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N,*N*′-Diethyl-*N*,*N*′-diphenyl-3-oxapentanediamide

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.089
Data-to-parameter ratio = 14.4

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

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The title compound, $C_{20}H_{24}N_2O_3$, is a kind of non-cyclic crown ether. It crystallizes as a zigzag chain with two slightly asymmetric terminal groups.

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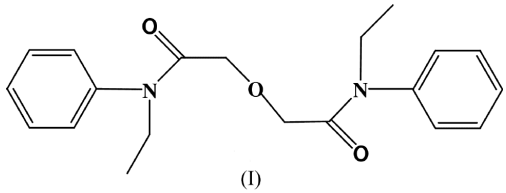
Comment

The title compound, (I), is a kind of non-cyclic ether-containing amide showing a highly selective complexation of lanthanide ions (Ding *et al.*, 1986; Liu *et al.*, 1996; Yang & Ding, 1982). To deepen our knowledge of the structural character of (I), and provide some information on the reactivity of the ligand with different lanthanide ions, we determined its crystal structure.



(I)

The framework of the molecule (Fig. 1) is composed of a zigzag chain (C2—C1—O1—C11—C12) with two ethylphenyl amide terminal groups. An interesting aspect of the molecular conformation concerns the two phenyl rings, which adopt opposite orientations with respect to the main chain. The C3—N1 distance is slightly longer than the C13—N2 distance [1.454 (2) and 1.446 (2) Å, while the angle C3—N1—C9 is smaller than the angle C13—N2—C19 [115.41 (17) and 115.86 (18)°, respectively]. This indicates that the two terminal groups in the zigzag chain are slightly asymmetric.

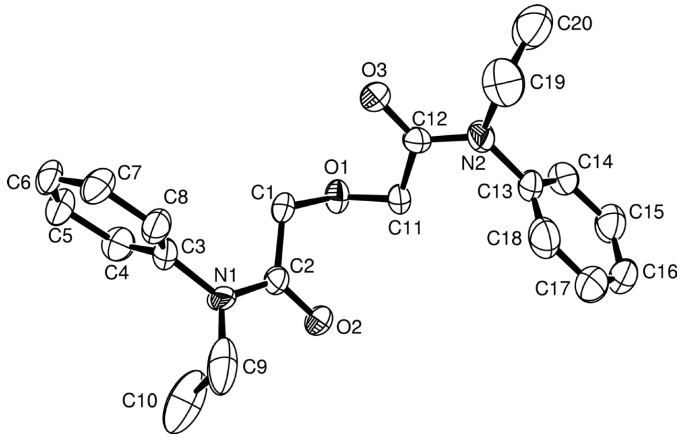


Figure 1
View of (I) shown with ellipsoids at the 50% probability level. H atoms have been omitted for clarity.

Experimental

The chemicals were purchased from commercial sources and were used without further purification. 3-Oxapentanedioic acid and 3-oxapentanedionyl chloride were prepared according to the method of Tan (1983). A solution of 3-oxapentanedionyl chloride (7.9 mmol) in anhydrous benzene (10 ml) was added dropwise to a solution of *N*-ethylphenylamine (23.7 mmol) and anhydrous pyridine (1 ml) in benzene (30 ml). The mixture was stirred at 313 K for 5 h, then the crude product was recrystallized from acetone (yield 50%). Single crystals were obtained by slow evaporation from MeCN over a period of several days. IR (KBr, pellet): 1672 (C═O, *s*), 1126 (C—O, *s*), 1268 (Ar-H, *s*), 1495, 1594 (Ar-ring, *s*), 3061 (Ar-H, *m*). ^{1}H NMR (acetone-d_6): δ 1.10 (6H, *t*), 3.87 (4H, *q*), 3.93 (4H, *s*), 7.36 (10H, *m*). MS: m/z = 341.

Crystal data

$C_{20}H_{24}N_2O_3$	D_x = 1.222 Mg m^{-3}
M_r = 340.41	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 25 reflections
a = 9.274 (2) Å	θ = 3.1–13.0°
b = 9.641 (1) Å	μ = 0.08 mm^{-1}
c = 20.746 (3) Å	T = 296 (2) K
β = 94.17 (2)°	Block, yellow
V = 1850.0 (5) Å^3	0.68 × 0.38 × 0.22 mm
Z = 4	

Data collection

KappaCCD diffractometer	$h = -11 \rightarrow 10$
ω scans	$k = 0 \rightarrow 11$
3250 measured reflections	$l = 0 \rightarrow 24$
3250 independent reflections	3 standard reflections every 97 reflections
2551 reflections with $I > 2\sigma(I)$	intensity decay: 1.8%
θ_{max} = 25.0°	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.01P)^2 + 0.51P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.089	$\Delta\rho_{max}$ = 0.47 e Å^{-3}
S = 1.01	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
3250 reflections	
226 parameters	
H-atom parameters not refined	

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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