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3-[2-(1,3-Dioxo-2,3-dihydro-1*H*-isoindol-2-yl)ethyl] 5-methyl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate

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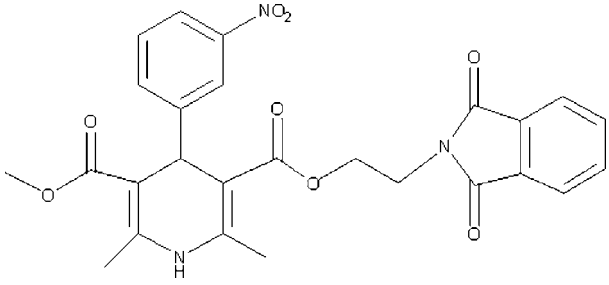
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.111; data-to-parameter ratio = 11.8.

The title compound, $C_{26}H_{23}N_3O_8$, is a nefidipine analogue. The dihydropyridine ring has a flattened boat conformation. No hydrogen bonds exist in the crystal packing.

Related literature

For related literature, see: Goldmann & Stoltefuss (1991); Hofmann & Cimiraglia (1990); Ramusino & Varì (1999); Sun *et al.* (2006); Yiu & Knaus (1999).



Experimental

Crystal data

$C_{26}H_{23}N_3O_8$
M_r = 505.47
Monoclinic, $P2_1/n$
a = 7.7713 (16) Å
b = 16.372 (3) Å
c = 17.945 (4) Å
β = 95.43 (3)°
V = 2273.0 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 (2) K
0.10 × 0.08 × 0.04 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.989, T_{max} = 0.996
13760 measured reflections
4009 independent reflections
3635 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.111
S = 1.10
4009 reflections
341 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2126).

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supplementary materials

Acta Cryst. (2007). E**63**, o3176 [**doi:10.1107/S1600536807028188**]

3-[2-(1,3-Dioxo-2,3-dihydro-1*H*-isoindol-2-yl)ethyl] 5-methyl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate

F.-X. Sun, X.-H. Chu and X.-M. Chen

Comment

4-Aryl-1,4-dihydropyridine-3,5-dicarboxylic diesters of the nefidipine type have become almost indispensable for the treatment of cardiovascular diseases since they first appeared on the market in 1975 (Yiu & Knaus, 1999; Goldmann & Stoltefuss, 1991). The compound, 2,6-dimethyl-4-(3-nitro-phenyl)-1,4-dihydro-pyridine- 3,5-dicarboxylic acid 3-[2-(1,3-dioxo-1,3-dihydro-isoindol-2-yl) -ethyl] ester 5-methyl ester, is a nefidipine analog. It can also be used as an intermediate for preparation of 2,6- dimethyl-4-(3-nitro-phenyl)-1,4-dihydro-pyridine-3,5-dicarboxylic acid 3-(2-amino-ethyl) ester 5-methyl ester. Fig.1 shows the structure of the title compound. The dihydropyridine ring has a flattened boat conformation. This compares well with the structure of 3-(2-acetoxyethyl) 5-methyl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine- 3,5-dicarboxylateand nefidipine (Sun *et al.*, 2006; Hofmann & Cimiraglia, 1990; Ramusino & Varì, 1999). The atoms C4 and N1 are displaced from the mean planes formed by the other atoms in the same ring by 0.281 (1) Å and 0.125 (1) Å, respectively. The dihedral angle between the benzene ring and the C3/C2/C6/C5 plane is 88.02 (1)°.

Experimental

The title compound was prepared from 2,6-dimethyl-4- (*m*-nitro-phenyl)-1,4-dihydro-pyridine-3,5-dicarboxylic acid monomethyl ester and 2-(2–2ydroxy-ethyl)-isoindole-1,3-dione in CH_2Cl_2. 2,6-Dimethyl-4- (*m*-nitro-phenyl)-1,4-dihydro-pyridine- 3,5-dicarboxylic acid mono-methyl ester (332 mg, 1 mmol) and 2-methyl-propan-1-ol (191 mg, 1 mmol) were dissolved in 20 ml CH_2Cl_2, dicyclohexylcarbodiimide (206 mg,1 mmol) and added to the solution at 278 K. The reaction mixture was stirred at 276–279 K for a further 5 h. The solvent was removed by vacuum evaporation. The product was purified by chromatography on silica gel column (eluted by ethyl acetate and petroleum ether, 1:4) at room temperature. The product (455 mg) was obtained in a yield of 90%. Suitable crystals were obtained by slow evaporation of a solution in ethyl acetate and petroleum ether (1:4).

Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H 0.97 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$ except for the H atom on N1 which was located in a Fourier map and freely refined.

Figures

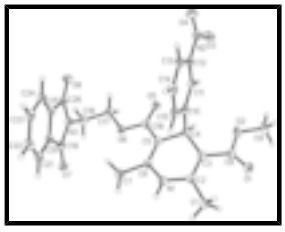


Fig. 1. A view of the title compound. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

3-[2-(1,3-Dioxo-2,3-dihydro-1*H*-isoindol-2-yl)ethyl] 5-methyl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate

Crystal data

$C_{26}H_{23}N_3O_8$	D_x = 1.474 Mg m^{-3}
M_r = 505.47	Melting point: 243-244 K
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.7713 (16) Å	Cell parameters from 2343 reflections
b = 16.372 (3) Å	θ = 2.3–22.5º
c = 17.945 (4) Å	μ = 0.11 mm^{-1}
β = 95.43 (3)º	T = 293 (2) K
V = 2273.0 (8) Å^3	Block, yellow
Z = 4	0.10 × 0.08 × 0.04 mm
F_{000} = 1056	

Data collection

Rigaku Saturn diffractometer	4009 independent reflections
Radiation source: rotating anode	3635 reflections with $I > 2\sigma(I)$
Monochromator: confocal	R_{int} = 0.035
T = 293(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	h = −9→8
T_{min} = 0.989, T_{max} = 0.996	k = −17→19
13760 measured reflections	l = −16→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.111	$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.7911P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} = 0.001$
4009 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
341 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.49383 (17)	0.38716 (8)	0.52148 (7)	0.0286 (3)
O2	0.21767 (16)	0.34959 (8)	0.49192 (7)	0.0249 (3)
O3	−0.22762 (16)	0.13687 (9)	0.55571 (8)	0.0320 (3)
O4	−0.15986 (17)	0.02564 (8)	0.61640 (8)	0.0305 (3)
O5	0.01803 (15)	0.14288 (7)	0.32204 (7)	0.0216 (3)
O6	0.19557 (14)	0.08248 (7)	0.24663 (7)	0.0201 (3)
O7	0.48119 (16)	−0.02815 (8)	0.13320 (7)	0.0243 (3)
O8	0.06068 (15)	−0.14941 (8)	0.25700 (8)	0.0277 (3)
N1	0.61576 (19)	0.19920 (9)	0.36933 (8)	0.0202 (3)
N2	−0.12398 (18)	0.08343 (9)	0.57705 (8)	0.0230 (3)
N3	0.23954 (17)	−0.07506 (9)	0.18687 (8)	0.0194 (3)
C1	0.7467 (2)	0.31005 (11)	0.44434 (10)	0.0221 (4)
H1A	0.7234	0.3671	0.4363	0.033*
H1B	0.8402	0.2937	0.4163	0.033*
H1C	0.7779	0.3004	0.4966	0.033*
C2	0.5881 (2)	0.26132 (10)	0.41896 (10)	0.0186 (4)
C3	0.4268 (2)	0.27317 (10)	0.43928 (9)	0.0182 (4)
C4	0.2811 (2)	0.21423 (10)	0.41495 (9)	0.0180 (4)
H4	0.1758	0.2463	0.4024	0.022*
C5	0.3193 (2)	0.16685 (10)	0.34544 (9)	0.0178 (4)
C6	0.4839 (2)	0.15767 (10)	0.32777 (10)	0.0188 (4)
C7	0.5472 (2)	0.10637 (11)	0.26678 (10)	0.0240 (4)
H7A	0.5237	0.0499	0.2760	0.036*
H7B	0.6694	0.1140	0.2658	0.036*
H7C	0.4889	0.1223	0.2195	0.036*
C8	0.3901 (2)	0.34176 (11)	0.48782 (10)	0.0200 (4)

C9	0.1646 (3)	0.41683 (12)	0.53670 (11)	0.0307 (5)
H9A	0.2016	0.4069	0.5885	0.046*
H9B	0.0410	0.4217	0.5304	0.046*
H9C	0.2159	0.4665	0.5210	0.046*
C10	0.2465 (2)	0.15458 (10)	0.47756 (9)	0.0177 (4)
C11	0.0819 (2)	0.14706 (10)	0.50058 (10)	0.0192 (4)
H11	−0.0075	0.1803	0.4802	0.023*
C12	0.0524 (2)	0.08944 (10)	0.55433 (9)	0.0190 (4)
C13	0.1800 (2)	0.03819 (11)	0.58675 (10)	0.0214 (4)
H13	0.1560	−0.0009	0.6219	0.026*
C14	0.3446 (2)	0.04740 (11)	0.56474 (10)	0.0234 (4)
H14	0.4343	0.0150	0.5862	0.028*
C15	0.3767 (2)	0.10468 (11)	0.51081 (10)	0.0214 (4)
H15	0.4882	0.1098	0.4965	0.026*
C16	0.1640 (2)	0.13082 (10)	0.30507 (9)	0.0178 (4)
C17	0.0471 (2)	0.03969 (11)	0.21084 (10)	0.0222 (4)
H17A	−0.0353	0.0782	0.1868	0.027*
H17B	−0.0098	0.0087	0.2475	0.027*
C18	0.1126 (2)	−0.01691 (11)	0.15341 (10)	0.0222 (4)
H18A	0.0159	−0.0466	0.1283	0.027*
H18B	0.1647	0.0152	0.1161	0.027*
C19	0.4159 (2)	−0.07257 (10)	0.17660 (10)	0.0186 (4)
C20	0.4994 (2)	−0.13393 (10)	0.22918 (9)	0.0184 (4)
C21	0.6719 (2)	−0.15324 (11)	0.24496 (10)	0.0210 (4)
H21	0.7568	−0.1284	0.2196	0.025*
C22	0.7138 (2)	−0.21128 (11)	0.30038 (10)	0.0233 (4)
H22	0.8288	−0.2256	0.3125	0.028*
C23	0.5864 (2)	−0.24808 (11)	0.33774 (10)	0.0243 (4)
H23	0.6180	−0.2868	0.3744	0.029*
C24	0.4130 (2)	−0.22880 (11)	0.32195 (10)	0.0221 (4)
H24	0.3279	−0.2537	0.3471	0.027*
C25	0.3725 (2)	−0.17085 (10)	0.26712 (10)	0.0184 (4)
C26	0.2036 (2)	−0.13412 (11)	0.23925 (10)	0.0199 (4)
H1	0.724 (3)	0.1938 (13)	0.3578 (12)	0.033 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0341 (7)	0.0245 (7)	0.0270 (7)	−0.0051 (6)	0.0015 (6)	−0.0079 (6)
O2	0.0263 (7)	0.0240 (7)	0.0240 (7)	0.0073 (5)	−0.0005 (5)	−0.0078 (5)
O3	0.0210 (7)	0.0389 (8)	0.0365 (8)	0.0058 (6)	0.0051 (6)	0.0092 (6)
O4	0.0312 (7)	0.0294 (8)	0.0316 (8)	−0.0078 (6)	0.0074 (6)	0.0046 (6)
O5	0.0185 (6)	0.0236 (7)	0.0225 (7)	0.0010 (5)	0.0012 (5)	−0.0010 (5)
O6	0.0184 (6)	0.0217 (7)	0.0198 (6)	−0.0013 (5)	−0.0012 (5)	−0.0047 (5)
O7	0.0299 (7)	0.0231 (7)	0.0203 (7)	−0.0034 (5)	0.0044 (5)	0.0018 (5)
O8	0.0160 (6)	0.0292 (7)	0.0385 (8)	−0.0026 (5)	0.0060 (6)	−0.0016 (6)
N1	0.0177 (8)	0.0205 (8)	0.0222 (8)	0.0002 (6)	0.0014 (6)	−0.0012 (6)
N2	0.0218 (8)	0.0253 (8)	0.0220 (8)	−0.0035 (7)	0.0028 (6)	−0.0005 (7)

N3	0.0183 (7)	0.0198 (8)	0.0198 (8)	0.0012 (6)	0.0003 (6)	−0.0015 (6)
C1	0.0204 (9)	0.0210 (9)	0.0242 (10)	−0.0019 (7)	−0.0010 (7)	0.0017 (8)
C2	0.0234 (9)	0.0168 (9)	0.0150 (8)	−0.0005 (7)	−0.0007 (7)	0.0024 (7)
C3	0.0227 (9)	0.0167 (9)	0.0147 (9)	0.0000 (7)	−0.0009 (7)	0.0016 (7)
C4	0.0182 (8)	0.0175 (9)	0.0180 (9)	0.0017 (7)	0.0007 (7)	−0.0021 (7)
C5	0.0202 (9)	0.0152 (8)	0.0175 (9)	−0.0002 (7)	−0.0008 (7)	−0.0003 (7)
C6	0.0212 (9)	0.0168 (9)	0.0182 (9)	0.0001 (7)	0.0001 (7)	0.0007 (7)
C7	0.0209 (9)	0.0276 (10)	0.0238 (10)	−0.0013 (8)	0.0034 (8)	−0.0063 (8)
C8	0.0249 (9)	0.0184 (9)	0.0163 (9)	0.0004 (7)	0.0011 (7)	0.0025 (7)
C9	0.0371 (11)	0.0297 (11)	0.0249 (10)	0.0143 (9)	0.0012 (9)	−0.0087 (8)
C10	0.0204 (9)	0.0170 (9)	0.0156 (9)	−0.0002 (7)	0.0005 (7)	−0.0049 (7)
C11	0.0201 (9)	0.0185 (9)	0.0188 (9)	0.0015 (7)	0.0004 (7)	−0.0037 (7)
C12	0.0182 (8)	0.0206 (9)	0.0185 (9)	−0.0012 (7)	0.0030 (7)	−0.0046 (7)
C13	0.0263 (9)	0.0184 (9)	0.0200 (9)	0.0019 (7)	0.0043 (8)	0.0007 (7)
C14	0.0231 (9)	0.0231 (10)	0.0237 (10)	0.0074 (7)	0.0002 (8)	0.0035 (8)
C15	0.0187 (9)	0.0241 (10)	0.0216 (9)	0.0016 (7)	0.0021 (7)	−0.0007 (7)
C16	0.0228 (9)	0.0159 (9)	0.0146 (9)	0.0008 (7)	0.0008 (7)	0.0015 (7)
C17	0.0176 (9)	0.0226 (9)	0.0251 (10)	0.0016 (7)	−0.0046 (7)	−0.0036 (8)
C18	0.0226 (9)	0.0216 (9)	0.0206 (9)	0.0040 (7)	−0.0069 (7)	−0.0031 (7)
C19	0.0208 (9)	0.0186 (9)	0.0165 (9)	−0.0027 (7)	0.0017 (7)	−0.0044 (7)
C20	0.0205 (9)	0.0184 (9)	0.0164 (9)	0.0001 (7)	0.0019 (7)	−0.0022 (7)
C21	0.0190 (9)	0.0226 (9)	0.0217 (9)	−0.0016 (7)	0.0034 (7)	−0.0020 (7)
C22	0.0199 (9)	0.0263 (10)	0.0229 (10)	0.0036 (7)	−0.0017 (7)	−0.0039 (8)
C23	0.0318 (10)	0.0204 (9)	0.0200 (10)	0.0048 (8)	−0.0013 (8)	0.0004 (7)
C24	0.0265 (9)	0.0191 (9)	0.0215 (9)	−0.0017 (7)	0.0064 (8)	0.0006 (7)
C25	0.0189 (9)	0.0168 (9)	0.0197 (9)	−0.0013 (7)	0.0036 (7)	−0.0034 (7)
C26	0.0189 (9)	0.0195 (9)	0.0213 (9)	−0.0012 (7)	0.0017 (7)	−0.0059 (7)

Geometric parameters (Å, °)

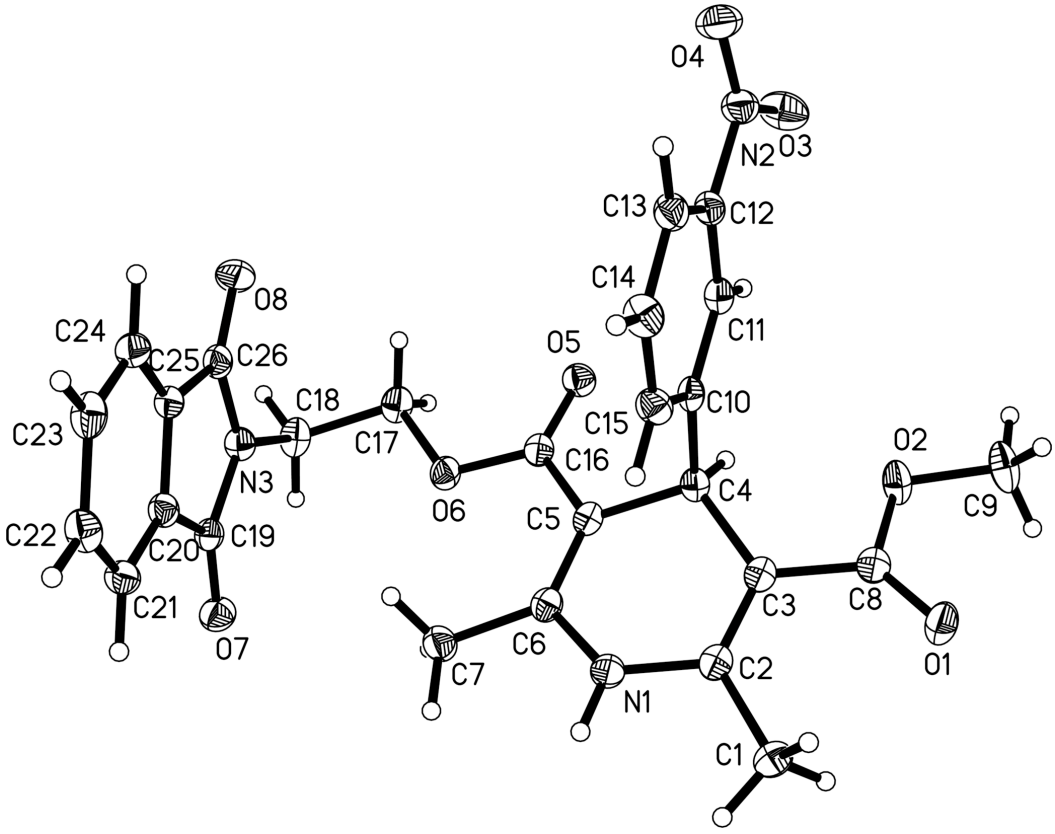
O1—C8	1.215 (2)	C7—H7C	0.9600
O2—C8	1.355 (2)	C9—H9A	0.9600
O2—C9	1.446 (2)	C9—H9B	0.9600
O3—N2	1.226 (2)	C9—H9C	0.9600
O4—N2	1.228 (2)	C10—C11	1.387 (2)
O5—C16	1.218 (2)	C10—C15	1.391 (2)
O6—C16	1.355 (2)	C11—C12	1.384 (2)
O6—C17	1.447 (2)	C11—H11	0.9300
O7—C19	1.211 (2)	C12—C13	1.385 (2)
O8—C26	1.210 (2)	C13—C14	1.382 (3)
N1—C2	1.382 (2)	C13—H13	0.9300
N1—C6	1.387 (2)	C14—C15	1.387 (3)
N1—H1	0.89 (2)	C14—H14	0.9300
N2—C12	1.470 (2)	C15—H15	0.9300
N3—C26	1.395 (2)	C17—C18	1.510 (2)
N3—C19	1.401 (2)	C17—H17A	0.9700
N3—C18	1.459 (2)	C17—H17B	0.9700
C1—C2	1.502 (2)	C18—H18A	0.9700
C1—H1A	0.9600	C18—H18B	0.9700

C1—H1B	0.9600	C19—C20	1.485 (2)
C1—H1C	0.9600	C20—C21	1.380 (2)
C2—C3	1.353 (2)	C20—C25	1.389 (2)
C3—C8	1.466 (2)	C21—C22	1.392 (3)
C3—C4	1.520 (2)	C21—H21	0.9300
C4—C5	1.522 (2)	C22—C23	1.385 (3)
C4—C10	1.532 (2)	C22—H22	0.9300
C4—H4	0.9800	C23—C24	1.387 (3)
C5—C6	1.355 (2)	C23—H23	0.9300
C5—C16	1.471 (2)	C24—C25	1.382 (3)
C6—C7	1.499 (2)	C24—H24	0.9300
C7—H7A	0.9600	C25—C26	1.487 (2)
C7—H7B	0.9600		
C8—O2—C9	115.98 (14)	C12—C11—H11	120.4
C16—O6—C17	115.54 (13)	C10—C11—H11	120.4
C2—N1—C6	123.74 (15)	C11—C12—C13	123.15 (16)
C2—N1—H1	115.5 (14)	C11—C12—N2	117.34 (15)
C6—N1—H1	119.5 (14)	C13—C12—N2	119.51 (15)
O3—N2—O4	123.44 (15)	C14—C13—C12	117.33 (16)
O3—N2—C12	117.91 (14)	C14—C13—H13	121.3
O4—N2—C12	118.64 (15)	C12—C13—H13	121.3
C26—N3—C19	111.71 (14)	C13—C14—C15	120.40 (16)
C26—N3—C18	123.98 (14)	C13—C14—H14	119.8
C19—N3—C18	123.96 (14)	C15—C14—H14	119.8
C2—C1—H1A	109.5	C14—C15—C10	121.64 (16)
C2—C1—H1B	109.5	C14—C15—H15	119.2
H1A—C1—H1B	109.5	C10—C15—H15	119.2
C2—C1—H1C	109.5	O5—C16—O6	121.97 (15)
H1A—C1—H1C	109.5	O5—C16—C5	123.50 (15)
H1B—C1—H1C	109.5	O6—C16—C5	114.53 (14)
C3—C2—N1	118.93 (16)	O6—C17—C18	107.07 (14)
C3—C2—C1	126.66 (16)	O6—C17—H17A	110.3
N1—C2—C1	114.41 (15)	C18—C17—H17A	110.3
C2—C3—C8	120.51 (16)	O6—C17—H17B	110.3
C2—C3—C4	121.06 (15)	C18—C17—H17B	110.3
C8—C3—C4	118.39 (14)	H17A—C17—H17B	108.6
C3—C4—C5	111.17 (14)	N3—C18—C17	112.23 (14)
C3—C4—C10	111.82 (14)	N3—C18—H18A	109.2
C5—C4—C10	109.73 (14)	C17—C18—H18A	109.2
C3—C4—H4	108.0	N3—C18—H18B	109.2
C5—C4—H4	108.0	C17—C18—H18B	109.2
C10—C4—H4	108.0	H18A—C18—H18B	107.9
C6—C5—C16	126.09 (16)	O7—C19—N3	125.22 (16)
C6—C5—C4	120.68 (15)	O7—C19—C20	129.07 (16)
C16—C5—C4	113.16 (14)	N3—C19—C20	105.71 (14)
C5—C6—N1	119.05 (16)	C21—C20—C25	121.37 (17)
C5—C6—C7	127.96 (16)	C21—C20—C19	130.00 (16)
N1—C6—C7	112.99 (15)	C25—C20—C19	108.56 (15)
C6—C7—H7A	109.5	C20—C21—C22	117.36 (16)

C6—C7—H7B	109.5	C20—C21—H21	121.3
H7A—C7—H7B	109.5	C22—C21—H21	121.3
C6—C7—H7C	109.5	C23—C22—C21	120.92 (17)
H7A—C7—H7C	109.5	C23—C22—H22	119.5
H7B—C7—H7C	109.5	C21—C22—H22	119.5
O1—C8—O2	121.89 (16)	C22—C23—C24	121.82 (17)
O1—C8—C3	127.38 (16)	C22—C23—H23	119.1
O2—C8—C3	110.73 (15)	C24—C23—H23	119.1
O2—C9—H9A	109.5	C25—C24—C23	116.93 (16)
O2—C9—H9B	109.5	C25—C24—H24	121.5
H9A—C9—H9B	109.5	C23—C24—H24	121.5
O2—C9—H9C	109.5	C24—C25—C20	121.60 (16)
H9A—C9—H9C	109.5	C24—C25—C26	130.64 (16)
H9B—C9—H9C	109.5	C20—C25—C26	107.72 (15)
C11—C10—C15	118.33 (16)	O8—C26—N3	124.62 (16)
C11—C10—C4	120.40 (15)	O8—C26—C25	129.12 (17)
C15—C10—C4	121.23 (15)	N3—C26—C25	106.26 (14)
C12—C11—C10	119.11 (16)		
C6—N1—C2—C3	12.7 (3)	C13—C14—C15—C10	0.3 (3)
C6—N1—C2—C1	−166.72 (15)	C11—C10—C15—C14	1.2 (3)
N1—C2—C3—C8	−175.91 (15)	C4—C10—C15—C14	−176.51 (16)
C1—C2—C3—C8	3.5 (3)	C17—O6—C16—O5	−6.1 (2)
N1—C2—C3—C4	6.4 (2)	C17—O6—C16—C5	173.91 (14)
C1—C2—C3—C4	−174.24 (16)	C6—C5—C16—O5	−177.82 (17)
C2—C3—C4—C5	−22.4 (2)	C4—C5—C16—O5	5.4 (2)
C8—C3—C4—C5	159.82 (14)	C6—C5—C16—O6	2.1 (2)
C2—C3—C4—C10	100.59 (18)	C4—C5—C16—O6	−174.63 (14)
C8—C3—C4—C10	−77.15 (19)	C16—O6—C17—C18	−174.08 (14)
C3—C4—C5—C6	22.5 (2)	C26—N3—C18—C17	63.0 (2)
C10—C4—C5—C6	−101.67 (18)	C19—N3—C18—C17	−109.65 (18)
C3—C4—C5—C16	−160.50 (14)	O6—C17—C18—N3	58.87 (19)
C10—C4—C5—C16	75.28 (17)	C26—N3—C19—O7	178.32 (16)
C16—C5—C6—N1	176.72 (15)	C18—N3—C19—O7	−8.2 (3)
C4—C5—C6—N1	−6.7 (2)	C26—N3—C19—C20	−1.94 (18)
C16—C5—C6—C7	−3.4 (3)	C18—N3—C19—C20	171.54 (15)
C4—C5—C6—C7	173.12 (16)	O7—C19—C20—C21	3.7 (3)
C2—N1—C6—C5	−12.5 (3)	N3—C19—C20—C21	−176.02 (17)
C2—N1—C6—C7	167.58 (16)	O7—C19—C20—C25	−179.33 (17)
C9—O2—C8—O1	2.0 (2)	N3—C19—C20—C25	0.94 (18)
C9—O2—C8—C3	−178.35 (14)	C25—C20—C21—C22	0.1 (3)
C2—C3—C8—O1	−9.6 (3)	C19—C20—C21—C22	176.70 (17)
C4—C3—C8—O1	168.13 (17)	C20—C21—C22—C23	0.2 (3)
C2—C3—C8—O2	170.75 (15)	C21—C22—C23—C24	−0.2 (3)
C4—C3—C8—O2	−11.5 (2)	C22—C23—C24—C25	−0.1 (3)
C3—C4—C10—C11	125.58 (17)	C23—C24—C25—C20	0.4 (3)
C5—C4—C10—C11	−110.58 (17)	C23—C24—C25—C26	−177.07 (17)
C3—C4—C10—C15	−56.8 (2)	C21—C20—C25—C24	−0.4 (3)
C5—C4—C10—C15	67.1 (2)	C19—C20—C25—C24	−177.65 (16)
C15—C10—C11—C12	−1.3 (2)	C21—C20—C25—C26	177.59 (16)

C4—C10—C11—C12	176.42 (15)	C19—C20—C25—C26	0.32 (19)
C10—C11—C12—C13	0.0 (3)	C19—N3—C26—O8	−178.54 (16)
C10—C11—C12—N2	−179.92 (15)	C18—N3—C26—O8	8.0 (3)
O3—N2—C12—C11	−10.4 (2)	C19—N3—C26—C25	2.14 (18)
O4—N2—C12—C11	169.81 (15)	C18—N3—C26—C25	−171.34 (14)
O3—N2—C12—C13	169.71 (16)	C24—C25—C26—O8	−3.0 (3)
O4—N2—C12—C13	−10.1 (2)	C20—C25—C26—O8	179.25 (18)
C11—C12—C13—C14	1.5 (3)	C24—C25—C26—N3	176.26 (17)
N2—C12—C13—C14	−178.62 (15)	C20—C25—C26—N3	−1.47 (18)
C12—C13—C14—C15	−1.6 (3)		

Fig. 1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