, A. Alegra Eroy-Reveles and Pradip K. Mascharak**

### S1. Comment

The structure determination of the title compound, 8[Mn($C_{18}H_{12}N_4O_2$)($C_7H_{10}N_2$)(NO)]·7$C_2H_5OH$·3.5$H_2O$, was found to involve a rotational twin. The structure is unusual in that there are eight molecules of the complex, [Mn(bpb)(DMAP)(NO)], (bpb = *N*,*N*′-*o*-phenylenebis(pyridine-2-carboxamidate; DMAP = dimethylaminopyridine) in the asymmetric unit. The structure also contains seven ethanol and 3.5 water solvent molecules in the asymmetric unit. The bpb ligand occupies the four equatorial coordination sites of the manganese ion. The axial sites are occupied by a nitrosyl group and DMAP, completing a distorted octahedral coordination of the metal ion. The two Mn—N bonds from pyridyl groups are slightly longer at 2.064[13] Å than the two from amido groups (1.950[10] Å), (average with average deviation from the mean in square brackets). This trend has been seen in a number of similar complexes (Ghosh *et al.*, 2004; Liang *et al.*, 2007; Eroy-Reveles *et al.*, 2008; Feng & Liao, 2008; Hoffman-Luca, *et al.*, 2009). The average Mn—$N_{(DMAP)}$ distance is 2.124[10] Å.

The geometry of the nitrosyl group does not vary a great deal from one complex to the next. It is nearly linear; the average Mn—N and N═O distances are 1.631[13] Å and 1.203[12] Å, respectively. The average Mn—N═O angle is 174.3[1.9] °. A notable difference concerns the rotation of the DMAP group, and this can be viewed in Fig. 1. In molecule **1**, the angle between the normal to the plane consisting of Mn1/N2/N4/N5 and the normal to the pyridine plane N6/C19/C20/C21/C22/C23 is 51.6 (2)°. For each of the eight molecules, the same angle is calculated. For the other seven molecules these angles are: **2**, 51.8 (2)°; **3**, 39.4 (2)°; **4**, 50.8 (2)°; **5**, 44.4 (2)°; **6**, 28.0 (2)°; **7**, 58.0 (3)°; **8**, 64.2 (3)°.

Hydrogen bonding interactions between the ethanol molecules and C═O groups of the bpb ligands are listed in Table 1. Additional hydrogen bonding that involves hydrate molecules is clearly present but not listed due to the difficulty in locating H atoms attached to the water molecules.

The oxidation state of Mn in the title compound, [Mn(bpb)(DMAP)(NO)], is most likely to be +II, *i.e.*, we can call the complex {Mn—NO}$^6$ (Enemark & Feltham, 1974). This nitrosyl has its N═O stretching frequency at 1730 $cm^{-1}$. A related complex of the deprotonated pentadentate ligand *N*,*N*-bis(2-pyridylmethyl)amine-*N*-ethyl-2-pyridine-2-carboxamide ($PaPy_3H$), was previously reported [Mn($PaPy_3$)(NO)]($ClO_4$) (Ghosh *et al.*, 2004). This is formally a $Mn^{II}$—NO or $Mn^{I}$—$NO^+$ species, and the N═O stretching frequency appears at 1745 $cm^{-1}$, while for the corresponding oxidized species [Mn($PaPy_3$)(NO)]($ClO_4$)$_2$, the N═O stretching frequency is at 1875 $cm^{-1}$. Also, in the present complex the Mn—$N_{(O)}$ distance is 1.631[13] Å. In [Mn($PaPy_3$)(NO)]($ClO_4$), this distance is 1.6601 (14) Å. It is also important to note that the average Mn—$N_{(py)}$ distance of the bpb ligand in the title complex is 2.064[13] Å while the same distance in [Mn($PaPy_3$)(NO)]($ClO_4$) is 1.9953 (15) Å. It is evident that the present complex more closely resembles the Mn(II) species.

### S2. Experimental

A portion of 100 mg (0.31 mmol) of the ligand $bpbH_2$ was dissolved in 25 ml of degassed EtOH in a 100 ml Schlenk flask and to it was added a batch of 17 mg (0.65 mmol) of NaH. The pale yellow solution was stirred under nitrogen. Next, a

batch of 86 mg (0.70 mmol) of DMAP (dimethylaminopyridine) was added to the solution and stirred. Once the solid was dissolved, the mixture was thoroughly degassed by two free-pump-thaw cycles. A batch of 114 mg (0.31 mmol) of $[Mn(H_2O)_6](ClO_4)_2$ was then added to the frozen mixture and it was allowed to thaw under dinitrogen. The color of the solution soon turned deep yellow and yellow solid separated out after 30 min. The headspace of the flask was then filled with NO(*g*) and the yellow-brown suspension was stirred under NO atmosphere for 2 h when the desired complex separated out as dark brown microcrystals. Anal. Calcd for [Mn(bpb)(DMAP)(NO)].EtOH.$H_2O$, $C_{27}H_{30}N_7O_5Mn$: %C 55.20, %H 5.15, %N 16.69. Found: %C 55.32, %H 5.08, %N 16.51. Selected FTIR data (KBr matrix): *ν*NO = 1730 $cm^{-1}$. Crystals of [Mn(bpb)(DMAP)(NO)] suitable for X-ray studies, were grown from EtOH *via* slow evaporation.

### S3. Refinement

The crystal was found to be a two-component twin, with a 179.9° rotation about the real axis [-0.535, 0.004, 1.000]. Integration was carried out with two components, and the absorption correction was applied with *TWINABS* (Sheldrick, 2005). For the HKLF 5 file, both components and composites were retained. The refined twin parameters were 0.32 (3) for the components and 0.12 (2) for and 0.08 (3) for racemic scale factors. In the final cycles of refinement, nextra was set to 75667 in order to better estimate the su's. Due to the large number of weak reflections in the dataset, it was not possible to refine all the atoms with anisotropic displacement parameters. Only the eight Mn atoms were assigned anisotropic displacement parameters. The seven molecules of ethanol were modeled using idealized geometry and treated as rigid groups in the final cycles of refinement. Three of the water molecules appeared to be at full occupancy, and a fourth was assigned the *ad hoc* value of 0.5 occupancy. The water hydrogen atoms could not be located with certainty and were not included in the model. Hydrogen atoms of the manganese complexes were added by geometry and refined as riding atoms with distances of H—C($sp^2$) = 0.95 and *H*—*C*(methyl) = 0.98 Å and with $U_{iso}$(H) set to 1.2 (1.5 for methyl) $U_{eq}$(C).

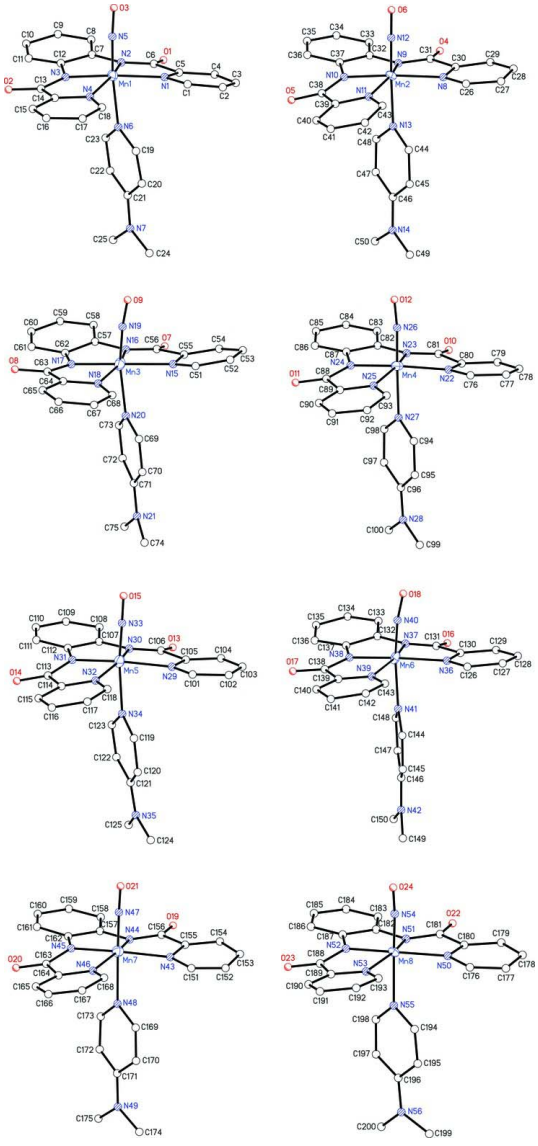

**Figure 1**

A view of the eight complexes in the asymmetric unit. The Mn atoms are shown with displacement parameters at the 35% probability level. Other atoms are assigned an arbitrary size. Ethanol and water molecules are not shown.

**octakis{[4-(dimethylamino)pyridine](nitrosyl)[*N*,*N*′-(*o*- phenylene)bis(pyridine-2-carboxamidato)]manganese(II)} ethanol heptasolvate 3.5-hydrate**

*Crystal data*

$[Mn(C_{18}H_{12}N_4O_2)(C_7H_{10}N_2)(NO)]_8 \cdot 7C_2H_6O \cdot 3.5H_2O$
$M_r = 571.63$
Monoclinic, *Pc*
Hall symbol: P -2yc
$a = 24.943$ (3) Å
$b = 14.4343$ (18) Å
$c = 29.688$ (4) Å
$\beta = 101.190$ (3)°
$V = 10486$ (2) Å$^3$
$Z = 16$
$F(000) = 4754$
$D_x = 1.448$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3191 reflections
$\theta = 2.2$–$20.6$°

$\mu$ = 0.55 mm$^{-1}$
$T$ = 90 K

Plate, brown
0.28 × 0.04 × 0.03 mm

*Data collection*

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2005)
$T_{min}$ = 0.861, $T_{max}$ = 0.984

158363 measured reflections
94844 independent reflections
26534 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.164
$\theta_{max}$ = 25.4°, $\theta_{min}$ = 1.7°
$h$ = −30→30
$k$ = −17→17
$l$ = −35→35

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.151
$S$ = 0.64
19177 reflections
1275 parameters
3166 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
$w = 1/[\sigma^2(F_o^2) + (0.0236P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.079
$\Delta\rho_{max}$ = 1.04 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.55 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Mn1 | 1.16133 (13) | 0.9554 (2) | 0.75887 (11) | 0.0182 (9) | |
| O1 | 1.2040 (5) | 1.2061 (8) | 0.7169 (4) | 0.022 (4)* | |
| O2 | 1.2120 (6) | 0.7182 (9) | 0.7044 (4) | 0.032 (4)* | |
| O3 | 1.0498 (5) | 0.9498 (9) | 0.7141 (4) | 0.026 (4)* | |
| N1 | 1.1457 (6) | 1.0674 (9) | 0.7954 (5) | 0.021 (4)* | |
| N2 | 1.1838 (6) | 1.0506 (9) | 0.7197 (5) | 0.023 (5)* | |
| N3 | 1.1924 (6) | 0.8743 (9) | 0.7187 (5) | 0.016 (4)* | |
| N4 | 1.1579 (6) | 0.8318 (8) | 0.7935 (4) | 0.013 (4)* | |
| N5 | 1.0977 (6) | 0.9503 (10) | 0.7323 (5) | 0.023 (5)* | |
| N6 | 1.2412 (5) | 0.9692 (9) | 0.7998 (4) | 0.012 (4)* | |
| N7 | 1.3994 (6) | 1.0009 (10) | 0.8792 (5) | 0.016 (4)* | |
| C1 | 1.1252 (7) | 1.0775 (11) | 0.8343 (5) | 0.016 (5)* | |
| H1 | 1.1119 | 1.0237 | 0.8469 | 0.019* | |
| C2 | 1.1224 (8) | 1.1608 (11) | 0.8569 (6) | 0.028 (6)* | |

| | | | | |
|---|---|---|---|---|
| H2 | 1.1078 | 1.1633 | 0.8841 | 0.034* |
| C3 | 1.1410 (8) | 1.2391 (13) | 0.8393 (6) | 0.029 (6)* |
| H3 | 1.1401 | 1.2963 | 0.8550 | 0.034* |
| C4 | 1.1612 (8) | 1.2370 (12) | 0.7991 (6) | 0.025 (6)* |
| H4 | 1.1728 | 1.2915 | 0.7858 | 0.030* |
| C5 | 1.1634 (8) | 1.1488 (11) | 0.7789 (6) | 0.021 (5)* |
| C6 | 1.1857 (9) | 1.1397 (12) | 0.7345 (6) | 0.029 (6)* |
| C7 | 1.1992 (9) | 1.0170 (11) | 0.6808 (6) | 0.015 (5)* |
| C8 | 1.2100 (9) | 1.0718 (13) | 0.6432 (6) | 0.034 (7)* |
| H8 | 1.2066 | 1.1374 | 0.6428 | 0.041* |
| C9 | 1.2262 (9) | 1.0224 (12) | 0.6064 (7) | 0.032 (7)* |
| H9 | 1.2321 | 1.0568 | 0.5805 | 0.038* |
| C10 | 1.2340 (9) | 0.9237 (13) | 0.6059 (7) | 0.039 (7)* |
| H10 | 1.2457 | 0.8936 | 0.5811 | 0.046* |
| C11 | 1.2239 (8) | 0.8757 (12) | 0.6429 (6) | 0.021 (6)* |
| H11 | 1.2297 | 0.8106 | 0.6439 | 0.025* |
| C12 | 1.2049 (8) | 0.9191 (11) | 0.6802 (6) | 0.017 (5)* |
| C13 | 1.1959 (8) | 0.7826 (11) | 0.7286 (6) | 0.026 (6)* |
| C14 | 1.1732 (8) | 0.7582 (11) | 0.7694 (6) | 0.016 (5)* |
| C15 | 1.1710 (8) | 0.6660 (12) | 0.7833 (6) | 0.028 (6)* |
| H15 | 1.1827 | 0.6174 | 0.7659 | 0.034* |
| C16 | 1.1522 (8) | 0.6473 (12) | 0.8213 (6) | 0.028 (6)* |
| H16 | 1.1483 | 0.5850 | 0.8305 | 0.034* |
| C17 | 1.1381 (8) | 0.7217 (12) | 0.8478 (6) | 0.027 (5)* |
| H17 | 1.1267 | 0.7108 | 0.8760 | 0.032* |
| C18 | 1.1416 (8) | 0.8092 (12) | 0.8316 (6) | 0.022 (5)* |
| H18 | 1.1312 | 0.8583 | 0.8494 | 0.026* |
| C19 | 1.2511 (8) | 0.9712 (12) | 0.8461 (6) | 0.023 (6)* |
| H19 | 1.2209 | 0.9620 | 0.8608 | 0.028* |
| C20 | 1.3005 (7) | 0.9853 (13) | 0.8730 (6) | 0.022 (6)* |
| H20 | 1.3036 | 0.9892 | 0.9053 | 0.026* |
| C21 | 1.3477 (7) | 0.9944 (13) | 0.8537 (5) | 0.015 (5)* |
| C22 | 1.3379 (7) | 0.9947 (13) | 0.8063 (6) | 0.023 (6)* |
| H22 | 1.3674 | 1.0043 | 0.7908 | 0.028* |
| C23 | 1.2857 (7) | 0.9811 (13) | 0.7812 (6) | 0.020 (6)* |
| H23 | 1.2810 | 0.9801 | 0.7487 | 0.024* |
| C24 | 1.4076 (8) | 1.0026 (14) | 0.9286 (5) | 0.023 (6)* |
| H24A | 1.3721 | 0.9994 | 0.9381 | 0.035* |
| H24B | 1.4262 | 1.0601 | 0.9401 | 0.035* |
| H24C | 1.4300 | 0.9494 | 0.9412 | 0.035* |
| C25 | 1.4465 (7) | 1.0031 (13) | 0.8581 (6) | 0.021 (6)* |
| H25A | 1.4349 | 1.0001 | 0.8246 | 0.031* |
| H25B | 1.4701 | 0.9501 | 0.8687 | 0.031* |
| H25C | 1.4668 | 1.0607 | 0.8665 | 0.031* |
| Mn2 | 1.05533 (13) | 1.4634 (2) | 0.70853 (11) | 0.0191 (9) |
| O4 | 1.0729 (5) | 1.2372 (8) | 0.6295 (4) | 0.031 (4)* |
| O5 | 1.0601 (5) | 1.7205 (9) | 0.6538 (4) | 0.041 (4)* |
| O6 | 1.1569 (5) | 1.4482 (9) | 0.7702 (4) | 0.031 (4)* |

| | | | | |
|---|---|---|---|---|
| N8 | 1.0300 (6) | 1.3369 (8) | 0.7292 (4) | 0.007 (4)* |
| N9 | 1.0714 (6) | 1.3892 (9) | 0.6584 (4) | 0.020 (4)* |
| N10 | 1.0732 (6) | 1.5647 (9) | 0.6708 (5) | 0.025 (5)* |
| N11 | 1.0316 (6) | 1.5753 (9) | 0.7427 (5) | 0.019 (4)* |
| N12 | 1.1137 (6) | 1.4543 (10) | 0.7433 (5) | 0.018 (4)* |
| N13 | 0.9752 (5) | 1.4773 (10) | 0.6706 (5) | 0.022 (5)* |
| N14 | 0.8138 (6) | 1.5220 (10) | 0.5973 (5) | 0.020 (4)* |
| C26 | 1.0097 (7) | 1.3107 (11) | 0.7656 (5) | 0.016 (5)* |
| H26 | 1.0022 | 1.3586 | 0.7854 | 0.019* |
| C27 | 0.9984 (8) | 1.2207 (11) | 0.7776 (6) | 0.021 (5)* |
| H27 | 0.9824 | 1.2074 | 0.8034 | 0.025* |
| C28 | 1.0128 (8) | 1.1485 (12) | 0.7481 (6) | 0.025 (5)* |
| H28 | 1.0083 | 1.0850 | 0.7549 | 0.030* |
| C29 | 1.0332 (8) | 1.1745 (12) | 0.7096 (6) | 0.036 (6)* |
| H29 | 1.0421 | 1.1284 | 0.6894 | 0.044* |
| C30 | 1.0407 (7) | 1.2687 (11) | 0.7003 (5) | 0.015 (5)* |
| C31 | 1.0644 (8) | 1.2953 (11) | 0.6581 (6) | 0.023 (5)* |
| C32 | 1.0962 (7) | 1.4355 (11) | 0.6273 (5) | 0.015 (5)* |
| C33 | 1.1166 (7) | 1.3933 (12) | 0.5906 (6) | 0.026 (5)* |
| H33 | 1.1135 | 1.3289 | 0.5839 | 0.031* |
| C34 | 1.1417 (8) | 1.4564 (12) | 0.5653 (6) | 0.030 (6)* |
| H34 | 1.1575 | 1.4317 | 0.5412 | 0.036* |
| C35 | 1.1458 (7) | 1.5489 (12) | 0.5720 (6) | 0.027 (5)* |
| H35 | 1.1634 | 1.5857 | 0.5526 | 0.032* |
| C36 | 1.1239 (8) | 1.5920 (13) | 0.6076 (6) | 0.046 (7)* |
| H36A | 1.1262 | 1.6571 | 0.6125 | 0.055* |
| C37 | 1.0981 (7) | 1.5331 (11) | 0.6358 (6) | 0.021 (5)* |
| C38 | 1.0575 (7) | 1.6486 (11) | 0.6777 (5) | 0.016 (5)* |
| C39 | 1.0352 (8) | 1.6566 (11) | 0.7193 (6) | 0.018 (5)* |
| C40 | 1.0173 (8) | 1.7386 (12) | 0.7348 (6) | 0.023 (5)* |
| H40 | 1.0186 | 1.7941 | 0.7178 | 0.028* |
| C41 | 0.9978 (9) | 1.7405 (14) | 0.7745 (7) | 0.046 (7)* |
| H41 | 0.9874 | 1.7981 | 0.7857 | 0.055* |
| C42 | 0.9925 (7) | 1.6597 (11) | 0.7993 (6) | 0.022 (5)* |
| H4A | 0.9772 | 1.6595 | 0.8262 | 0.026* |
| C43 | 1.0115 (7) | 1.5793 (11) | 0.7815 (5) | 0.020 (5)* |
| H43 | 1.0101 | 1.5233 | 0.7980 | 0.023* |
| C44 | 0.9316 (7) | 1.4741 (12) | 0.6905 (6) | 0.016 (5)* |
| H44 | 0.9379 | 1.4620 | 0.7226 | 0.019* |
| C45 | 0.8782 (7) | 1.4870 (11) | 0.6680 (5) | 0.012 (5)* |
| H45 | 0.8496 | 1.4807 | 0.6848 | 0.014* |
| C46 | 0.8652 (6) | 1.5087 (12) | 0.6222 (5) | 0.016 (5)* |
| C47 | 0.9117 (6) | 1.5135 (11) | 0.6007 (6) | 0.014 (5)* |
| H47 | 0.9067 | 1.5270 | 0.5688 | 0.016* |
| C48 | 0.9629 (7) | 1.4991 (12) | 0.6251 (6) | 0.025 (5)* |
| H48 | 0.9924 | 1.5047 | 0.6094 | 0.030* |
| C49 | 0.7681 (7) | 1.5197 (13) | 0.6224 (6) | 0.027 (6)* |
| H49A | 0.7824 | 1.5068 | 0.6549 | 0.041* |

| | | | | |
|---|---|---|---|---|
| H49B | 0.7423 | 1.4710 | 0.6095 | 0.041* |
| H49C | 0.7495 | 1.5798 | 0.6193 | 0.041* |
| C50 | 0.8045 (7) | 1.5414 (12) | 0.5487 (5) | 0.026 (5)* |
| H50A | 0.8396 | 1.5422 | 0.5384 | 0.038* |
| H50B | 0.7868 | 1.6020 | 0.5427 | 0.038* |
| H50C | 0.7810 | 1.4934 | 0.5319 | 0.038* |
| Mn3 | 0.29953 (13) | 0.2148 (2) | 0.51169 (10) | 0.0238 (9) |
| O7 | 0.1781 (6) | 0.3926 (9) | 0.4549 (4) | 0.034 (4)* |
| O8 | 0.2765 (6) | −0.0687 (9) | 0.4950 (5) | 0.043 (4)* |
| O9 | 0.2911 (6) | 0.2230 (10) | 0.6054 (4) | 0.039 (4)* |
| N15 | 0.3158 (6) | 0.3573 (8) | 0.5188 (5) | 0.019 (4)* |
| N16 | 0.2273 (5) | 0.2614 (10) | 0.4854 (5) | 0.024 (5)* |
| N17 | 0.2662 (6) | 0.0932 (9) | 0.4924 (5) | 0.028 (5)* |
| N18 | 0.3674 (5) | 0.1272 (9) | 0.5283 (5) | 0.017 (4)* |
| N19 | 0.2922 (7) | 0.2155 (11) | 0.5649 (5) | 0.033 (5)* |
| N20 | 0.3240 (6) | 0.2342 (10) | 0.4470 (4) | 0.019 (4)* |
| N21 | 0.3700 (6) | 0.2714 (11) | 0.3209 (5) | 0.022 (4)* |
| C51 | 0.3593 (8) | 0.4005 (12) | 0.5436 (6) | 0.027 (6)* |
| H51 | 0.3910 | 0.3664 | 0.5568 | 0.032* |
| C52 | 0.3574 (7) | 0.4972 (11) | 0.5497 (6) | 0.010 (5)* |
| H52 | 0.3889 | 0.5274 | 0.5664 | 0.012* |
| C53 | 0.3106 (8) | 0.5517 (13) | 0.5323 (7) | 0.034 (6)* |
| H53 | 0.3096 | 0.6165 | 0.5378 | 0.040* |
| C54 | 0.2668 (8) | 0.5055 (11) | 0.5068 (6) | 0.017 (5)* |
| H54 | 0.2352 | 0.5389 | 0.4926 | 0.021* |
| C55 | 0.2688 (7) | 0.4072 (11) | 0.5015 (7) | 0.026 (6)* |
| C56 | 0.2189 (8) | 0.3521 (12) | 0.4784 (7) | 0.031 (6)* |
| C57 | 0.1859 (8) | 0.1916 (13) | 0.4719 (7) | 0.042 (7)* |
| C58 | 0.1292 (9) | 0.2093 (16) | 0.4599 (8) | 0.070 (9)* |
| H58 | 0.1142 | 0.2696 | 0.4610 | 0.084* |
| C59 | 0.0962 (9) | 0.1297 (15) | 0.4460 (7) | 0.066 (8)* |
| H59 | 0.0580 | 0.1371 | 0.4359 | 0.079* |
| C60 | 0.1188 (9) | 0.0408 (15) | 0.4469 (7) | 0.059 (8)* |
| H60 | 0.0945 | −0.0093 | 0.4375 | 0.071* |
| C61 | 0.1743 (8) | 0.0200 (13) | 0.4605 (7) | 0.037 (6)* |
| H61 | 0.1879 | −0.0417 | 0.4620 | 0.044* |
| C62 | 0.2094 (7) | 0.0997 (13) | 0.4722 (7) | 0.041 (7)* |
| C63 | 0.2935 (7) | 0.0159 (12) | 0.5007 (7) | 0.027 (6)* |
| C64 | 0.3509 (7) | 0.0354 (11) | 0.5234 (6) | 0.020 (5)* |
| C65 | 0.3868 (7) | −0.0363 (12) | 0.5348 (6) | 0.025 (5)* |
| H65 | 0.3752 | −0.0990 | 0.5310 | 0.030* |
| C66 | 0.4411 (8) | −0.0135 (13) | 0.5522 (7) | 0.042 (6)* |
| H66 | 0.4667 | −0.0620 | 0.5609 | 0.050* |
| C67 | 0.4592 (7) | 0.0787 (11) | 0.5572 (6) | 0.020 (5)* |
| H67 | 0.4965 | 0.0939 | 0.5684 | 0.024* |
| C68 | 0.4201 (7) | 0.1455 (12) | 0.5448 (6) | 0.023 (6)* |
| H68 | 0.4311 | 0.2085 | 0.5482 | 0.028* |
| C69 | 0.3759 (7) | 0.2533 (12) | 0.4450 (6) | 0.017 (5)* |

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|---|---|---|---|---|
| H69 | 0.4021 | 0.2595 | 0.4727 | 0.020* |
| C70 | 0.3920 (8) | 0.2641 (13) | 0.4042 (5) | 0.028 (6)* |
| H70 | 0.4295 | 0.2744 | 0.4041 | 0.034* |
| C71 | 0.3555 (7) | 0.2605 (12) | 0.3627 (5) | 0.011 (5)* |
| C72 | 0.2991 (7) | 0.2479 (12) | 0.3646 (6) | 0.016 (5)* |
| H72 | 0.2718 | 0.2482 | 0.3374 | 0.019* |
| C73 | 0.2857 (7) | 0.2355 (12) | 0.4069 (5) | 0.018 (5)* |
| H73 | 0.2483 | 0.2275 | 0.4086 | 0.021* |
| C74 | 0.4263 (7) | 0.2735 (14) | 0.3170 (6) | 0.029 (6)* |
| H74A | 0.4491 | 0.2843 | 0.3473 | 0.043* |
| H74B | 0.4320 | 0.3235 | 0.2961 | 0.043* |
| H74C | 0.4362 | 0.2141 | 0.3049 | 0.043* |
| C75 | 0.3299 (7) | 0.2577 (13) | 0.2786 (5) | 0.019 (5)* |
| H75A | 0.2930 | 0.2581 | 0.2854 | 0.029* |
| H75B | 0.3365 | 0.1980 | 0.2649 | 0.029* |
| H75C | 0.3332 | 0.3076 | 0.2569 | 0.029* |
| Mn4 | 0.54984 (13) | 0.5246 (2) | 0.47811 (10) | 0.0200 (9) |
| O10 | 0.4962 (6) | 0.7669 (9) | 0.5250 (4) | 0.032 (4)* |
| O11 | 0.5037 (6) | 0.2800 (9) | 0.5276 (4) | 0.040 (4)* |
| O12 | 0.6608 (6) | 0.5207 (9) | 0.5241 (5) | 0.035 (4)* |
| N22 | 0.5555 (6) | 0.6439 (8) | 0.4426 (4) | 0.012 (4)* |
| N23 | 0.5231 (6) | 0.6133 (9) | 0.5182 (4) | 0.016 (4)* |
| N24 | 0.5253 (6) | 0.4355 (9) | 0.5190 (4) | 0.013 (4)* |
| N25 | 0.5604 (6) | 0.4040 (8) | 0.4427 (4) | 0.014 (4)* |
| N26 | 0.6143 (6) | 0.5258 (10) | 0.5035 (5) | 0.021 (5)* |
| N27 | 0.4701 (5) | 0.5163 (10) | 0.4370 (5) | 0.022 (5)* |
| N28 | 0.3132 (6) | 0.5041 (11) | 0.3555 (5) | 0.016 (4)* |
| C76 | 0.5772 (8) | 0.6601 (12) | 0.4052 (6) | 0.021 (5)* |
| H76 | 0.5898 | 0.6082 | 0.3906 | 0.025* |
| C77 | 0.5825 (8) | 0.7486 (11) | 0.3860 (6) | 0.027 (6)* |
| H77 | 0.5994 | 0.7565 | 0.3602 | 0.032* |
| C78 | 0.5619 (8) | 0.8231 (12) | 0.4067 (6) | 0.023 (5)* |
| H78 | 0.5625 | 0.8836 | 0.3941 | 0.027* |
| C79 | 0.5406 (7) | 0.8091 (11) | 0.4455 (5) | 0.013 (5)* |
| H79 | 0.5285 | 0.8602 | 0.4610 | 0.015* |
| C80 | 0.5368 (9) | 0.7169 (12) | 0.4625 (6) | 0.031 (6)* |
| C81 | 0.5174 (8) | 0.7030 (11) | 0.5065 (6) | 0.020 (5)* |
| C82 | 0.5090 (8) | 0.5732 (11) | 0.5572 (6) | 0.018 (5)* |
| C83 | 0.4965 (8) | 0.6205 (12) | 0.5949 (6) | 0.026 (6)* |
| H83 | 0.4976 | 0.6863 | 0.5956 | 0.031* |
| C84 | 0.4825 (8) | 0.5717 (12) | 0.6319 (6) | 0.022 (6)* |
| H84 | 0.4722 | 0.6046 | 0.6566 | 0.026* |
| C85 | 0.4836 (8) | 0.4767 (11) | 0.6324 (6) | 0.017 (6)* |
| H85 | 0.4756 | 0.4449 | 0.6584 | 0.021* |
| C86 | 0.4964 (8) | 0.4246 (12) | 0.5955 (6) | 0.026 (6)* |
| H86 | 0.4953 | 0.3588 | 0.5956 | 0.031* |
| C87 | 0.5110 (9) | 0.4742 (11) | 0.5582 (6) | 0.020 (6)* |
| C88 | 0.5220 (9) | 0.3461 (12) | 0.5071 (6) | 0.027 (6)* |

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|---|---|---|---|---|
| C89 | 0.5420 (8) | 0.3301 (11) | 0.4641 (6) | 0.022 (6)* |
| C90 | 0.5435 (8) | 0.2436 (12) | 0.4474 (6) | 0.029 (6)* |
| H90 | 0.5316 | 0.1926 | 0.4632 | 0.035* |
| C91 | 0.5626 (7) | 0.2293 (12) | 0.4068 (6) | 0.025 (5)* |
| H91 | 0.5640 | 0.1687 | 0.3947 | 0.030* |
| C92 | 0.5798 (7) | 0.3064 (11) | 0.3840 (6) | 0.016 (5)* |
| H92 | 0.5921 | 0.2996 | 0.3559 | 0.019* |
| C93 | 0.5780 (8) | 0.3924 (13) | 0.4045 (6) | 0.037 (6)* |
| H93 | 0.5902 | 0.4451 | 0.3901 | 0.044* |
| C94 | 0.4622 (7) | 0.5138 (12) | 0.3905 (5) | 0.016 (5)* |
| H94 | 0.4932 | 0.5170 | 0.3764 | 0.019* |
| C95 | 0.4115 (7) | 0.5069 (13) | 0.3629 (6) | 0.014 (5)* |
| H95 | 0.4088 | 0.5031 | 0.3306 | 0.016* |
| C96 | 0.3633 (7) | 0.5054 (14) | 0.3811 (5) | 0.015 (5)* |
| C97 | 0.3748 (7) | 0.5025 (13) | 0.4289 (5) | 0.014 (5)* |
| H97 | 0.3452 | 0.4944 | 0.4444 | 0.016* |
| C98 | 0.4260 (7) | 0.5106 (13) | 0.4546 (6) | 0.020 (5)* |
| H98 | 0.4300 | 0.5123 | 0.4871 | 0.023* |
| C99 | 0.3037 (8) | 0.5038 (14) | 0.3063 (6) | 0.024 (6)* |
| H99A | 0.3387 | 0.4989 | 0.2961 | 0.036* |
| H99B | 0.2854 | 0.5614 | 0.2946 | 0.036* |
| H99C | 0.2805 | 0.4508 | 0.2946 | 0.036* |
| C100 | 0.2656 (8) | 0.5064 (14) | 0.3780 (7) | 0.031 (6)* |
| H10B | 0.2320 | 0.5021 | 0.3547 | 0.047* |
| H10C | 0.2657 | 0.5646 | 0.3950 | 0.047* |
| H10D | 0.2675 | 0.4541 | 0.3993 | 0.047* |
| Mn5 | 0.65198 (14) | 1.0340 (2) | 0.52464 (11) | 0.0229 (10) |
| O13 | 0.6322 (5) | 0.8118 (8) | 0.6036 (4) | 0.028 (4)* |
| O14 | 0.6501 (5) | 1.2919 (9) | 0.5800 (4) | 0.037 (4)* |
| O15 | 0.5565 (5) | 1.0268 (9) | 0.4557 (4) | 0.030 (4)* |
| N29 | 0.6767 (6) | 0.9055 (9) | 0.5062 (5) | 0.025 (5)* |
| N30 | 0.6276 (6) | 0.9600 (8) | 0.5711 (4) | 0.016 (4)* |
| N31 | 0.6325 (6) | 1.1352 (9) | 0.5619 (4) | 0.016 (4)* |
| N32 | 0.6817 (6) | 1.1411 (9) | 0.4917 (5) | 0.023 (4)* |
| N33 | 0.5960 (6) | 1.0275 (10) | 0.4864 (5) | 0.019 (5)* |
| N34 | 0.7322 (5) | 1.0344 (10) | 0.5646 (5) | 0.016 (5)* |
| N35 | 0.8882 (6) | 1.0084 (10) | 0.6471 (5) | 0.022 (4)* |
| C101 | 0.6992 (7) | 0.8808 (11) | 0.4722 (6) | 0.020 (5)* |
| H101 | 0.7085 | 0.9282 | 0.4528 | 0.024* |
| C102 | 0.7109 (8) | 0.7879 (12) | 0.4619 (6) | 0.024 (6)* |
| H102 | 0.7273 | 0.7724 | 0.4366 | 0.029* |
| C103 | 0.6966 (7) | 0.7206 (11) | 0.4912 (5) | 0.013 (5)* |
| H103 | 0.7035 | 0.6571 | 0.4860 | 0.016* |
| C104 | 0.6725 (7) | 0.7447 (10) | 0.5280 (5) | 0.012 (5)* |
| H104 | 0.6618 | 0.6989 | 0.5474 | 0.015* |
| C105 | 0.6647 (8) | 0.8387 (11) | 0.5352 (6) | 0.024 (6)* |
| C106 | 0.6382 (7) | 0.8694 (10) | 0.5750 (5) | 0.012 (5)* |
| C107 | 0.6040 (8) | 1.0132 (11) | 0.6033 (6) | 0.022 (5)* |

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|---|---|---|---|---|
| C108 | 0.5763 (8) | 0.9757 (13) | 0.6362 (6) | 0.043 (6)* |
| H108 | 0.5720 | 0.9108 | 0.6395 | 0.052* |
| C109 | 0.5546 (8) | 1.0423 (11) | 0.6645 (6) | 0.021 (6)* |
| H109 | 0.5378 | 1.0196 | 0.6884 | 0.025* |
| C110 | 0.5571 (8) | 1.1353 (12) | 0.6587 (6) | 0.034 (6)* |
| H110 | 0.5416 | 1.1761 | 0.6779 | 0.041* |
| C111 | 0.5825 (7) | 1.1706 (13) | 0.6245 (6) | 0.034 (6)* |
| H111 | 0.5831 | 1.2356 | 0.6195 | 0.041* |
| C112 | 0.6072 (8) | 1.1104 (12) | 0.5974 (6) | 0.032 (6)* |
| C113 | 0.6526 (8) | 1.2200 (12) | 0.5554 (6) | 0.025 (5)* |
| C114 | 0.6788 (7) | 1.2230 (11) | 0.5143 (5) | 0.019 (5)* |
| C115 | 0.6947 (8) | 1.3075 (12) | 0.4998 (6) | 0.026 (6)* |
| H115 | 0.6898 | 1.3630 | 0.5157 | 0.032* |
| C116 | 0.7185 (8) | 1.3086 (13) | 0.4605 (6) | 0.034 (6)* |
| H116 | 0.7323 | 1.3644 | 0.4502 | 0.041* |
| C117 | 0.7212 (8) | 1.2236 (12) | 0.4368 (6) | 0.037 (6)* |
| H117 | 0.7350 | 1.2218 | 0.4091 | 0.044* |
| C118 | 0.7035 (7) | 1.1442 (12) | 0.4548 (6) | 0.025 (5)* |
| H118 | 0.7073 | 1.0874 | 0.4395 | 0.030* |
| C119 | 0.7773 (7) | 1.0340 (12) | 0.5471 (6) | 0.023 (6)* |
| H119 | 0.7732 | 1.0371 | 0.5147 | 0.027* |
| C120 | 0.8296 (7) | 1.0293 (12) | 0.5726 (5) | 0.018 (5)* |
| H120 | 0.8601 | 1.0329 | 0.5579 | 0.021* |
| C121 | 0.8377 (6) | 1.0191 (12) | 0.6209 (5) | 0.015 (5)* |
| C122 | 0.7905 (6) | 1.0244 (12) | 0.6396 (6) | 0.020 (5)* |
| H122 | 0.7932 | 1.0208 | 0.6720 | 0.023* |
| C123 | 0.7408 (7) | 1.0346 (12) | 0.6117 (5) | 0.026 (6)* |
| H123 | 0.7099 | 1.0425 | 0.6256 | 0.032* |
| C124 | 0.9356 (7) | 1.0031 (12) | 0.6254 (6) | 0.013 (5)* |
| H12D | 0.9244 | 1.0153 | 0.5924 | 0.020* |
| H12E | 0.9518 | 0.9411 | 0.6300 | 0.020* |
| H12F | 0.9627 | 1.0494 | 0.6391 | 0.020* |
| C125 | 0.8955 (8) | 0.9973 (13) | 0.6962 (5) | 0.033 (6)* |
| H12G | 0.9346 | 0.9938 | 0.7095 | 0.049* |
| H12H | 0.8775 | 0.9402 | 0.7031 | 0.049* |
| H12I | 0.8794 | 1.0503 | 0.7093 | 0.049* |
| Mn6 | 0.76186 (12) | 0.2699 (2) | 0.75693 (10) | 0.0207 (8) |
| O16 | 0.8851 (5) | 0.0955 (8) | 0.8075 (4) | 0.027 (4)* |
| O17 | 0.7896 (6) | 0.5496 (9) | 0.7533 (4) | 0.030 (4)* |
| O18 | 0.6994 (5) | 0.2506 (8) | 0.8257 (4) | 0.032 (4)* |
| N36 | 0.7484 (6) | 0.1305 (8) | 0.7459 (5) | 0.025 (4)* |
| N37 | 0.8296 (5) | 0.2237 (9) | 0.7942 (4) | 0.019 (4)* |
| N38 | 0.7968 (6) | 0.3888 (8) | 0.7701 (5) | 0.021 (4)* |
| N39 | 0.7034 (6) | 0.3519 (9) | 0.7172 (5) | 0.023 (4)* |
| N40 | 0.7269 (5) | 0.2649 (9) | 0.7978 (4) | 0.014 (4)* |
| N41 | 0.7989 (5) | 0.2630 (9) | 0.6982 (4) | 0.013 (4)* |
| N42 | 0.8757 (6) | 0.2560 (10) | 0.5832 (4) | 0.025 (4)* |
| C126 | 0.7035 (8) | 0.0857 (12) | 0.7240 (6) | 0.032 (6)* |

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|---|---|---|---|---|
| H126 | 0.6734 | 0.1197 | 0.7074 | 0.038* |
| C127 | 0.7013 (8) | −0.0121 (12) | 0.7257 (6) | 0.033 (6)* |
| H127 | 0.6685 | −0.0426 | 0.7120 | 0.039* |
| C128 | 0.7462 (7) | −0.0654 (13) | 0.7470 (6) | 0.032 (6)* |
| H128 | 0.7452 | −0.1312 | 0.7464 | 0.039* |
| C129 | 0.7927 (8) | −0.0173 (11) | 0.7694 (6) | 0.024 (6)* |
| H129 | 0.8238 | −0.0497 | 0.7853 | 0.029* |
| C130 | 0.7922 (7) | 0.0822 (11) | 0.7677 (6) | 0.015 (5)* |
| C131 | 0.8420 (7) | 0.1359 (11) | 0.7925 (6) | 0.029 (6)* |
| C132 | 0.8648 (6) | 0.2918 (10) | 0.8158 (5) | 0.011 (4)* |
| C133 | 0.9102 (7) | 0.2757 (12) | 0.8488 (5) | 0.024 (5)* |
| H133 | 0.9193 | 0.2148 | 0.8599 | 0.028* |
| C134 | 0.9434 (8) | 0.3524 (12) | 0.8661 (6) | 0.033 (6)* |
| H134 | 0.9767 | 0.3424 | 0.8873 | 0.040* |
| C135 | 0.9272 (7) | 0.4449 (12) | 0.8520 (6) | 0.027 (6)* |
| H135 | 0.9487 | 0.4955 | 0.8657 | 0.032* |
| C136 | 0.8806 (7) | 0.4623 (12) | 0.8186 (6) | 0.030 (6)* |
| H136 | 0.8706 | 0.5233 | 0.8082 | 0.036* |
| C137 | 0.8487 (7) | 0.3838 (11) | 0.8010 (6) | 0.025 (5)* |
| C138 | 0.7736 (7) | 0.4645 (11) | 0.7495 (6) | 0.021 (5)* |
| C139 | 0.7184 (6) | 0.4414 (11) | 0.7202 (5) | 0.015 (5)* |
| C140 | 0.6848 (7) | 0.5115 (13) | 0.6984 (6) | 0.034 (6)* |
| H140 | 0.6949 | 0.5749 | 0.7023 | 0.040* |
| C141 | 0.6364 (8) | 0.4846 (14) | 0.6710 (7) | 0.052 (7)* |
| H141 | 0.6146 | 0.5287 | 0.6518 | 0.062* |
| C142 | 0.6187 (8) | 0.3913 (13) | 0.6712 (6) | 0.042 (6)* |
| H142 | 0.5829 | 0.3737 | 0.6565 | 0.050* |
| C143 | 0.6546 (7) | 0.3280 (12) | 0.6932 (6) | 0.031 (6)* |
| H143 | 0.6445 | 0.2644 | 0.6914 | 0.037* |
| C144 | 0.7709 (7) | 0.2633 (12) | 0.6543 (5) | 0.019 (5)* |
| H144 | 0.7322 | 0.2639 | 0.6498 | 0.023* |
| C145 | 0.7936 (7) | 0.2629 (12) | 0.6151 (5) | 0.024 (5)* |
| H145 | 0.7708 | 0.2675 | 0.5856 | 0.029* |
| C146 | 0.8502 (7) | 0.2557 (15) | 0.6195 (6) | 0.017 (4)* |
| C147 | 0.8791 (7) | 0.2540 (11) | 0.6642 (5) | 0.021 (5)* |
| H147 | 0.9178 | 0.2497 | 0.6694 | 0.025* |
| C148 | 0.8537 (7) | 0.2584 (13) | 0.7013 (6) | 0.027 (6)* |
| H148 | 0.8761 | 0.2583 | 0.7311 | 0.033* |
| C149 | 0.8437 (7) | 0.2641 (14) | 0.5360 (5) | 0.032 (6)* |
| H14J | 0.8683 | 0.2612 | 0.5141 | 0.048* |
| H14K | 0.8241 | 0.3233 | 0.5327 | 0.048* |
| H14L | 0.8173 | 0.2130 | 0.5301 | 0.048* |
| C150 | 0.9348 (6) | 0.2651 (13) | 0.5877 (6) | 0.025 (5)* |
| H15B | 0.9443 | 0.2624 | 0.5572 | 0.038* |
| H15C | 0.9530 | 0.2145 | 0.6067 | 0.038* |
| H15D | 0.9466 | 0.3246 | 0.6022 | 0.038* |
| Mn7 | 0.94975 (12) | 0.18291 (19) | 0.99417 (10) | 0.0211 (8) |
| O19 | 0.9299 (6) | −0.0997 (9) | 1.0005 (4) | 0.039 (4)* |

| | | | | |
|---|---|---|---|---|
| O20 | 0.8235 (5) | 0.3430 (8) | 0.9297 (4) | 0.028 (4)* |
| O21 | 1.0195 (5) | 0.1780 (7) | 0.9291 (4) | 0.023 (3)* |
| N43 | 1.0043 (5) | 0.1079 (9) | 1.0425 (4) | 0.022 (4)* |
| N44 | 0.9165 (6) | 0.0568 (9) | 0.9853 (5) | 0.019 (4)* |
| N45 | 0.8836 (5) | 0.2209 (9) | 0.9516 (4) | 0.024 (4)* |
| N46 | 0.9592 (6) | 0.3255 (8) | 1.0001 (5) | 0.025 (4)* |
| N47 | 0.9893 (6) | 0.1773 (9) | 0.9545 (4) | 0.016 (4)* |
| N48 | 0.9073 (5) | 0.2051 (9) | 1.0491 (4) | 0.016 (4)* |
| N49 | 0.8244 (6) | 0.2470 (10) | 1.1580 (4) | 0.025 (4)* |
| C151 | 1.0478 (7) | 0.1347 (12) | 1.0741 (6) | 0.029 (6)* |
| H151 | 1.0565 | 0.1987 | 1.0778 | 0.034* |
| C152 | 1.0795 (7) | 0.0714 (12) | 1.1008 (6) | 0.034 (6)* |
| H152 | 1.1081 | 0.0920 | 1.1247 | 0.041* |
| C153 | 1.0706 (8) | −0.0230 (13) | 1.0938 (6) | 0.043 (6)* |
| H153 | 1.0944 | −0.0661 | 1.1118 | 0.052* |
| C154 | 1.0279 (7) | −0.0550 (12) | 1.0613 (6) | 0.026 (5)* |
| H154 | 1.0215 | −0.1191 | 1.0554 | 0.031* |
| C155 | 0.9946 (7) | 0.0137 (11) | 1.0376 (5) | 0.020 (5)* |
| C156 | 0.9425 (8) | −0.0178 (12) | 1.0046 (6) | 0.032 (6)* |
| C157 | 0.8689 (7) | 0.0579 (10) | 0.9503 (5) | 0.018 (5)* |
| C158 | 0.8403 (7) | −0.0243 (12) | 0.9321 (6) | 0.023 (5)* |
| H158 | 0.8516 | −0.0840 | 0.9437 | 0.027* |
| C159 | 0.7942 (7) | −0.0121 (11) | 0.8959 (5) | 0.014 (5)* |
| H159 | 0.7748 | −0.0656 | 0.8831 | 0.017* |
| C160 | 0.7761 (8) | 0.0748 (12) | 0.8784 (6) | 0.034 (6)* |
| H160 | 0.7444 | 0.0795 | 0.8548 | 0.040* |
| C161 | 0.8043 (7) | 0.1542 (12) | 0.8955 (6) | 0.032 (6)* |
| H161 | 0.7936 | 0.2132 | 0.8827 | 0.038* |
| C162 | 0.8497 (6) | 0.1454 (10) | 0.9324 (5) | 0.008 (4)* |
| C163 | 0.8683 (7) | 0.3104 (11) | 0.9507 (6) | 0.017 (5)* |
| C164 | 0.9127 (7) | 0.3710 (11) | 0.9767 (6) | 0.025 (5)* |
| C165 | 0.9107 (9) | 0.4687 (12) | 0.9737 (7) | 0.040 (7)* |
| H165 | 0.8793 | 0.4987 | 0.9567 | 0.048* |
| C166 | 0.9542 (7) | 0.5195 (12) | 0.9956 (6) | 0.030 (5)* |
| H166 | 0.9530 | 0.5853 | 0.9943 | 0.036* |
| C167 | 0.9991 (8) | 0.4756 (12) | 1.0192 (6) | 0.026 (6)* |
| H167 | 1.0288 | 0.5111 | 1.0352 | 0.031* |
| C168 | 1.0022 (7) | 0.3790 (11) | 1.0201 (6) | 0.027 (6)* |
| H168 | 1.0351 | 0.3500 | 1.0351 | 0.033* |
| C169 | 0.9338 (8) | 0.2354 (12) | 1.0916 (5) | 0.031 (6)* |
| H169 | 0.9720 | 0.2468 | 1.0961 | 0.037* |
| C170 | 0.9082 (6) | 0.2495 (11) | 1.1269 (6) | 0.024 (5)* |
| H170 | 0.9289 | 0.2688 | 1.1556 | 0.029* |
| C171 | 0.8518 (7) | 0.2365 (12) | 1.1223 (5) | 0.013 (4)* |
| C172 | 0.8250 (7) | 0.2033 (11) | 1.0802 (5) | 0.023 (5)* |
| H172 | 0.7870 | 0.1904 | 1.0750 | 0.027* |
| C173 | 0.8536 (6) | 0.1895 (11) | 1.0464 (5) | 0.015 (5)* |
| H173 | 0.8338 | 0.1664 | 1.0181 | 0.018* |

| | | | | |
|---|---|---|---|---|
| C174 | 0.8531 (7) | 0.2715 (12) | 1.2043 (5) | 0.024 (5)* |
| H174 | 0.8921 | 0.2798 | 1.2043 | 0.036* |
| H17F | 0.8484 | 0.2219 | 1.2257 | 0.036* |
| H17G | 0.8381 | 0.3294 | 1.2139 | 0.036* |
| C175 | 0.7658 (6) | 0.2302 (12) | 1.1519 (5) | 0.020 (5)* |
| H17H | 0.7511 | 0.2155 | 1.1197 | 0.030* |
| H17I | 0.7477 | 0.2857 | 1.1607 | 0.030* |
| H17J | 0.7592 | 0.1781 | 1.1713 | 0.030* |
| Mn8 | 0.40525 (12) | 0.2861 (2) | 0.71914 (10) | 0.0155 (8) |
| O22 | 0.4102 (5) | 0.5681 (8) | 0.7363 (4) | 0.017 (3)* |
| O23 | 0.5350 (5) | 0.1283 (8) | 0.7780 (4) | 0.025 (4)* |
| O24 | 0.4176 (6) | 0.2747 (9) | 0.6270 (4) | 0.036 (4)* |
| N50 | 0.3334 (5) | 0.3592 (9) | 0.7019 (5) | 0.015 (4)* |
| N51 | 0.4321 (5) | 0.4098 (8) | 0.7389 (5) | 0.010 (4)* |
| N52 | 0.4801 (5) | 0.2514 (9) | 0.7465 (4) | 0.006 (4)* |
| N53 | 0.3980 (6) | 0.1439 (8) | 0.7156 (5) | 0.012 (4)* |
| N54 | 0.4133 (6) | 0.2876 (9) | 0.6666 (4) | 0.014 (4)* |
| N55 | 0.3843 (5) | 0.2639 (10) | 0.7838 (4) | 0.011 (4)* |
| N56 | 0.3342 (6) | 0.2341 (11) | 0.9105 (5) | 0.018 (4)* |
| C176 | 0.2817 (7) | 0.3347 (12) | 0.6866 (6) | 0.020 (5)* |
| H176 | 0.2750 | 0.2701 | 0.6825 | 0.024* |
| C177 | 0.2369 (7) | 0.3906 (12) | 0.6761 (6) | 0.027 (6)* |
| H177 | 0.2013 | 0.3661 | 0.6660 | 0.032* |
| C178 | 0.2465 (7) | 0.4890 (11) | 0.6811 (6) | 0.018 (5)* |
| H178 | 0.2171 | 0.5316 | 0.6736 | 0.021* |
| C179 | 0.2994 (6) | 0.5202 (11) | 0.6969 (5) | 0.009 (4)* |
| H179 | 0.3076 | 0.5845 | 0.7000 | 0.011* |
| C180 | 0.3409 (6) | 0.4519 (11) | 0.7084 (6) | 0.015 (5)* |
| C181 | 0.3991 (7) | 0.4843 (11) | 0.7295 (6) | 0.018 (5)* |
| C182 | 0.4898 (6) | 0.4131 (10) | 0.7558 (6) | 0.008 (5)* |
| C183 | 0.5199 (7) | 0.4952 (11) | 0.7696 (6) | 0.013 (5)* |
| H183 | 0.5026 | 0.5541 | 0.7679 | 0.015* |
| C184 | 0.5758 (7) | 0.4853 (11) | 0.7857 (6) | 0.018 (5)* |
| H18D | 0.5971 | 0.5387 | 0.7955 | 0.021* |
| C185 | 0.6012 (7) | 0.3996 (11) | 0.7879 (6) | 0.019 (5)* |
| H185 | 0.6398 | 0.3971 | 0.7977 | 0.023* |
| C186 | 0.5736 (6) | 0.3186 (11) | 0.7767 (5) | 0.014 (5)* |
| H186 | 0.5917 | 0.2603 | 0.7797 | 0.017* |
| C187 | 0.5170 (7) | 0.3259 (11) | 0.7603 (6) | 0.020 (6)* |
| C188 | 0.4909 (7) | 0.1642 (11) | 0.7569 (6) | 0.020 (5)* |
| C189 | 0.4454 (7) | 0.1005 (11) | 0.7357 (6) | 0.012 (5)* |
| C190 | 0.4493 (7) | 0.0084 (11) | 0.7343 (6) | 0.015 (5)* |
| H190 | 0.4820 | −0.0207 | 0.7495 | 0.018* |
| C191 | 0.4067 (7) | −0.0459 (12) | 0.7113 (6) | 0.016 (5)* |
| H191 | 0.4099 | −0.1114 | 0.7100 | 0.019* |
| C192 | 0.3589 (8) | −0.0002 (12) | 0.6901 (6) | 0.019 (5)* |
| H192 | 0.3287 | −0.0341 | 0.6735 | 0.022* |
| C193 | 0.3563 (7) | 0.0951 (11) | 0.6938 (6) | 0.015 (5)* |

| | | | | |
|---|---|---|---|---|
| H193 | 0.3236 | 0.1262 | 0.6803 | 0.018* |
| C194 | 0.3321 (7) | 0.2399 (12) | 0.7866 (5) | 0.013 (5)* |
| H194 | 0.3065 | 0.2288 | 0.7589 | 0.016* |
| C195 | 0.3150 (7) | 0.2311 (12) | 0.8273 (5) | 0.011 (5)* |
| H195 | 0.2777 | 0.2171 | 0.8269 | 0.013* |
| C196 | 0.3508 (7) | 0.2421 (13) | 0.8698 (5) | 0.016 (5)* |
| C197 | 0.4049 (7) | 0.2640 (13) | 0.8674 (6) | 0.026 (6)* |
| H197 | 0.4319 | 0.2709 | 0.8945 | 0.031* |
| C198 | 0.4176 (7) | 0.2751 (12) | 0.8245 (5) | 0.019 (5)* |
| H198 | 0.4542 | 0.2927 | 0.8238 | 0.022* |
| C199 | 0.2753 (7) | 0.2260 (15) | 0.9103 (7) | 0.041 (7)* |
| H19J | 0.2554 | 0.2176 | 0.8787 | 0.061* |
| H19K | 0.2625 | 0.2825 | 0.9232 | 0.061* |
| H19L | 0.2688 | 0.1726 | 0.9289 | 0.061* |
| C200 | 0.3712 (7) | 0.2454 (14) | 0.9543 (6) | 0.031 (6)* |
| H20A | 0.4089 | 0.2497 | 0.9493 | 0.046* |
| H20B | 0.3680 | 0.1919 | 0.9739 | 0.046* |
| H20C | 0.3619 | 0.3021 | 0.9692 | 0.046* |
| O25 | 0.4001 (4) | −0.2744 (7) | 0.6831 (3) | 0.025 (3)* |
| C201 | 0.3580 (5) | −0.2891 (10) | 0.6437 (4) | 0.033 (6)* |
| C202 | 0.3672 (7) | −0.2217 (11) | 0.6068 (3) | 0.024 (5)* |
| H20D | 0.3952 | −0.3166 | 0.7072 | 0.029* |
| H20E | 0.3176 | −0.2778 | 0.6523 | 0.029* |
| H20F | 0.3593 | −0.3608 | 0.6314 | 0.029* |
| H20G | 0.3359 | −0.2304 | 0.5757 | 0.029* |
| H20H | 0.3657 | −0.1503 | 0.6187 | 0.029* |
| H20I | 0.4072 | −0.2331 | 0.5978 | 0.029* |
| O26 | 0.2449 (4) | 0.2389 (8) | 1.0157 (4) | 0.027 (3)* |
| C203 | 0.1915 (4) | 0.2476 (11) | 0.9879 (4) | 0.036 (6)* |
| C204 | 0.1508 (4) | 0.2097 (12) | 1.0150 (5) | 0.036 (6)* |
| H20J | 0.2555 | 0.1854 | 1.0092 | 0.044* |
| H20K | 0.1890 | 0.2088 | 0.9557 | 0.044* |
| H20L | 0.1825 | 0.3206 | 0.9790 | 0.044* |
| H20M | 0.1091 | 0.2148 | 0.9951 | 0.044* |
| H20N | 0.1594 | 0.1369 | 1.0237 | 0.047* |
| H20O | 0.1529 | 0.2483 | 1.0470 | 0.044* |
| O27 | 0.9582 (6) | 0.9557 (9) | 0.8031 (4) | 0.042 (5)* |
| C205 | 0.9927 (5) | 0.9722 (12) | 0.8468 (4) | 0.042 (7)* |
| C206 | 0.9597 (8) | 0.9527 (13) | 0.8836 (4) | 0.047 (7)* |
| H20P | 0.9311 | 0.9914 | 0.7998 | 0.056* |
| H20Q | 1.0071 | 1.0443 | 0.8491 | 0.056* |
| H20R | 1.0288 | 0.9270 | 0.8514 | 0.056* |
| H20S | 0.9844 | 0.9644 | 0.9177 | 0.056* |
| H20T | 0.9239 | 0.9979 | 0.8793 | 0.056* |
| H20U | 0.9455 | 0.8809 | 0.8816 | 0.056* |
| O28 | 0.5659 (6) | −0.0216 (9) | 0.8341 (5) | 0.056 (5)* |
| C207 | 0.6229 (6) | −0.0043 (10) | 0.8366 (7) | 0.078 (9)* |
| C208 | 0.6486 (7) | −0.0922 (14) | 0.8228 (8) | 0.099 (10)* |

| | | | | | |
|---|---|---|---|---|---|
| H20V | 0.5559 | 0.0251 | 0.8169 | 0.119* | |
| H20W | 0.6423 | 0.0159 | 0.8717 | 0.119* | |
| H20X | 0.6287 | 0.0530 | 0.8136 | 0.119* | |
| H20Y | 0.6923 | −0.0824 | 0.8242 | 0.119* | |
| H21A | 0.6432 | −0.1492 | 0.8457 | 0.119* | |
| H21B | 0.6296 | −0.1122 | 0.7878 | 0.119* | |
| O29 | 0.7486 (6) | 0.4730 (8) | 0.9401 (4) | 0.033 (4)* | |
| C209 | 0.7173 (5) | 0.4668 (11) | 0.8945 (4) | 0.040 (7)* | |
| C21F | 0.7372 (8) | 0.5019 (13) | 0.8595 (4) | 0.045 (7)* | |
| H21C | 0.7785 | 0.4452 | 0.9415 | 0.054* | |
| H21D | 0.7097 | 0.4004 | 0.8878 | 0.054* | |
| H21E | 0.6817 | 0.4972 | 0.8944 | 0.054* | |
| H21G | 0.7109 | 0.4919 | 0.8308 | 0.054* | |
| H21H | 0.7717 | 0.4710 | 0.8577 | 0.054* | |
| H21I | 0.7436 | 0.5684 | 0.8643 | 0.054* | |
| O30 | 0.1495 (6) | 0.4560 (10) | 0.8991 (5) | 0.061 (6)* | |
| C211 | 0.0914 (6) | 0.4647 (16) | 0.8920 (5) | 0.081 (10)* | |
| C212 | 0.0741 (8) | 0.4444 (16) | 0.9371 (7) | 0.093 (10)* | |
| H21J | 0.1589 | 0.5023 | 0.9165 | 0.111* | |
| H21K | 0.0718 | 0.4159 | 0.8654 | 0.111* | |
| H21L | 0.0788 | 0.5350 | 0.8802 | 0.111* | |
| H21M | 0.0297 | 0.4502 | 0.9334 | 0.111* | |
| H21N | 0.0862 | 0.3743 | 0.9489 | 0.111* | |
| H21O | 0.0932 | 0.4931 | 0.9636 | 0.111* | |
| O31 | 0.6384 (6) | 0.7631 (9) | 0.6988 (5) | 0.059 (5)* | |
| C213 | 0.5881 (7) | 0.7158 (11) | 0.6988 (7) | 0.091 (9)* | |
| C214 | 0.5545 (8) | 0.7745 (19) | 0.7253 (9) | 0.161 (15)* | |
| H21P | 0.6371 | 0.7769 | 0.6707 | 0.193* | |
| H21Q | 0.5959 | 0.6473 | 0.7148 | 0.193* | |
| H21R | 0.5658 | 0.7052 | 0.6634 | 0.193* | |
| H21S | 0.5154 | 0.7411 | 0.7263 | 0.193* | |
| H21T | 0.5763 | 0.7848 | 0.7606 | 0.193* | |
| H21U | 0.5463 | 0.8426 | 0.7093 | 0.193* | |
| O1W | 0.7376 (8) | 0.7106 (13) | 0.7660 (6) | 0.106 (7)* | |
| O2W | 0.7816 (8) | 1.2427 (14) | 0.3413 (7) | 0.144 (8)* | |
| O3W | 0.9659 (9) | 0.7383 (14) | 0.9704 (7) | 0.137 (9)* | |
| O4W | 0.8654 (14) | 1.290 (2) | 0.3861 (11) | 0.092 (12)* | 0.50 |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Mn1 | 0.016 (2) | 0.0150 (19) | 0.023 (2) | −0.0001 (16) | 0.0020 (17) | −0.0018 (15) |
| Mn2 | 0.016 (2) | 0.019 (2) | 0.019 (2) | 0.0029 (16) | −0.0028 (18) | 0.0059 (16) |
| Mn3 | 0.032 (3) | 0.021 (2) | 0.018 (2) | −0.0079 (18) | 0.0026 (18) | 0.0002 (16) |
| Mn4 | 0.016 (2) | 0.025 (2) | 0.018 (2) | −0.0020 (16) | 0.0000 (17) | −0.0014 (16) |
| Mn5 | 0.022 (3) | 0.023 (2) | 0.024 (2) | 0.0039 (18) | 0.0067 (19) | −0.0044 (17) |
| Mn6 | 0.022 (2) | 0.0148 (18) | 0.0259 (19) | 0.0074 (16) | 0.0062 (16) | −0.0039 (15) |
| Mn7 | 0.023 (2) | 0.0208 (19) | 0.0193 (19) | −0.0006 (16) | 0.0031 (16) | −0.0021 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| Mn8 | 0.019 (2) | 0.0127 (18) | 0.015 (2) | −0.0014 (16) | 0.0026 (16) | 0.0012 (15) |

*Bond lengths (Å)*

| | | | |
|---|---|---|---|
| Mn1—N5 | 1.632 (14) | C104—C105 | 1.393 (17) |
| Mn1—N3 | 1.937 (12) | C104—H104 | 0.9500 |
| Mn1—N2 | 1.950 (12) | C105—C106 | 1.528 (17) |
| Mn1—N1 | 2.026 (12) | C107—C108 | 1.408 (18) |
| Mn1—N4 | 2.069 (12) | C107—C112 | 1.419 (18) |
| Mn1—N6 | 2.132 (12) | C108—C109 | 1.450 (19) |
| O1—C6 | 1.220 (16) | C108—H108 | 0.9500 |
| O2—C13 | 1.285 (16) | C109—C110 | 1.357 (18) |
| O3—N5 | 1.211 (15) | C109—H109 | 0.9500 |
| N1—C1 | 1.357 (16) | C110—C111 | 1.393 (18) |
| N1—C5 | 1.379 (17) | C110—H110 | 0.9500 |
| N2—C6 | 1.357 (17) | C111—C112 | 1.406 (18) |
| N2—C7 | 1.374 (16) | C111—H111 | 0.9500 |
| N3—C13 | 1.355 (17) | C113—C114 | 1.493 (17) |
| N3—C12 | 1.402 (16) | C114—C115 | 1.377 (18) |
| N4—C18 | 1.316 (16) | C115—C116 | 1.407 (18) |
| N4—C14 | 1.377 (16) | C115—H115 | 0.9500 |
| N6—C23 | 1.345 (17) | C116—C117 | 1.425 (19) |
| N6—C19 | 1.347 (16) | C116—H116 | 0.9500 |
| N7—C21 | 1.366 (17) | C117—C118 | 1.374 (18) |
| N7—C25 | 1.436 (17) | C117—H117 | 0.9500 |
| N7—C24 | 1.441 (16) | C118—H118 | 0.9500 |
| C1—C2 | 1.385 (18) | C119—C120 | 1.376 (18) |
| C1—H1 | 0.9500 | C119—H119 | 0.9500 |
| C2—C3 | 1.363 (19) | C120—C121 | 1.414 (17) |
| C2—H2 | 0.9500 | C120—H120 | 0.9500 |
| C3—C4 | 1.384 (17) | C121—C122 | 1.399 (17) |
| C3—H3 | 0.9500 | C122—C123 | 1.360 (18) |
| C4—C5 | 1.413 (18) | C122—H122 | 0.9500 |
| C4—H4 | 0.9500 | C123—H123 | 0.9500 |
| C5—C6 | 1.533 (18) | C124—H12D | 0.9800 |
| C7—C12 | 1.421 (18) | C124—H12E | 0.9800 |
| C7—C8 | 1.437 (18) | C124—H12F | 0.9800 |
| C8—C9 | 1.427 (19) | C125—H12G | 0.9800 |
| C8—H8 | 0.9500 | C125—H12H | 0.9800 |
| C9—C10 | 1.437 (19) | C125—H12I | 0.9800 |
| C9—H9 | 0.9500 | Mn6—N40 | 1.629 (11) |
| C10—C11 | 1.362 (19) | Mn6—N38 | 1.930 (12) |
| C10—H10 | 0.9500 | Mn6—N37 | 1.950 (12) |
| C11—C12 | 1.431 (18) | Mn6—N36 | 2.056 (12) |
| C11—H11 | 0.9500 | Mn6—N39 | 2.062 (13) |
| C13—C14 | 1.475 (18) | Mn6—N41 | 2.127 (11) |
| C14—C15 | 1.398 (18) | O16—C131 | 1.229 (16) |
| C15—C16 | 1.329 (18) | O17—C138 | 1.290 (16) |

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| C15—H15 | 0.9500 | O18—N40 | 1.190 (12) |
| C16—C17 | 1.415 (19) | N36—C126 | 1.345 (18) |
| C16—H16 | 0.9500 | N36—C130 | 1.351 (17) |
| C17—C18 | 1.360 (18) | N37—C131 | 1.308 (17) |
| C17—H17 | 0.9500 | N37—C132 | 1.390 (16) |
| C18—H18 | 0.9500 | N38—C138 | 1.329 (17) |
| C19—C20 | 1.349 (18) | N38—C137 | 1.436 (17) |
| C19—H19 | 0.9500 | N39—C143 | 1.331 (17) |
| C20—C21 | 1.410 (18) | N39—C139 | 1.343 (16) |
| C20—H20 | 0.9500 | N41—C148 | 1.354 (17) |
| C21—C22 | 1.382 (18) | N41—C144 | 1.355 (16) |
| C22—C23 | 1.384 (19) | N42—C146 | 1.355 (17) |
| C22—H22 | 0.9500 | N42—C150 | 1.459 (17) |
| C23—H23 | 0.9500 | N42—C149 | 1.475 (17) |
| C24—H24A | 0.9800 | C126—C127 | 1.414 (18) |
| C24—H24B | 0.9800 | C126—H126 | 0.9500 |
| C24—H24C | 0.9800 | C127—C128 | 1.41 (2) |
| C25—H25A | 0.9800 | C127—H127 | 0.9500 |
| C25—H25B | 0.9800 | C128—C129 | 1.403 (19) |
| C25—H25C | 0.9800 | C128—H128 | 0.9500 |
| Mn2—N12 | 1.619 (13) | C129—C130 | 1.437 (18) |
| Mn2—N9 | 1.939 (12) | C129—H129 | 0.9500 |
| Mn2—N10 | 1.947 (13) | C130—C131 | 1.526 (18) |
| Mn2—N11 | 2.056 (12) | C132—C133 | 1.366 (17) |
| Mn2—N8 | 2.065 (12) | C132—C137 | 1.432 (17) |
| Mn2—N13 | 2.106 (13) | C133—C134 | 1.417 (18) |
| O4—C31 | 1.240 (15) | C133—H133 | 0.9500 |
| O5—C38 | 1.266 (16) | C134—C135 | 1.434 (18) |
| O6—N12 | 1.213 (15) | C134—H134 | 0.9500 |
| N8—C26 | 1.333 (16) | C135—C136 | 1.397 (19) |
| N8—C30 | 1.366 (16) | C135—H135 | 0.9500 |
| N9—C31 | 1.366 (16) | C136—C137 | 1.424 (18) |
| N9—C32 | 1.378 (16) | C136—H136 | 0.9500 |
| N10—C38 | 1.301 (16) | C138—C139 | 1.517 (19) |
| N10—C37 | 1.387 (16) | C139—C140 | 1.389 (18) |
| N11—C43 | 1.343 (15) | C140—C141 | 1.38 (2) |
| N11—C39 | 1.375 (16) | C140—H140 | 0.9500 |
| N13—C44 | 1.335 (16) | C141—C142 | 1.417 (19) |
| N13—C48 | 1.360 (17) | C141—H141 | 0.9500 |
| N14—C46 | 1.364 (16) | C142—C143 | 1.353 (19) |
| N14—C50 | 1.445 (16) | C142—H142 | 0.9500 |
| N14—C49 | 1.476 (17) | C143—H143 | 0.9500 |
| C26—C27 | 1.390 (18) | C144—C145 | 1.388 (17) |
| C26—H26 | 0.9500 | C144—H144 | 0.9500 |
| C27—C28 | 1.452 (18) | C145—C146 | 1.395 (18) |
| C27—H27 | 0.9500 | C145—H145 | 0.9500 |
| C28—C29 | 1.390 (18) | C146—C147 | 1.383 (19) |
| C28—H28 | 0.9500 | C147—C148 | 1.374 (17) |

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| C29—C30 | 1.408 (18) | C147—H147 | 0.9500 |
| C29—H29 | 0.9500 | C148—H148 | 0.9500 |
| C30—C31 | 1.535 (18) | C149—H14J | 0.9800 |
| C32—C33 | 1.426 (17) | C149—H14K | 0.9800 |
| C32—C37 | 1.429 (18) | C149—H14L | 0.9800 |
| C33—C34 | 1.403 (19) | C150—H15B | 0.9800 |
| C33—H33 | 0.9500 | C150—H15C | 0.9800 |
| C34—C35 | 1.351 (18) | C150—H15D | 0.9800 |
| C34—H34 | 0.9500 | Mn7—N47 | 1.679 (12) |
| C35—C36 | 1.424 (19) | Mn7—N45 | 1.952 (13) |
| C35—H35 | 0.9500 | Mn7—N44 | 1.997 (13) |
| C36—C37 | 1.430 (18) | Mn7—N46 | 2.076 (12) |
| C36—H36A | 0.9500 | Mn7—N43 | 2.078 (12) |
| C38—C39 | 1.456 (17) | Mn7—N48 | 2.135 (11) |
| C39—C40 | 1.376 (18) | O19—C156 | 1.222 (16) |
| C40—C41 | 1.358 (18) | O20—C163 | 1.259 (16) |
| C40—H40 | 0.9500 | O21—N47 | 1.165 (13) |
| C41—C42 | 1.399 (19) | N43—C151 | 1.347 (17) |
| C41—H41 | 0.9500 | N43—C155 | 1.383 (16) |
| C42—C43 | 1.395 (17) | N44—C156 | 1.328 (17) |
| C42—H4A | 0.9500 | N44—C157 | 1.417 (17) |
| C43—H43 | 0.9500 | N45—C163 | 1.346 (16) |
| C44—C45 | 1.383 (18) | N45—C162 | 1.429 (16) |
| C44—H44 | 0.9500 | N46—C168 | 1.361 (17) |
| C45—C46 | 1.374 (17) | N46—C164 | 1.395 (17) |
| C45—H45 | 0.9500 | N48—C173 | 1.345 (16) |
| C46—C47 | 1.430 (17) | N48—C169 | 1.375 (17) |
| C47—C48 | 1.356 (18) | N49—C171 | 1.378 (16) |
| C47—H47 | 0.9500 | N49—C175 | 1.459 (16) |
| C48—H48 | 0.9500 | N49—C174 | 1.464 (16) |
| C49—H49A | 0.9800 | C151—C152 | 1.359 (18) |
| C49—H49B | 0.9800 | C151—H151 | 0.9500 |
| C49—H49C | 0.9800 | C152—C153 | 1.391 (19) |
| C50—H50A | 0.9800 | C152—H152 | 0.9500 |
| C50—H50B | 0.9800 | C153—C154 | 1.370 (19) |
| C50—H50C | 0.9800 | C153—H153 | 0.9500 |
| Mn3—N19 | 1.624 (13) | C154—C155 | 1.394 (18) |
| Mn3—N16 | 1.940 (13) | C154—H154 | 0.9500 |
| Mn3—N17 | 1.978 (13) | C155—C156 | 1.537 (19) |
| Mn3—N18 | 2.093 (12) | C157—C162 | 1.418 (17) |
| Mn3—N15 | 2.099 (12) | C157—C158 | 1.434 (18) |
| Mn3—N20 | 2.143 (12) | C158—C159 | 1.425 (19) |
| O7—C56 | 1.260 (17) | C158—H158 | 0.9500 |
| O8—C63 | 1.294 (17) | C159—C160 | 1.400 (18) |
| O9—N19 | 1.213 (14) | C159—H159 | 0.9500 |
| N15—C51 | 1.340 (18) | C160—C161 | 1.388 (19) |
| N15—C55 | 1.387 (18) | C160—H160 | 0.9500 |
| N16—C56 | 1.335 (17) | C161—C162 | 1.420 (18) |

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| N16—C57 | 1.443 (18) | C161—H161 | 0.9500 |
| N17—C63 | 1.306 (17) | C163—C164 | 1.502 (18) |
| N17—C62 | 1.430 (18) | C164—C165 | 1.414 (18) |
| N18—C68 | 1.337 (17) | C165—C166 | 1.36 (2) |
| N18—C64 | 1.387 (17) | C165—H165 | 0.9500 |
| N20—C69 | 1.337 (17) | C166—C167 | 1.358 (19) |
| N20—C73 | 1.373 (17) | C166—H166 | 0.9500 |
| N21—C71 | 1.368 (15) | C167—C168 | 1.396 (18) |
| N21—C74 | 1.431 (17) | C167—H167 | 0.9500 |
| N21—C75 | 1.461 (17) | C168—H168 | 0.9500 |
| C51—C52 | 1.410 (18) | C169—C170 | 1.345 (17) |
| C51—H51 | 0.9500 | C169—H169 | 0.9500 |
| C52—C53 | 1.419 (19) | C170—C171 | 1.400 (19) |
| C52—H52 | 0.9500 | C170—H170 | 0.9500 |
| C53—C54 | 1.375 (19) | C171—C172 | 1.383 (18) |
| C53—H53 | 0.9500 | C172—C173 | 1.351 (16) |
| C54—C55 | 1.430 (19) | C172—H172 | 0.9500 |
| C54—H54 | 0.9500 | C173—H173 | 0.9500 |
| C55—C56 | 1.523 (19) | C174—H174 | 0.9800 |
| C57—C58 | 1.41 (2) | C174—H17F | 0.9800 |
| C57—C62 | 1.451 (19) | C174—H17G | 0.9800 |
| C58—C59 | 1.43 (2) | C175—H17H | 0.9800 |
| C58—H58 | 0.9500 | C175—H17I | 0.9800 |
| C59—C60 | 1.40 (2) | C175—H17J | 0.9800 |
| C59—H59 | 0.9500 | Mn8—N54 | 1.611 (12) |
| C60—C61 | 1.40 (2) | Mn8—N52 | 1.951 (12) |
| C60—H60 | 0.9500 | Mn8—N51 | 1.957 (12) |
| C61—C62 | 1.45 (2) | Mn8—N50 | 2.056 (13) |
| C61—H61 | 0.9500 | Mn8—N53 | 2.062 (12) |
| C63—C64 | 1.486 (19) | Mn8—N55 | 2.108 (11) |
| C64—C65 | 1.367 (18) | O22—C181 | 1.249 (16) |
| C65—C66 | 1.39 (2) | O23—C188 | 1.267 (17) |
| C65—H65 | 0.9500 | O24—N54 | 1.215 (14) |
| C66—C67 | 1.404 (19) | N50—C176 | 1.330 (17) |
| C66—H66 | 0.9500 | N50—C180 | 1.361 (17) |
| C67—C68 | 1.370 (18) | N51—C181 | 1.350 (17) |
| C67—H67 | 0.9500 | N51—C182 | 1.428 (16) |
| C68—H68 | 0.9500 | N52—C188 | 1.311 (17) |
| C69—C70 | 1.357 (17) | N52—C187 | 1.424 (17) |
| C69—H69 | 0.9500 | N53—C193 | 1.318 (17) |
| C70—C71 | 1.381 (18) | N53—C189 | 1.367 (17) |
| C70—H70 | 0.9500 | N55—C198 | 1.338 (16) |
| C71—C72 | 1.431 (17) | N55—C194 | 1.366 (16) |
| C72—C73 | 1.374 (17) | N56—C196 | 1.357 (16) |
| C72—H72 | 0.9500 | N56—C200 | 1.450 (17) |
| C73—H73 | 0.9500 | N56—C199 | 1.474 (17) |
| C74—H74A | 0.9800 | C176—C177 | 1.363 (18) |
| C74—H74B | 0.9800 | C176—H176 | 0.9500 |

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| C74—H74C | 0.9800 | C177—C178 | 1.442 (18) |
| C75—H75A | 0.9800 | C177—H177 | 0.9500 |
| C75—H75B | 0.9800 | C178—C179 | 1.389 (18) |
| C75—H75C | 0.9800 | C178—H178 | 0.9500 |
| Mn4—N26 | 1.637 (14) | C179—C180 | 1.423 (17) |
| Mn4—N24 | 1.947 (12) | C179—H179 | 0.9500 |
| Mn4—N23 | 1.951 (12) | C180—C181 | 1.537 (19) |
| Mn4—N22 | 2.040 (12) | C182—C183 | 1.419 (17) |
| Mn4—N25 | 2.075 (12) | C182—C187 | 1.425 (17) |
| Mn4—N27 | 2.126 (13) | C183—C184 | 1.392 (19) |
| O10—C81 | 1.243 (16) | C183—H183 | 0.9500 |
| O11—C88 | 1.263 (17) | C184—C185 | 1.386 (18) |
| O12—N26 | 1.204 (15) | C184—H18D | 0.9500 |
| N22—C80 | 1.336 (17) | C185—C186 | 1.366 (18) |
| N22—C76 | 1.346 (16) | C185—H185 | 0.9500 |
| N23—C81 | 1.342 (16) | C186—C187 | 1.404 (18) |
| N23—C82 | 1.398 (16) | C186—H186 | 0.9500 |
| N24—C88 | 1.337 (17) | C188—C189 | 1.501 (18) |
| N24—C87 | 1.396 (16) | C189—C190 | 1.334 (18) |
| N25—C93 | 1.305 (17) | C190—C191 | 1.388 (19) |
| N25—C89 | 1.367 (17) | C190—H190 | 0.9500 |
| N27—C98 | 1.308 (17) | C191—C192 | 1.402 (19) |
| N27—C94 | 1.358 (16) | C191—H191 | 0.9500 |
| N28—C96 | 1.331 (17) | C192—C193 | 1.382 (18) |
| N28—C99 | 1.432 (17) | C192—H192 | 0.9500 |
| N28—C100 | 1.473 (17) | C193—H193 | 0.9500 |
| C76—C77 | 1.415 (18) | C194—C195 | 1.363 (17) |
| C76—H76 | 0.9500 | C194—H194 | 0.9500 |
| C77—C78 | 1.386 (18) | C195—C196 | 1.407 (18) |
| C77—H77 | 0.9500 | C195—H195 | 0.9500 |
| C78—C79 | 1.374 (17) | C196—C197 | 1.398 (18) |
| C78—H78 | 0.9500 | C197—C198 | 1.383 (17) |
| C79—C80 | 1.433 (18) | C197—H197 | 0.9500 |
| C79—H79 | 0.9500 | C198—H198 | 0.9500 |
| C80—C81 | 1.491 (18) | C199—H19J | 0.9800 |
| C82—C83 | 1.398 (17) | C199—H19K | 0.9800 |
| C82—C87 | 1.430 (17) | C199—H19L | 0.9800 |
| C83—C84 | 1.404 (18) | C200—H20A | 0.9800 |
| C83—H83 | 0.9500 | C200—H20B | 0.9800 |
| C84—C85 | 1.372 (18) | C200—H20C | 0.9800 |
| C84—H84 | 0.9500 | O25—C201 | 1.4297 |
| C85—C86 | 1.416 (18) | O25—H20D | 0.9641 |
| C85—H85 | 0.9500 | C201—C202 | 1.5153 |
| C86—C87 | 1.425 (18) | C201—H20E | 1.0990 |
| C86—H86 | 0.9500 | C201—H20F | 1.0990 |
| C88—C89 | 1.474 (18) | C202—H20G | 1.0939 |
| C89—C90 | 1.347 (18) | C202—H20H | 1.0928 |
| C90—C91 | 1.395 (18) | C202—H20I | 1.0927 |

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| C90—H90 | 0.9500 | O26—C203 | 1.4297 |
| C91—C92 | 1.411 (18) | O26—H20J | 0.8491 |
| C91—H91 | 0.9500 | C203—C204 | 1.5153 |
| C92—C93 | 1.387 (18) | C203—H20K | 1.0991 |
| C92—H92 | 0.9500 | C203—H20L | 1.0990 |
| C93—H93 | 0.9500 | C204—H20M | 1.0940 |
| C94—C95 | 1.369 (18) | C204—H20N | 1.0927 |
| C94—H94 | 0.9500 | C204—H20O | 1.0928 |
| C95—C96 | 1.411 (18) | O27—C205 | 1.4298 |
| C95—H95 | 0.9500 | O27—H20P | 0.8400 |
| C96—C97 | 1.393 (17) | C205—C206 | 1.5153 |
| C97—C98 | 1.361 (18) | C205—H20Q | 1.0990 |
| C97—H97 | 0.9500 | C205—H20R | 1.0990 |
| C98—H98 | 0.9500 | C206—H20S | 1.0940 |
| C99—H99A | 0.9800 | C206—H20T | 1.0927 |
| C99—H99B | 0.9800 | C206—H20U | 1.0928 |
| C99—H99C | 0.9800 | O28—C207 | 1.4297 |
| C100—H10B | 0.9800 | O28—H20V | 0.8521 |
| C100—H10C | 0.9800 | C207—C208 | 1.5153 |
| C100—H10D | 0.9800 | C207—H20W | 1.0991 |
| Mn5—N33 | 1.624 (14) | C207—H20X | 1.0989 |
| Mn5—N30 | 1.934 (12) | C208—H20Y | 1.0940 |
| Mn5—N31 | 1.950 (12) | C208—H21A | 1.0928 |
| Mn5—N32 | 2.043 (12) | C208—H21B | 1.0928 |
| Mn5—N29 | 2.061 (13) | O29—C209 | 1.4298 |
| Mn5—N34 | 2.119 (13) | O29—H21C | 0.8400 |
| O13—C106 | 1.217 (15) | C209—C21F | 1.3350 |
| O14—C113 | 1.277 (16) | C209—H21D | 0.9900 |
| O15—N33 | 1.205 (15) | C209—H21E | 0.9900 |
| N29—C101 | 1.298 (16) | C21F—H21G | 0.9800 |
| N29—C105 | 1.363 (17) | C21F—H21H | 0.9800 |
| N30—C106 | 1.334 (16) | C21F—H21I | 0.9800 |
| N30—C107 | 1.438 (16) | O30—C211 | 1.4297 |
| N31—C113 | 1.350 (17) | O30—H21J | 0.8505 |
| N31—C112 | 1.379 (16) | C211—C212 | 1.5152 |
| N32—C118 | 1.316 (16) | C211—H21K | 1.0990 |
| N32—C114 | 1.369 (17) | C211—H21L | 1.0990 |
| N34—C119 | 1.327 (17) | C212—H21M | 1.0940 |
| N34—C123 | 1.370 (16) | C212—H21N | 1.0928 |
| N35—C121 | 1.354 (16) | C212—H21O | 1.0928 |
| N35—C125 | 1.443 (16) | O31—C213 | 1.4297 |
| N35—C124 | 1.456 (16) | O31—H21P | 0.8497 |
| C101—C102 | 1.419 (18) | C213—C214 | 1.5153 |
| C101—H101 | 0.9500 | C213—H21Q | 1.0990 |
| C102—C103 | 1.397 (17) | C213—H21R | 1.0991 |
| C102—H102 | 0.9500 | C214—H21S | 1.0939 |
| C103—C104 | 1.388 (17) | C214—H21T | 1.0928 |
| C103—H103 | 0.9500 | C214—H21U | 1.0928 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O25—H20*D*···O22$^{i}$ | 0.96 | 1.88 | 2.751 (15) | 149 |
| O26—H20*J*···O8$^{ii}$ | 0.85 | 1.84 | 2.686 (17) | 178 |
| O27—H20*P*···O16$^{iii}$ | 0.84 | 1.93 | 2.739 (18) | 161 |
| O28—H20*V*···O23 | 0.85 | 1.89 | 2.747 (19) | 179 |
| O29—H21*C*···O20 | 0.84 | 1.93 | 2.709 (17) | 154 |
| O30—H21*J*···O7$^{iv}$ | 0.85 | 1.90 | 2.75 (2) | 178 |
| O31—H21*P*···O13 | 0.85 | 2.04 | 2.887 (17) | 179 |

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