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Bis[4-(2-hydroxyethylamino)phenyl] sulfone

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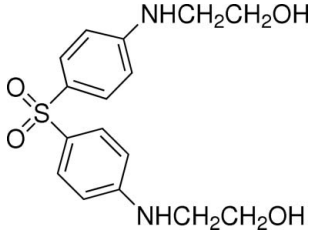
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.110; data-to-parameter ratio = 12.6.

The title compound, $C_{16}H_{20}N_2O_4S$, exhibits a V-shape structure with a dihedral angle of 77.5 (11)° formed by the two benzenel rings. The molecular packing is stabilized by intramolecular and intermolecular hydrogen bonds as well as π–π [3.738 (3) Å] and C—H$\cdots\pi$ interactions.

Related literature

For related literature, see: Shahsafi *et al.* (1987).



Experimental

Crystal data

$C_{16}H_{20}N_2O_4S$
M_r = 336.40
Monoclinic, $C2/c$
a = 25.643 (17) Å
b = 8.118 (6) Å
c = 15.340 (11) Å
β = 102.989 (12)°
V = 3112 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 294 (2) K
0.20 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.953, T_{max} = 0.966
7793 measured reflections
2742 independent reflections
1982 reflections with $I > 2\sigma$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.110
S = 1.03
2742 reflections
218 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C14—H14$\cdots$O3	0.93	2.59	2.919 (3)	101
C10—H10$\cdots$O2	0.93	2.57	2.915 (3)	102
C7—H7$\cdots$O3	0.93	2.47	2.854 (3)	105
O1—H1$\cdots$O3^{i}	0.82	1.87	2.683 (3)	175
O1—H1$\cdots$S1^{i}	0.82	2.88	3.638 (2)	154
O4—H4$\cdots$O2^{ii}	0.82	2.13	2.945 (3)	177
N1—H1*C*$\cdots$O4^{iii}	0.892 (10)	2.185 (11)	3.066 (3)	169 (2)
N2—H2*C*$\cdots$O1^{iv}	0.895 (10)	2.027 (11)	2.917 (3)	172 (2)
C10—H10$\cdots$*Cg*2	0.93	2.97	3.762(4)	144

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2122).

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supplementary materials

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Bis[4-(2-hydroxyethylamino)phenyl] sulfone

G.-F. Chen, G.-C. Ma, J. Hu and W.-Q. Zhang

Comment

The derivatives of diphenyl sulphone are used as precursors in the organic synthesis. Several derivatives of aminosulphones have been shown to possess strong tuberculostatic, antileprotic and anticonvulsant activities (Shahsafi, *et al.*, 1987). The crystal structure determination of the title compound, (I), was carried out in order to elucidate its molecular conformation.

The V-shape structure of the molecule is supported by the two phenyl rings with a dihedral angle of 77.5 (11)°.

The molecular packing is stabilized by intramolecular and intermolecular hydrogen bonds (Table 1) as well as weak π-π and C—H..π interactions.

Experimental

The title compound, (I), was synthesized by the reaction of 4,4'-dichlorodiphenyl sulfone (5.74 g, 0.02 mol) with 2-amino-ethanol (9.76 g, 0.16 mol). The mixture was refluxed for 6 h and cooled to room temperature. After dilution with water, it was filtered off, washed thoroughly with water, and recrystallized from dimethylformamide and water (4:1 *v*/*v*) to give the product as fine white needles (5.5 g, yield 81.8%). The pure product (0.1 g) was dissolved in 15 ml dimethylformamide and water (4:1 *v*/*v*). Single crystals were obtained from this solution by slow evaporation over a period of 7 days at room temperature (m.p. 464–466 K).

Refinement

The H atom involved in the hydrogen bonds was found in difference Fourier maps. All other H atoms were positioned geometrically and refined using a during refinement, fix at O–H distances of 0.82 Å and its U_{iso} value was set at 1.2 U_{eq} (O). H atoms bonded to C atoms were included in the refinement in the riding model approximation, with C–H = 0.93 Å. and U_{iso} (H) = 1.2 U_{eq} (C atom).

Figures

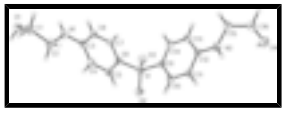


Fig. 1. A view of the structure of (I), showing the atom-numbering Scheme; displacement ellipsoids were drawn at the 30% probability level.

Bis[4-(2-hydroxyethylamino)phenyl] sulfone

Crystal data

$C_{16}H_{20}N_2O_4S$ F_{000} = 1424

M_r = 336.40	D_x = 1.436 Mg m^{-3}
Monoclinic, *C*2/*c*	Melting point: 465(1) K
Hall symbol: -C 2yc	Mo *K*α radiation λ = 0.71073 Å
a = 25.643 (17) Å	Cell parameters from 2679 reflections
b = 8.118 (6) Å	θ = 2.6–26.4º
c = 15.340 (11) Å	μ = 0.23 mm^{-1}
β = 102.989 (12)º	*T* = 294 (2) K
V = 3112 (4) Å^3	Needle, colorless
Z = 8	0.20 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2742 independent reflections
Radiation source: fine-focus sealed tube	1982 reflections with $I > 2\sigma$
Monochromator: graphite	R_{int} = 0.033
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −26→30
T_{min} = 0.953, T_{max} = 0.966	*k* = −9→9
7793 measured reflections	*l* = −15→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.037	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.110	$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 1.5895P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.005
2742 reflections	$\Delta\rho_{max}$ = 0.22 e Å^{-3}
218 parameters	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
S1	0.13804 (2)	0.13061 (7)	0.27577 (4)	0.0437 (2)
O1	−0.11464 (7)	0.7991 (2)	0.07807 (12)	0.0614 (5)
H1	−0.1153	0.8496	0.1241	0.092*
O2	0.16477 (7)	0.1933 (2)	0.36085 (10)	0.0575 (5)
O3	0.11181 (7)	−0.0265 (2)	0.27233 (11)	0.0551 (5)
O4	0.37876 (7)	−0.1123 (3)	0.00979 (13)	0.0656 (5)
H4	0.3659	−0.1633	0.0460	0.098*
N1	−0.02318 (8)	0.5964 (3)	0.09390 (13)	0.0496 (5)
N2	0.29293 (8)	0.0802 (3)	0.05074 (14)	0.0479 (5)
C1	−0.06999 (11)	0.8469 (3)	0.04713 (18)	0.0605 (7)
H1A	−0.0667	0.9659	0.0504	0.073*
H1B	−0.0749	0.8150	−0.0151	0.073*
C2	−0.01965 (10)	0.7710 (3)	0.09995 (18)	0.0541 (7)
H2A	0.0106	0.8089	0.0771	0.065*
H2B	−0.0140	0.8045	0.1621	0.065*
C3	0.01441 (8)	0.4931 (3)	0.13841 (14)	0.0395 (5)
C4	0.06235 (9)	0.5465 (3)	0.19253 (16)	0.0455 (6)
H4A	0.0692	0.6588	0.1996	0.055*
C5	0.09948 (9)	0.4366 (3)	0.23534 (16)	0.0452 (6)
H5	0.1314	0.4743	0.2712	0.054*
C6	0.09002 (8)	0.2708 (3)	0.22587 (14)	0.0370 (5)
C7	0.04241 (9)	0.2161 (3)	0.17295 (15)	0.0436 (6)
H7	0.0358	0.1036	0.1664	0.052*
C8	0.00543 (9)	0.3235 (3)	0.13085 (15)	0.0449 (6)
H8	−0.0267	0.2844	0.0961	0.054*
C9	0.18453 (8)	0.1155 (3)	0.21042 (14)	0.0380 (5)
C10	0.23154 (9)	0.2043 (3)	0.23028 (15)	0.0441 (6)
H10	0.2389	0.2729	0.2801	0.053*
C11	0.26711 (9)	0.1918 (3)	0.17704 (16)	0.0450 (6)
H11	0.2989	0.2510	0.1914	0.054*
C12	0.25677 (9)	0.0920 (3)	0.10144 (14)	0.0378 (5)
C13	0.20852 (8)	0.0063 (3)	0.08150 (15)	0.0407 (5)
H13	0.2002	−0.0593	0.0305	0.049*
C14	0.17353 (9)	0.0173 (3)	0.13568 (15)	0.0424 (6)
H14	0.1418	−0.0423	0.1221	0.051*
C15	0.28658 (9)	−0.0244 (3)	−0.02587 (15)	0.0465 (6)
H15A	0.2595	0.0214	−0.0743	0.056*
H15B	0.2745	−0.1321	−0.0115	0.056*
C16	0.33752 (10)	−0.0418 (4)	−0.05525 (17)	0.0554 (7)
H16A	0.3313	−0.1096	−0.1087	0.066*

H16B	0.3489	0.0661	−0.0709	0.066*
H1C	−0.0542 (6)	0.548 (3)	0.0693 (15)	0.053 (7)*
H2C	0.3197 (7)	0.153 (2)	0.0623 (15)	0.049 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0429 (3)	0.0529 (4)	0.0352 (3)	0.0069 (3)	0.0084 (2)	0.0087 (3)
O1	0.0496 (10)	0.0687 (12)	0.0647 (12)	0.0064 (9)	0.0100 (9)	−0.0226 (10)
O2	0.0570 (10)	0.0800 (13)	0.0318 (9)	0.0134 (10)	0.0023 (8)	0.0028 (8)
O3	0.0590 (10)	0.0523 (10)	0.0570 (11)	−0.0009 (9)	0.0190 (9)	0.0179 (8)
O4	0.0422 (10)	0.0902 (15)	0.0653 (12)	0.0090 (10)	0.0144 (9)	0.0052 (11)
N1	0.0434 (12)	0.0531 (13)	0.0481 (12)	0.0080 (11)	0.0016 (10)	−0.0008 (10)
N2	0.0427 (11)	0.0510 (12)	0.0521 (12)	−0.0059 (10)	0.0150 (10)	−0.0089 (10)
C1	0.0681 (18)	0.0621 (17)	0.0520 (16)	0.0196 (15)	0.0147 (14)	0.0100 (14)
C2	0.0517 (15)	0.0544 (16)	0.0578 (16)	0.0082 (13)	0.0157 (12)	0.0068 (13)
C3	0.0367 (12)	0.0505 (14)	0.0329 (12)	0.0077 (11)	0.0113 (10)	0.0001 (10)
C4	0.0424 (13)	0.0445 (14)	0.0500 (14)	0.0024 (11)	0.0111 (11)	0.0014 (11)
C5	0.0362 (12)	0.0540 (15)	0.0442 (13)	−0.0014 (11)	0.0064 (10)	0.0011 (11)
C6	0.0331 (11)	0.0470 (13)	0.0325 (11)	0.0049 (10)	0.0103 (9)	0.0036 (10)
C7	0.0421 (13)	0.0457 (14)	0.0436 (13)	0.0019 (12)	0.0110 (11)	−0.0027 (11)
C8	0.0359 (12)	0.0553 (15)	0.0413 (13)	0.0018 (11)	0.0043 (10)	−0.0075 (11)
C9	0.0347 (11)	0.0411 (12)	0.0361 (12)	0.0082 (10)	0.0034 (9)	0.0048 (10)
C10	0.0430 (13)	0.0439 (14)	0.0426 (13)	0.0038 (11)	0.0040 (10)	−0.0037 (11)
C11	0.0371 (12)	0.0441 (13)	0.0518 (15)	−0.0028 (11)	0.0060 (11)	−0.0040 (12)
C12	0.0361 (11)	0.0375 (12)	0.0386 (12)	0.0050 (10)	0.0059 (10)	0.0038 (10)
C13	0.0358 (12)	0.0420 (13)	0.0414 (13)	0.0036 (10)	0.0024 (10)	−0.0050 (11)
C14	0.0316 (11)	0.0459 (13)	0.0472 (13)	0.0030 (10)	0.0034 (10)	0.0023 (11)
C15	0.0424 (13)	0.0533 (15)	0.0428 (13)	0.0017 (11)	0.0073 (11)	−0.0014 (11)
C16	0.0544 (15)	0.0697 (18)	0.0444 (14)	−0.0022 (14)	0.0158 (12)	−0.0033 (13)

Geometric parameters (Å, °)

S1—O2	1.4249 (18)	C4—H4A	0.9300
S1—O3	1.4371 (19)	C5—C6	1.370 (3)
S1—C6	1.724 (2)	C5—H5	0.9300
S1—C9	1.726 (2)	C6—C7	1.379 (3)
O1—C1	1.390 (3)	C7—C8	1.342 (3)
O1—H1	0.8200	C7—H7	0.9300
O4—C16	1.402 (3)	C8—H8	0.9300
O4—H4	0.8200	C9—C14	1.373 (3)
N1—C3	1.343 (3)	C9—C10	1.379 (3)
N1—C2	1.422 (3)	C10—C11	1.358 (3)
N1—H1C	0.892 (10)	C10—H10	0.9300
N2—C12	1.341 (3)	C11—C12	1.390 (3)
N2—C15	1.429 (3)	C11—H11	0.9300
N2—H2C	0.895 (10)	C12—C13	1.393 (3)
C1—C2	1.494 (4)	C13—C14	1.356 (3)
C1—H1A	0.9700	C13—H13	0.9300

C1—H1B	0.9700	C14—H14	0.9300
C2—H2A	0.9700	C15—C16	1.481 (3)
C2—H2B	0.9700	C15—H15A	0.9700
C3—C4	1.389 (3)	C15—H15B	0.9700
C3—C8	1.396 (3)	C16—H16A	0.9700
C4—C5	1.361 (3)	C16—H16B	0.9700
O2—S1—O3	118.39 (11)	C7—C6—S1	119.89 (18)
O2—S1—C6	108.63 (11)	C8—C7—C6	120.7 (2)
O3—S1—C6	106.71 (11)	C8—C7—H7	119.7
O2—S1—C9	107.72 (11)	C6—C7—H7	119.7
O3—S1—C9	107.12 (11)	C7—C8—C3	121.0 (2)
C6—S1—C9	107.85 (11)	C7—C8—H8	119.5
C1—O1—H1	109.5	C3—C8—H8	119.5
C16—O4—H4	109.5	C14—C9—C10	119.6 (2)
C3—N1—C2	124.2 (2)	C14—C9—S1	119.16 (18)
C3—N1—H1C	114.2 (16)	C10—C9—S1	121.22 (18)
C2—N1—H1C	120.3 (16)	C11—C10—C9	120.0 (2)
C12—N2—C15	123.6 (2)	C11—C10—H10	120.0
C12—N2—H2C	115.9 (15)	C9—C10—H10	120.0
C15—N2—H2C	119.8 (15)	C10—C11—C12	121.2 (2)
O1—C1—C2	112.2 (2)	C10—C11—H11	119.4
O1—C1—H1A	109.2	C12—C11—H11	119.4
C2—C1—H1A	109.2	N2—C12—C11	119.9 (2)
O1—C1—H1B	109.2	N2—C12—C13	122.2 (2)
C2—C1—H1B	109.2	C11—C12—C13	117.9 (2)
H1A—C1—H1B	107.9	C14—C13—C12	120.7 (2)
N1—C2—C1	109.9 (2)	C14—C13—H13	119.7
N1—C2—H2A	109.7	C12—C13—H13	119.7
C1—C2—H2A	109.7	C13—C14—C9	120.7 (2)
N1—C2—H2B	109.7	C13—C14—H14	119.7
C1—C2—H2B	109.7	C9—C14—H14	119.7
H2A—C2—H2B	108.2	N2—C15—C16	111.2 (2)
N1—C3—C4	123.1 (2)	N2—C15—H15A	109.4
N1—C3—C8	119.2 (2)	C16—C15—H15A	109.4
C4—C3—C8	117.7 (2)	N2—C15—H15B	109.4
C5—C4—C3	120.9 (2)	C16—C15—H15B	109.4
C5—C4—H4A	119.6	H15A—C15—H15B	108.0
C3—C4—H4A	119.6	O4—C16—C15	113.5 (2)
C4—C5—C6	120.3 (2)	O4—C16—H16A	108.9
C4—C5—H5	119.8	C15—C16—H16A	108.9
C6—C5—H5	119.8	O4—C16—H16B	108.9
C5—C6—C7	119.4 (2)	C15—C16—H16B	108.9
C5—C6—S1	120.64 (18)	H16A—C16—H16B	107.7
C3—N1—C2—C1	−175.9 (2)	O2—S1—C9—C14	161.83 (17)
O1—C1—C2—N1	60.4 (3)	O3—S1—C9—C14	33.5 (2)
C2—N1—C3—C4	−3.1 (3)	C6—S1—C9—C14	−81.1 (2)
C2—N1—C3—C8	176.8 (2)	O2—S1—C9—C10	−20.3 (2)
N1—C3—C4—C5	−179.1 (2)	O3—S1—C9—C10	−148.70 (18)

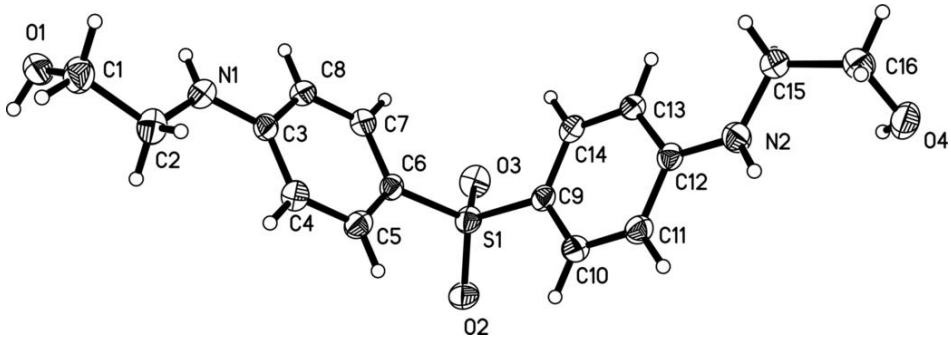
C8—C3—C4—C5	1.0 (3)	C6—S1—C9—C10	96.8 (2)
C3—C4—C5—C6	−0.2 (3)	C14—C9—C10—C11	−1.3 (3)
C4—C5—C6—C7	−0.4 (3)	S1—C9—C10—C11	−179.14 (18)
C4—C5—C6—S1	177.07 (17)	C9—C10—C11—C12	0.9 (3)
O2—S1—C6—C5	37.3 (2)	C15—N2—C12—C11	177.4 (2)
O3—S1—C6—C5	166.02 (17)	C15—N2—C12—C13	−2.2 (3)
C9—S1—C6—C5	−79.2 (2)	C10—C11—C12—N2	−179.1 (2)
O2—S1—C6—C7	−145.26 (17)	C10—C11—C12—C13	0.5 (3)
O3—S1—C6—C7	−16.6 (2)	N2—C12—C13—C14	178.0 (2)
C9—S1—C6—C7	98.25 (19)	C11—C12—C13—C14	−1.6 (3)
C5—C6—C7—C8	0.0 (3)	C12—C13—C14—C9	1.2 (3)
S1—C6—C7—C8	−177.44 (17)	C10—C9—C14—C13	0.3 (3)
C6—C7—C8—C3	0.9 (3)	S1—C9—C14—C13	178.15 (17)
N1—C3—C8—C7	178.8 (2)	C12—N2—C15—C16	−166.6 (2)
C4—C3—C8—C7	−1.4 (3)	N2—C15—C16—O4	61.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O3	0.93	2.59	2.919 (3)	101
C10—H10···O2	0.93	2.57	2.915 (3)	102
C7—H7···O3	0.93	2.47	2.854 (3)	105
O1—H1···O3^{i}	0.82	1.87	2.683 (3)	175
O1—H1···S1^{i}	0.82	2.88	3.638 (2)	154
O4—H4···O2^{ii}	0.82	2.13	2.945 (3)	177
N1—H1C···O4^{iii}	0.892 (10)	2.185 (11)	3.066 (3)	169 (2)
N2—H2C···O1^{iv}	0.895 (10)	2.027 (11)	2.917 (3)	172 (2)
C10—H10···Cg2^{v}	0.93	2.97	3.762 (4)	144

Symmetry codes: (i) −*x*, *y*+1, −*z*+1/2; (ii) −*x*+1/2, *y*−1/2, −*z*+1/2; (iii) *x*−1/2, *y*+1/2, *z*; (iv) *x*+1/2, *y*−1/2, *z*; (v) −*x*+1/2, *y*+1/2, −*z*+1/2.

Fig. 1


O1
C1
N1
C8
C7
C3
C2
C6
O3
C14
C13
C15
C16
N2
O4
C12
C9
C4
C5
S1
C11
C10
O2