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N,*N*′-Bis(2-methoxyphenyl)-3,6-dioxaoctanediamide

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.098
Data-to-parameter ratio = 16.5

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

The title compound, $C_{24}H_{24}N_2O_6$, has a centre of symmetry and belongs to the monoclinic space group $P2_1/c$. The two benzene rings are almost parallel to each other and perpendicular to the ether chain.

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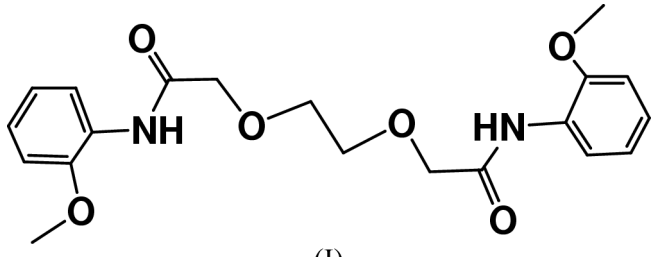
Comment

Glycol-*O*,*O*′-diacetamide compounds are excellent extractors and have been widely studied in the extraction of rare earths and some actinide ions (Ding *et al.*, 1986). For example, *N*,*N*,*N*′,*N*′-tetraphenyl-3,6-dioxaoctanediamide (TDD) has a large separation factor, and both the separation factor and distribution ratio of lighter lanthanide ions for TDD are larger than those for dicyclohexyl-18-crown-6 (Gao & Ni, 1983), if picrate is used as the accompanying ion. Further research into these compounds can help us design better extractors, exploring the relationship between structure and properties, and acquiring better property data (Yang *et al.*, 1984).

As part of a systematic investigation of a new extractor of rare earths, the present paper reports the crystal structure of *N*,*N*′-bis(2-methoxyphenyl)-3,6-dioxaoctanediamide, (I) (Fig. 1), which can act as a tetradentate ligand. In the molecule, two carbonyl O atoms and two ether O atoms can coordinate to a metal ion. There is a centre of symmetry and a zigzag skeleton, indicating that the ligand has good flexibility. In this structure, the average C—O(ether) distance is 1.4017 Å, longer than the C—O(carbonyl) distance of 1.2138 Å. The two benzene rings are almost parallel to each other and perpendicular to the ether chain. When coordinating to a metal ion, this kind of ligand can form half-ring coordination structures (Fan *et al.*, 1999; S.–X. Liu *et al.*, 1997; W.–S. Liu *et al.*, 1997). The size of the cavity will change with different terminal groups, so that the extractive properties will be different for different metal ions. A study of the selectivity of this ligand to *s*- and *f*-block metal ions is in progress. A packing diagram for molecules of (I) is shown in Fig. 2.



(I)

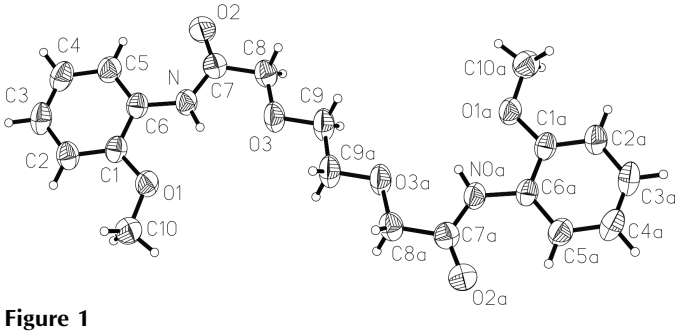


Figure 1
The structure of *N,N′*-bis(2-methoxyphenyl)-3,6-dioxaoctanediamide showing the atom labelling and displacement ellipsoids at the 50% probability level.

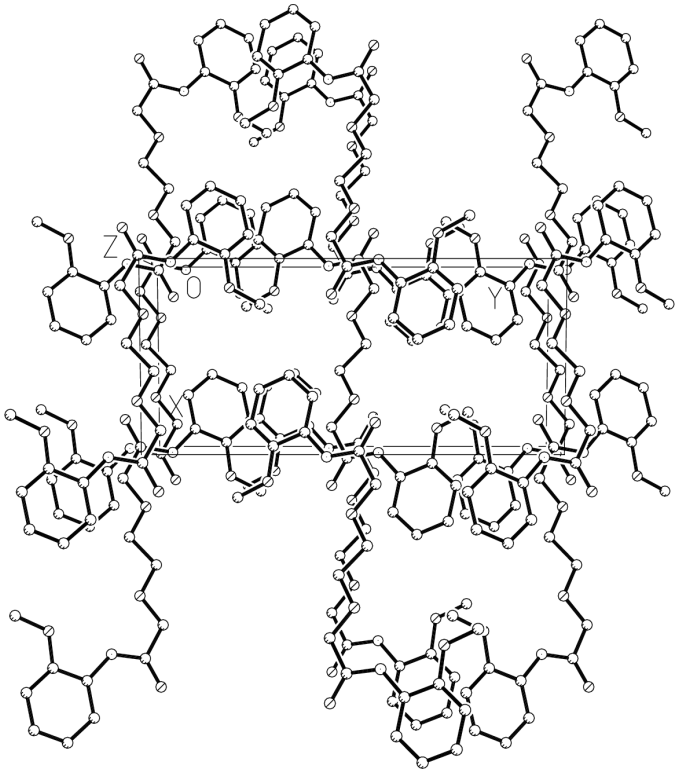


Figure 2
The packing of the title compound.

Experimental

The title compound was prepared according to the literature method of Ding *et al.* (1986). Single crystals suitable for X-ray determination were obtained by slow evaporation of an MeCN solution over a period of several days.

Crystal data

$C_{20}H_{24}N_2O_6$	D_x = 1.324 Mg m^{-3}
M_r = 388.41	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 19 reflections
a = 7.4670 (10) Å	θ = 4.3–14.9°
b = 16.002 (2) Å	μ = 0.10 mm^{-1}
c = 8.2560 (10) Å	T = 296 (2) K
β = 98.960 (10)°	Block, white
V = 974.4 (2) Å^3	0.48 × 0.46 × 0.42 mm
Z = 2	

Data collection

Siemens *P*4 diffractometer	$h = 0 \rightarrow 9$
ω scans	$k = 0 \rightarrow 20$
2458 measured reflections	$l = -10 \rightarrow 10$
2129 independent reflections	3 standard reflections
1354 reflections with $I > 2\sigma(I)$	every 97 reflections
R_{int} = 0.014	intensity decay: 6.0%
θ_{max} = 27.0°	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.098	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
S = 0.94	$\Delta\rho_{min}$ = −0.11 e Å^{-3}
2129 reflections	Extinction correction: *SHELXL*97
129 parameters	Extinction coefficient: 0.086 (6)
H-atom parameters constrained	

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL-Plus* (Siemens, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXTL-Plus*.

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