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(*S*)-3-[(*R*)-2,4-Dimethylpent-4-enoyl]-4-isopropyl-5,5-diphenyl-1,3-oxazolidin-2-one

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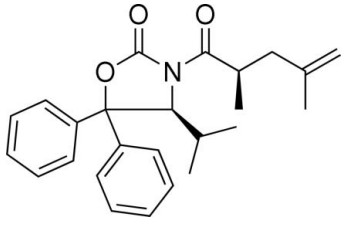
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.009 Å; R factor = 0.032; wR factor = 0.086; data-to-parameter ratio = 8.5.

The title compound, $C_{25}H_{29}NO_3$, was prepared in the course of the generation of depsipeptide libraries resembling the Jasplakinolide family of natural products. The dihedral angle between the phenyl ring planes is 74.1 (3)° The oxazolidinone ring adopts a slightly distorted ^4E conformation with an axial projection of the isopropyl substituent, which is easily rationalized by pseudo-allylic strain exerted by the exocyclic imide carbonyl. The two carbonyl groups adopt a noncolinear S-shaped conformation.

Related literature

For related literature, see: Evans & Takacs (1980); Hintermann & Seebach (1998); Hu *et al.* (2007).



Experimental

Crystal data

$C_{25}H_{29}NO_3$
M_r = 391.49
Orthorhombic, $P2_12_12_1$
a = 8.7567 (11) Å
b = 10.0467 (17) Å
c = 24.921 (5) Å
V = 2192.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 291 (1) K
0.25 × 0.25 × 0.23 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: none
15624 measured reflections
2223 independent reflections
628 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.086
S = 1.01
2223 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2580).

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supplementary materials

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(*S*)-3-[(*R*)-2,4-Dimethylpent-4-enoyl]-4-isopropyl-5,5-diphenyl-1,3-oxazolidin-2-one

R. Tannert, M. Schürmann, H. Preut, H.-D. Arndt and H. Waldmann

Comment

The title compound, (I), was synthesized in the course of the generation of depsipeptide libraries resembling the Jasplakinolide family of natural products (Hu *et al.*, 2007). The relative configuration of (I) is in accordance with the model for diastereoselective alkylation of acylated chiral oxazolidinones derived from amino acids (Evans & Takacs, 1980) and their modified diphenyl analogs (Hintermann & Seebach, 1998). The stereogenic centres were assigned based on the known chirality of the starting material (C3 S and C7 *R*).

Experimental

To a solution of (*S*)-4-isopropyl-5,5-diphenyl-3-propionyloxazolidin-2-one (1.6 g, 4.8 mmol, 1.0 eq) in 20 ml dry THF was added dropwise *via* syringe a freshly prepared solution of lithium diisoproylamide (6.2 mmol, 1.3 eq) in 12 ml dry THF at 195 K. The solution was stirred at 195 K for 30 min and then a solution of 1.4 g (6.2 mmol dry $ZnBr_2$ in 12 ml dry THF was added *via* syringe at 195 K. After stirring for 30 min at 195 K 5.1 ml (50 mmol, 10 eq) 3-bromo-2-methylprop-1-ene were added in one portion *via* syringe. The mixture was allowed to warm to 258 K and stirred at 258 K for 20 h, treated with 20 ml saturated aqueous NH_4Cl solution and diluted with 50 ml Et_2O. The organic layer was separated and washed with 5% aqueous HCl solution (2 × 20 ml), 5% aqueous NaOH solution (2 × 20 ml) and brine (1 × 15 ml). The solution was dried with $MgSO_4$, filtered and concentrated to give 1.9 g of a light yellow solid. Recrystallization with Et_2O/pentane afforded 1.4 g (75%) of (I) as colourless blocks.

$[\alpha]^{273}_D$ −190.5 (c 1.0, $CHCl_3$); mp 392.5–393.0 K; R_f = 0.43 (cyclohexane/ethyl acetate 19:1); ^{1}H NMR (500.1 MHz, $CDCl_3$) δ = 7.46 (d, J = 8.2 Hz, 2H), 7.40 (d, J = 7.7 Hz, 2H), 7.34 (dd, J = 16.4, 8.1 Hz, 4H), 7.30–7.25 (m, 2H, *p*-phenyl), 5.38 (d, J = 3.0 Hz, 1H, NCH) 4.77 (s, 1H, =C**H**H), 4.74 (s, 1H, =CH**H**), 3.96–3.87 (m, 1H, O=C—CH), 2.57 (dd, J = 14.0, 7.2 Hz, 1H, C**H**H), 2.02 (dd, J = 14.0, 7.5 Hz, 1H, CH**H**), 1.99–1.92 (m, 1H, CH_3—C**H**-CH_3), 1.76 (s, 3H, =C—C**H**$_3$), 0.86 (d, J = 7.0 Hz, 3H, O=C—C—C**H**$_3$), 0.80 (d, J = 6.8 Hz, 3H, C**H**$_3$-CH—CH_3), 0.76 (d, J = 6.7 Hz, 3H, CH_3—CH—C**H**$_3$); ^{13}C NMR (125.8 MHz, $CDCl_3$) δ = 176.6 (C=O), 152.9 (C=O), 143.0 (quart. arom. C), 142.4 (quart. arom. C), 138.2 (C=CH_2), 128.8 (2x, arom. CH), 128.5 (arom. CH), 128.4 (2x, arom. CH), 127.9 (arom. CH), 125.9 (2x, arom. CH), 125.6 (2x, arom. CH), 112.2 (C=CH_2), 64.5 (CH), 41.7 (CH2), 35.4 (CH), 29.8 (CH), 22.2 (CH_3), 21.7 (CH_3), 16.3 (CH_3), 16.3(CH_3); HRMS (FAB): m/*z* calculated for $C_{25}H_{30}NO_3$; $[M+H]^+$: 392.2220; found: 392.2244.

Refinement

Anomalous dispersion was negligible and Friedel pairs were merged before refinement.

The H atoms were placed in calculated positions, with C—H = 0.93–0.98 Å and were refined as riding, with U_{iso}(H)= 1.5U_{eq}(C) for methyl and 1.2U_{eq}(C) for all other H atoms; the methyl groups were allowed to rotate but not to tip to best fit the electron density.

Figures

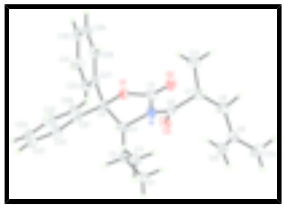


Fig. 1. : The molecular structure of (I). Displacement ellipsoids for the non-hydrogen atoms are shown at the 20% probability level.

(*S*)-3-[(*R*)-2,4-Dimethylpent-4-enoyl]-4-isopropyl-5,5-diphenyl- 1,3-oxazolidin-2-one

Crystal data

$C_{25}H_{29}NO_3$	F_{000} = 840
M_r = 391.49	D_x = 1.186 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 15624 reflections
a = 8.7567 (11) Å	θ = 3.1–25.0º
b = 10.0467 (17) Å	μ = 0.08 mm^{-1}
c = 24.921 (5) Å	T = 291 (1) K
V = 2192.4 (6) Å^3	Block, colourless
Z = 4	0.25 × 0.25 × 0.23 mm

Data collection

Nonius KappaCCD area-detector diffractometer	2223 independent reflections
Radiation source: fine-focus sealed tube	628 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.064
Detector resolution: 19 vertical, 18 horizontal pixels mm^{-1}	θ_{max} = 25.0º
T = 291(1) K	θ_{min} = 3.1º
338 frames via ω–rotation (Δω = 1%) and two times 20 s per frame (three sets at different κ–angles) scans	h = −10→10
Absorption correction: none	k = −11→11
15624 measured reflections	l = −29→29

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained
$wR(F^2) = 0.086$	$[1.0 \exp(7.90(\sin\theta/\lambda)^2)]/[\sigma^2(F_o^2)]$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
2223 reflections	$\Delta\rho_{max} = 0.10$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.13$ 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	0.2130 (4)	0.6030 (4)	0.84026 (17)	0.0393 (11)
O2	0.3031 (5)	0.4620 (4)	0.77804 (16)	0.0449 (12)
O3	0.6121 (5)	0.3935 (4)	0.90646 (18)	0.0455 (13)
N	0.4382 (5)	0.5084 (5)	0.85736 (18)	0.0387 (14)
C1	0.6965 (6)	0.7027 (6)	0.8894 (2)	0.055 (2)
H1A	0.7582	0.7774	0.8790	0.083*
H1B	0.7215	0.6274	0.8674	0.083*
H1C	0.7155	0.6816	0.9263	0.083*
C2	0.5262 (7)	0.7379 (6)	0.8820 (2)	0.0410 (17)
H2A	0.5021	0.8103	0.9069	0.049*
C3	0.4273 (6)	0.6170 (6)	0.8977 (2)	0.0384 (17)
H3A	0.4581	0.5839	0.9330	0.046*
C4	0.2510 (6)	0.6376 (6)	0.8961 (3)	0.0402 (18)
C5	0.3168 (8)	0.5165 (6)	0.8208 (3)	0.0427 (18)
C6	0.5360 (8)	0.3987 (7)	0.8662 (3)	0.0458 (19)
C7	0.5342 (7)	0.2882 (6)	0.8239 (2)	0.0381 (17)
H7A	0.5001	0.3252	0.7896	0.046*
C8	0.6941 (7)	0.2323 (6)	0.8174 (2)	0.0461 (19)
H8A	0.6878	0.1522	0.7957	0.055*
H8B	0.7316	0.2065	0.8525	0.055*
C9	0.8104 (8)	0.3254 (7)	0.7918 (3)	0.049 (2)
C10	0.7793 (8)	0.4454 (7)	0.7734 (2)	0.054 (2)
H10A	0.6803	0.4785	0.7756	0.065*
H10B	0.8563	0.4969	0.7583	0.065*
C11	0.4984 (7)	0.7896 (6)	0.8246 (2)	0.052 (2)

H11A	0.5617	0.8660	0.8182	0.078*
H11B	0.3930	0.8142	0.8207	0.078*
H11C	0.5230	0.7211	0.7992	0.078*
C12	0.4201 (6)	0.1795 (6)	0.8422 (2)	0.057 (2)
H12A	0.4171	0.1096	0.8160	0.086*
H12B	0.3203	0.2178	0.8459	0.086*
H12C	0.4524	0.1437	0.8761	0.086*
C13	0.9699 (7)	0.2650 (6)	0.7874 (2)	0.062 (2)
H13A	1.0378	0.3283	0.7711	0.093*
H13B	0.9657	0.1862	0.7657	0.093*
H13C	1.0067	0.2426	0.8225	0.093*
C21	0.1919 (7)	0.7761 (7)	0.9059 (3)	0.0411 (17)
C22	0.2239 (7)	0.8402 (7)	0.9540 (3)	0.048 (2)
H22A	0.2860	0.7991	0.9794	0.057*
C23	0.1631 (7)	0.9663 (7)	0.9646 (3)	0.055 (2)
H23A	0.1856	1.0092	0.9967	0.066*
C24	0.0692 (8)	1.0271 (7)	0.9271 (3)	0.058 (2)
H24A	0.0279	1.1106	0.9340	0.070*
C25	0.0375 (8)	0.9627 (7)	0.8796 (3)	0.059 (2)
H25A	−0.0237	1.0041	0.8540	0.071*
C26	0.0958 (7)	0.8368 (7)	0.8694 (3)	0.049 (2)
H26A	0.0701	0.7930	0.8378	0.059*
C27	0.1700 (7)	0.5358 (6)	0.9326 (3)	0.0373 (17)
C28	0.0354 (7)	0.4759 (6)	0.9156 (2)	0.0416 (17)
H28A	−0.0045	0.4956	0.8819	0.050*
C29	−0.0390 (7)	0.3871 (7)	0.9487 (3)	0.0485 (19)
H29A	−0.1289	0.3475	0.9369	0.058*
C30	0.0162 (7)	0.3552 (6)	0.9990 (3)	0.052 (2)
H30A	−0.0341	0.2942	1.0208	0.062*
C31	0.1508 (8)	0.4179 (7)	1.0162 (3)	0.056 (2)
H31A	0.1902	0.3990	1.0500	0.067*
C32	0.2255 (7)	0.5080 (7)	0.9831 (3)	0.049 (2)
H32A	0.3137	0.5499	0.9952	0.059*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.039 (3)	0.041 (3)	0.038 (3)	0.006 (3)	0.001 (2)	−0.005 (2)
O2	0.048 (3)	0.056 (3)	0.031 (3)	0.004 (3)	0.000 (3)	−0.005 (3)
O3	0.054 (3)	0.039 (3)	0.043 (3)	0.005 (3)	−0.010 (3)	−0.005 (3)
N	0.038 (3)	0.039 (4)	0.039 (4)	0.010 (3)	−0.005 (3)	−0.004 (3)
C1	0.050 (4)	0.056 (5)	0.059 (5)	−0.011 (4)	0.003 (4)	−0.006 (4)
C2	0.047 (4)	0.036 (4)	0.040 (5)	0.004 (4)	0.004 (4)	−0.002 (4)
C3	0.042 (4)	0.041 (4)	0.032 (4)	−0.004 (4)	−0.004 (3)	−0.009 (4)
C4	0.039 (4)	0.042 (5)	0.040 (5)	0.001 (4)	−0.007 (4)	−0.002 (4)
C5	0.050 (5)	0.035 (5)	0.043 (5)	−0.008 (4)	−0.006 (5)	0.010 (4)
C6	0.043 (5)	0.047 (5)	0.047 (5)	−0.012 (5)	0.018 (4)	−0.007 (5)
C7	0.040 (4)	0.039 (4)	0.036 (5)	0.011 (4)	0.001 (4)	0.001 (4)

C8	0.059 (5)	0.041 (4)	0.038 (4)	0.002 (4)	−0.007 (4)	−0.007 (4)
C9	0.051 (5)	0.050 (5)	0.045 (5)	−0.005 (5)	0.000 (4)	−0.011 (4)
C10	0.065 (5)	0.051 (5)	0.047 (5)	0.001 (4)	0.010 (4)	−0.002 (4)
C11	0.058 (5)	0.042 (5)	0.057 (5)	−0.001 (4)	0.005 (4)	0.003 (4)
C12	0.056 (5)	0.052 (5)	0.063 (5)	−0.014 (4)	−0.007 (4)	−0.007 (4)
C13	0.046 (5)	0.075 (6)	0.066 (6)	0.002 (5)	−0.004 (4)	0.005 (5)
C21	0.041 (4)	0.046 (5)	0.037 (5)	0.001 (4)	0.015 (4)	0.006 (4)
C22	0.054 (5)	0.047 (5)	0.042 (5)	0.004 (4)	0.002 (4)	−0.002 (4)
C23	0.061 (6)	0.046 (5)	0.058 (5)	−0.006 (5)	0.015 (4)	−0.011 (5)
C24	0.064 (5)	0.043 (5)	0.067 (6)	0.010 (5)	0.024 (5)	−0.005 (5)
C25	0.066 (5)	0.045 (5)	0.067 (6)	0.007 (5)	0.008 (5)	0.013 (5)
C26	0.056 (5)	0.041 (5)	0.051 (5)	0.011 (4)	0.006 (4)	−0.012 (4)
C27	0.039 (4)	0.033 (4)	0.039 (5)	0.011 (4)	0.005 (4)	0.001 (4)
C28	0.044 (4)	0.037 (4)	0.043 (4)	0.010 (4)	−0.006 (4)	0.001 (4)
C29	0.047 (4)	0.042 (5)	0.056 (5)	−0.005 (4)	−0.011 (4)	−0.008 (4)
C30	0.048 (5)	0.047 (5)	0.061 (6)	0.005 (4)	0.010 (4)	0.005 (4)
C31	0.062 (6)	0.063 (6)	0.041 (5)	−0.010 (5)	−0.011 (4)	0.008 (4)
C32	0.049 (5)	0.055 (5)	0.044 (5)	−0.014 (4)	0.001 (4)	−0.003 (4)

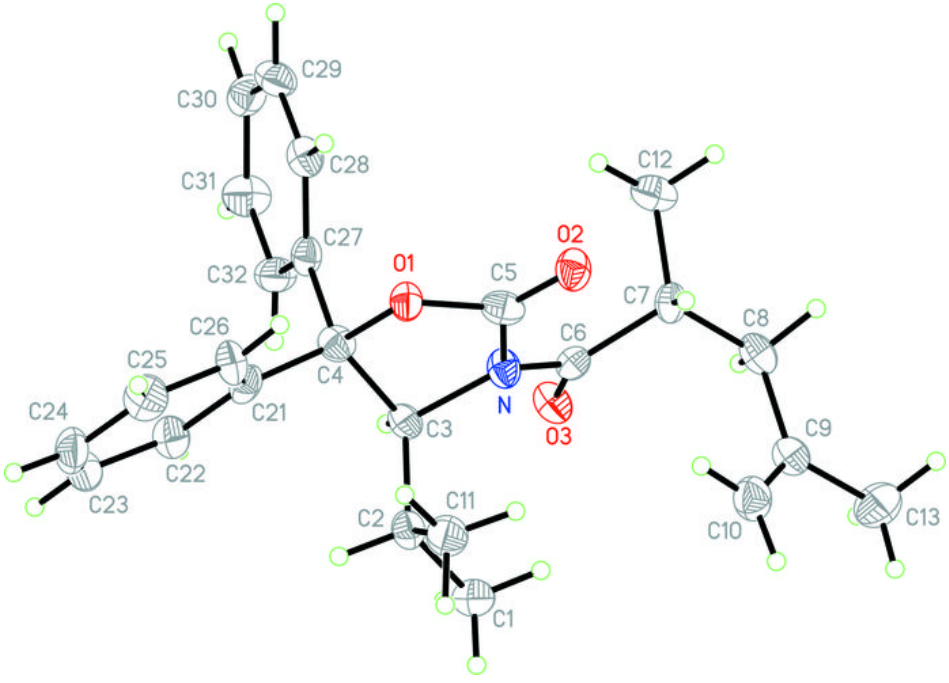
Geometric parameters (Å, °)

O1—C5	1.348 (7)	C11—H11B	0.9600
O1—C4	1.471 (7)	C11—H11C	0.9600
O2—C5	1.203 (7)	C12—H12A	0.9600
O3—C6	1.205 (7)	C12—H12B	0.9600
N—C5	1.404 (7)	C12—H12C	0.9600
N—C6	1.413 (7)	C13—H13A	0.9600
N—C3	1.486 (6)	C13—H13B	0.9600
C1—C2	1.543 (7)	C13—H13C	0.9600
C1—H1A	0.9600	C21—C26	1.382 (8)
C1—H1B	0.9600	C21—C22	1.390 (8)
C1—H1C	0.9600	C22—C23	1.399 (8)
C2—C11	1.541 (7)	C22—H22A	0.9300
C2—C3	1.542 (7)	C23—C24	1.387 (8)
C2—H2A	0.9800	C23—H23A	0.9300
C3—C4	1.558 (7)	C24—C25	1.377 (7)
C3—H3A	0.9800	C24—H24A	0.9300
C4—C21	1.505 (8)	C25—C26	1.388 (7)
C4—C27	1.541 (8)	C25—H25A	0.9300
C6—C7	1.531 (8)	C26—H26A	0.9300
C7—C8	1.517 (7)	C27—C32	1.379 (7)
C7—C12	1.549 (7)	C27—C28	1.390 (7)
C7—H7A	0.9800	C28—C29	1.380 (7)
C8—C9	1.523 (8)	C28—H28A	0.9300
C8—H8A	0.9700	C29—C30	1.381 (8)
C8—H8B	0.9700	C29—H29A	0.9300
C9—C10	1.318 (7)	C30—C31	1.403 (7)
C9—C13	1.527 (7)	C30—H30A	0.9300
C10—H10A	0.9300	C31—C32	1.387 (8)

C10—H10B	0.9300	C31—H31A	0.9300
C11—H11A	0.9600	C32—H32A	0.9300
C5—O1—C4	109.9 (5)	C2—C11—H11B	109.5
C5—N—C6	127.3 (6)	H11A—C11—H11B	109.5
C5—N—C3	110.4 (5)	C2—C11—H11C	109.5
C6—N—C3	120.4 (5)	H11A—C11—H11C	109.5
C2—C1—H1A	109.5	H11B—C11—H11C	109.5
C2—C1—H1B	109.5	C7—C12—H12A	109.5
H1A—C1—H1B	109.5	C7—C12—H12B	109.5
C2—C1—H1C	109.5	H12A—C12—H12B	109.5
H1A—C1—H1C	109.5	C7—C12—H12C	109.5
H1B—C1—H1C	109.5	H12A—C12—H12C	109.5
C11—C2—C1	110.0 (5)	H12B—C12—H12C	109.5
C11—C2—C3	114.3 (5)	C9—C13—H13A	109.5
C1—C2—C3	109.4 (5)	C9—C13—H13B	109.5
C11—C2—H2A	107.6	H13A—C13—H13B	109.5
C1—C2—H2A	107.6	C9—C13—H13C	109.5
C3—C2—H2A	107.6	H13A—C13—H13C	109.5
N—C3—C2	111.7 (5)	H13B—C13—H13C	109.5
N—C3—C4	98.3 (5)	C26—C21—C22	119.1 (6)
C2—C3—C4	116.5 (5)	C26—C21—C4	120.7 (6)
N—C3—H3A	109.9	C22—C21—C4	120.0 (7)
C2—C3—H3A	109.9	C21—C22—C23	120.4 (7)
C4—C3—H3A	109.9	C21—C22—H22A	119.8
O1—C4—C21	107.2 (5)	C23—C22—H22A	119.8
O1—C4—C27	107.3 (5)	C24—C23—C22	119.8 (7)
C21—C4—C27	111.0 (5)	C24—C23—H23A	120.1
O1—C4—C3	102.5 (5)	C22—C23—H23A	120.1
C21—C4—C3	117.3 (5)	C25—C24—C23	119.5 (7)
C27—C4—C3	110.6 (5)	C25—C24—H24A	120.3
O2—C5—O1	123.1 (7)	C23—C24—H24A	120.3
O2—C5—N	128.6 (7)	C24—C25—C26	120.7 (7)
O1—C5—N	108.3 (6)	C24—C25—H25A	119.6
O3—C6—N	119.9 (6)	C26—C25—H25A	119.6
O3—C6—C7	123.2 (7)	C21—C26—C25	120.4 (7)
N—C6—C7	116.9 (6)	C21—C26—H26A	119.8
C8—C7—C6	109.5 (5)	C25—C26—H26A	119.8
C8—C7—C12	111.4 (5)	C32—C27—C28	119.3 (6)
C6—C7—C12	108.4 (5)	C32—C27—C4	120.8 (6)
C8—C7—H7A	109.2	C28—C27—C4	119.8 (6)
C6—C7—H7A	109.2	C29—C28—C27	119.9 (6)
C12—C7—H7A	109.2	C29—C28—H28A	120.1
C7—C8—C9	115.8 (5)	C27—C28—H28A	120.1
C7—C8—H8A	108.3	C28—C29—C30	121.9 (6)
C9—C8—H8A	108.3	C28—C29—H29A	119.0
C7—C8—H8B	108.3	C30—C29—H29A	119.0
C9—C8—H8B	108.3	C29—C30—C31	117.8 (7)
H8A—C8—H8B	107.4	C29—C30—H30A	121.1
C10—C9—C8	124.7 (7)	C31—C30—H30A	121.1

C10—C9—C13	121.8 (7)	C32—C31—C30	120.5 (6)
C8—C9—C13	113.5 (6)	C32—C31—H31A	119.7
C9—C10—H10A	120.0	C30—C31—H31A	119.7
C9—C10—H10B	120.0	C27—C32—C31	120.6 (6)
H10A—C10—H10B	120.0	C27—C32—H32A	119.7
C2—C11—H11A	109.5	C31—C32—H32A	119.7
C5—N—C3—C2	−95.7 (5)	C12—C7—C8—C9	171.5 (5)
C6—N—C3—C2	99.1 (6)	C7—C8—C9—C10	−3.3 (9)
C5—N—C3—C4	27.2 (6)	C7—C8—C9—C13	178.8 (5)
C6—N—C3—C4	−138.1 (5)	O1—C4—C21—C26	11.1 (7)
C11—C2—C3—N	51.9 (7)	C27—C4—C21—C26	−105.8 (7)
C1—C2—C3—N	−71.9 (6)	C3—C4—C21—C26	125.6 (6)
C11—C2—C3—C4	−59.9 (7)	O1—C4—C21—C22	−174.0 (5)
C1—C2—C3—C4	176.3 (5)	C27—C4—C21—C22	69.1 (7)
C5—O1—C4—C21	151.1 (5)	C3—C4—C21—C22	−59.5 (8)
C5—O1—C4—C27	−89.6 (5)	C26—C21—C22—C23	−1.9 (9)
C5—O1—C4—C3	27.0 (6)	C4—C21—C22—C23	−176.8 (6)
N—C3—C4—O1	−30.9 (6)	C21—C22—C23—C24	0.6 (9)
C2—C3—C4—O1	88.4 (6)	C22—C23—C24—C25	−0.4 (10)
N—C3—C4—C21	−148.0 (6)	C23—C24—C25—C26	1.4 (10)
C2—C3—C4—C21	−28.6 (8)	C22—C21—C26—C25	2.8 (9)
N—C3—C4—C27	83.2 (6)	C4—C21—C26—C25	177.8 (6)
C2—C3—C4—C27	−157.4 (5)	C24—C25—C26—C21	−2.6 (10)
C4—O1—C5—O2	172.0 (6)	O1—C4—C27—C32	154.9 (5)
C4—O1—C5—N	−10.2 (6)	C21—C4—C27—C32	−88.3 (7)
C6—N—C5—O2	−30.7 (10)	C3—C4—C27—C32	43.8 (8)
C3—N—C5—O2	165.3 (6)	O1—C4—C27—C28	−28.2 (7)
C6—N—C5—O1	151.7 (5)	C21—C4—C27—C28	88.6 (7)
C3—N—C5—O1	−12.3 (6)	C3—C4—C27—C28	−139.3 (5)
C5—N—C6—O3	−163.2 (6)	C32—C27—C28—C29	−1.6 (9)
C3—N—C6—O3	−0.6 (9)	C4—C27—C28—C29	−178.5 (6)
C5—N—C6—C7	14.5 (9)	C27—C28—C29—C30	0.1 (10)
C3—N—C6—C7	177.1 (5)	C28—C29—C30—C31	1.0 (10)
O3—C6—C7—C8	−38.4 (9)	C29—C30—C31—C32	−0.5 (10)
N—C6—C7—C8	144.0 (5)	C28—C27—C32—C31	2.0 (9)
O3—C6—C7—C12	83.4 (7)	C4—C27—C32—C31	178.9 (6)
N—C6—C7—C12	−94.3 (6)	C30—C31—C32—C27	−1.0 (10)
C6—C7—C8—C9	−68.6 (7)		

Fig. 1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