Nitrato(5,10,15,20-tetraphenylporphinato)-manganese(III)–benzene–n-hexane (2/1/1)

Hongli Cao,* Junwen Wang* and Jianfeng Li*

*Key Laboratory of Magnetic Molecules, Magnetic Information Materials, Ministry of Education, School of Chemical and Material Science, Shanxi Normal University, Taiyu Road, Taiyuan 030022, People’s Republic of China, and College of Materials Science and Opto-electronic Technology, CAS Center for Excellence in Topological Quantum Computation & Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Yanqi Lake, Huairou District, Beijing 101408, People’s Republic of China. *Correspondence e-mail: wangjunwen2013@126.com, jfl@ucas.ac.cn

The crystal structure of solvated [Mn(TPP)(NO₃)] (TPP = 5,10,15,20-tetraphenylporphyrinato, C₄₄H₂₈N₄), [Mn(C₄₄H₂₈N₄O₃)(NO₃)]·0.5C₆H₁₄·0.5C₆H₆, has been determined in the space group Pccn. The MnIII atom has a distorted square-pyramidal environment, being coordinated by four pyrrole N atoms of the porphyrin ligand in the basal plane and an O atom of the nitrate ligand in the apical site. The MnIII atom is displaced out of the porphyrin plane by 0.22 (4) Å with the average Mn—Np distance being 2.011 (6) Å (where Np is a porphyrin N atom). The Mn—O bond length is 2.1246 (18) Å. Two kinds of intermolecular C—H⋯O hydrogen bonds exist in the crystal structure, with the apical nitrate ligands interacting with solvent molecules and adjacent molecules, respectively.

Structure description

Interactions between metalloporphyrins and nitrate ligands occur in many areas of bioinorganic chemistry. Nitrates play a key role in fixing atmospheric nitrogen into a more bioavailable form, as detailed in the nitrogen cycle (Averill, 1996). A series of nitrate-coordinating FeIII derivatives have been reported, whereby the denticity of the nitrate ligands shows differences for complexes of the general type [Fe(Por)(NO₃)] (where Por is porphyrin). Among them, [Fe(OEP)(NO₃)] (OEP = 2,3,7,8,12,13,17,18-octaethylporphyrinato, space group P2₁/c; Ellison et al., 1996), [Fe(OEP)(NO₃)] (space group P2₁/c; Wyllie et al., 2007) and [Fe(4-Me-TTP)(NO₃)] (TTP = 5,10,15,20-tetrakis(4-methylphenyl)porphyrinato; Bhuyan & Sarkar, 2013) have a nitrate group monodentately binding to the central metal cation, while [Fe(TPP)(NO₃)] (Wyllie et al., 2007),
20 f4

Cao et al. / C15 [Mn(C44H28N4O3)(NO3)]0.5C6H140.5C6H6 IUCrData (2022). 7, x220386

data reports

Table 1
Selected structural parameters (Å) for related metalloporphyrin nitrate complexes.

| Complex | $\Delta_4$ | $\Delta_24$ | $M-O$ | $N-O1$ | $M-N_p$ | Ref. |
|---------|------------|------------|-------|--------|---------|------|
| [Mn(TPP)(NO3)] (Pccn) benzene and n-hexane hemisolvate | 0.23 | 0.22 | 2.1246 (18) | 1.260 (3) 1.236 (3) 1.230 (3) 2.011 (6) | This work |
| [Mn(TPP)(NO3)] ($P_2_1/c$) benzene disolvate | 0.21 | 0.20 | 2.101 (3) | 1.298 (4) 1.226 (5) 1.226 (5) 2.007 (9) | (Suslick & Watson, 1991) |
| [Fe(OEP)(NO3)] ($P_2_1/c$) | 0.40 | 0.45 | 1.966 (2) | 1.301 (3) 1.199 (3) 1.212 (3) 2.047 (6) | (Wyllie et al., 2007) |
| [Fe(TpivPP)(NO3)] ($P_2_1/c$) | 0.46 | 0.50 | 2.016 (3) | 1.206 (5) 1.198 (4) 1.208 (6) 2.056 (1) | (Ellison et al., 1996) |
| [Fe(TPP)(NO3)] | 0.47 | 0.53 | 1.971 (3) | 1.262 (5) 1.252 (5) 1.221 (4) 2.063 (13) | (Bhuyan & Sarkar, 2013) |
| [Fe(TpivPP)(NO3)] | 0.54 | 0.63 | 2.121 (6) 2.19 (10) | 1.27 (10) 1.285 (21) 1.217 (3) 2.085 (10) | (Wyllie et al., 2007) |
| [Fe(4-OMe-TPP)(NO3)] | 0.54 | 0.62 | 2.169 (5) 2.169 (5) | 1.216 (5) 1.276 (8) 1.216 (5) 2.05 (3) | (Bhuyan & Sarkar, 2013) |

In the crystal structure of the title five-coordinate manganese(III) nitrate complex (Fig. 1), the asymmetric unit contains one porphyrin molecule, half of a benzene solvate molecule, and half of an $n$-hexane solvate molecule. The Mn$^{III}$ atom has a distorted square-pyramidal environment, defined by the four pyrrole N atoms of the porphyrin ligand in the basal plane and an O atom of the nitrato ligand in the apical site. Additional quantitative information about the structure is given in Fig. 2, which includes the displacement of each porphyrin core atom (in units of 0.01 Å) from the 24-atom mean plane. Averaged values of the chemically unique bond lengths (in Å) and angles ($^\circ$) are also shown. The

Figure 1
The molecular structure of the title compound, drawn with displacement ellipsoids at the 50% probability level. Only one of the two orientations of the disordered benzene solvate molecules is shown. [Symmetry code: (i) $-x+\frac{1}{2}, -y+\frac{1}{2}, z$.]

Figure 2
A formal diagram of the porphyrin core of the title compound. Averaged values of the chemically unique bond lengths (Å) and angles ($^\circ$) are shown. The perpendicular displacements (in units of 0.01 Å) of the porphyrin core atoms from the 24-atom mean plane are also displayed. The positive numbers indicate a displacement towards the nitrate ligand, the dashed line indicates the plane of the nitrate ligand on the unhindered porphyrin side.
mean absolute core-atom displacements of $C_a$, $C_b$, $C_m$ and $C_{av}$ are 0.11 (2), 0.28 (3), 0.04 (2) and 0.16 (10) Å, respectively, and the monodentate nitrato ligand forms a dihedral angle of 43.69 (13)° with the plane defined by the Mn1, N3 and O1 atoms.

The porphyrin core shows a characteristic saddle-shaped distortion and the Mn$^{III}$ atom is displaced by 0.22 (4) Å from the 24-atom porphyrin plane in the direction of the nitrato ligand. This value is smaller than the displacement of the iron atom (0.63 Å) in [Fe(TPP)(NO)₃] reported by Wyllie et al. (2007). This difference is explained by the high-spin configuration of 3d⁵ Fe$^{III}$ where the occupied d$(x²−y²)$ orbital ‘pushes’ the metal out of the porphyrin plane, and the empty d$(x²−y²)$ orbital of 3d⁴ Mn$^{III}$ allows a more in-plane conformation (Suslick & Watson, 1991).

In the title compound, C—H···O hydrogen-bonding interactions are found between the disordered benzene solvent molecule (C4S) and the apical nitrato ligand (O3), as illustrated in Fig. 3 and detailed in Table 2. All these structural parameters are consistent with literature data where C—H···O bonds range from 3.00–4.00 Å (Desiraju, 1996), with angles of 120–180° (Steiner & Desiraju, 1998). The molecular packing of the title compound is shown in Fig. 5.

**Synthesis and crystallization**

**General information.** All experimental manipulations were performed under a purified nitrogen atmosphere using Schlenk techniques. Except for the solvent used in column chromatography, all solvents used in the experimental process were treated under dry conditions and exclusion of oxygen. Benzene and n-hexane were distilled under argon protection, and then refluxed over sodium/benzophenone and potassium–sodium alloy, respectively. All solvents used in the anhydrous and anaerobic operation (Schlenk system) were treated with the pump–freeze–thaw method three times before use.

The title compound was obtained serendipitously in an unsuccessful attempt to isolate the five-coordinate manganese(II) nitrosyl species [Mn(TPP)(NO)]. [Mn(TPP)OH] was prepared according to a reported method (He et al., 2016). The purple [Mn(TPP)OH] powder (10 mg, 0.0015 mmol) was reduced by ethyl mercaptan for 48 h with benzene as solvent, then the solution was evaporated to dryness. NO gas was then bubbled slowly in a solution of the residue in degassed benzene for 5 minutes under an argon atmosphere. There was a dramatic color change from greenish yellow to red. The red solution was finally layered with hexanes. Black, block-shaped crystals were obtained several weeks later.

**Table 2**

| $D$—H···$A$   | $D$—H | $H$···$A$ | $D$···$A$ | $D$—H···$A$ |
|---------------|--------|------------|-----------|-------------|
| C4S—H4S···O3  | 0.95   | 2.38       | 3.177 (8) | 141         |
| C10—H10···O2ii| 0.95   | 2.50       | 3.182 (3) | 129         |
| C17—H17···O2ii| 0.95   | 2.53       | 3.350 (4) | 145         |
| C22—H22···O2ii| 0.95   | 2.49       | 3.085 (3) | 120         |

Symmetry codes: (i) $x$, $−y+1$, $−z+1$; (ii) $x$, $−y+3/2$, $z+1/2$; (iii) $x+1/2$, $y+1$, $z+1/2$.

**Figure 3**

The C—H···O interactions between the apical nitrato ligand and the benzene solvent molecule.

**Figure 4**

C—H···O hydrogen-bonding interactions between adjacent porphyrin molecules (dashed lines).

**Figure 5**

A view of the molecular packing of the title compound in the crystal structure, as seen in a projection along [100]. H atoms have been omitted for clarity.
Table 3
Experimental details.

| Crystal data |       |
|--------------|-------|
| Chemical formula | [Mn(C_{44}H_{28}N_{4}O_{3})(NO_{3})]—0.5C_{6}H_{14}·0.5C_{6}H_{6} |
| M_r          | 811.79 |
| Crystal system, space group | Orthorhombic, Pccn |
| Temperature (K) | 100 |
| a, b, c (Å)  | 20.1021 (10), 21.5505 (9), 17.9807 (9) |
| V (Å^3)      | 7789.4 (6) |
| Z            | 8 |
| Radiation type | Mo Kα |
| μ (mm⁻¹)     | 0.39 |
| Crystal size (mm) | 0.33 × 0.29 × 0.12 |

Data collection

| Diffractometer | Bruker APEXII CCD |
|----------------|-------------------|
| Absorption correction | Multi-scan (SADABS; Krause et al., 2015) |
| T_min, T_max | 0.763, 0.865 |
| No. of measured, independent and observed [I > 2σ(I)] reflections | 58775, 8270, 6163 |
| R_{int}                | 0.058 |
| (sinθ/λ)_{max} (Å⁻¹)  | 0.633 |

Refinement

| R(F^2 > 2σ(F^2)), wR(F^2), S | 0.050, 0.148, 1.07 |
| No. of reflections          | 8270 |
| No. of parameters           | 560 |
| No. of restraints           | 37 |
| H-atom treatment            | H-atom parameters constrained |
| Δρ_{max}, Δρ_{min} (e Å⁻³) | 0.80, −0.48 |

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full crystallographic data

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Nitrato(5,10,15,20-tetraphenylporphinato)manganese(III)–benzene–n-hexane (2/1/1)

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Crystal data

[Mn(C44H28N4O3)(NO3)]·0.5C6H14·0.5C6H6  
Mr = 811.79
Orthorhombic, Pccn
a = 20.1021 (10) Å  
b = 21.5505 (9) Å  
c = 17.9807 (9) Å  
V = 7789.4 (6) Å³  
Z = 8  
F(000) = 3376

Dₐ = 1.384 Mg m⁻³  
Mo Kα radiation, λ = 0.71073 Å

Cell parameters from 9845 reflections
θ = 2.5–26.7°  
µ = 0.39 mm⁻¹  
T = 100 K

0.33 × 0.29 × 0.12 mm

Data collection

Bruker APEXII CCD

φ and ω scans

Absorption correction: multi-scan  
(SADABS; Krause et al., 2015)

T = 0.763, T = 0.865  
58775 measured reflections

8270 independent reflections  
6163 reflections with I > 2σ(I)

R_int = 0.058  
θ_max = 26.7°, θ_min = 2.3°

8270 reflections  
560 parameters  
37 restraints

Refinement

Refinement on F²

Least-squares matrix: full
R[F² > 2σ(F²)] = 0.050  
wR(F²) = 0.148
S = 1.07

8270 reflections  
560 parameters  
37 restraints

Hydrogen site location: inferred from

neighbouring sites

H-atom parameters constrained

w = 1/[(σ(F²)² + (0.0686P)² + 10.1161P)]

where P = (F² + 2Fc²)/3

(Δ/σ)max = 0.097  
Δρ_max = 0.80 e Å⁻³

Δρ_min = −0.48 e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.
|    | x       | y       | z       | U₁₀₀/¹eq | Occ. (<1) |
|----|---------|---------|---------|----------|-----------|
| Mn1| 0.42182 (2) | 0.50321 (2) | 0.38016 (2) | 0.01235 (11) |
| O1 | 0.42711 (8)  | 0.52498 (8)  | 0.26507 (10) | 0.0206 (4)   |
| O2 | 0.41592 (10) | 0.58633 (9)  | 0.17166 (11) | 0.0311 (5)   |
| O3 | 0.42351 (12) | 0.62345 (10) | 0.28275 (12) | 0.0416 (6)   |
| N1 | 0.49166 (9)  | 0.43691 (8)  | 0.36975 (11) | 0.0144 (4)   |
| N2 | 0.35071 (9)  | 0.43777 (8)  | 0.36889 (11) | 0.0148 (4)   |
| N3 | 0.35138 (9)  | 0.56361 (9)  | 0.41173 (11) | 0.0151 (4)   |
| N4 | 0.49211 (9)  | 0.56102 (8)  | 0.41874 (11) | 0.0147 (4)   |
| N5 | 0.42152 (11) | 0.57920 (11) | 0.23960 (13) | 0.0259 (5)   |
| C1 | 0.42051 (11) | 0.28091 (11) | 0.31319 (15) | 0.0183 (5)   |
| C2 | 0.44918 (13) | 0.23571 (11) | 0.35761 (16) | 0.0259 (6)   |
| H2 | 0.467963     | 0.247013    | 0.404159    | 0.031       |
| C3 | 0.45086 (14) | 0.17416 (12) | 0.33504 (18) | 0.0304 (6)   |
| H3 | 0.470578     | 0.143610    | 0.366108    | 0.036       |
| C4 | 0.42397 (14) | 0.15745 (12) | 0.26773 (19) | 0.0341 (7)   |
| H4 | 0.425615     | 0.115394    | 0.251982    | 0.041       |
| C5 | 0.39436 (16) | 0.20192 (13) | 0.22261 (18) | 0.0369 (7)   |
| H5 | 0.375509     | 0.190271    | 0.176218    | 0.044       |
| C6 | 0.39240 (14) | 0.26347 (12) | 0.24550 (16) | 0.0298 (6)   |
| H6 | 0.371794     | 0.293805    | 0.214858    | 0.036       |
| C7 | 0.17559 (12) | 0.50079 (10) | 0.38931 (13) | 0.0158 (5)   |
| C8 | 0.14138 (12) | 0.47327 (11) | 0.44853 (15) | 0.0198 (5)   |
| H8 | 0.165523     | 0.456573    | 0.489306    | 0.024       |
| C9 | 0.07229 (12) | 0.47019 (12) | 0.44807 (16) | 0.0243 (6)   |
| H9 | 0.049340     | 0.451340    | 0.488358    | 0.029       |
| C10| 0.03678 (13) | 0.49480 (12) | 0.38843 (15) | 0.0244 (6)   |
| H10| −0.010419    | 0.492704    | 0.387856    | 0.029       |
| C11| 0.07056 (13) | 0.52232 (13) | 0.33002 (16) | 0.0256 (6)   |
| H11| 0.046353     | 0.539209    | 0.289402    | 0.031       |
| C12| 0.13958 (12) | 0.52542 (11) | 0.33034 (15) | 0.0217 (5)   |
| H12| 0.162274     | 0.544480    | 0.290016    | 0.026       |
| C13| 0.42453 (11) | 0.72160 (11) | 0.45726 (15) | 0.0189 (5)   |
| C14| 0.45003 (16) | 0.75859 (13) | 0.4016 (2)  | 0.0404 (8)   |
| H14| 0.466560     | 0.740272    | 0.357213    | 0.048       |
| C15| 0.45157 (18) | 0.82290 (14) | 0.4103 (2)  | 0.0527 (10)  |
| H15| 0.468977     | 0.848052    | 0.371515    | 0.063       |
| C16| 0.42877 (14) | 0.84987 (13) | 0.4729 (2)  | 0.0398 (8)   |
| H16| 0.429418     | 0.893761    | 0.477800    | 0.048       |
| C17| 0.40443 (17) | 0.81338 (14) | 0.5299 (2)  | 0.0430 (9)   |
| H17| 0.389609     | 0.832124    | 0.574726    | 0.052       |
| C18| 0.40157 (16) | 0.74907 (13) | 0.52169 (17) | 0.0338 (7)   |
| H18| 0.383801     | 0.724157    | 0.560487    | 0.041       |
| C19| 0.66708 (12) | 0.50305 (10) | 0.38165 (13) | 0.0154 (5)   |
| C20| 0.70957 (12) | 0.45885 (11) | 0.41236 (14) | 0.0198 (5)   |
| H20| 0.691967     | 0.426573    | 0.442483    | 0.024       |
|  | x | y | z | e |
|---|---|---|---|---|
| C21 | 0.77752 (13) | 0.46181 (13) | 0.39912 (15) | 0.0256 (6) |
| H21 | 0.806087 | 0.431261 | 0.419872 | 0.031* |
| C22 | 0.80410 (13) | 0.50902 (13) | 0.35582 (16) | 0.0271 (6) |
| H22 | 0.850647 | 0.510865 | 0.346956 | 0.032* |
| C23 | 0.76238 (13) | 0.55324 (13) | 0.32574 (15) | 0.0277 (6) |
| H23 | 0.780381 | 0.585843 | 0.296427 | 0.033* |
| C24 | 0.69414 (13) | 0.55040 (12) | 0.33805 (15) | 0.0226 (5) |
| H24 | 0.665777 | 0.580821 | 0.316693 | 0.027* |
| C(A1) | 0.55989 (11) | 0.44641 (10) | 0.36743 (13) | 0.0146 (5) |
| C(A2) | 0.48166 (12) | 0.37726 (10) | 0.34335 (13) | 0.0157 (5) |
| C(A3) | 0.35993 (12) | 0.37606 (10) | 0.35121 (14) | 0.0169 (5) |
| C(A4) | 0.28251 (12) | 0.44579 (10) | 0.37543 (13) | 0.0159 (5) |
| C(A5) | 0.28327 (12) | 0.55656 (11) | 0.40428 (14) | 0.0174 (5) |
| C(A6) | 0.36142 (12) | 0.62527 (10) | 0.43015 (14) | 0.0173 (5) |
| C(A7) | 0.48260 (12) | 0.62090 (10) | 0.44399 (13) | 0.0162 (5) |
| C(A8) | 0.56024 (11) | 0.55124 (10) | 0.42006 (13) | 0.0150 (5) |
| C(B1) | 0.59185 (12) | 0.39247 (11) | 0.33697 (14) | 0.0194 (5) |
| H(B1) | 0.638168 | 0.387514 | 0.328321 | 0.023* |
| C(B2) | 0.54403 (12) | 0.35015 (11) | 0.32289 (14) | 0.0191 (5) |
| H(B2) | 0.550561 | 0.309748 | 0.303040 | 0.023* |
| C(B3) | 0.29657 (12) | 0.34533 (11) | 0.34796 (15) | 0.0216 (5) |
| H(B3) | 0.289310 | 0.302652 | 0.337501 | 0.026* |
| C(B4) | 0.24941 (12) | 0.38788 (11) | 0.36239 (15) | 0.0213 (5) |
| H(B4) | 0.202762 | 0.380878 | 0.363712 | 0.026* |
| C(B5) | 0.25083 (13) | 0.61474 (11) | 0.41847 (15) | 0.0230 (6) |
| H(B5) | 0.204257 | 0.622200 | 0.417728 | 0.028* |
| C(B6) | 0.29864 (12) | 0.65671 (11) | 0.43303 (16) | 0.0230 (6) |
| H(B6) | 0.291982 | 0.699496 | 0.443361 | 0.028* |
| C(B7) | 0.54509 (12) | 0.64704 (11) | 0.46568 (14) | 0.0182 (5) |
| H(B7) | 0.551968 | 0.687212 | 0.486043 | 0.022* |
| C(B8) | 0.59258 (12) | 0.60410 (11) | 0.45188 (14) | 0.0176 (5) |
| H(B8) | 0.638833 | 0.608255 | 0.461525 | 0.021* |
| C(M1) | 0.42063 (12) | 0.34755 (10) | 0.33679 (13) | 0.0162 (5) |
| C(M2) | 0.25010 (12) | 0.50150 (10) | 0.38919 (13) | 0.0153 (5) |
| C(M3) | 0.42232 (11) | 0.65274 (10) | 0.44520 (14) | 0.0168 (5) |
| C(M4) | 0.59319 (12) | 0.49958 (10) | 0.39124 (13) | 0.0145 (5) |
| C1S | 0.28678 (18) | 0.23978 (17) | 0.4985 (2) | 0.0488 (9) |
| H1SA | 0.315264 | 0.276355 | 0.508279 | 0.059* |
| H1SB | 0.298393 | 0.223535 | 0.448647 | 0.059* |
| C2S | 0.30152 (18) | 0.18932 (17) | 0.5575 (2) | 0.0509 (9) |
| H2SA | 0.289087 | 0.204976 | 0.607336 | 0.061* |
| H2SB | 0.274282 | 0.152072 | 0.546955 | 0.061* |
| C3S | 0.37423 (19) | 0.17186 (17) | 0.5572 (2) | 0.0571 (10) |
| H3SA | 0.387512 | 0.159787 | 0.506761 | 0.086* |
| H3SB | 0.381507 | 0.136996 | 0.591202 | 0.086* |
| H3SC | 0.400895 | 0.207461 | 0.573341 | 0.086* |
| C4S | 0.3238 (4) | 0.7350 (3) | 0.2525 (4) | 0.0454 (15) | 0.5 |
| H4S | 0.363543 | 0.718301 | 0.272952 | 0.054* | 0.5 |
| Atomic displacement parameters (Å²) |
|-----------------------------------|
|  | $U^{11}$ | $U^{12}$ | $U^{13}$ | $U^{22}$ | $U^{23}$ | $U^{33}$ |
| Mn1 | 0.01075 (19) | 0.00928 (18) | 0.0170 (2) | 0.00011 (12) | $-0.00051$ (13) | $-0.00002$ (13) |
| O1 | 0.0168 (9) | 0.0267 (9) | 0.0183 (9) | 0.0015 (7) | $-0.0016$ (7) | 0.0008 (7) |
| O2 | 0.0329 (11) | 0.0353 (11) | 0.0252 (11) | $-0.0007$ (8) | $-0.0020$ (8) | 0.0095 (9) |
| O3 | 0.0610 (15) | 0.0309 (11) | 0.0328 (12) | $-0.0039$ (10) | 0.0025 (10) | $-0.0002$ (9) |
| N1 | 0.0149 (10) | 0.0101 (9) | 0.0181 (10) | $-0.0040$ (7) | $-0.0014$ (8) | $-0.0002$ (8) |
| N2 | 0.0134 (10) | 0.0104 (9) | 0.0206 (11) | $-0.0002$ (9) | 0.0007 (8) | 0.0002 (8) |
| N3 | 0.0117 (9) | 0.0115 (9) | 0.0220 (11) | $-0.0004$ (7) | 0.0000 (8) | 0.0009 (8) |
| N4 | 0.0149 (10) | 0.0100 (9) | 0.0191 (11) | 0.0013 (7) | 0.0001 (8) | 0.0005 (8) |
| N5 | 0.0201 (11) | 0.0309 (12) | 0.0268 (13) | $-0.0047$ (9) | 0.0010 (9) | $-0.0002$ (10) |
| C1 | 0.0126 (11) | 0.0137 (11) | 0.0286 (14) | $-0.0017$ (9) | 0.0024 (10) | $-0.0036$ (10) |
| C2 | 0.0255 (14) | 0.0180 (12) | 0.0342 (15) | 0.0028 (10) | $-0.0041$ (12) | $-0.0024$ (11) |
| C3 | 0.0262 (14) | 0.0138 (12) | 0.0511 (19) | 0.0033 (10) | $-0.0036$ (13) | $-0.0017$ (12) |
| C4 | 0.0252 (14) | 0.0164 (13) | 0.061 (2) | 0.0002 (11) | $-0.0031$ (14) | $-0.0159$ (13) |
| C5 | 0.0428 (18) | 0.0290 (15) | 0.0390 (18) | $-0.0024$ (13) | $-0.0086$ (14) | $-0.0149$ (13) |
| C6 | 0.0345 (15) | 0.0233 (14) | 0.0317 (16) | 0.0017 (11) | $-0.0060$ (13) | $-0.0038$ (11) |
| C7 | 0.0138 (11) | 0.0128 (11) | 0.0209 (12) | $-0.0001$ (8) | 0.0010 (9) | $-0.0044$ (9) |
| C8 | 0.0176 (12) | 0.0173 (12) | 0.0247 (13) | $-0.0006$ (9) | $-0.0012$ (10) | 0.0000 (10) |
| C9 | 0.0196 (13) | 0.0219 (13) | 0.0313 (15) | $-0.0043$ (10) | 0.0077 (11) | $-0.0043$ (11) |
| C10 | 0.0120 (12) | 0.0269 (14) | 0.0343 (16) | $-0.0011$ (10) | 0.0009 (10) | $-0.0107$ (11) |
| C11 | 0.0172 (13) | 0.0303 (14) | 0.0293 (15) | 0.0033 (10) | $-0.0036$ (11) | $-0.0083$ (12) |
| C12 | 0.0183 (13) | 0.0225 (12) | 0.0243 (14) | 0.0032 (10) | 0.0001 (10) | 0.0005 (10) |
| C13 | 0.0128 (11) | 0.0130 (11) | 0.0309 (14) | 0.0013 (9) | $-0.0068$ (10) | $-0.0024$ (10) |
| C14 | 0.0412 (18) | 0.0175 (14) | 0.062 (2) | 0.0008 (12) | 0.0178 (16) | 0.0018 (14) |
| C15 | 0.044 (2) | 0.0170 (14) | 0.097 (3) | $-0.0012$ (13) | 0.024 (2) | 0.0097 (17) |
| C16 | 0.0225 (14) | 0.0127 (12) | 0.084 (3) | 0.0005 (11) | $-0.0136$ (15) | $-0.0049$ (15) |
| C17 | 0.052 (2) | 0.0296 (16) | 0.048 (2) | 0.0194 (14) | $-0.0259$ (16) | $-0.0189$ (15) |
| C18 | 0.0496 (18) | 0.0196 (13) | 0.0321 (16) | 0.0122 (12) | $-0.0080$ (14) | $-0.0017$ (12) |
| C19 | 0.0110 (11) | 0.0159 (11) | 0.0173 (12) | $-0.0024$ (9) | 0.0003 (9) | $-0.0027$ (9) |
| C20 | 0.0194 (13) | 0.0184 (12) | 0.0216 (13) | 0.0013 (9) | $-0.0010$ (10) | $-0.0002$ (10) |
| C21 | 0.0183 (13) | 0.0278 (14) | 0.0308 (15) | 0.0066 (10) | $-0.0019$ (11) | $-0.0055$ (11) |
| C22 | 0.0155 (13) | 0.0340 (15) | 0.0317 (15) | $-0.0039$ (10) | 0.0045 (11) | $-0.0089$ (12) |
| C23 | 0.0241 (14) | 0.0313 (14) | 0.0276 (14) | $-0.0080$ (11) | 0.0063 (11) | 0.0013 (12) |
| C24 | 0.0212 (13) | 0.0217 (13) | 0.0249 (14) | $-0.0017$ (10) | $-0.0010$ (10) | 0.0026 (10) |
| C(A1) | 0.0141 (11) | 0.0130 (11) | 0.0167 (12) | 0.0011 (8) | 0.0011 (9) | 0.0022 (9) |
|     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|
| C(A2) | 0.0184 (12) | 0.0117 (10) | 0.0171 (12) | 0.0026 (9) | −0.0004 (9) | 0.0006 (9) |
| C(A3) | 0.0170 (12) | 0.0122 (11) | 0.0214 (13) | −0.0010 (9) | −0.0021 (10) | 0.0002 (9) |
| C(A4) | 0.0148 (11) | 0.0143 (11) | 0.0185 (12) | −0.0012 (9) | −0.0007 (9) | 0.0010 (9) |
| C(A5) | 0.0150 (12) | 0.0139 (11) | 0.0232 (13) | 0.0020 (9) | 0.0011 (10) | 0.0011 (9) |
| C(A6) | 0.0165 (12) | 0.0126 (11) | 0.0227 (13) | 0.0011 (9) | 0.0008 (10) | 0.0011 (9) |
| C(A7) | 0.0167 (12) | 0.0127 (11) | 0.0191 (12) | 0.0001 (9) | −0.0012 (9) | −0.0002 (9) |
| C(A8) | 0.0132 (11) | 0.0139 (11) | 0.0180 (12) | −0.0005 (8) | −0.0014 (9) | 0.0016 (9) |
| C(B1) | 0.0176 (12) | 0.0161 (11) | 0.0245 (14) | 0.0023 (9) | 0.0023 (10) | −0.0003 (10) |
| C(B2) | 0.0182 (12) | 0.0133 (11) | 0.0258 (13) | 0.0031 (9) | 0.0009 (10) | −0.0029 (10) |
| C(B3) | 0.0175 (12) | 0.0138 (11) | 0.0336 (15) | −0.0041 (9) | −0.0002 (11) | −0.0024 (10) |
| C(B4) | 0.0149 (12) | 0.0170 (11) | 0.0320 (15) | −0.0030 (9) | 0.0005 (10) | −0.0003 (10) |
| C(B5) | 0.0147 (12) | 0.0158 (11) | 0.0386 (16) | 0.0022 (9) | −0.0011 (11) | −0.0022 (11) |
| C(B6) | 0.0162 (12) | 0.0141 (11) | 0.0386 (16) | 0.0024 (9) | −0.0017 (11) | −0.0025 (11) |
| C(B7) | 0.0192 (12) | 0.0131 (11) | 0.0224 (13) | −0.0021 (9) | −0.0011 (10) | −0.0018 (9) |
| C(B8) | 0.0156 (12) | 0.0170 (11) | 0.0202 (13) | −0.0011 (9) | −0.0021 (9) | −0.0007 (9) |
| C(M1) | 0.0179 (12) | 0.0112 (10) | 0.0196 (13) | 0.0007 (9) | −0.0016 (9) | 0.0001 (9) |
| C(M2) | 0.0135 (11) | 0.0149 (11) | 0.0175 (12) | 0.0002 (9) | −0.0002 (9) | 0.0025 (9) |
| C(M3) | 0.0173 (12) | 0.0114 (10) | 0.0215 (13) | 0.0006 (9) | −0.0012 (10) | −0.0003 (9) |
| C(M4) | 0.0119 (11) | 0.0145 (11) | 0.0170 (12) | 0.0007 (8) | −0.0007 (8) | 0.0019 (9) |
| C1S  | 0.059 (2) | 0.0438 (19) | 0.043 (2) | 0.0006 (17) | −0.0063 (17) | −0.0030 (16) |
| C2S  | 0.049 (2) | 0.046 (2) | 0.057 (2) | −0.0065 (16) | 0.0016 (18) | −0.0077 (17) |
| C3S  | 0.060 (2) | 0.045 (2) | 0.067 (3) | −0.0008 (18) | −0.001 (2) | −0.0046 (18) |
| C4S  | 0.050 (4) | 0.048 (4) | 0.038 (4) | 0.001 (3) | 0.003 (3) | 0.004 (3) |
| C5S  | 0.074 (10) | 0.046 (7) | 0.087 (12) | 0.001 (6) | −0.014 (9) | −0.015 (8) |
| C6S  | 0.068 (6) | 0.060 (5) | 0.104 (8) | −0.016 (4) | −0.024 (5) | −0.012 (5) |
| C7S  | 0.046 (7) | 0.077 (9) | 0.103 (11) | 0.010 (6) | −0.043 (7) | −0.015 (8) |
| C8S  | 0.044 (4) | 0.053 (4) | 0.059 (5) | −0.001 (3) | −0.006 (4) | −0.011 (4) |
| C9S  | 0.042 (3) | 0.044 (3) | 0.038 (4) | 0.004 (3) | 0.006 (3) | −0.001 (3) |

**Geometric parameters (Å, °)**

|     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|
| Mn1—O1 | 2.1246 (18) | C21—H21 | 0.9500 |
| Mn1—N1 | 2.0119 (19) | C21—C22 | 1.388 (4) |
| Mn1—N2 | 2.0184 (19) | C22—H22 | 0.9500 |
| Mn1—N3 | 2.0052 (19) | C22—C23 | 1.380 (4) |
| Mn1—N4 | 2.0074 (19) | C23—H23 | 0.9500 |
| O1—N5 | 1.260 (3) | C23—C24 | 1.391 (4) |
| O2—N5 | 1.236 (3) | C24—H24 | 0.9500 |
| O3—N5 | 1.230 (3) | C(A1)—C(B1) | 1.437 (3) |
| N1—C(A1) | 1.387 (3) | C(A1)—C(M4) | 1.394 (3) |
| N1—C(A2) | 1.385 (3) | C(A2)—C(B2) | 1.431 (3) |
| N2—C(A3) | 1.380 (3) | C(A2)—C(M1) | 1.389 (3) |
| N2—C(A4) | 1.387 (3) | C(A3)—C(B3) | 1.437 (3) |
| N3—C(A5) | 1.384 (3) | C(A3)—C(M1) | 1.391 (3) |
| N3—C(A6) | 1.384 (3) | C(A4)—C(B4) | 1.434 (3) |
| N4—C(A7) | 1.381 (3) | C(A4)—C(M2) | 1.388 (3) |
| N4—C(A8) | 1.386 (3) | C(A5)—C(B5) | 1.436 (3) |
| C1—C2 | 1.385 (4) | C(A5)—C(M2) | 1.388 (3) |
| Bond       | Distance (Å) | Bond       | Distance (Å) |
|------------|--------------|------------|--------------|
| C1—C6      | 1.394 (4)    | C(A6—C(B6)| 1.433 (3)    |
| C1—C(M1)   | 1.497 (3)    | C(A6—C(M3)| 1.386 (3)    |
| C2—H2      | 0.9500       | C(A7—C(B7)| 1.431 (3)    |
| C2—C3      | 1.388 (3)    | C(A7—C(M3)| 1.393 (3)    |
| C3—H3      | 0.9500       | C(A8—C(B8)| 1.431 (3)    |
| C3—C4      | 1.374 (4)    | C(A8—C(M4)| 1.395 (3)    |
| C4—H4      | 0.9500       | C(B1—H(B1)| 0.9500       |
| C4—C5      | 1.390 (4)    | C(B1—C(B2)| 1.349 (3)    |
| C5—H5      | 0.9500       | C(B2—H(B2)| 0.9500       |
| C5—C6      | 1.389 (4)    | C(B3—H(B3)| 0.9500       |
| C6—H6      | 0.9500       | C(B3—C(B4)| 1.344 (3)    |
| C7—C8      | 1.399 (3)    | C(B4—H(B4)| 0.9500       |
| C7—C12     | 1.389 (3)    | C(B5—H(B5)| 0.9500       |
| C7—C(M2)   | 1.498 (3)    | C(B5—C(B6)| 1.346 (3)    |
| C8—H8      | 0.9500       | C(B6—H(B6)| 0.9500       |
| C8—C9      | 1.391 (3)    | C(B7—H(B7)| 0.9500       |
| C9—H9      | 0.9500       | C(B7—C(B8)| 1.353 (3)    |
| C9—C10     | 1.393 (4)    | C(B8—H(B8)| 0.9500       |
| C10—H10    | 0.9500       | C1S—C1S'   | 1.543 (7)    |
| C10—C11    | 1.384 (4)    | C1S—H1SA  | 0.9900       |
| C11—H11    | 0.9500       | C1S—H1SB  | 0.9900       |
| C11—C12    | 1.389 (4)    | C1S—C2S   | 1.548 (5)    |
| C12—H12    | 0.9500       | C2S—H2SA  | 0.9900       |
| C13—C14    | 1.379 (4)    | C2S—H2SB  | 0.9900       |
| C13—C18    | 1.380 (4)    | C2S—C3S   | 1.509 (5)    |
| C13—C(M3)  | 1.500 (3)    | C3S—H3SA  | 0.9800       |
| C14—H14    | 0.9500       | C3S—H3SB  | 0.9800       |
| C14—C15    | 1.395 (4)    | C3S—H3SC  | 0.9800       |
| C15—H15    | 0.9500       | C4S—H4S   | 0.9500       |
| C15—C16    | 1.347 (5)    | C4S—C5S   | 1.38 (2)     |
| C16—H16    | 0.9500       | C4S—C9S   | 1.372 (9)    |
| C16—C17    | 1.381 (5)    | C5S—H5S   | 0.9500       |
| C17—H17    | 0.9500       | C5S—C6S   | 1.33 (2)     |
| C17—C18    | 1.395 (4)    | C6S—H6S   | 0.9500       |
| C18—H18    | 0.9500       | C6S—C7S   | 1.49 (3)     |
| C19—C20    | 1.393 (3)    | C7S—H7S   | 0.9500       |
| C19—C24    | 1.397 (3)    | C7S—C8S   | 1.37 (2)     |
| C19—C(M4)  | 1.497 (3)    | C8S—H8S   | 0.9500       |
| C20—H20    | 0.9500       | C8S—C9S   | 1.342 (10)   |
| C20—C21    | 1.388 (4)    | C9S—H9S   | 0.9500       |

N1—Mn1—O1  | 91.79 (7)    | C23—C24—H24 | 119.8
N1—Mn1—N2  | 89.34 (8)    | N1—C(A1—C(B1)| 109.5 (2)
N2—Mn1—O1  | 95.27 (7)    | N1—C(A1—C(M4)| 125.9 (2)
N3—Mn1—O1  | 99.66 (7)    | C(M4—C(A1—C(B1)| 124.6 (2)
N3—Mn1—N1  | 168.53 (8)   | N1—C(A2—C(B2)| 109.9 (2)
N3—Mn1—N2  | 88.96 (8)    | N1—C(A2—C(M1)| 125.8 (2)
N3—Mn1—N4  | 89.79 (8)    | C(M1—C(A2—C(B2)| 124.3 (2)
N4—Mn1—O1 99.46 (7)  N2—C(A3)—C(B3) 109.5 (2)
N4—Mn1—N1 88.95 (8)  N2—C(A3)—C(M1) 125.9 (2)
N4—Mn1—N2 165.21 (8)  C(M1)—C(A3)—C(B3) 124.5 (2)
N5—Mn1 123.66 (15)  N2—C(A4)—C(B4) 109.7 (2)
C(A1)—N1—Mn1 126.01 (15)  N2—C(A4)—C(M2) 125.9 (2)
C(A2)—N1—Mn1 126.15 (15)  C(M2)—C(A4)—C(B4) 124.3 (2)
C(A2)—N1—C(A1) 105.67 (18)  N3—C(A5)—C(B5) 109.7 (2)
C(A3)—N2—Mn1 126.98 (16)  N3—C(A5)—C(M2) 126.0 (2)
C(A3)—N2—C(A4) 105.81 (19)  C(M2)—C(A5)—C(B5) 124.3 (2)
C(A4)—N2—Mn1 127.19 (15)  N3—C(A6)—C(B6) 109.5 (2)
C(A5)—N3—Mn1 126.86 (16)  N3—C(A6)—C(M3) 125.8 (2)
C(A6)—N3—Mn1 126.00 (15)  C(M3)—C(A6)—C(B6) 124.6 (2)
C(A6)—N3—C(A5) 105.82 (18)  N4—C(A7)—C(B7) 109.6 (2)
C(A7)—N4—Mn1 126.58 (15)  N4—C(A7)—C(M3) 125.9 (2)
C(A7)—N4—C(A8) 105.85 (18)  C(M3)—C(A7)—C(B7) 124.4 (2)
C(A8)—N4—Mn1 127.38 (15)  N4—C(A8)—C(B8) 109.6 (2)
O2—N5—O1 118.8 (2)  N4—C(A8)—C(M4) 125.7 (2)
O3—N5—O1 119.1 (2)  C(A1)—C(B1)—H(B1) 126.3
C2—C1—C6 118.9 (2)  C(B2)—C(B1)—C(A1) 107.5 (2)
C2—C1—C(M1) 120.7 (2)  C(B2)—C(B1)—H(B1) 126.3
C6—C1—C(M1) 120.5 (2)  C(A2)—C(B2)—H(B2) 126.3
C1—C2—H2 119.5  C(B1)—C(B2)—C(A2) 107.4 (2)
C1—C2—C3 120.9 (3)  C(B1)—C(B2)—H(B2) 126.3
C3—C2—H2 119.5  C(A3)—C(B3)—H(B3) 126.2
C2—C3—C6 120.0  C(B4)—C(B3)—C(A3) 107.6 (2)
C4—C3—C2 119.9 (3)  C(B4)—C(B3)—H(B3) 126.2
C4—C3—H3 120.0  C(A4)—C(B4)—H(B4) 126.3
C3—C4—H4 119.9  C(B3)—C(B4)—C(A4) 107.3 (2)
C3—C4—C5 120.1 (2)  C(B3)—C(B4)—H(B4) 126.3
C5—C4—H4 119.9  C(A5)—C(B5)—H(B5) 126.4
C4—C5—H5 120.1  C(B6)—C(B5)—C(A5) 107.3 (2)
C6—C5—C4 119.9 (3)  C(B6)—C(B5)—H(B5) 126.4
C6—C5—H5 120.1  C(A6)—C(B6)—H(B6) 126.1
C1—C6—H6 119.8  C(B5)—C(B6)—C(A6) 107.7 (2)
C5—C6—C1 120.3 (3)  C(B5)—C(B6)—H(B6) 126.2
C5—C6—H6 119.8  C(A7)—C(B7)—H(B7) 126.3
C8—C7—C(M2) 119.8 (2)  C(B8)—C(B7)—C(A7) 107.5 (2)
C12—C7—C8 119.1 (2)  C(B8)—C(B7)—H(B7) 126.3
C12—C7—C(M2) 121.1 (2)  C(A8)—C(B8)—H(B8) 126.3
C7—C8—H8 119.8  C(B7)—C(B8)—C(A8) 107.3 (2)
C9—C8—C7 120.4 (2)  C(B7)—C(B8)—H(B8) 126.3
C9—C8—H8 119.8  C(A2)—C(M1)—C1 117.9 (2)
C8—C9—H9 120.1  C(A2)—C(M1)—C(A3) 123.7 (2)
C8—C9—C10 119.9 (2)  C(A3)—C(M1)—C1 118.4 (2)
C10—C9—H9 120.1  C(A4)—C(M2)—C7 117.4 (2)
C9—C10—H10 120.1  C(A5)—C(M2)—C7 119.3 (2)
C11—C10—C9 119.7 (2)  C(A5)—C(M2)—C(A4) 123.3 (2)
| Bond Pairs                      | Distance (Å) | Angle (°) | Reference |
|--------------------------------|--------------|-----------|-----------|
| C11—C10—H10                   | 120.1        | 118.5     | (2)       |
| C10—C11—H11                   | 119.8        | 119.8     |           |
| C10—C11—C12                   | 120.5 (3)    | 119.8     |           |
| C12—C11—H11                   | 119.8        | 119.8     |           |
| C7—C12—H12                    | 119.8        | 119.8     |           |
| C11—C12—C7                    | 120.3 (2)    | 119.8     |           |
| C11—C12—H12                   | 119.8        | 119.8     |           |
| C14—C13—C18                   | 119.1 (2)    | 119.8     |           |
| C14—C13—C(M3)                 | 118.5 (2)    | 119.8     |           |
| C18—C13—C(M3)                 | 122.4 (2)    | 119.8     |           |
| C13—C14—H14                   | 120.0        | 119.8     |           |
| C13—C14—C15                   | 120.1 (3)    | 119.8     |           |
| C15—C14—H14                   | 120.0        | 119.8     |           |
| C14—C15—H15                   | 119.5        | 119.8     |           |
| C16—C15—C14                   | 121.0 (3)    | 119.8     |           |
| C16—C15—H15                   | 119.5        | 119.8     |           |
| C15—C16—H16                   | 120.2        | 119.8     |           |
| C15—C16—C17                   | 119.6 (3)    | 119.8     |           |
| C16—C17—H17                   | 120.2        | 119.8     |           |
| C16—C17—C18                   | 119.9        | 119.8     |           |
| C18—C17—H17                   | 119.9        | 119.8     |           |
| C13—C18—H18                   | 120.0        | 119.8     |           |
| C17—C18—H18                   | 120.0        | 119.8     |           |
| C20—C19—C24                   | 118.9 (2)    | 119.8     |           |
| C20—C19—C(M4)                 | 121.9 (2)    | 119.8     |           |
| C24—C19—C(M4)                 | 119.2 (2)    | 119.8     |           |
| C19—C20—H20                   | 119.9        | 119.8     |           |
| C21—C20—C19                   | 120.3 (2)    | 119.8     |           |
| C21—C20—H20                   | 119.9        | 119.8     |           |
| C20—C21—H21                   | 119.7        | 119.8     |           |
| C22—C21—C20                   | 120.6 (2)    | 119.8     |           |
| C22—C21—H21                   | 119.7        | 119.8     |           |
| C21—C22—H22                   | 120.3        | 119.8     |           |
| C23—C22—C21                   | 119.5 (2)    | 119.8     |           |
| C23—C22—H22                   | 120.3        | 119.8     |           |
| C22—C23—H23                   | 119.8        | 119.8     |           |
| C22—C23—C24                   | 120.4 (2)    | 119.8     |           |
| Mn1—O1—N5—O2                  | -169.95 (16) | 119.8     | (2)       |
| Mn1—O1—N5—O3                  | 11.9 (3)     | 119.8     |           |
| Mn1—N1—C(A1—C(B1)             | -162.14 (16) | 119.8     |           |
| Mn1—N1—C(A1—C(M4)             | 18.3 (3)     | 119.8     |           |
| Mn1—N1—C(A2—C(B2)             | 162.58 (16)  | 119.8     |           |
Mn1—N1—C(A2—C(M1 −17.0 (3) C20—C21—C22—C23 −0.1 (4)  
Mn1—N2—C(A3—C(M1 −179.46 (17) C21—C22—C23—C24 −0.6 (4)  
Mn1—N2—C(A4—C(M2 −0.9 (4) C22—C23—C24—C19 0.6 (4)  
Mn1—N2—C(M1—C(M2 1.9 (4) C24—C19—C(A1—C(B1 1.8 (3)  
Mn1—N3—C(A6—C(M3 −14.5 (4) C(A1—N1—C(A2—C(B2 −1.3 (3)  
Mn1—N3—C(A6—C(M4 −2.0 (4) C(A1—N1—C(A2—C(M1 179.1 (2)  
Mn1—N3—C(A6—C(M3 −177.4 (2) C(A1—C(B1—C(B2—C(A2 0.8 (3)  
Mn1—N4—C(A7—C(M3 −3.7 (4) C(A7—N4—C(A8—C(B8 179.5 (2)  
N1—C(A1—C(B1—C(B2 −1.6 (3) C(A3—C(B3—C(B4—C(A4 −0.4 (3)  
N1—C(A1—C(M4—C1 −174.8 (2) C(A5—C(B5—C(B6—C(A6 −1.5 (3)  
N1—C(A1—C(M4—C(A8 −1.0 (4) C(A5—C(B5—C(B6—C(A6 −1.5 (3)  
N2—C(A4—C(M2—C7 −165.7 (2) C(B1—C(A1—C(M4—C1 179.5 (2)  
N2—C(A4—C(M2—C(A5 9.0 (4) C(B1—C(A1—C(M4—C19 179.5 (2)  
N2—C(A4—C(M2—C(A6 −3.5 (3) C(B1—C(A1—C(M4—C(A8 −10.0 (4)  
N2—C(A4—C(M2—C(A7 166.2 (2) C(B1—C(A1—C(M4—C(A8 −10.0 (4)  
C1—C2—C3—C4 0.2 (4) C(B6—C(A6—C(M3—C(A7 178.2 (2)  
C2—C1—C6—C5 −1.2 (4) C(B7—C(A7—C(M3—C(A7 11.0 (4)  
C2—C1—C(M1—C(A2 64.2 (3) C(B7—C(A7—C(M3—C(A8 −174.2 (2)  
C2—C1—C(M1—C(A3 −115.5 (3) C(B8—C(A8—C(M4—C19 −10.0 (4)  
C2—C3—C4—C5 −0.8 (5) C(B8—C(A8—C(M4—C(A1 173.5 (2)  
C3—C4—C5—C6 0.4 (5) C(M1—C1—C2—C3 −178.2 (2)  
C4—C5—C6—C1 0.6 (5) C(M1—C1—C6—C5 177.8 (3)  
C6—C1—C2—C3 0.8 (4) C(M1—C2—C(B2—C(B1 180.0 (2)  
C6—C1—C(M1—C(A2 −114.8 (3) C(M1—C2—C(B2—C(B1 180.0 (2)  
C6—C1—C(M1—C(A3 65.5 (3) C(M1—C2—C(B2—C(B1 180.0 (2)  
C7—C8—C9—C10 −0.2 (4) C(M2—C7—C12—C11 177.6 (2)
| C8—C7—C12—C11 | -0.5 (4) | C(M2—C(A4—C(B4—C(B3) | 177.2 (2) |
| C8—C7—C(M2—C(A4) | 72.7 (3) | C(M2—C(A5—C(B5—C(B6) | 178.1 (2) |
| C8—C7—C(M2—C(A5) | -105.9 (3) | C(M3—C13—C14—C15 | 178.7 (3) |
| C8—C9—C10—C11 | -0.1 (4) | C(M3—C13—C18—C17 | -179.6 (3) |
| C9—C10—C11—C12 | 0.2 (4) | C(M3—C(A6—C(B6—C(B5) | -177.3 (3) |
| C10—C11—C12—C7 | 0.1 (4) | C(M3—C(A7—C(B7—C(B8) | -175.6 (2) |
| C12—C7—C8—C9 | 0.5 (3) | C(M4—C19—C20—C21 | 176.7 (2) |
| C12—C7—C(M2—C(A4) | -105.3 (3) | C(M4—C19—C24—C23 | -177.4 (2) |
| C12—C7—C(M2—C(A5) | 76.1 (3) | C(M4—C(A1—C(B1—C(B2) | 177.9 (2) |
| C13—C14—C15—C16 | 0.4 (6) | C(M4—C(A8—C(B8—C(B7) | 173.2 (2) |
| C14—C13—C18—C17 | -0.1 (4) | C1S—C1S—C2S—C3S | -178.4 (3) |
| C14—C13—C(M3—C(A6) | -105.4 (3) | C4S—C5S—C6S—C7S | -6 (3) |
| C14—C13—C(M3—C(A7) | 69.6 (3) | C5S—C4S—C9S—C8S | -0.6 (15) |
| C14—C15—C16—C17 | 1.0 (5) | C5S—C6S—C7S—C8S | 5 (3) |
| C15—C16—C17—C18 | -2.0 (5) | C6S—C7S—C8S—C9S | -2 (3) |
| C16—C17—C18—C13 | 1.5 (5) | C7S—C8S—C9S—C4S | -0.2 (19) |
| C18—C13—C14—C15 | -0.8 (5) | C9S—C4S—C5S—C6S | 4 (3) |
| C18—C13—C(M3—C(A6) | 74.1 (3) |

Symmetry code: (i) -x+1/2, -y+1/2, z.

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| C4S—H4S···O3 | 0.95 | 2.38 | 3.177 (8) | 141 |
| C10—H10···O2ii | 0.95 | 2.50 | 3.182 (3) | 129 |
| C17—H17···O2iii | 0.95 | 2.53 | 3.350 (4) | 145 |
| C22—H22···O2iv | 0.95 | 2.49 | 3.085 (3) | 120 |

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