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11,18-Diphenoxy-3,26-dioxa-13,16-diazahexacyclo[26.2.2.0^{4,9}.0^{10,13}.0^{16,19}.0^{20,25}]dotriaconta-1(31),4,6,8,20,22,24,28(32),29-nonaene-12,17-dione. Corrigendum

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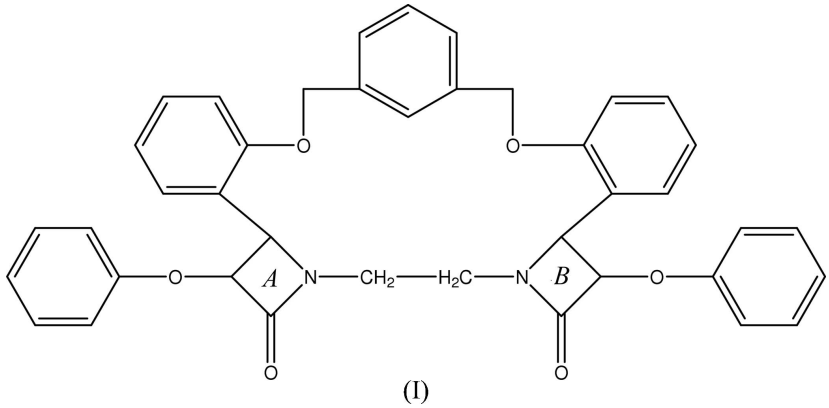
In the paper by Gayathri, Latha, Velmurugan, Ravikumar & Arumugam [*Acta Cryst.* (2006), E**62**, o3082–o3084], the title and chemical diagram are incorrect. The correct systematic name for the title compound is '11,18-Diphenoxy-3,26-dioxa-13,16-diazahexacyclo[26.3.1.0^{4,9}.0^{10,13}.0^{16,19}.0^{20,25}]dotriaconta-1(31),4,6,8,20,22,24,28(32),29-nonaene-12,17-dione' and the correct chemical diagram is given below.



(I)

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11,18-Diphenoxy-3,26-dioxa-13,16-diaza-hexacyclo[26.2.2.0^{4,9}.0^{10,13}.0^{16,19}.0^{20,25}]-dotriaconta-1(31),4,6,8,20,22,24,28(32),29-nonaene-12,17-dione

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The crystal structure of the title compound, $C_{30}H_{34}N_2O_6$, is stabilized by C—H···O interactions. The C—H···O interactions result in the formation of a centrosymmetric dimer and a chain of glide-related molecules.

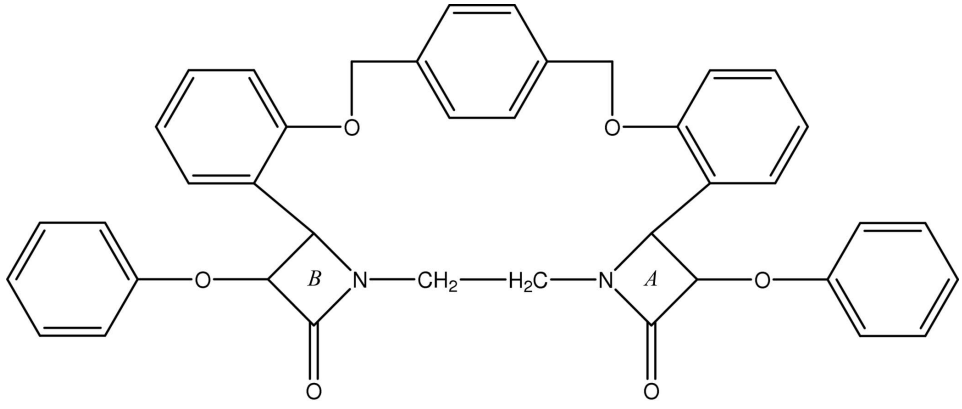
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.103
Data-to-parameter ratio = 13.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The β-lactam ring (2-azetidinone) is an important structural element in antimicrobial agents such as penicillin. The activity and selectivity of β-lactam antibiotics can be influenced decisively by the substituents attached to the β-lactam ring (Kumar *et al.*, 1993; Sharma *et al.*, 1994). Since substitution at the N atom is relatively easy, β-lactam rings are widely employed in the synthesis of bicyclic β-lactam antibiotics.



(I)

The internal angles of the four-membered rings of the title compound, (I), vary from 85.4 (1) to 96.1 (1)° (Table 1). The sums of the bond angles at the N atoms are 358.8 and 359.6° for N1 and N2, respectively. The conformation is stabilized by weak intramolecular C—H···O and C—H···N interactions (Table 2). The crystal structure is stabilized by intermolecular C—H···O interactions.

Experimental

A solution of phenoxyacetylcholine (1 mmol) in dry dichloromethane (20 ml) was slowly added to a solution of *N*,*N*′-bis(triphenylmethylene)-8,12-dioxaethane-1,4-diamine (1 mmol) and triethylamine (3.5 mmol) in dichloromethane (20 ml) at 273 K. After completion of the reaction, the solvent was removed under reduced pressure. The crude material was purified by column chromatography, yielding the title compound. The compound was recrystallized from ethyl acetate.

Crystal data

$C_{40}H_{34}N_2O_6$
M_r = 638.69
Monoclinic, $P2_1/n$
a = 8.3548 (6) Å
b = 18.1540 (13) Å
c = 22.0663 (16) Å
β = 90.528 (1)°
V = 3346.7 (4) Å^3
Z = 4
D_x = 1.268 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colorless
0.29 × 0.26 × 0.25 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: none
31839 measured reflections
5885 independent reflections
4751 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.103
S = 1.03
5885 reflections
433 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2 + 0.7548P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.378 (2)	C12—C13	1.528 (2)
C7—O1	1.402 (2)	C13—O4	1.405 (2)
C7—C8	1.525 (2)	C13—C14	1.566 (2)
C7—C9	1.567 (2)	C14—N2	1.473 (2)
C8—N1	1.348 (2)	C15—O4	1.385 (2)
C9—N1	1.477 (2)	C26—O5	1.365 (2)
C10—N1	1.443 (2)	C27—O5	1.430 (2)
C11—N2	1.447 (2)	C34—O6	1.425 (2)
C12—N2	1.343 (2)	C35—O6	1.365 (2)
C8—N1—C10	130.8 (1)	C12—N2—C11	132.4 (1)
C8—N1—C9	96.0 (1)	C12—N2—C14	96.3 (1)
C10—N1—C9	132.0 (1)	C11—N2—C14	130.9 (1)
C9—C7—C8—N1	3.2 (1)	C7—C8—N1—C9	−3.4 (1)
C8—C7—C9—N1	−2.9 (1)	C7—C9—N1—C8	3.3 (1)
N2—C12—C13—C14	5.9 (1)	C13—C12—N2—C14	−6.3 (1)
C12—C13—C14—N2	−5.4 (1)	C13—C14—N2—C12	6.2 (1)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···O5	0.98	2.35	2.738 (2)	103
C22—H22···N2	0.93	2.63	2.936 (2)	100
C22—H22···O3^{i}	0.93	2.58	3.179 (2)	123
C34—H34A···O2^{ii}	0.97	2.53	3.393 (2)	148

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

All H atoms were positioned geometrically and allowed to ride on their parent C atoms, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

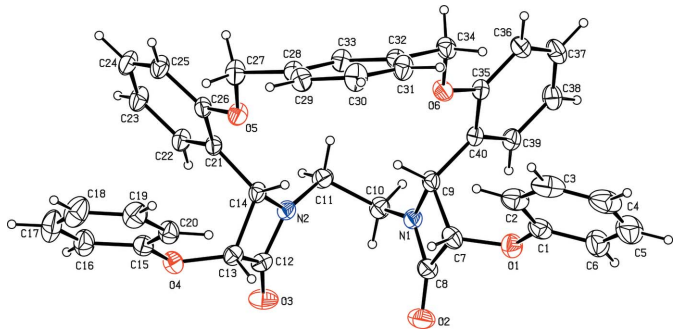


Figure 1
The molecular structure of the title compound, showing 20% probability displacement ellipsoids.

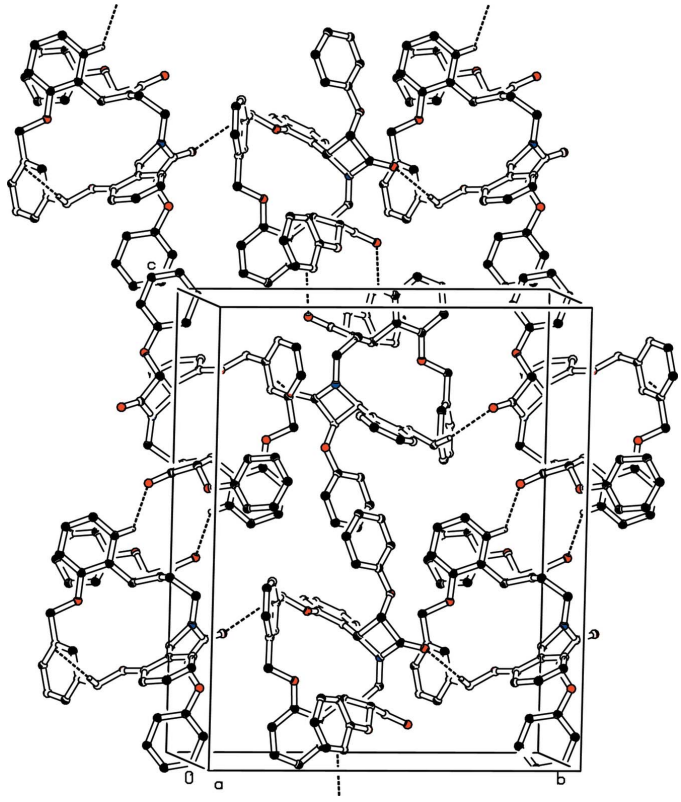


Figure 2
The molecular packing of (I), viewed approximately down the *a* axis, showing C—H···O interactions (dashed lines). For clarity, H atoms not involved in the hydrogen bonds have been omitted.

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