# organic compounds

# $N$-Morpholino-$\Delta^8$-dihydroabietamide

## Xiao-Ping Rao

Institute of Chemical Industry of Forest Products, Chinese Academy of Forestry, Nanjing 210042, People's Republic of China
Correspondence e-mail: rxping2001@163.com

The title compound, $C_{24}H_{39}NO_2$ (systematic name: 4-{[1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,5,6,7,8,9,10,10a-dodeca-hydrophenanthren-1-yl]carbonyl}morpholine), has been synthesized from $\Delta^8$-dihydroabietic acid. Two cyclohexene rings adopt half-chair conformations, whereas the cyclohexane and morpholine rings are each in the chair conformation. Two methyl groups are in an axial position with respect to the tricyclic hydrophenanthrene nuclei.

## Related literature

For literature on $\Delta^8$-dihydroabietic acid, see: Rao *et al.* (2009). For the biological activity of rosin acid derivatives, see Fonseca *et al.* (2004); Sepulveda *et al.* (2005).
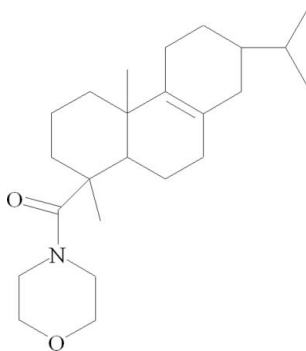


## Experimental

### Crystal data

| | |
|---|---|
| $C_{24}H_{39}NO_2$ | $V = 2147.1$ (7) Å$^3$ |
| $M_r = 373.56$ | $Z = 4$ |
| Orthorhombic, $P2_12_12_1$ | Mo $K\alpha$ radiation |
| $a = 7.8683$ (16) Å | $\mu = 0.07$ mm$^{-1}$ |
| $b = 11.036$ (2) Å | $T = 293$ K |
| $c = 24.726$ (5) Å | $0.42 \times 0.34 \times 0.25$ mm |

### Data collection

| | |
|---|---|
| Rigaku R-AXIS RAPID diffractometer | 16937 measured reflections |
| Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995) | 2186 independent reflections |
| | 1957 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.352$, $T_{max} = 0.497$ | $R_{int} = 0.029$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | 248 parameters |
| $wR(F^2) = 0.117$ | H-atom parameters constrained |
| $S = 1.37$ | $\Delta\rho_{max} = 0.23$ e Å$^{-3}$ |
| 2186 reflections | $\Delta\rho_{min} = -0.26$ e Å$^{-3}$ |

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2277).

## References

Fonseca, T., Gigante, B., Marques, M. M., Gilchrist, T. L. & Clercq, E. C. (2004). *Bioorg. Med. Chem.* **12**, 103–112.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rao, X.-P., Song, Z.-Q., Shang, S.-B. & Wu, Y. (2009). *Acta Cryst.* E**65**, o2804.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sepulveda, B., Astudillo, L., Rodriguez, J., Yanez, T., Theoduloz, C. & Schmeda, G. (2005). *Pharm. Res.* **52**, 429–437.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

## *N*-Morpholino-Δ⁸-dihydroabietamide

### Xiao-Ping Rao

### S1. Comment

$\Delta^8$-Dihydroabietic acid is one of the main component of hydrogenated rosin. It is more stable to air oxidation than abietic acid (Rao *et al.*, 2009). Rosin acid derivatives exhibit wide range of biological activities, such as antifungal and antitumor (Fonseca *et al.*, 2004), nitrogen derivatives of rosin acid have been studied as gastroprotective and cytotoxic reagents and they are found to have high activity in reducing blood serum cholesterol levels in animals (Sepulveda *et al.*, 2005). In this work, we describe the crystal structure of the title compound.

   Two cyclohexene rings adopt a half-chair conformations, and the cyclohexane and morpholine rings are in the chair conformation. Two methyl groups are in an axial position of the tricyclic hydrophenanthrene nuclei. The absolute configuration cannot be assigned on a basis of the value of the Flack parameter due to its high deviation. The Friedel opposite reflections were not measured.

### S2. Experimental

A mixture of $\Delta^8$-dihydroabietic acid (0.1 mol), trichloro phosphorous (6 ml) and chloroform (40 ml) was stirred at 333 K for 3 h, after distilled off the solvent, the residue was added to the morpholine (0.2 mol) in toluene (60 ml) solution, the mixture was reacted for 24 h at room temperature, then the solvent was distilled off, upon recrystallization from acetone, white crystals of the title compound were obtained (yield 40%, m.p.394 K). Single crystals were grown from acetone.

### S3. Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.96Å and $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl H atoms, and C—H = 0.97–0.98Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) for all other H atoms.
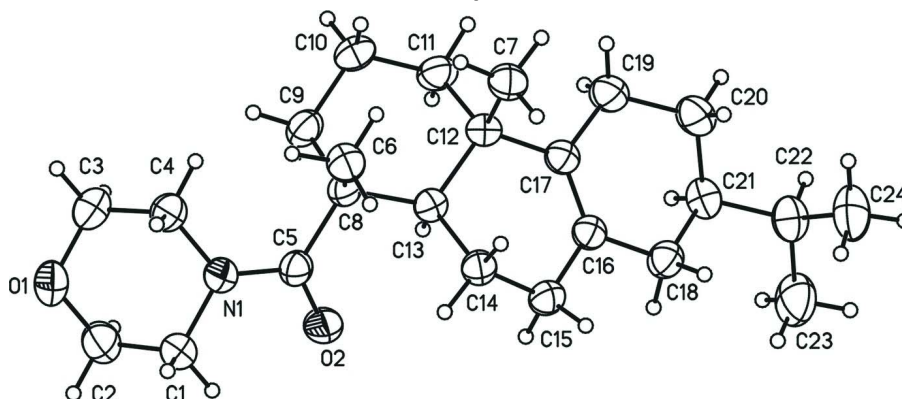


**Figure 1**
Molecular structure of the title compound, with H atoms represented by small spheres of arbitrary radius and displacement ellipsoids at the 30% probability level.

**4-{[1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,5,6,7,8,9,10,10a- dodecahydrophenanthren-1-yl]carbonyl}morpholine**

*Crystal data*

| | |
|---|---|
| $C_{24}H_{39}NO_2$ | $F(000) = 824$ |
| $M_r = 373.56$ | $D_x = 1.156$ Mg m$^{-3}$ |
| Orthorhombic, $P2_12_12_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: P 2ac 2ab | Cell parameters from 16603 reflections |
| $a = 7.8683$ (16) Å | $\theta = 3.1–27.4°$ |
| $b = 11.036$ (2) Å | $\mu = 0.07$ mm$^{-1}$ |
| $c = 24.726$ (5) Å | $T = 293$ K |
| $V = 2147.1$ (7) Å$^3$ | Block, colorless |
| $Z = 4$ | $0.42 \times 0.34 \times 0.25$ mm |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS RAPID diffractometer | 16937 measured reflections |
| Radiation source: fine-focus sealed tube | 2186 independent reflections |
| Graphite monochromator | 1957 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 0 pixels mm$^{-1}$ | $R_{int} = 0.029$ |
| $\omega$ scans | $\theta_{max} = 25.0°$, $\theta_{min} = 3.1°$ |
| Absorption correction: multi-scan | $h = -9{\rightarrow}9$ |
| (*ABSCOR*; Higashi, 1995) | $k = -13{\rightarrow}13$ |
| $T_{min} = 0.352$, $T_{max} = 0.497$ | $l = -29{\rightarrow}29$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | $w = 1/[\sigma^2(F_o^2) + (0.0672P)^2]$ |
| $wR(F^2) = 0.117$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.37$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 2186 reflections | $\Delta\rho_{max} = 0.23$ e Å$^{-3}$ |
| 248 parameters | $\Delta\rho_{min} = -0.26$ e Å$^{-3}$ |
| 0 restraints | Absolute structure: Flack (1983), **??? Friedel pairs** |
| Primary atom site location: structure-invariant direct methods | Absolute structure parameter: 0 (10) |
| Secondary atom site location: difference Fourier map | |

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 1.1743 (3) | 0.85945 (18) | 0.01582 (7) | 0.0661 (6) |

| | | | | |
|---|---|---|---|---|
| O2 | 0.9634 (2) | 0.83691 (14) | 0.19288 (7) | 0.0528 (5) |
| N1 | 1.0754 (3) | 0.75942 (19) | 0.11701 (8) | 0.0523 (6) |
| C1 | 1.1939 (4) | 0.8606 (3) | 0.11335 (10) | 0.0577 (7) |
| H1A | 1.3095 | 0.8301 | 0.1132 | 0.069* |
| H1B | 1.1805 | 0.9126 | 0.1447 | 0.069* |
| C2 | 1.1629 (4) | 0.9328 (3) | 0.06276 (10) | 0.0627 (8) |
| H2A | 1.0508 | 0.9693 | 0.0645 | 0.075* |
| H2B | 1.2458 | 0.9977 | 0.0605 | 0.075* |
| C3 | 1.0545 (4) | 0.7641 (3) | 0.01898 (10) | 0.0586 (7) |
| H3A | 1.0628 | 0.7147 | −0.0134 | 0.070* |
| H3B | 0.9409 | 0.7981 | 0.0203 | 0.070* |
| C4 | 1.0817 (4) | 0.6852 (2) | 0.06789 (9) | 0.0501 (6) |
| H4A | 0.9944 | 0.6233 | 0.0694 | 0.060* |
| H4B | 1.1913 | 0.6453 | 0.0654 | 0.060* |
| C5 | 0.9656 (3) | 0.75310 (19) | 0.16034 (9) | 0.0404 (5) |
| C6 | 0.9513 (3) | 0.52216 (19) | 0.16245 (10) | 0.0467 (6) |
| H6A | 1.0593 | 0.5390 | 0.1460 | 0.070* |
| H6B | 0.8898 | 0.4655 | 0.1404 | 0.070* |
| H6C | 0.9688 | 0.4882 | 0.1978 | 0.070* |
| C7 | 0.6449 (4) | 0.4303 (2) | 0.23662 (10) | 0.0492 (6) |
| H7A | 0.7448 | 0.4175 | 0.2582 | 0.074* |
| H7B | 0.6643 | 0.4004 | 0.2007 | 0.074* |
| H7C | 0.5508 | 0.3879 | 0.2525 | 0.074* |
| C8 | 0.8477 (3) | 0.64162 (18) | 0.16745 (8) | 0.0371 (5) |
| C9 | 0.7048 (3) | 0.6567 (2) | 0.12412 (9) | 0.0467 (6) |
| H9A | 0.6655 | 0.7400 | 0.1246 | 0.056* |
| H9B | 0.7526 | 0.6410 | 0.0886 | 0.056* |
| C10 | 0.5535 (3) | 0.5732 (2) | 0.13276 (10) | 0.0509 (6) |
| H10A | 0.4685 | 0.5895 | 0.1053 | 0.061* |
| H10B | 0.5899 | 0.4898 | 0.1287 | 0.061* |
| C11 | 0.4745 (3) | 0.5901 (2) | 0.18848 (9) | 0.0478 (6) |
| H11A | 0.3801 | 0.5343 | 0.1926 | 0.057* |
| H11B | 0.4302 | 0.6718 | 0.1915 | 0.057* |
| C12 | 0.6045 (3) | 0.56781 (19) | 0.23426 (9) | 0.0373 (5) |
| C13 | 0.7604 (3) | 0.65211 (18) | 0.22398 (8) | 0.0344 (5) |
| H13A | 0.7140 | 0.7345 | 0.2250 | 0.041* |
| C14 | 0.8810 (3) | 0.6454 (2) | 0.27262 (9) | 0.0391 (5) |
| H14A | 0.9105 | 0.5616 | 0.2799 | 0.047* |
| H14B | 0.9847 | 0.6895 | 0.2648 | 0.047* |
| C15 | 0.7940 (3) | 0.7000 (2) | 0.32151 (9) | 0.0448 (6) |
| H15A | 0.7983 | 0.7876 | 0.3187 | 0.054* |
| H15B | 0.8562 | 0.6768 | 0.3538 | 0.054* |
| C16 | 0.6101 (3) | 0.66108 (19) | 0.32775 (9) | 0.0376 (5) |
| C17 | 0.5253 (3) | 0.60145 (18) | 0.28917 (9) | 0.0381 (5) |
| C18 | 0.5310 (3) | 0.6973 (2) | 0.38098 (9) | 0.0456 (6) |
| H18A | 0.5529 | 0.7828 | 0.3869 | 0.055* |
| H18B | 0.5875 | 0.6530 | 0.4097 | 0.055* |
| C19 | 0.3437 (3) | 0.5623 (3) | 0.29822 (11) | 0.0539 (6) |

| | | | | |
|---|---|---|---|---|
| H19A | 0.3275 | 0.4824 | 0.2826 | 0.065* |
| H19B | 0.2685 | 0.6179 | 0.2796 | 0.065* |
| C20 | 0.2957 (4) | 0.5583 (3) | 0.35748 (11) | 0.0563 (7) |
| H20A | 0.1746 | 0.5435 | 0.3608 | 0.068* |
| H20B | 0.3551 | 0.4919 | 0.3749 | 0.068* |
| C21 | 0.3398 (3) | 0.6757 (2) | 0.38580 (10) | 0.0458 (6) |
| H21A | 0.2847 | 0.7404 | 0.3651 | 0.055* |
| C22 | 0.2693 (4) | 0.6842 (2) | 0.44366 (10) | 0.0553 (7) |
| H22A | 0.1454 | 0.6785 | 0.4406 | 0.066* |
| C23 | 0.3069 (5) | 0.8059 (3) | 0.46971 (13) | 0.0773 (10) |
| H23A | 0.2579 | 0.8082 | 0.5052 | 0.116* |
| H23B | 0.2590 | 0.8695 | 0.4480 | 0.116* |
| H23C | 0.4277 | 0.8170 | 0.4723 | 0.116* |
| C24 | 0.3247 (5) | 0.5812 (3) | 0.48076 (12) | 0.0782 (9) |
| H24A | 0.4457 | 0.5842 | 0.4857 | 0.117* |
| H24B | 0.2938 | 0.5050 | 0.4648 | 0.117* |
| H24C | 0.2695 | 0.5894 | 0.5152 | 0.117* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0850 (15) | 0.0717 (11) | 0.0416 (9) | −0.0148 (11) | 0.0137 (10) | 0.0019 (9) |
| O2 | 0.0659 (12) | 0.0420 (8) | 0.0504 (9) | −0.0102 (8) | 0.0087 (9) | −0.0097 (8) |
| N1 | 0.0661 (14) | 0.0536 (11) | 0.0370 (10) | −0.0205 (11) | 0.0084 (10) | −0.0062 (9) |
| C1 | 0.0629 (17) | 0.0646 (15) | 0.0457 (13) | −0.0236 (14) | 0.0031 (13) | −0.0030 (13) |
| C2 | 0.078 (2) | 0.0529 (13) | 0.0566 (16) | −0.0142 (14) | 0.0135 (16) | −0.0022 (13) |
| C3 | 0.0667 (17) | 0.0687 (16) | 0.0403 (13) | −0.0044 (14) | 0.0025 (13) | −0.0082 (12) |
| C4 | 0.0550 (15) | 0.0503 (13) | 0.0448 (13) | −0.0032 (11) | 0.0071 (12) | −0.0088 (11) |
| C5 | 0.0461 (13) | 0.0393 (10) | 0.0357 (11) | −0.0004 (10) | −0.0029 (10) | 0.0020 (10) |
| C6 | 0.0499 (14) | 0.0411 (11) | 0.0490 (13) | 0.0025 (10) | 0.0043 (12) | −0.0013 (11) |
| C7 | 0.0593 (16) | 0.0358 (11) | 0.0525 (14) | −0.0042 (11) | 0.0030 (13) | −0.0037 (10) |
| C8 | 0.0419 (12) | 0.0346 (10) | 0.0348 (11) | −0.0007 (9) | −0.0026 (9) | 0.0002 (9) |
| C9 | 0.0538 (14) | 0.0511 (13) | 0.0352 (11) | −0.0002 (12) | −0.0066 (11) | −0.0010 (11) |
| C10 | 0.0480 (15) | 0.0608 (14) | 0.0440 (12) | −0.0039 (12) | −0.0159 (11) | −0.0033 (12) |
| C11 | 0.0412 (13) | 0.0555 (13) | 0.0466 (13) | −0.0047 (11) | −0.0083 (11) | −0.0049 (11) |
| C12 | 0.0360 (12) | 0.0359 (10) | 0.0400 (11) | −0.0019 (9) | −0.0018 (10) | −0.0025 (9) |
| C13 | 0.0349 (11) | 0.0329 (9) | 0.0355 (11) | 0.0024 (9) | −0.0037 (8) | 0.0009 (9) |
| C14 | 0.0330 (11) | 0.0451 (11) | 0.0392 (12) | 0.0017 (10) | −0.0043 (9) | 0.0036 (10) |
| C15 | 0.0401 (13) | 0.0548 (13) | 0.0396 (12) | −0.0050 (10) | −0.0048 (10) | −0.0014 (11) |
| C16 | 0.0381 (12) | 0.0364 (10) | 0.0385 (11) | 0.0008 (9) | −0.0006 (9) | 0.0001 (9) |
| C17 | 0.0358 (12) | 0.0379 (10) | 0.0406 (11) | −0.0020 (9) | −0.0004 (10) | 0.0000 (10) |
| C18 | 0.0514 (14) | 0.0454 (11) | 0.0401 (12) | 0.0020 (10) | 0.0006 (11) | −0.0022 (11) |
| C19 | 0.0433 (14) | 0.0643 (14) | 0.0541 (15) | −0.0108 (12) | 0.0053 (12) | −0.0092 (13) |
| C20 | 0.0472 (15) | 0.0633 (15) | 0.0585 (15) | −0.0120 (13) | 0.0121 (13) | −0.0016 (13) |
| C21 | 0.0469 (13) | 0.0437 (12) | 0.0469 (13) | 0.0016 (10) | 0.0056 (11) | 0.0054 (11) |
| C22 | 0.0543 (16) | 0.0597 (15) | 0.0520 (14) | 0.0023 (12) | 0.0118 (13) | 0.0056 (12) |
| C23 | 0.100 (3) | 0.0742 (19) | 0.0581 (17) | 0.0018 (18) | 0.0266 (19) | −0.0087 (15) |
| C24 | 0.095 (3) | 0.085 (2) | 0.0553 (17) | 0.0004 (19) | 0.0128 (17) | 0.0227 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C3 | 1.415 (3) | C11—H11B | 0.9700 |
| O1—C2 | 1.418 (3) | C12—C17 | 1.539 (3) |
| O2—C5 | 1.226 (3) | C12—C13 | 1.561 (3) |
| N1—C5 | 1.378 (3) | C13—C14 | 1.534 (3) |
| N1—C1 | 1.458 (3) | C13—H13A | 0.9800 |
| N1—C4 | 1.466 (3) | C14—C15 | 1.514 (3) |
| C1—C2 | 1.503 (4) | C14—H14A | 0.9700 |
| C1—H1A | 0.9700 | C14—H14B | 0.9700 |
| C1—H1B | 0.9700 | C15—C16 | 1.517 (3) |
| C2—H2A | 0.9700 | C15—H15A | 0.9700 |
| C2—H2B | 0.9700 | C15—H15B | 0.9700 |
| C3—C4 | 1.505 (3) | C16—C17 | 1.337 (3) |
| C3—H3A | 0.9700 | C16—C18 | 1.510 (3) |
| C3—H3B | 0.9700 | C17—C19 | 1.509 (3) |
| C4—H4A | 0.9700 | C18—C21 | 1.528 (4) |
| C4—H4B | 0.9700 | C18—H18A | 0.9700 |
| C5—C8 | 1.551 (3) | C18—H18B | 0.9700 |
| C6—C8 | 1.555 (3) | C19—C20 | 1.514 (4) |
| C6—H6A | 0.9600 | C19—H19A | 0.9700 |
| C6—H6B | 0.9600 | C19—H19B | 0.9700 |
| C6—H6C | 0.9600 | C20—C21 | 1.513 (4) |
| C7—C12 | 1.552 (3) | C20—H20A | 0.9700 |
| C7—H7A | 0.9600 | C20—H20B | 0.9700 |
| C7—H7B | 0.9600 | C21—C22 | 1.537 (3) |
| C7—H7C | 0.9600 | C21—H21A | 0.9800 |
| C8—C9 | 1.562 (3) | C22—C23 | 1.519 (4) |
| C8—C13 | 1.562 (3) | C22—C24 | 1.524 (4) |
| C9—C10 | 1.520 (3) | C22—H22A | 0.9800 |
| C9—H9A | 0.9700 | C23—H23A | 0.9600 |
| C9—H9B | 0.9700 | C23—H23B | 0.9600 |
| C10—C11 | 1.523 (3) | C23—H23C | 0.9600 |
| C10—H10A | 0.9700 | C24—H24A | 0.9600 |
| C10—H10B | 0.9700 | C24—H24B | 0.9600 |
| C11—C12 | 1.545 (3) | C24—H24C | 0.9600 |
| C11—H11A | 0.9700 | | |
| | | | |
| C3—O1—C2 | 109.73 (19) | C17—C12—C13 | 108.54 (17) |
| C5—N1—C1 | 119.21 (19) | C11—C12—C13 | 107.85 (17) |
| C5—N1—C4 | 129.6 (2) | C7—C12—C13 | 115.32 (19) |
| C1—N1—C4 | 110.79 (19) | C14—C13—C12 | 109.26 (17) |
| N1—C1—C2 | 110.7 (2) | C14—C13—C8 | 115.23 (17) |
| N1—C1—H1A | 109.5 | C12—C13—C8 | 116.57 (17) |
| C2—C1—H1A | 109.5 | C14—C13—H13A | 104.8 |
| N1—C1—H1B | 109.5 | C12—C13—H13A | 104.8 |
| C2—C1—H1B | 109.5 | C8—C13—H13A | 104.8 |
| H1A—C1—H1B | 108.1 | C15—C14—C13 | 109.08 (18) |

| | | | |
|---|---|---|---|
| O1—C2—C1 | 111.6 (2) | C15—C14—H14A | 109.9 |
| O1—C2—H2A | 109.3 | C13—C14—H14A | 109.9 |
| C1—C2—H2A | 109.3 | C15—C14—H14B | 109.9 |
| O1—C2—H2B | 109.3 | C13—C14—H14B | 109.9 |
| C1—C2—H2B | 109.3 | H14A—C14—H14B | 108.3 |
| H2A—C2—H2B | 108.0 | C14—C15—C16 | 113.57 (19) |
| O1—C3—C4 | 112.3 (2) | C14—C15—H15A | 108.9 |
| O1—C3—H3A | 109.1 | C16—C15—H15A | 108.9 |
| C4—C3—H3A | 109.1 | C14—C15—H15B | 108.9 |
| O1—C3—H3B | 109.1 | C16—C15—H15B | 108.9 |
| C4—C3—H3B | 109.1 | H15A—C15—H15B | 107.7 |
| H3A—C3—H3B | 107.9 | C17—C16—C18 | 123.2 (2) |
| N1—C4—C3 | 109.75 (19) | C17—C16—C15 | 122.8 (2) |
| N1—C4—H4A | 109.7 | C18—C16—C15 | 114.00 (19) |
| C3—C4—H4A | 109.7 | C16—C17—C19 | 120.5 (2) |
| N1—C4—H4B | 109.7 | C16—C17—C12 | 123.1 (2) |
| C3—C4—H4B | 109.7 | C19—C17—C12 | 116.39 (19) |
| H4A—C4—H4B | 108.2 | C16—C18—C21 | 115.6 (2) |
| O2—C5—N1 | 118.7 (2) | C16—C18—H18A | 108.4 |
| O2—C5—C8 | 121.0 (2) | C21—C18—H18A | 108.4 |
| N1—C5—C8 | 120.22 (19) | C16—C18—H18B | 108.4 |
| C8—C6—H6A | 109.5 | C21—C18—H18B | 108.4 |
| C8—C6—H6B | 109.5 | H18A—C18—H18B | 107.4 |
| H6A—C6—H6B | 109.5 | C17—C19—C20 | 112.8 (2) |
| C8—C6—H6C | 109.5 | C17—C19—H19A | 109.0 |
| H6A—C6—H6C | 109.5 | C20—C19—H19A | 109.0 |
| H6B—C6—H6C | 109.5 | C17—C19—H19B | 109.0 |
| C12—C7—H7A | 109.5 | C20—C19—H19B | 109.0 |
| C12—C7—H7B | 109.5 | H19A—C19—H19B | 107.8 |
| H7A—C7—H7B | 109.5 | C21—C20—C19 | 111.5 (2) |
| C12—C7—H7C | 109.5 | C21—C20—H20A | 109.3 |
| H7A—C7—H7C | 109.5 | C19—C20—H20A | 109.3 |
| H7B—C7—H7C | 109.5 | C21—C20—H20B | 109.3 |
| C5—C8—C6 | 110.49 (18) | C19—C20—H20B | 109.3 |
| C5—C8—C9 | 105.57 (17) | H20A—C20—H20B | 108.0 |
| C6—C8—C9 | 114.40 (18) | C20—C21—C18 | 108.9 (2) |
| C5—C8—C13 | 107.80 (17) | C20—C21—C22 | 113.6 (2) |
| C6—C8—C13 | 111.38 (17) | C18—C21—C22 | 114.7 (2) |
| C9—C8—C13 | 106.83 (18) | C20—C21—H21A | 106.3 |
| C10—C9—C8 | 113.76 (19) | C18—C21—H21A | 106.3 |
| C10—C9—H9A | 108.8 | C22—C21—H21A | 106.3 |
| C8—C9—H9A | 108.8 | C23—C22—C24 | 110.4 (2) |
| C10—C9—H9B | 108.8 | C23—C22—C21 | 112.2 (2) |
| C8—C9—H9B | 108.8 | C24—C22—C21 | 114.3 (2) |
| H9A—C9—H9B | 107.7 | C23—C22—H22A | 106.4 |
| C11—C10—C9 | 111.89 (19) | C24—C22—H22A | 106.4 |
| C11—C10—H10A | 109.2 | C21—C22—H22A | 106.4 |
| C9—C10—H10A | 109.2 | C22—C23—H23A | 109.5 |

| | | | |
|---|---|---|---|
| C11—C10—H10B | 109.2 | C22—C23—H23B | 109.5 |
| C9—C10—H10B | 109.2 | H23A—C23—H23B | 109.5 |
| H10A—C10—H10B | 107.9 | C22—C23—H23C | 109.5 |
| C10—C11—C12 | 111.9 (2) | H23A—C23—H23C | 109.5 |
| C10—C11—H11A | 109.2 | H23B—C23—H23C | 109.5 |
| C12—C11—H11A | 109.2 | C22—C24—H24A | 109.5 |
| C10—C11—H11B | 109.2 | C22—C24—H24B | 109.5 |
| C12—C11—H11B | 109.2 | H24A—C24—H24B | 109.5 |
| H11A—C11—H11B | 107.9 | C22—C24—H24C | 109.5 |
| C17—C12—C11 | 109.88 (19) | H24A—C24—H24C | 109.5 |
| C17—C12—C7 | 106.60 (18) | H24B—C24—H24C | 109.5 |
| C11—C12—C7 | 108.60 (19) | | |