Table 3. *Selected geometric parameters* (Å, °) *for* (I) *and* (II)

	(I)	(II)		(I)	(II)
O1—N3	1.220 (2)	1.223 (3)	C2—C3	1.349 (2)	1.352 (4)
O2—N3	1.218 (2)	1.215 (3)	C4—C5	1.368 (2)	1.374 (4)
N1—C3	1.352 (2)	1.354 (3)	C4—C9	1.379 (2)	1.369 (4)
N1—C1	1.377 (2)	1.378 (3)	C5—C6	1.377 (2)	1.383 (4)
N1—C4	1.429 (2)	1.436 (3)	C6—C7	1.367 (3)	1.374 (4)
N2—C1	1.307 (2)	1.315 (3)	C7—C8	1.365 (3)	1.386 (4)
N2—C2	1.351 (2)	1.359 (3)	C7—C11	–	1.500 (4)
N3—C2	1.416 (2)	1.417 (3)	C8—C9	1.375 (3)	1.374 (4)
C1—C10	1.474 (3)	1.469 (4)			

	(I)	(II)
C3—N1—C1	107.42 (12)	107.6 (2)
C3—N1—C4	123.96 (12)	124.6 (2)
C1—N1—C4	128.56 (12)	127.8 (2)
C1—N2—C2	104.24 (12)	105.0 (2)
O2—N3—O1	123.30 (15)	123.2 (2)
O2—N3—C2	117.85 (14)	119.3 (2)
O1—N3—C2	118.9 (2)	117.5 (2)
N2—C1—N1	111.02 (14)	110.4 (2)
N2—C1—C10	124.76 (14)	125.2 (2)
N1—C1—C10	124.22 (14)	124.3 (2)
C3—C2—N2	112.98 (13)	112.0 (2)
C3—C2—N3	125.4 (2)	126.6 (2)
N2—C2—N3	121.58 (13)	121.4 (2)
C2—C3—N1	104.33 (13)	105.0 (2)
C5—C4—C9	120.98 (15)	120.5 (2)
C5—C4—N1	120.03 (13)	119.3 (2)
C9—C4—N1	118.96 (14)	120.2 (2)
C4—C5—C6	119.0 (2)	119.2 (2)
C7—C6—C5	120.6 (2)	121.4 (2)
C8—C7—C6	120.0 (2)	118.0 (2)
C6—C7—C11	–	121.0 (3)
C8—C7—C11	–	120.9 (3)
C7—C8—C9	120.4 (2)	121.2 (2)
C8—C9—C4	119.1 (2)	119.6 (2)

Unit-cell parameters and space groups were found from oscillation and Weissenberg photographs and confirmed by preliminary diffractometer data collection. All non-H atom positions were found using direct methods and refined. H-atom positions were calculated from geometry and also refined (not using any restrains).

For both compounds, data collection: *Kuma KM*4 *Software* (1989); program(s) used to solve structures: *SHELXS*86 (Sheldrick, 1985); program(s) used to refine structures: *SHELXL*93 (Sheldrick, 1993); molecular graphics: *ORTEP*II (Johnson, 1976).

The author wishes to thank Professor J. Suwiński for samples of compounds.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1197). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Methyl 6-[(4-Bromobenzoyloxy)(5,5,8,8-tetramethyl-5,6,7,8-tetrahydro-2-naphthyl)methyl]-2-naphthalenecarboxylate

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Abstract

The structure of the title compound, $C_{34}H_{33}BrO_4$, determined using direct methods and refined including the anomalous scattering from the Br atoms, shows that the absolute configuration at the C14 atom is *R*. High displacement parameters of several C atoms indicate conformational disorder of the saturated ring in the tetramethyltetrahydronaphthyl group. The packing of the molecules is stabilized by van der Waal's forces.

Comment

Retinoic acid is known to exert its biological effects through gene regulation mediated by at least two classes of nuclear receptors: retinoic acid receptors (RAR α,β,γ) and retinoid X receptors (RXR α,β,γ) (Lehmann *et al.*, 1992). In attempts to identify biological functions of each receptor, recent efforts have focused on finding receptor-specific ligands for these receptors (Bernard *et al.*, 1992; Shroot, 1991; Lehmann, Dawson, Hobbs, Husmann & Pfahl, 1991). Graupner *et al.* (1991) have reported that the racemate of the 2-naphthoate derivative (1) is an RAR β,γ-selective agonist. We have synthesized both enantiomers of (1) and tested their biological activity (Reczek *et al.*, 1994).

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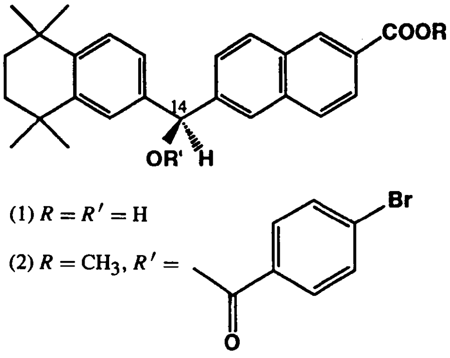
In order to correlate the three-dimensional structures of these enantiomers with biological activity, we have determined the absolute configuration of (1) by X-ray analysis of its *p*-bromobenzoate ester (2). Here we report the results of the single-crystal analysis.



(1) $R = R' = \mathrm{H}$

(2) $R = \mathrm{CH_3}, R' =$

Though the difference between the two *R* values for the two enantiomers appears significant, an *R*-factor test was performed (Hamilton, 1965) to confirm the absolute configuration. The results revealed that the absolute stereochemistry at the asymmetric atom C14 is *R*. The dihedral angle between the best least-squares plane containing the tetramethyltetrahydronaphthyl group and the plane containing the naphthyl group is 75.5 (1)°. The bromobenzyl group is tilted by 26.8 (3)° with respect to the tetramethyltetrahydronaphthyl group and by 93.59 (9)° to the naphthyl group. Most bond lengths and angles are generally as expected. Several C—C single bonds of the saturated ring in the tetramethyltetrahydronaphthyl group are short, especially C19—C20 [1.401 (1) Å]. This is the result of conformational disorder, indicated by large displacement parameters for C19, C20 and the four methyl C atoms at C18 and C21. Abnormally high displacement parameters and shortened C—C bonds in this ring have been common observations in other retinoidal analogs (Yoshiharu, Kasuya & Itai, 1990; Gao, 1992). Although the molecular packing is stabilized by van der Waals forces, there are no short contacts involving the Br atom.

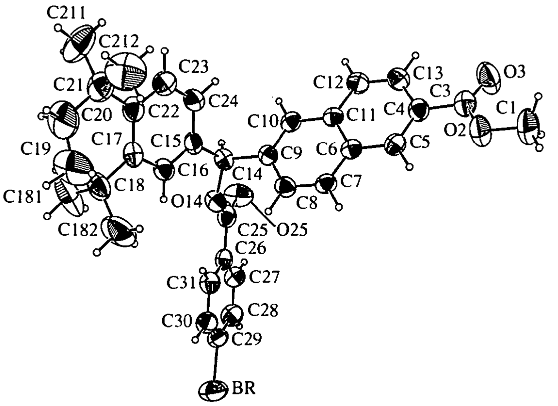


Fig. 1. *ORTEP*II (Johnson, 1976) drawing of the molecule showing the atomic labeling scheme. Displacement ellipsoids are shown at the 50% probability level; H atoms are drawn as small circles of arbitrary radii.

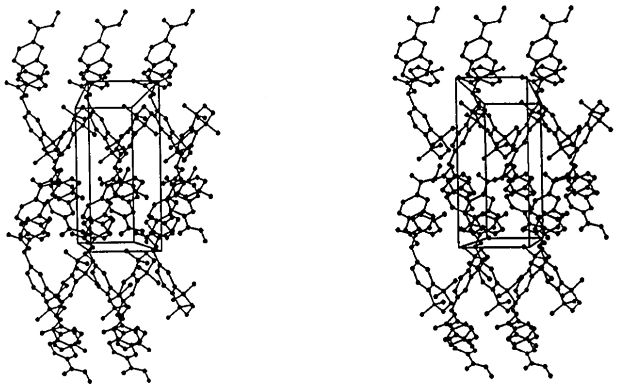


Fig. 2. Stereoscopic diagram (Sheldrick, 1990) of the molecular packing in the crystal viewed along the *c* axis.

Experimental

The synthesis of the title compound has been reported elsewhere (Reczek *et al.*, 1994). Crystals were grown from EtOAc.

Crystal data

$\mathrm{C_{34}H_{33}BrO_4}$
$M_r = 585.538$
Orthorhombic
$P2_12_12_1$
$a = 5.916\,(1)$ Å
$b = 13.808\,(2)$ Å
$c = 35.841\,(5)$ Å
$V = 2927.8\,(7)$ Å^3
$Z = 4$
$D_x = 1.328$ Mg m^{-3}

Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å
Cell parameters from 25 reflections
$\theta = 17.12–40.95°$
$\mu = 2.18$ mm^{-1}
$T = 290$ K
Rod
0.40 × 0.25 × 0.12 mm
Colorless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: ψ scan
$T_{\min} = 0.767$, $T_{\max} = 0.998$
3221 measured reflections
3221 independent reflections

2767 observed reflections $[I \geq 3\sigma(I)]$
$\theta_{\max} = 70°$
$h = -7 \rightarrow 0$
$k = -16 \rightarrow 0$
$l = -43 \rightarrow 0$
3 standard reflections
frequency: 120 min
intensity decay: 0.03% h^{-1}

Refinement

Refinement on F
$R = 0.045$
$wR = 0.057$
$S = 1.643$
2767 reflections

$(\Delta/\sigma)_{\max} = 0.01$
$\Delta\rho_{\max} = 0.342$ e Å^{-3}
$\Delta\rho_{\min} = -0.456$ e Å^{-3}
Extinction correction: $|F_c|/(1 + gI_c)$

353 parameters
H-atom parameters not refined
$w = 1/\sigma^2(F)$
Extinction coefficient: $g = 8.77 \times 10^{-7}$
Atomic scattering factors from *MolEN* (Fair, 1990)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
Br	0.9749 (1)	0.18191 (4)	0.90024 (2)	6.36 (1)
O2	1.0425 (6)	0.4113 (2)	1.25020 (9)	5.10 (7)
O3	0.7025 (7)	0.4301 (3)	1.2764 (1)	6.57 (9)
O14	0.6291 (5)	−0.0002 (2)	1.06548 (7)	3.78 (5)
O25	0.3186 (6)	0.0876 (3)	1.05454 (9)	5.53 (7)
C1	1.130 (1)	0.4857 (4)	1.2743 (2)	6.4 (1)
C3	0.8220 (9)	0.3899 (3)	1.2542 (1)	4.19 (9)
C4	0.7490 (7)	0.3118 (3)	1.2286 (1)	3.69 (8)
C5	0.8791 (7)	0.2809 (3)	1.1995 (1)	3.47 (7)
C6	0.8033 (6)	0.2069 (3)	1.1752 (1)	2.97 (7)
C7	0.9332 (7)	0.1737 (3)	1.1449 (1)	3.43 (7)
C8	0.8576 (8)	0.1013 (3)	1.1224 (1)	3.62 (8)
C9	0.6410 (7)	0.0596 (3)	1.1283 (1)	3.14 (7)
C10	0.5105 (7)	0.0900 (3)	1.1575 (1)	3.25 (7)
C11	0.5872 (6)	0.1646 (3)	1.18199 (9)	2.96 (6)
C12	0.4578 (7)	0.1978 (3)	1.2123 (1)	3.98 (8)
C13	0.5325 (8)	0.2699 (3)	1.2345 (1)	4.16 (8)
C14	0.5606 (7)	−0.0209 (3)	1.1033 (1)	3.46 (7)
C15	0.6586 (8)	−0.1182 (3)	1.1142 (1)	3.49 (8)
C16	0.8009 (7)	−0.1704 (3)	1.0916 (1)	3.62 (8)
C17	0.8907 (8)	−0.2603 (3)	1.1018 (1)	3.95 (8)
C18	1.0388 (9)	−0.3148 (3)	1.0741 (1)	5.2 (1)
C19	1.171 (1)	−0.3938 (5)	1.0943 (2)	11.4 (2)
C20	1.058 (2)	−0.4467 (4)	1.1219 (2)	9.6 (2)
C21	0.935 (1)	−0.3922 (3)	1.1522 (1)	5.6 (1)
C22	0.8380 (9)	−0.2972 (3)	1.1368 (1)	4.12 (9)
C23	0.692 (1)	−0.2445 (3)	1.1595 (1)	5.0 (1)
C24	0.6008 (9)	−0.1567 (3)	1.1488 (1)	4.24 (9)
C25	0.5051 (8)	0.0601 (3)	1.0452 (1)	3.72 (8)
C26	0.6209 (7)	0.0901 (3)	1.0107 (1)	3.28 (7)
C27	0.5173 (8)	0.1548 (3)	0.9863 (1)	4.09 (8)
C28	0.6200 (9)	0.1823 (3)	0.9535 (1)	4.56 (9)
C29	0.8289 (8)	0.1455 (3)	0.9450 (1)	4.04 (8)
C30	0.9392 (8)	0.0826 (3)	0.9690 (1)	4.29 (9)
C31	0.8365 (8)	0.0555 (3)	1.0016 (1)	3.93 (8)
C181	0.894 (1)	−0.3540 (5)	1.0435 (2)	9.7 (2)
C182	1.217 (1)	−0.2499 (6)	1.0565 (2)	8.4 (2)
C211	0.746 (1)	−0.4565 (4)	1.1672 (2)	8.8 (2)
C212	1.098 (1)	−0.3694 (6)	1.1841 (2)	8.9 (2)

Table 2. *Selected geometric parameters* (Å, °)

Br—C29	1.892 (4)	C15—C24	1.394 (6)
O2—C1	1.440 (6)	C16—C17	1.400 (6)
O2—C3	1.349 (6)	C17—C18	1.524 (6)
O3—C3	1.200 (6)	C17—C22	1.394 (6)
O14—C14	1.443 (4)	C18—C19	1.528 (9)
O14—C25	1.327 (5)	C18—C181	1.493 (9)
O25—C25	1.216 (6)	C18—C182	1.524 (9)
C3—C4	1.483 (6)	C19—C20	1.40 (1)
C4—C5	1.365 (6)	C20—C21	1.510 (9)
C4—C13	1.424 (6)	C21—C22	1.534 (6)
C5—C6	1.417 (5)	C21—C211	1.525 (9)
C6—C7	1.409 (5)	C21—C212	1.533 (9)
C6—C11	1.429 (5)	C22—C23	1.393 (7)
C7—C8	1.362 (6)	C23—C24	1.381 (6)
C8—C9	1.424 (6)	C25—C26	1.476 (6)
C9—C10	1.368 (5)	C26—C27	1.393 (6)
C9—C14	1.507 (5)	C26—C31	1.403 (6)
C10—C11	1.428 (5)	C27—C28	1.380 (6)
C11—C12	1.406 (5)	C28—C29	1.374 (7)
C12—C13	1.351 (6)	C29—C30	1.387 (6)
C14—C15	1.515 (5)	C30—C31	1.370 (6)
C15—C16	1.376 (7)		
C1—O2—C3	116.1 (4)	C17—C18—C181	109.1 (5)
C14—O14—C25	118.8 (3)	C17—C18—C182	112.2 (4)
O2—C3—O3	122.8 (4)	C19—C18—C181	112.7 (5)
O2—C3—C4	112.1 (4)	C19—C18—C182	105.1 (5)
O3—C3—C4	125.1 (5)	C181—C18—C182	107.9 (5)
C3—C4—C5	122.4 (4)	C18—C19—C20	117.5 (7)
C3—C4—C13	117.8 (4)	C19—C20—C21	118.6 (5)
C5—C4—C13	119.8 (4)	C20—C21—C22	110.5 (4)
C4—C5—C6	121.0 (4)	C20—C21—C211	108.5 (5)
C5—C6—C7	122.4 (4)	C11—C12—C13	121.1 (4)
C5—C6—C11	118.4 (3)	C22—C21—C211	110.5 (5)
C7—C6—C11	119.2 (3)	C22—C21—C212	109.2 (4)
C6—C7—C8	121.1 (4)	C211—C21—C212	108.6 (5)
C7—C8—C9	120.3 (4)	C17—C22—C21	123.6 (4)
C8—C9—C10	120.1 (3)	C17—C22—C23	118.3 (4)
C8—C9—C14	119.7 (3)	C21—C22—C23	118.1 (4)
C10—C9—C14	120.2 (4)	C22—C23—C24	122.8 (4)
C9—C10—C11	120.8 (4)	C15—C24—C23	119.0 (4)
C6—C11—C10	118.4 (3)	O14—C25—O25	123.4 (4)
C6—C11—C12	119.2 (3)	O14—C25—C26	112.1 (4)
C10—C11—C12	122.4 (4)	O25—C25—C26	124.5 (4)
C4—C13—C12	120.4 (4)	C20—C21—C212	109.5 (6)
O14—C14—C9	108.9 (3)	C25—C26—C27	120.1 (4)
O14—C14—C15	108.1 (3)	C25—C26—C31	121.6 (4)
C9—C14—C15	112.2 (3)	C27—C26—C31	118.3 (4)
C14—C15—C16	123.2 (3)	C26—C27—C28	121.2 (4)
C14—C15—C24	118.4 (4)	C27—C28—C29	119.0 (4)
C16—C15—C24	118.4 (4)	Br—C29—C28	120.2 (3)
C15—C16—C17	123.0 (4)	Br—C29—C30	118.5 (4)
C16—C17—C18	119.2 (4)	C28—C29—C30	121.3 (4)
C16—C17—C22	118.4 (4)	C29—C30—C31	119.4 (4)
C18—C17—C22	122.4 (4)	C26—C31—C30	120.7 (4)
C1—O2—C3—O3	0.4 (6)	C1—O2—C3—C4	−179.3 (4)
O2—C3—C4—C5	−12.6 (6)	O3—C3—C4—C5	167.7 (4)
C3—C4—C5—C6	−179.2 (4)	C8—C9—C14—O14	−39.4 (5)
C8—C9—C14—C15	80.3 (4)	C9—C14—C15—C16	−115.8 (4)
C14—C15—C24—C23	−178.9 (4)	C14—O14—C25—O25	−11.7 (6)
C14—O14—C25—C26	167.8 (3)	O14—C14—C15—C16	4.3 (5)
O14—C25—C26—C27	−178.8 (3)	C15—C16—C17—C18	177.3 (4)
C16—C17—C18—C19	163.5 (5)	C16—C17—C22—C21	−176.8 (4)
C17—C18—C19—C20	40.5 (8)	C17—C22—C23—C24	−1.3 (8)
C18—C17—C22—C21	4.2 (7)	C18—C17—C22—C23	−176.6 (4)
C18—C19—C20—C21	−51.5 (10)	C19—C20—C21—C22	33.2 (9)
C20—C21—C22—C17	−9.9 (7)	C20—C21—C22—C23	170.9 (5)
C22—C17—C18—C19	−17.4 (7)	O25—C25—C26—C27	0.7 (6)
C25—O14—C14—C9	−81.8 (4)	C25—O14—C14—C15	156.0 (3)

The positions of all H atoms were calculated from an idealized geometry with standard bond lengths and angles. Including the anomalous-scattering effect of the Br atom, the refinements on the *S* enantiomer gave $R = 0.053$ and $wR = 0.067$, while $R = 0.045$ and $wR = 0.057$ for the *R* enantiomer.

The structure was solved by direct methods using program *SHELXS*86 (Sheldrick, 1990) and was refined by full-matrix least-squares techniques using *MolEN* (Fair, 1990). Molecular graphics were drawn using *ORTEP*II (Johnson, 1976).

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: PT1000). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Three Stereoisomers of a Novel and Selective μ-Opioid Analgesic

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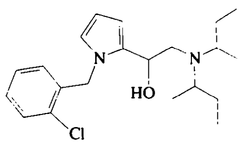
Abstract

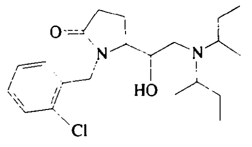
The crystal structures of the following three stereoisomers have been determined: (1*S*)-2-[(1*R*,1′*R*)-, (1*S*)-2-[(1*S*,1′*S*)- and (1*S*)-2-[(1*R*,1′*S*)-bis(1-methylpropyl)-amino]-1-[(5*S*)-1-[(2-chlorophenyl)methyl]-2-oxo-5-pyrrolidinyl]ethanol, $C_{21}H_{33}ClN_2O_2$. The configurations at the stereocentres strongly influence both the hydrogen-bonding behaviour of the OH group and the packing. The conformations of the central N—C—C(OH)—C—N chains are particularly relevant to this behaviour and to the pharmacological activity.

Comment

In the past few years research on new μ-opioid analgesics has been developed by modifying the structure of viminol, (1) (Chiarino, Della Bella, Jommi & Veneziani, 1978), a central analgesic compound developed in our laboratories in the 1970's. This has led to the synthesis and the pharmacological evaluation of all stereoisomers of 5-[2-bis(1-methylpropyl)amino]-1-hydroxyethyl]-1-[(2-chlorophenyl)methyl]-2-pyrrolidinone, (2) (Napoletano *et al.*, 1995).



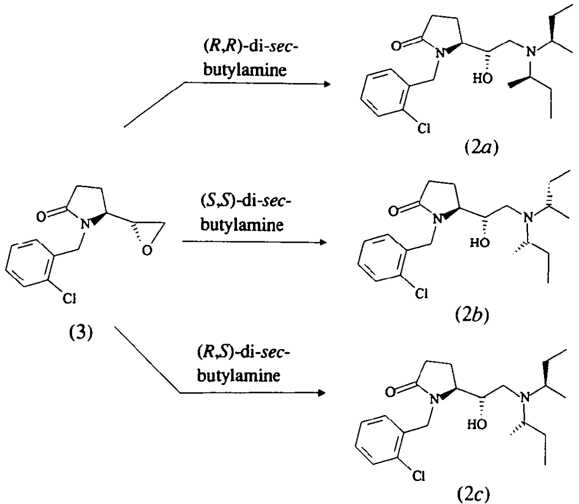
Viminol (1)



(2)

The biological data clearly showed how the stereochemistry of compounds (2) deeply influenced their affinity towards the opioid receptors and the related analgesic activity.

Elucidation of the influence of the stereogenic centres of the di-*sec*-butyl chains on the conformation of the whole molecule may provide an explanation of the stereochemical requirements for binding to the receptor. Accordingly, X-ray crystal structure analyses of isomers (1*S*)-2-[(1*R*,1′*R*)-, (2*a*), (1*S*)-2-[(1*S*,1′*S*)-, (2*b*), and (1*S*)-2-[(1*R*,1′*S*)-bis(1-methylpropyl)amino]-1-[(5*S*)-1-[(2-chlorophenyl)methyl]-2-oxo-5-pyrrolidinyl]-ethanol, (2*c*), have been carried out and the results are illustrated here. These compounds were prepared starting from (3) (Napoletano, Grancini, Veneziani & Chiarino, 1992) and sterically pure di-*sec*-butylamines according to the scheme shown below.



(II)

Fig. 1 contains drawings of the three molecules and Tables 4, 5 and 6 present some selected bond distances and angles. As can be seen from Fig. 1, the most relevant differences involve the conformation about the central C11—C12(O2)—C13—N2 chain. The orientation of the C—OH group with respect to the plane through the pyrrolidinone ring is defined by the torsion angle τ_1 = N1—C11—C12—O2: with respect

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