Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Mesaconitine

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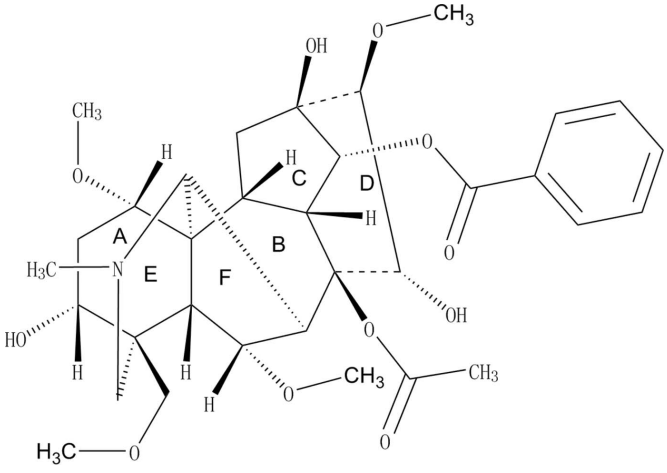
Received 26 April 2008; accepted 4 May 2008

Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.038; $wR$ factor = 0.082; data-to-parameter ratio = 8.9.

The title compound, (1$\alpha$,3$\alpha$,6$\alpha$,14$\alpha$,15$\alpha$,16$\beta$)-3,8,13,14,15-pentahydroxy-1,6,16-trimethoxy-4-methoxymethyl-20-methylaconitan-8,14-diyl 8-acetate 14-benzoate, $C_{33}H_{45}NO_{11}$, a $C_{19}$ diterpenoid alkaloid, obtained from the roots of *Aconitum kusnezoffii*, has been crystallographically characterized in this study. Rings *A*, *B* and *E* have chair conformations, rings *C* and *F* display envelope conformations, and ring *D* adopts a boat conformation. There are inter- and intramolecular O—H···O hydrogen bonds, the latter resulting in the formation of a non-planar seven-membered ring. The intermolecular interactions link the molecules into a two-dimensional network.

## Related literature

For general background, see: Hikino *et al.* (1980); Li *et al.* (1997); Mitamura *et al.* (2002); Saito *et al.* (1982); For ring conformation details, see: Codding (1982); De Camp & Pelletier (1977); Parvez *et al.* (1999); Pelletier *et al.* (1982). For related literature, see: Pelletier & Djarmati (1976); Tsuda & Marion (1963); Zhapova *et al.* (1986).



## Experimental

### Crystal data

$C_{33}H_{45}NO_{11}$
$M_r$ = 631.70
Orthorhombic, $P2_12_12_1$
$a$ = 12.6820 (6) Å
$b$ = 15.3848 (7) Å
$c$ = 15.6110 (7) Å
$V$ = 3045.9 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 173 (2) K
0.46 × 0.35 × 0.12 mm

### Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min}$ = 0.954, $T_{max}$ = 0.988
18319 measured reflections
3713 independent reflections
3026 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.081
$S$ = 1.07
3713 reflections
418 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O10—H10$A$···O2 | 0.84 | 2.11 | 2.788 (3) | 138 |
| O7—H7···O8 | 0.84 | 2.04 | 2.560 (3) | 120 |
| O4—H4···O11$^{i}$ | 0.84 | 2.20 | 3.018 (3) | 163 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank Guangdong Provincial Natural Science Foundation of China (No. 04300531) for financial assistance.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2256).

## References

Bruker (2001). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Codding, P. W. (1982). *Acta Cryst.* B**38**, 2519–2522.
De Camp, W. H. & Pelletier, S. W. (1977). *Acta Cryst.* B**33**, 722–727.
Hikino, H., Konno, C., Takata, H., Yamada, Y., Yamada, C., Ohizumi, Y., Sugio, K. & Fujimura, H. (1980). *J. Pharm. Dyn.* **3**, 514–525.
Li, Z. B., Lu, G. H., Chen, D. L. & Wang, F. P. (1997). *Nat. Prod. Res. Dev.* **9**, 9-14.
Mitamura, M., Horie, S., Sakaguchi, M., Someya, A., Tsuchiya, S. V., Murayama, T. & Watanabe, K. (2002). *Eur. J. Pharmacol.* **436**, 217–225.
Parvez, M., Gul, W., Atta-ur-Rahman, Choudhary, M. I., Nasreen, A. & Fatima, N. (1999). *Acta Cryst.* C**55**, 72–74.
Pelletier, S. W. & Djarmati, Z. (1976). *J Am Chem Soc.* **98**, 2626–2636.
Pelletier, S. W., Finer-Moore, J., Desai, R. C., Mody, N. V. & Desai, H. K. (1982). *J. Org. Chem.* **47**, 5290–5297.

Saito, H., Ueyama, T., Naka, N., Yagi, J. & Okamoto, T. (1982). *Chem. Pharm. Bull.* **30**, 1844–1850.
Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tsuda, Y. & Marion, L. (1963). *Can. J. Chem*. **41**, 1485-1489.
Zhapova, T., Modonova, L. D. & Semenov, A. A. (1986). *Chem Nat Compd*, **21**, 7678–679.

# supporting information

*Acta Cryst.* (2008). E**64**, o1033–o1034 [doi:10.1107/S1600536808013147]

## Mesaconitine

**Dao-Hang He, Yong-Chuang Zhu and Ai-Xi Hu**

### S1. Comment

As an important Chinese herbal medicine belonging to the genus *Aconitum*, *A. kusnzoffii* has been therapeutically used to treat rheumatic pain, paralysis due to stroke, rheumatoid arthritis and some other inflammations. Mesaconitine, a $C_{19}$ diterpenoid alkaloid, is pharmacologically one of the most active components obtained from the roots of *A. kusnezoffii* (Li *et al.*, 1997). Mesaconitine has been reported to have an anti-inflammatory activity (Hikino *et al.*,1980; Saito *et al.*, 1982), and the vasorelaxant effect of mesaconitine may contribute to the therapeutical effectiveness on persons with a weak constitution and poor metabolism, by improving peripheral blood circulation (Mitamura *et al.*, 2002). The three-dimensional structure of most biologically active molecules plays a role in governing their interactions and activities. It is important to obtain information on the mode of action and selectivity of mesaconitine so that it can be used safely and efficiently. Many X-ray crystal structure determinations of $C_{19}$ diterpenoid alkaloids have been reported, such as pseudaconitine, delphinine (Parvez *et al.*, 1999; Pelletier *et al.*, 1982.). However, the crystal structure of mesaconitine has not been reported. In view of this, the crystal structure determination of the title compound was carried out and the results are presented here.

The structure of mesaconitine is similar to that of aconitine (Codding, 1982). The only difference between aconitine and mesaconitine is a methylene group at the tertiary nitrogen atom. The bond lengths and angles in the title compound are in good agreement with expected values. In the molecule of the title compound, (Fig. 1), rings A, B and E have a chair conformation, rings C and F display an envelope conformation, ring D adopts a boat conformation. The packing of the title compound is shown in Fig. 2. In the crystal structure, there are inter- and intramolecular O—H···O hydrogen bonds. The former link the molecules into a two-dimensional network, while the latter results in the formation of a non-planar seven-membered ring. These intramolecular hydrogen bonds may be effective in the stabilization of the structure.

### S2. Experimental

The title compound was isolated from the roots of *A. kusnezoffii* according to the literature procedure of Li *et al.* (1997) and crystals of X-ray quality were grown from methanol at room temperature by slow evaporation.

### S3. Refinement

The H atom attached to C2 was located and refined freely [C—H = 0.97 (2) Å]. Other H atoms were included in the refinement at idealized positions and refin ed as riding, with C—H = 0.95 (aromatic), 0.98 ($CH_2$), 1.00 (CH), O—H = 0.84 Å. $U_{iso}(H) = xU_{eq}$(carrier atom), where x = 1.5 for O and methyl, 1.2 for all other H atoms. In the absence of significant anomalous scattering effects, Friedel pairs were merged. The absolute configuration was assigned on the basis of the related literature (Pelletier & Djarmati, 1976; Tsuda & Marion, 1963; Zhapova *et al.*, 1986).

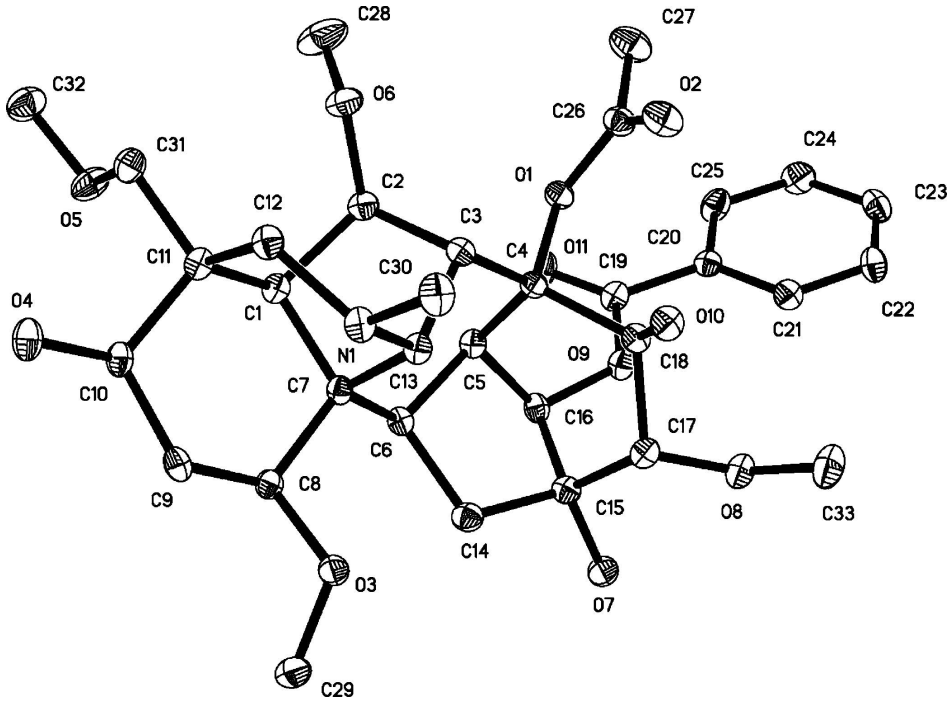



**Figure 1**

A view of the structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

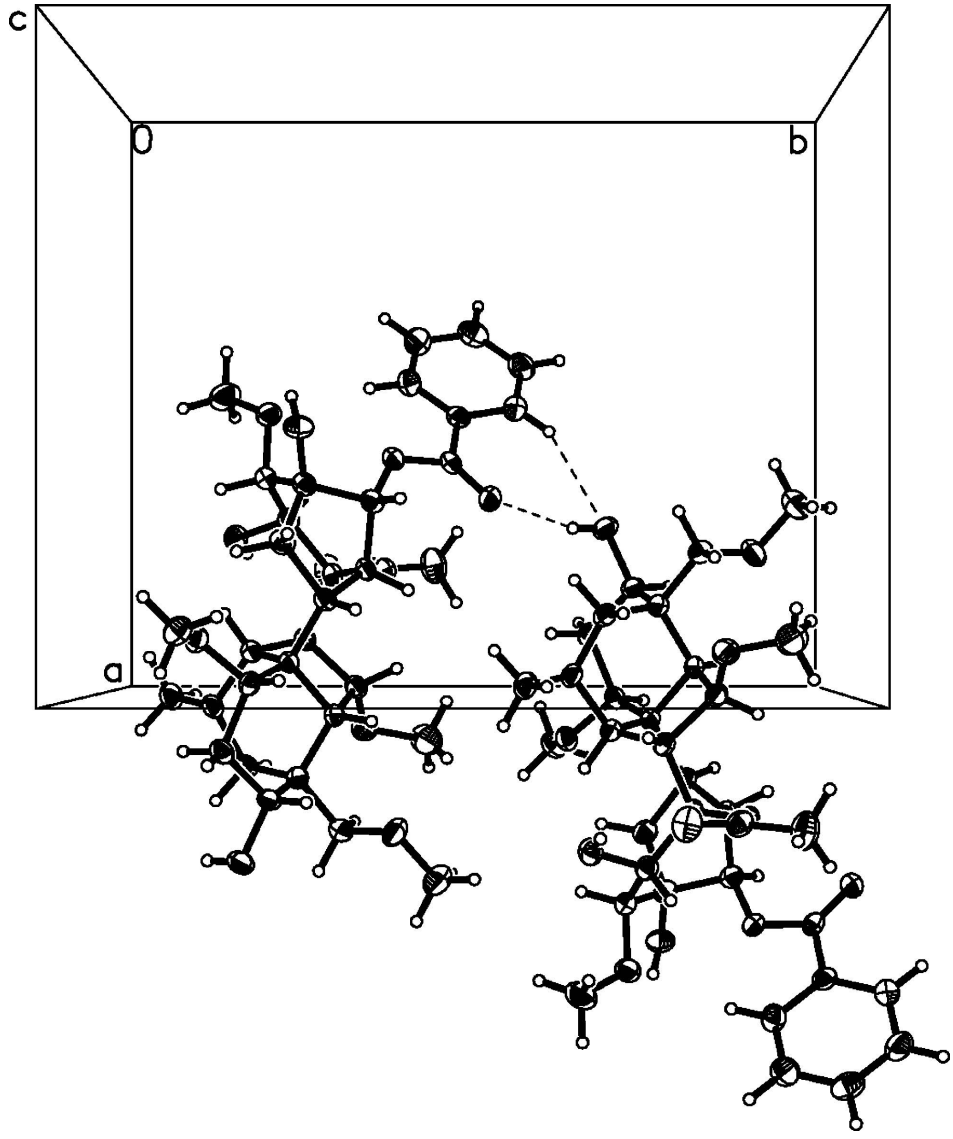



**Figure 2**

The packing of molecules of the title compound, viewed down the *c* axis. Dashed lines indicate hydrogen bonds.

### 3,8,13,14,15-pentahydroxy-1*α*,3*α*,6*α*,14*α*,15*α*,16*β*-20-methyl-1,6,16- trimethoxy-4-methoxymethylaconitan-8,14-diyl 8-acetate 14-benzoate

*Crystal data*

$C_{33}H_{45}NO_{11}$
$M_r = 631.70$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 12.6820\ (6)$ Å
$b = 15.3848\ (7)$ Å
$c = 15.6110\ (7)$ Å
$V = 3045.9\ (2)$ Å$^3$
$Z = 4$
$F(000) = 1352$
$D_x = 1.378$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6314 reflections
$\theta = 2.5–26.8°$
$\mu = 0.10$ mm$^{-1}$
$T = 173$ K
Block, colorless
0.46 × 0.35 × 0.12 mm

*Data collection*

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min}$ = 0.954, $T_{max}$ = 0.988
18319 measured reflections
3713 independent reflections
3026 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042
$\theta_{max}$ = 27.0°, $\theta_{min}$ = 1.9°
$h$ = −16→15
$k$ = −16→19
$l$ = −16→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.081
$S$ = 1.07
3713 reflections
418 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0245P)^2 + 1.2755P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | −0.0391 (2) | 0.81198 (18) | 0.21029 (19) | 0.0220 (6) |
| H1 | −0.0477 | 0.8647 | 0.1734 | 0.026* |
| C2 | 0.0052 (2) | 0.8377 (2) | 0.3007 (2) | 0.0246 (7) |
| C3 | 0.0859 (2) | 0.76493 (18) | 0.32284 (18) | 0.0218 (6) |
| H3 | 0.0727 | 0.7412 | 0.3815 | 0.026* |
| C4 | 0.1968 (2) | 0.80413 (18) | 0.31663 (18) | 0.0209 (6) |
| C5 | 0.2045 (2) | 0.85444 (18) | 0.23165 (18) | 0.0219 (6) |
| H5 | 0.1701 | 0.9126 | 0.2373 | 0.026* |
| C6 | 0.1544 (2) | 0.80248 (19) | 0.15592 (18) | 0.0220 (6) |
| H6 | 0.1380 | 0.8456 | 0.1099 | 0.026* |
| C7 | 0.0505 (2) | 0.75172 (18) | 0.17449 (18) | 0.0207 (6) |
| C8 | 0.0175 (2) | 0.70445 (19) | 0.09137 (19) | 0.0226 (6) |
| H8 | 0.0235 | 0.7470 | 0.0432 | 0.027* |
| C9 | −0.0936 (2) | 0.6672 (2) | 0.0894 (2) | 0.0256 (7) |
| H9A | −0.1126 | 0.6534 | 0.0294 | 0.031* |

| | | | | |
|---|---|---|---|---|
| H9B | −0.0949 | 0.6123 | 0.1225 | 0.031* |
| C10 | −0.1744 (2) | 0.72861 (19) | 0.12591 (19) | 0.0241 (6) |
| H10 | −0.1762 | 0.7807 | 0.0877 | 0.029* |
| C11 | −0.1439 (2) | 0.76086 (19) | 0.21596 (19) | 0.0236 (6) |
| C12 | −0.1281 (2) | 0.68527 (19) | 0.2794 (2) | 0.0254 (7) |
| H12A | −0.1312 | 0.7082 | 0.3386 | 0.030* |
| H12B | −0.1866 | 0.6432 | 0.2724 | 0.030* |
| C13 | 0.0663 (2) | 0.69431 (18) | 0.25371 (18) | 0.0226 (6) |
| H13 | 0.1306 | 0.6574 | 0.2466 | 0.027* |
| C14 | 0.2486 (2) | 0.7463 (2) | 0.1230 (2) | 0.0275 (7) |
| H14A | 0.2335 | 0.6837 | 0.1313 | 0.033* |
| H14B | 0.2606 | 0.7570 | 0.0612 | 0.033* |
| C15 | 0.3455 (2) | 0.7728 (2) | 0.17473 (18) | 0.0247 (6) |
| C16 | 0.3180 (2) | 0.86471 (19) | 0.20170 (19) | 0.0242 (6) |
| H16 | 0.3214 | 0.9048 | 0.1513 | 0.029* |
| C17 | 0.3584 (2) | 0.71420 (19) | 0.25396 (19) | 0.0253 (7) |
| H17 | 0.3397 | 0.6533 | 0.2376 | 0.030* |
| C18 | 0.2910 (2) | 0.74092 (19) | 0.33247 (18) | 0.0240 (6) |
| H18 | 0.3398 | 0.7717 | 0.3726 | 0.029* |
| C19 | 0.3869 (2) | 0.97097 (19) | 0.3007 (2) | 0.0257 (7) |
| C20 | 0.4690 (2) | 0.98015 (19) | 0.3682 (2) | 0.0250 (6) |
| C21 | 0.5301 (3) | 0.9093 (2) | 0.3930 (2) | 0.0299 (7) |
| H21 | 0.5187 | 0.8540 | 0.3677 | 0.036* |
| C22 | 0.6072 (3) | 0.9198 (2) | 0.4544 (2) | 0.0356 (8) |
| H22 | 0.6489 | 0.8715 | 0.4713 | 0.043* |
| C23 | 0.6240 (3) | 0.9998 (2) | 0.4915 (2) | 0.0365 (8) |
| H23 | 0.6767 | 1.0065 | 0.5342 | 0.044* |
| C24 | 0.5643 (3) | 1.0702 (2) | 0.4664 (2) | 0.0401 (9) |
| H24 | 0.5768 | 1.1255 | 0.4914 | 0.048* |
| C25 | 0.4865 (3) | 1.0608 (2) | 0.4053 (2) | 0.0362 (8) |
| H25 | 0.4451 | 1.1094 | 0.3887 | 0.043* |
| C26 | 0.2065 (2) | 0.8593 (2) | 0.46489 (19) | 0.0284 (7) |
| C27 | 0.2139 (3) | 0.9414 (2) | 0.5150 (2) | 0.0452 (9) |
| H27A | 0.1483 | 0.9745 | 0.5086 | 0.068* |
| H27B | 0.2731 | 0.9762 | 0.4937 | 0.068* |
| H27C | 0.2251 | 0.9277 | 0.5756 | 0.068* |
| C28 | −0.0892 (3) | 0.9341 (3) | 0.3905 (3) | 0.0584 (12) |
| H28A | −0.0235 | 0.9626 | 0.4079 | 0.088* |
| H28B | −0.1399 | 0.9362 | 0.4378 | 0.088* |
| H28C | −0.1187 | 0.9641 | 0.3406 | 0.088* |
| C29 | 0.1046 (3) | 0.6183 (2) | −0.0140 (2) | 0.0339 (8) |
| H29A | 0.0383 | 0.5980 | −0.0393 | 0.051* |
| H29B | 0.1589 | 0.5735 | −0.0212 | 0.051* |
| H29C | 0.1272 | 0.6718 | −0.0427 | 0.051* |
| C30 | −0.0119 (3) | 0.5751 (2) | 0.3337 (2) | 0.0311 (7) |
| H30A | 0.0555 | 0.5451 | 0.3248 | 0.047* |
| H30B | −0.0696 | 0.5328 | 0.3315 | 0.047* |
| H30C | −0.0115 | 0.6038 | 0.3897 | 0.047* |

| | | | | |
|---|---|---|---|---|
| C31 | −0.2345 (2) | 0.81935 (19) | 0.2462 (2) | 0.0284 (7) |
| H31A | −0.3027 | 0.7887 | 0.2400 | 0.034* |
| H31B | −0.2249 | 0.8348 | 0.3073 | 0.034* |
| C32 | −0.3153 (3) | 0.9539 (2) | 0.2150 (2) | 0.0399 (8) |
| H32A | −0.3834 | 0.9252 | 0.2058 | 0.060* |
| H32B | −0.3104 | 1.0054 | 0.1783 | 0.060* |
| H32C | −0.3092 | 0.9714 | 0.2751 | 0.060* |
| C33 | 0.5015 (3) | 0.6510 (2) | 0.3335 (2) | 0.0445 (9) |
| H33A | 0.4696 | 0.6603 | 0.3899 | 0.067* |
| H33B | 0.5785 | 0.6529 | 0.3386 | 0.067* |
| H33C | 0.4800 | 0.5941 | 0.3113 | 0.067* |
| N1 | −0.02662 (19) | 0.63950 (15) | 0.26699 (16) | 0.0239 (5) |
| O1 | 0.20493 (15) | 0.87584 (12) | 0.38022 (12) | 0.0241 (4) |
| O2 | 0.2048 (2) | 0.78785 (15) | 0.49642 (14) | 0.0402 (6) |
| O3 | 0.08940 (16) | 0.63488 (13) | 0.07442 (13) | 0.0263 (5) |
| O4 | −0.27732 (15) | 0.68993 (14) | 0.12299 (15) | 0.0316 (5) |
| H4 | −0.2766 | 0.6427 | 0.1499 | 0.047* |
| O5 | −0.23341 (17) | 0.89599 (14) | 0.19455 (15) | 0.0349 (6) |
| O6 | −0.06838 (16) | 0.84649 (14) | 0.36913 (14) | 0.0328 (5) |
| O7 | 0.43716 (15) | 0.76827 (15) | 0.12268 (13) | 0.0309 (5) |
| H7 | 0.4897 | 0.7566 | 0.1534 | 0.046* |
| O8 | 0.46752 (16) | 0.71676 (14) | 0.27663 (14) | 0.0305 (5) |
| O9 | 0.39220 (15) | 0.89139 (13) | 0.26615 (14) | 0.0257 (5) |
| O10 | 0.25977 (17) | 0.66318 (13) | 0.37478 (14) | 0.0290 (5) |
| H10A | 0.2344 | 0.6755 | 0.4230 | 0.044* |
| O11 | 0.32507 (17) | 1.02599 (13) | 0.27820 (16) | 0.0349 (5) |
| H2 | 0.037 (2) | 0.8949 (9) | 0.297 (2) | 0.042* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0223 (14) | 0.0175 (14) | 0.0261 (15) | −0.0007 (12) | 0.0000 (12) | 0.0027 (12) |
| C2 | 0.0242 (15) | 0.0225 (15) | 0.0272 (16) | −0.0032 (12) | 0.0023 (13) | −0.0019 (13) |
| C3 | 0.0241 (14) | 0.0210 (14) | 0.0204 (14) | −0.0024 (12) | 0.0003 (12) | 0.0007 (12) |
| C4 | 0.0231 (14) | 0.0190 (14) | 0.0207 (14) | −0.0019 (12) | −0.0004 (12) | −0.0012 (12) |
| C5 | 0.0216 (14) | 0.0180 (14) | 0.0261 (15) | −0.0037 (12) | −0.0013 (12) | 0.0012 (12) |
| C6 | 0.0224 (14) | 0.0220 (15) | 0.0215 (15) | −0.0024 (12) | −0.0015 (12) | 0.0018 (12) |
| C7 | 0.0203 (14) | 0.0180 (14) | 0.0239 (15) | −0.0014 (11) | −0.0029 (12) | −0.0007 (12) |
| C8 | 0.0251 (15) | 0.0201 (15) | 0.0227 (14) | 0.0031 (12) | −0.0018 (12) | 0.0023 (12) |
| C9 | 0.0263 (15) | 0.0254 (16) | 0.0251 (16) | −0.0045 (13) | −0.0068 (13) | −0.0003 (13) |
| C10 | 0.0192 (14) | 0.0249 (15) | 0.0283 (15) | −0.0032 (12) | −0.0032 (12) | 0.0052 (13) |
| C11 | 0.0217 (14) | 0.0211 (15) | 0.0281 (15) | −0.0004 (12) | −0.0001 (12) | 0.0029 (13) |
| C12 | 0.0231 (14) | 0.0248 (15) | 0.0282 (16) | −0.0053 (12) | −0.0001 (13) | 0.0023 (13) |
| C13 | 0.0218 (14) | 0.0198 (14) | 0.0263 (16) | −0.0016 (12) | −0.0013 (12) | 0.0010 (13) |
| C14 | 0.0273 (15) | 0.0290 (16) | 0.0263 (15) | −0.0029 (14) | 0.0031 (13) | −0.0012 (13) |
| C15 | 0.0242 (14) | 0.0255 (15) | 0.0243 (15) | −0.0033 (13) | 0.0022 (12) | 0.0001 (13) |
| C16 | 0.0244 (15) | 0.0248 (15) | 0.0235 (15) | −0.0030 (13) | −0.0028 (12) | 0.0058 (12) |
| C17 | 0.0230 (15) | 0.0217 (15) | 0.0311 (16) | −0.0013 (12) | 0.0002 (13) | −0.0003 (13) |

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|---|---|---|---|---|---|---|
| C18 | 0.0259 (15) | 0.0225 (15) | 0.0237 (15) | −0.0018 (13) | 0.0000 (13) | 0.0021 (12) |
| C19 | 0.0233 (15) | 0.0203 (15) | 0.0337 (18) | −0.0055 (13) | 0.0016 (13) | 0.0034 (13) |
| C20 | 0.0217 (14) | 0.0266 (15) | 0.0267 (16) | −0.0045 (13) | 0.0035 (13) | 0.0004 (13) |
| C21 | 0.0336 (17) | 0.0256 (16) | 0.0307 (18) | −0.0019 (14) | −0.0003 (14) | 0.0026 (14) |
| C22 | 0.0373 (18) | 0.0350 (19) | 0.0343 (19) | 0.0011 (16) | −0.0072 (15) | 0.0090 (16) |
| C23 | 0.0339 (18) | 0.047 (2) | 0.0284 (18) | −0.0087 (16) | −0.0056 (15) | 0.0040 (16) |
| C24 | 0.0358 (19) | 0.036 (2) | 0.049 (2) | −0.0075 (16) | −0.0028 (17) | −0.0144 (17) |
| C25 | 0.0302 (17) | 0.0269 (17) | 0.051 (2) | 0.0008 (14) | −0.0034 (16) | −0.0027 (16) |
| C26 | 0.0288 (16) | 0.0304 (18) | 0.0260 (16) | −0.0039 (14) | 0.0002 (14) | −0.0031 (14) |
| C27 | 0.064 (3) | 0.035 (2) | 0.036 (2) | −0.0062 (19) | −0.0018 (19) | −0.0077 (16) |
| C28 | 0.043 (2) | 0.050 (2) | 0.082 (3) | −0.0042 (19) | 0.019 (2) | −0.034 (2) |
| C29 | 0.0347 (17) | 0.0335 (18) | 0.0335 (18) | 0.0068 (15) | 0.0028 (15) | −0.0042 (15) |
| C30 | 0.0338 (17) | 0.0234 (16) | 0.0362 (18) | −0.0041 (14) | −0.0038 (15) | 0.0080 (14) |
| C31 | 0.0241 (15) | 0.0279 (16) | 0.0332 (17) | −0.0026 (13) | 0.0009 (13) | 0.0014 (14) |
| C32 | 0.041 (2) | 0.0364 (19) | 0.043 (2) | 0.0109 (16) | 0.0066 (17) | 0.0022 (17) |
| C33 | 0.0345 (19) | 0.045 (2) | 0.054 (2) | 0.0089 (17) | −0.0026 (17) | 0.0134 (19) |
| N1 | 0.0250 (13) | 0.0197 (12) | 0.0269 (13) | −0.0043 (11) | −0.0018 (11) | 0.0047 (11) |
| O1 | 0.0270 (10) | 0.0215 (10) | 0.0238 (11) | −0.0029 (9) | −0.0012 (9) | −0.0031 (9) |
| O2 | 0.0527 (15) | 0.0367 (14) | 0.0313 (12) | −0.0038 (12) | 0.0017 (11) | 0.0005 (11) |
| O3 | 0.0290 (11) | 0.0230 (11) | 0.0270 (11) | 0.0031 (9) | −0.0036 (9) | −0.0029 (9) |
| O4 | 0.0239 (11) | 0.0305 (12) | 0.0405 (13) | −0.0063 (9) | −0.0056 (10) | 0.0057 (11) |
| O5 | 0.0348 (12) | 0.0273 (12) | 0.0424 (14) | 0.0098 (10) | 0.0107 (11) | 0.0074 (10) |
| O6 | 0.0293 (11) | 0.0338 (12) | 0.0354 (12) | −0.0005 (10) | 0.0084 (10) | −0.0081 (11) |
| O7 | 0.0232 (10) | 0.0401 (13) | 0.0293 (11) | −0.0012 (10) | 0.0048 (9) | 0.0014 (11) |
| O8 | 0.0248 (11) | 0.0300 (12) | 0.0367 (12) | 0.0019 (9) | 0.0003 (10) | 0.0067 (10) |
| O9 | 0.0231 (10) | 0.0224 (10) | 0.0318 (12) | −0.0035 (9) | −0.0030 (9) | 0.0003 (9) |
| O10 | 0.0326 (11) | 0.0249 (11) | 0.0297 (12) | −0.0004 (9) | 0.0023 (10) | 0.0080 (10) |
| O11 | 0.0287 (12) | 0.0229 (11) | 0.0532 (15) | 0.0023 (10) | −0.0106 (11) | 0.0011 (11) |

*Geometric parameters (Å, º)*

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| C1—C11 | 1.547 (4) | C18—O10 | 1.422 (3) |
| C1—C7 | 1.570 (4) | C18—H18 | 1.0000 |
| C1—C2 | 1.570 (4) | C19—O11 | 1.206 (3) |
| C1—H1 | 1.0000 | C19—O9 | 1.339 (3) |
| C2—O6 | 1.424 (4) | C19—C20 | 1.489 (4) |
| C2—C3 | 1.556 (4) | C20—C25 | 1.387 (4) |
| C2—H2 | 0.970 (16) | C20—C21 | 1.391 (4) |
| C3—C4 | 1.533 (4) | C21—C22 | 1.379 (4) |
| C3—C13 | 1.551 (4) | C21—H21 | 0.9500 |
| C3—H3 | 1.0000 | C22—C23 | 1.376 (5) |
| C4—O1 | 1.488 (3) | C22—H22 | 0.9500 |
| C4—C5 | 1.539 (4) | C23—C24 | 1.377 (5) |
| C4—C18 | 1.560 (4) | C23—H23 | 0.9500 |
| C5—C16 | 1.522 (4) | C24—C25 | 1.380 (5) |
| C5—C6 | 1.562 (4) | C24—H24 | 0.9500 |
| C5—H5 | 1.0000 | C25—H25 | 0.9500 |
| C6—C7 | 1.559 (4) | C26—O2 | 1.204 (4) |

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| C6—C14 | 1.561 (4) | C26—O1 | 1.346 (4) |
| C6—H6 | 1.0000 | C26—C27 | 1.490 (4) |
| C7—C13 | 1.533 (4) | C27—H27A | 0.9800 |
| C7—C8 | 1.545 (4) | C27—H27B | 0.9800 |
| C8—O3 | 1.431 (3) | C27—H27C | 0.9800 |
| C8—C9 | 1.521 (4) | C28—O6 | 1.413 (4) |
| C8—H8 | 1.0000 | C28—H28A | 0.9800 |
| C9—C10 | 1.506 (4) | C28—H28B | 0.9800 |
| C9—H9A | 0.9900 | C28—H28C | 0.9800 |
| C9—H9B | 0.9900 | C29—O3 | 1.417 (4) |
| C10—O4 | 1.435 (3) | C29—H29A | 0.9800 |
| C10—C11 | 1.540 (4) | C29—H29B | 0.9800 |
| C10—H10 | 1.0000 | C29—H29C | 0.9800 |
| C11—C31 | 1.534 (4) | C30—N1 | 1.449 (4) |
| C11—C12 | 1.540 (4) | C30—H30A | 0.9800 |
| C12—N1 | 1.480 (4) | C30—H30B | 0.9800 |
| C12—H12A | 0.9900 | C30—H30C | 0.9800 |
| C12—H12B | 0.9900 | C31—O5 | 1.429 (4) |
| C13—N1 | 1.464 (4) | C31—H31A | 0.9900 |
| C13—H13 | 1.0000 | C31—H31B | 0.9900 |
| C14—C15 | 1.526 (4) | C32—O5 | 1.405 (4) |
| C14—H14A | 0.9900 | C32—H32A | 0.9800 |
| C14—H14B | 0.9900 | C32—H32B | 0.9800 |
| C15—O7 | 1.420 (3) | C32—H32C | 0.9800 |
| C15—C16 | 1.516 (4) | C33—O8 | 1.413 (4) |
| C15—C17 | 1.539 (4) | C33—H33A | 0.9800 |
| C16—O9 | 1.437 (3) | C33—H33B | 0.9800 |
| C16—H16 | 1.0000 | C33—H33C | 0.9800 |
| C17—O8 | 1.429 (3) | O4—H4 | 0.8400 |
| C17—C18 | 1.550 (4) | O7—H7 | 0.8400 |
| C17—H17 | 1.0000 | O10—H10A | 0.8400 |

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| C11—C1—C7 | 110.0 (2) | O9—C16—H16 | 110.3 |
| C11—C1—C2 | 112.6 (2) | C15—C16—H16 | 110.3 |
| C7—C1—C2 | 102.1 (2) | C5—C16—H16 | 110.3 |
| C11—C1—H1 | 110.6 | O8—C17—C15 | 106.6 (2) |
| C7—C1—H1 | 110.6 | O8—C17—C18 | 109.3 (2) |
| C2—C1—H1 | 110.6 | C15—C17—C18 | 114.9 (2) |
| O6—C2—C3 | 109.5 (2) | O8—C17—H17 | 108.6 |
| O6—C2—C1 | 117.6 (2) | C15—C17—H17 | 108.6 |
| C3—C2—C1 | 104.7 (2) | C18—C17—H17 | 108.6 |
| O6—C2—H2 | 104 (2) | O10—C18—C17 | 107.3 (2) |
| C3—C2—H2 | 113 (2) | O10—C18—C4 | 112.6 (2) |
| C1—C2—H2 | 109 (2) | C17—C18—C4 | 117.6 (2) |
| C4—C3—C13 | 112.2 (2) | O10—C18—H18 | 106.2 |
| C4—C3—C2 | 107.8 (2) | C17—C18—H18 | 106.2 |
| C13—C3—C2 | 104.1 (2) | C4—C18—H18 | 106.2 |
| C4—C3—H3 | 110.8 | O11—C19—O9 | 123.9 (3) |

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|---|---|---|---|
| C13—C3—H3 | 110.8 | O11—C19—C20 | 126.5 (3) |
| C2—C3—H3 | 110.8 | O9—C19—C20 | 109.7 (2) |
| O1—C4—C3 | 108.3 (2) | C25—C20—C21 | 119.7 (3) |
| O1—C4—C5 | 101.4 (2) | C25—C20—C19 | 119.5 (3) |
| C3—C4—C5 | 108.1 (2) | C21—C20—C19 | 120.8 (3) |
| O1—C4—C18 | 107.7 (2) | C22—C21—C20 | 119.7 (3) |
| C3—C4—C18 | 116.6 (2) | C22—C21—H21 | 120.1 |
| C5—C4—C18 | 113.7 (2) | C20—C21—H21 | 120.1 |
| C16—C5—C4 | 112.2 (2) | C23—C22—C21 | 120.5 (3) |
| C16—C5—C6 | 101.9 (2) | C23—C22—H22 | 119.8 |
| C4—C5—C6 | 111.7 (2) | C21—C22—H22 | 119.8 |
| C16—C5—H5 | 110.3 | C22—C23—C24 | 119.9 (3) |
| C4—C5—H5 | 110.3 | C22—C23—H23 | 120.1 |
| C6—C5—H5 | 110.3 | C24—C23—H23 | 120.1 |
| C7—C6—C14 | 115.5 (2) | C23—C24—C25 | 120.4 (3) |
| C7—C6—C5 | 117.3 (2) | C23—C24—H24 | 119.8 |
| C14—C6—C5 | 102.8 (2) | C25—C24—H24 | 119.8 |
| C7—C6—H6 | 106.8 | C24—C25—C20 | 119.8 (3) |
| C14—C6—H6 | 106.8 | C24—C25—H25 | 120.1 |
| C5—C6—H6 | 106.8 | C20—C25—H25 | 120.1 |
| C13—C7—C8 | 116.2 (2) | O2—C26—O1 | 125.0 (3) |
| C13—C7—C6 | 109.1 (2) | O2—C26—C27 | 124.1 (3) |
| C8—C7—C6 | 108.0 (2) | O1—C26—C27 | 110.8 (3) |
| C13—C7—C1 | 98.5 (2) | C26—C27—H27A | 109.5 |
| C8—C7—C1 | 112.4 (2) | C26—C27—H27B | 109.5 |
| C6—C7—C1 | 112.5 (2) | H27A—C27—H27B | 109.5 |
| O3—C8—C9 | 107.7 (2) | C26—C27—H27C | 109.5 |
| O3—C8—C7 | 109.5 (2) | H27A—C27—H27C | 109.5 |
| C9—C8—C7 | 116.4 (2) | H27B—C27—H27C | 109.5 |
| O3—C8—H8 | 107.6 | O6—C28—H28A | 109.5 |
| C9—C8—H8 | 107.6 | O6—C28—H28B | 109.5 |
| C7—C8—H8 | 107.6 | H28A—C28—H28B | 109.5 |
| C10—C9—C8 | 112.7 (2) | O6—C28—H28C | 109.5 |
| C10—C9—H9A | 109.0 | H28A—C28—H28C | 109.5 |
| C8—C9—H9A | 109.0 | H28B—C28—H28C | 109.5 |
| C10—C9—H9B | 109.0 | O3—C29—H29A | 109.5 |
| C8—C9—H9B | 109.0 | O3—C29—H29B | 109.5 |
| H9A—C9—H9B | 107.8 | H29A—C29—H29B | 109.5 |
| O4—C10—C9 | 110.3 (2) | O3—C29—H29C | 109.5 |
| O4—C10—C11 | 113.0 (2) | H29A—C29—H29C | 109.5 |
| C9—C10—C11 | 112.1 (2) | H29B—C29—H29C | 109.5 |
| O4—C10—H10 | 107.0 | N1—C30—H30A | 109.5 |
| C9—C10—H10 | 107.0 | N1—C30—H30B | 109.5 |
| C11—C10—H10 | 107.0 | H30A—C30—H30B | 109.5 |
| C31—C11—C10 | 106.4 (2) | N1—C30—H30C | 109.5 |
| C31—C11—C12 | 110.0 (2) | H30A—C30—H30C | 109.5 |
| C10—C11—C12 | 112.1 (2) | H30B—C30—H30C | 109.5 |
| C31—C11—C1 | 111.3 (2) | O5—C31—C11 | 107.6 (2) |

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| C10—C11—C1 | 109.1 (2) | O5—C31—H31A | 110.2 |
| C12—C11—C1 | 108.0 (2) | C11—C31—H31A | 110.2 |
| N1—C12—C11 | 112.9 (2) | O5—C31—H31B | 110.2 |
| N1—C12—H12A | 109.0 | C11—C31—H31B | 110.2 |
| C11—C12—H12A | 109.0 | H31A—C31—H31B | 108.5 |
| N1—C12—H12B | 109.0 | O5—C32—H32A | 109.5 |
| C11—C12—H12B | 109.0 | O5—C32—H32B | 109.5 |
| H12A—C12—H12B | 107.8 | H32A—C32—H32B | 109.5 |
| N1—C13—C7 | 109.9 (2) | O5—C32—H32C | 109.5 |
| N1—C13—C3 | 115.7 (2) | H32A—C32—H32C | 109.5 |
| C7—C13—C3 | 100.3 (2) | H32B—C32—H32C | 109.5 |
| N1—C13—H13 | 110.2 | O8—C33—H33A | 109.5 |
| C7—C13—H13 | 110.2 | O8—C33—H33B | 109.5 |
| C3—C13—H13 | 110.2 | H33A—C33—H33B | 109.5 |
| C15—C14—C6 | 107.1 (2) | O8—C33—H33C | 109.5 |
| C15—C14—H14A | 110.3 | H33A—C33—H33C | 109.5 |
| C6—C14—H14A | 110.3 | H33B—C33—H33C | 109.5 |
| C15—C14—H14B | 110.3 | C30—N1—C13 | 113.1 (2) |
| C6—C14—H14B | 110.3 | C30—N1—C12 | 110.1 (2) |
| H14A—C14—H14B | 108.5 | C13—N1—C12 | 116.4 (2) |
| O7—C15—C16 | 113.1 (2) | C26—O1—C4 | 121.0 (2) |
| O7—C15—C14 | 110.1 (2) | C29—O3—C8 | 113.7 (2) |
| C16—C15—C14 | 102.2 (2) | C10—O4—H4 | 109.5 |
| O7—C15—C17 | 110.1 (2) | C32—O5—C31 | 112.8 (2) |
| C16—C15—C17 | 110.4 (2) | C28—O6—C2 | 112.9 (3) |
| C14—C15—C17 | 110.8 (2) | C15—O7—H7 | 109.5 |
| O9—C16—C15 | 108.1 (2) | C33—O8—C17 | 115.5 (2) |
| O9—C16—C5 | 115.7 (2) | C19—O9—C16 | 120.7 (2) |
| C15—C16—C5 | 101.9 (2) | C18—O10—H10A | 109.5 |

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| C11—C1—C2—O6 | −26.0 (4) | C2—C3—C13—C7 | 40.7 (3) |
| C7—C1—C2—O6 | −143.9 (2) | C7—C6—C14—C15 | −133.1 (2) |
| C11—C1—C2—C3 | 95.8 (3) | C5—C6—C14—C15 | −4.0 (3) |
| C7—C1—C2—C3 | −22.2 (3) | C6—C14—C15—O7 | −145.6 (2) |
| O6—C2—C3—C4 | −124.5 (2) | C6—C14—C15—C16 | −25.2 (3) |
| C1—C2—C3—C4 | 108.5 (2) | C6—C14—C15—C17 | 92.4 (3) |
| O6—C2—C3—C13 | 116.1 (2) | O7—C15—C16—O9 | −73.8 (3) |
| C1—C2—C3—C13 | −10.9 (3) | C14—C15—C16—O9 | 167.8 (2) |
| C13—C3—C4—O1 | 175.3 (2) | C17—C15—C16—O9 | 50.0 (3) |
| C2—C3—C4—O1 | 61.2 (3) | O7—C15—C16—C5 | 163.8 (2) |
| C13—C3—C4—C5 | 66.2 (3) | C14—C15—C16—C5 | 45.5 (3) |
| C2—C3—C4—C5 | −47.9 (3) | C17—C15—C16—C5 | −72.4 (3) |
| C13—C3—C4—C18 | −63.2 (3) | C4—C5—C16—O9 | −45.8 (3) |
| C2—C3—C4—C18 | −177.4 (2) | C6—C5—C16—O9 | −165.3 (2) |
| O1—C4—C5—C16 | 89.2 (3) | C4—C5—C16—C15 | 71.2 (3) |
| C3—C4—C5—C16 | −157.1 (2) | C6—C5—C16—C15 | −48.4 (3) |
| C18—C4—C5—C16 | −26.0 (3) | O7—C15—C17—O8 | 33.8 (3) |
| O1—C4—C5—C6 | −157.2 (2) | C16—C15—C17—O8 | −91.8 (3) |

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| C3—C4—C5—C6 | −43.5 (3) | C14—C15—C17—O8 | 155.8 (2) |
| C18—C4—C5—C6 | 87.6 (3) | O7—C15—C17—C18 | 155.1 (2) |
| C16—C5—C6—C7 | 159.5 (2) | C16—C15—C17—C18 | 29.5 (3) |
| C4—C5—C6—C7 | 39.7 (3) | C14—C15—C17—C18 | −82.9 (3) |
| C16—C5—C6—C14 | 31.6 (3) | O8—C17—C18—O10 | −95.0 (3) |
| C4—C5—C6—C14 | −88.3 (3) | C15—C17—C18—O10 | 145.2 (2) |
| C14—C6—C7—C13 | 69.8 (3) | O8—C17—C18—C4 | 136.9 (3) |
| C5—C6—C7—C13 | −51.7 (3) | C15—C17—C18—C4 | 17.0 (4) |
| C14—C6—C7—C8 | −57.4 (3) | O1—C4—C18—O10 | 104.2 (3) |
| C5—C6—C7—C8 | −178.9 (2) | C3—C4—C18—O10 | −17.5 (3) |
| C14—C6—C7—C1 | 178.0 (2) | C5—C4—C18—O10 | −144.3 (2) |
| C5—C6—C7—C1 | 56.5 (3) | O1—C4—C18—C17 | −130.2 (2) |
| C11—C1—C7—C13 | −72.6 (3) | C3—C4—C18—C17 | 108.0 (3) |
| C2—C1—C7—C13 | 47.1 (2) | C5—C4—C18—C17 | −18.7 (3) |
| C11—C1—C7—C8 | 50.4 (3) | O11—C19—C20—C25 | −6.9 (5) |
| C2—C1—C7—C8 | 170.1 (2) | O9—C19—C20—C25 | 172.2 (3) |
| C11—C1—C7—C6 | 172.5 (2) | O11—C19—C20—C21 | 174.7 (3) |
| C2—C1—C7—C6 | −67.8 (3) | O9—C19—C20—C21 | −6.2 (4) |
| C13—C7—C8—O3 | −52.6 (3) | C25—C20—C21—C22 | 0.2 (5) |
| C6—C7—C8—O3 | 70.3 (3) | C19—C20—C21—C22 | 178.6 (3) |
| C1—C7—C8—O3 | −165.0 (2) | C20—C21—C22—C23 | 0.1 (5) |
| C13—C7—C8—C9 | 69.9 (3) | C21—C22—C23—C24 | −0.7 (5) |
| C6—C7—C8—C9 | −167.2 (2) | C22—C23—C24—C25 | 0.9 (5) |
| C1—C7—C8—C9 | −42.5 (3) | C23—C24—C25—C20 | −0.6 (5) |
| O3—C8—C9—C10 | 166.8 (2) | C21—C20—C25—C24 | 0.0 (5) |
| C7—C8—C9—C10 | 43.4 (3) | C19—C20—C25—C24 | −178.4 (3) |
| C8—C9—C10—O4 | −179.6 (2) | C10—C11—C31—O5 | −68.7 (3) |
| C8—C9—C10—C11 | −52.7 (3) | C12—C11—C31—O5 | 169.7 (2) |
| O4—C10—C11—C31 | −52.4 (3) | C1—C11—C31—O5 | 50.1 (3) |
| C9—C10—C11—C31 | −177.8 (2) | C7—C13—N1—C30 | 172.1 (2) |
| O4—C10—C11—C12 | 67.9 (3) | C3—C13—N1—C30 | −75.2 (3) |
| C9—C10—C11—C12 | −57.5 (3) | C7—C13—N1—C12 | −59.0 (3) |
| O4—C10—C11—C1 | −172.6 (2) | C3—C13—N1—C12 | 53.7 (3) |
| C9—C10—C11—C1 | 62.0 (3) | C11—C12—N1—C30 | 174.3 (2) |
| C7—C1—C11—C31 | −177.0 (2) | C11—C12—N1—C13 | 44.0 (3) |
| C2—C1—C11—C31 | 69.9 (3) | O2—C26—O1—C4 | 2.3 (5) |
| C7—C1—C11—C10 | −59.9 (3) | C27—C26—O1—C4 | −179.4 (3) |
| C2—C1—C11—C10 | −173.0 (2) | C3—C4—O1—C26 | 69.5 (3) |
| C7—C1—C11—C12 | 62.2 (3) | C5—C4—O1—C26 | −176.9 (2) |
| C2—C1—C11—C12 | −51.0 (3) | C18—C4—O1—C26 | −57.3 (3) |
| C31—C11—C12—N1 | −165.4 (2) | C9—C8—O3—C29 | 84.5 (3) |
| C10—C11—C12—N1 | 76.4 (3) | C7—C8—O3—C29 | −148.0 (2) |
| C1—C11—C12—N1 | −43.8 (3) | C11—C31—O5—C32 | 178.3 (3) |
| C8—C7—C13—N1 | −51.9 (3) | C3—C2—O6—C28 | 136.2 (3) |
| C6—C7—C13—N1 | −174.2 (2) | C1—C2—O6—C28 | −104.5 (3) |
| C1—C7—C13—N1 | 68.3 (3) | C15—C17—O8—C33 | −164.5 (3) |
| C8—C7—C13—C3 | −174.2 (2) | C18—C17—O8—C33 | 70.7 (3) |
| C6—C7—C13—C3 | 63.4 (3) | O11—C19—O9—C16 | −3.7 (4) |

| | | | |
|---|---|---|---|
| C1—C7—C13—C3 | −54.0 (2) | C20—C19—O9—C16 | 177.3 (2) |
| C4—C3—C13—N1 | 166.2 (2) | C15—C16—O9—C19 | 179.1 (2) |
| C2—C3—C13—N1 | −77.4 (3) | C5—C16—O9—C19 | −67.5 (3) |
| C4—C3—C13—C7 | −75.7 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O10—H10*A*···O2 | 0.84 | 2.11 | 2.788 (3) | 138 |
| O7—H7···O8 | 0.84 | 2.04 | 2.560 (3) | 120 |
| O4—H4···O11$^{i}$ | 0.84 | 2.20 | 3.018 (3) | 163 |

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