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1-(3,4-Dimethoxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one

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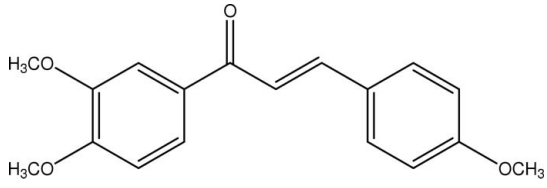
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.001 Å; R factor = 0.049; wR factor = 0.157; data-to-parameter ratio = 31.7.

In the title compound, $C_{18}H_{18}O_4$, the molecule is slightly twisted with a dihedral angle of 17.49 (5)° between the two benzene rings. All of the methoxy substituents lie almost in the planes of the benzene rings to which they are attached. The crystal structure is stabilized by intermolecular C—H···O, C—H···π and π–π interactions.

Related literature

For related literature on hydrogen-bonding motifs, see Bernstein *et al.* (1995) and on values of bond lengths and angles, see Allen *et al.* (1987). For a related structure, see Ng *et al.* (2006).



Experimental

Crystal data

$C_{18}H_{18}O_4$
M_r = 298.32
Triclinic, $P\overline{1}$
a = 8.6745 (2) Å
b = 8.8452 (2) Å
c = 11.3132 (2) Å
α = 108.314 (1)°
β = 102.391 (1)°
γ = 107.237 (1)°
V = 740.35 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100.0 (1) K
0.59 × 0.51 × 0.25 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.883, T_{max} = 0.977
19236 measured reflections
6413 independent reflections
5074 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.157
S = 1.07
6413 reflections
202 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···O1	0.93	2.42	2.775 (1)	102
C11—H11A···O1^{i}	0.93	2.34	3.245 (1)	165
C18—H18B···O1^{ii}	0.96	2.44	3.250 (2)	142
C5—H5A···$Cg2$^{iii}	0.93	3.30	3.604 (1)	102

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $x-1, y, z$; (iii) $x+1, y, z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2294).

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supplementary materials

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1-(3,4-Dimethoxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one

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Comment

We report here the molecular and supramolecular structure of the title compound, (I) (Figure 1).

The bond lengths and angles in (I) have normal values (Allen *et al.*, 1987) and are comparable with those in a related structure (Ng *et al.*, 2006). The molecule is slightly twisted about the C6—C7 bond with the dihedral angle between the two benzene rings (C1—C6 and C10—C15) being 17.49 (5)°. The methoxy groups attached at C3, C4 and C13 lie almost in the planes of the benzene rings to which they are attached (C1—C6 and C10—C15) [C17—O3—C4—C5 = 5.31 (13), C16—O2—C3—C2 = -3.87 (13) and C18—O4—C13—C12 = -0.56 (13)°].

The O1 atom is involved in both intramolecular and intermolecular interactions. An intramolecular C9—H9A···O1 interaction (Table 1 and Figure 1) generates an S(5) ring motif (Bernstein *et al.*, 1995). In the crystal structure, the molecules are linked by intermolecular C11—H11A···O1^{i} hydrogen bonds into cyclic centrosymmetric $R^2_2(14)$ dimers (Bernstein *et al.*, 1995). The dimers are then interlinked by intermolecular C18—H18B···O1^{ii} interactions. The crystal structure is further stablized by intermolecular π···π interactions involving the C1—C6 benzene ring (Centroid Cg1) with a Cg1···Cg1^{iv} distance of 3.5267 (6)Å [symmetry code : (iv) 1-x, 1-y, -z]. In addition, the crystal packing is also stabilized by weak intermolecular C—H···π interactions involving C10—C15 (Centroid Cg2) (Table 1).

Experimental

4-Methoxybenzaldehyde (0.01 mol) and 3,4-dimethoxyacetophenone (0.01 mol) were stirred in 60 ml of methanol at room temperature. 10 ml of 10% aqueous NaOH solution was added and the mixture was stirred for 4 h. The precipitate was filtered, washed with water, dried and the crude product recrystallized from acetone. Crystals suitable for X-ray analysis were grown by slow evaporation of an acetone solution at room temperature.

Refinement

H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.96 Å. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms.

Figures

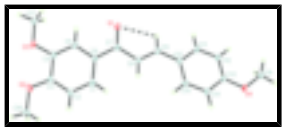

Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The dashed line indicates an intramolecular hydrogen bond.

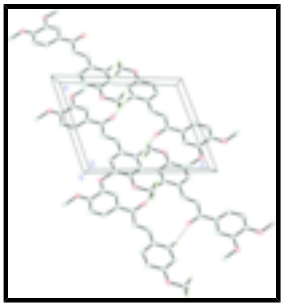

Fig. 2. The crystal packing of (I), viewed down the *b* axis. Intermolecular C—H···O hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

1-(3,4-Dimethoxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one

Crystal data

$C_{18}H_{18}O_4$	$Z = 2$
$M_r = 298.32$	$F_{000} = 316$
Triclinic, $P\overline{1}$	$D_x = 1.338$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.6745$ (2) Å	Cell parameters from 4878 reflections
$b = 8.8452$ (2) Å	$\theta = 2.0$–35.0^o
$c = 11.3132$ (2) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 108.314$ (1)º	$T = 100.0$ (1) K
$\beta = 102.391$ (1)º	Block, yellow
$\gamma = 107.237$ (1)º	0.59 × 0.51 × 0.25 mm
$V = 740.35$ (3) Å^3	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	6413 independent reflections
Radiation source: fine-focus sealed tube	5074 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.035$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 35.0^o$
$T = 297$(2) K	$\theta_{min} = 2.0^o$
ω scans	$h = -13 \rightarrow 13$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$k = -14 \rightarrow 14$
$T_{min} = 0.883$, $T_{max} = 0.977$	$l = -18 \rightarrow 18$
19236 measured reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0906P)^2 + 0.0805P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.050$	$(\Delta/\sigma)_{max} < 0.001$

$wR(F^2) = 0.157$

$S = 1.07$

6413 reflections

202 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$\Delta\rho_{max} = 0.34$ e Å^{-3}

$\Delta\rho_{min} = -0.39$ e Å^{-3}

Extinction correction: none

Special details

Experimental. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
O1	0.60249 (9)	0.91155 (10)	0.34039 (7)	0.02048 (14)
O2	0.68372 (9)	0.50985 (10)	−0.19431 (7)	0.02111 (14)
O3	0.86081 (9)	0.58127 (10)	0.04335 (7)	0.02213 (15)
O4	−0.18166 (9)	1.28476 (10)	0.31923 (7)	0.02137 (15)
C1	0.47983 (11)	0.77178 (12)	−0.01605 (9)	0.01705 (16)
H1A	0.3956	0.8150	−0.0322	0.020*
C2	0.51867 (11)	0.67691 (12)	−0.12132 (9)	0.01841 (16)
H2A	0.4607	0.6580	−0.2073	0.022*
C3	0.64301 (11)	0.61069 (11)	−0.09870 (9)	0.01643 (15)
C4	0.73710 (11)	0.64655 (12)	0.03273 (9)	0.01661 (15)
C5	0.69780 (11)	0.74036 (12)	0.13624 (9)	0.01642 (15)
H5A	0.7587	0.7633	0.2226	0.020*
C6	0.56670 (10)	0.80193 (11)	0.11301 (8)	0.01507 (15)
C7	0.52360 (11)	0.89143 (11)	0.22823 (8)	0.01578 (15)
C8	0.38377 (11)	0.95373 (12)	0.20778 (9)	0.01766 (16)
H8A	0.3353	0.9534	0.1259	0.021*
C9	0.32676 (11)	1.01090 (12)	0.30768 (9)	0.01699 (15)
H9A	0.3795	1.0073	0.3869	0.020*
C10	0.19162 (10)	1.07816 (11)	0.30654 (8)	0.01582 (15)
C11	0.14495 (11)	1.12011 (12)	0.41977 (9)	0.01748 (16)
H11A	0.1991	1.1027	0.4917	0.021*
C12	0.01963 (11)	1.18722 (12)	0.42755 (9)	0.01821 (16)

H12A	−0.0104	1.2132	0.5034	0.022*
C13	−0.06058 (11)	1.21513 (12)	0.32035 (8)	0.01630 (15)
C14	−0.01674 (11)	1.17283 (12)	0.20553 (9)	0.01796 (16)
H14A	−0.0707	1.1910	0.1339	0.022*
C15	0.10662 (11)	1.10416 (12)	0.19840 (9)	0.01709 (15)
H15A	0.1338	1.0748	0.1213	0.021*
C16	0.58389 (14)	0.46028 (14)	−0.32809 (9)	0.02451 (19)
H16A	0.6087	0.3718	−0.3856	0.037*
H16B	0.6115	0.5590	−0.3502	0.037*
H16D	0.4642	0.4166	−0.3386	0.037*
C17	0.94934 (12)	0.59903 (13)	0.17186 (10)	0.02154 (18)
H17A	1.0356	0.5522	0.1670	0.032*
H17D	0.8694	0.5375	0.2042	0.032*
H17B	1.0027	0.7193	0.2309	0.032*
C18	−0.22757 (12)	1.32908 (13)	0.43559 (9)	0.02108 (17)
H18D	−0.3110	1.3791	0.4243	0.032*
H18A	−0.1274	1.4112	0.5102	0.032*
H18B	−0.2752	1.2268	0.4504	0.032*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0224 (3)	0.0271 (3)	0.0163 (3)	0.0155 (3)	0.0059 (2)	0.0091 (3)
O2	0.0253 (3)	0.0256 (3)	0.0189 (3)	0.0158 (3)	0.0120 (2)	0.0086 (3)
O3	0.0213 (3)	0.0314 (4)	0.0223 (3)	0.0196 (3)	0.0094 (2)	0.0117 (3)
O4	0.0239 (3)	0.0321 (4)	0.0195 (3)	0.0212 (3)	0.0110 (2)	0.0124 (3)
C1	0.0180 (3)	0.0192 (4)	0.0180 (3)	0.0113 (3)	0.0065 (3)	0.0087 (3)
C2	0.0213 (4)	0.0216 (4)	0.0168 (3)	0.0127 (3)	0.0071 (3)	0.0089 (3)
C3	0.0186 (3)	0.0181 (4)	0.0174 (3)	0.0100 (3)	0.0093 (3)	0.0083 (3)
C4	0.0155 (3)	0.0191 (4)	0.0201 (4)	0.0102 (3)	0.0079 (3)	0.0095 (3)
C5	0.0156 (3)	0.0193 (4)	0.0177 (3)	0.0104 (3)	0.0059 (3)	0.0082 (3)
C6	0.0156 (3)	0.0163 (3)	0.0164 (3)	0.0088 (3)	0.0065 (3)	0.0073 (3)
C7	0.0160 (3)	0.0172 (4)	0.0172 (3)	0.0095 (3)	0.0062 (3)	0.0076 (3)
C8	0.0174 (3)	0.0213 (4)	0.0177 (3)	0.0116 (3)	0.0061 (3)	0.0083 (3)
C9	0.0162 (3)	0.0195 (4)	0.0184 (3)	0.0101 (3)	0.0062 (3)	0.0084 (3)
C10	0.0149 (3)	0.0181 (4)	0.0166 (3)	0.0090 (3)	0.0058 (3)	0.0071 (3)
C11	0.0188 (3)	0.0216 (4)	0.0159 (3)	0.0119 (3)	0.0064 (3)	0.0084 (3)
C12	0.0198 (3)	0.0239 (4)	0.0160 (3)	0.0136 (3)	0.0080 (3)	0.0085 (3)
C13	0.0163 (3)	0.0192 (4)	0.0171 (3)	0.0110 (3)	0.0070 (3)	0.0073 (3)
C14	0.0187 (3)	0.0237 (4)	0.0165 (3)	0.0128 (3)	0.0073 (3)	0.0093 (3)
C15	0.0177 (3)	0.0215 (4)	0.0164 (3)	0.0115 (3)	0.0079 (3)	0.0081 (3)
C16	0.0313 (5)	0.0269 (5)	0.0176 (4)	0.0143 (4)	0.0105 (3)	0.0076 (3)
C17	0.0193 (4)	0.0255 (4)	0.0237 (4)	0.0140 (3)	0.0064 (3)	0.0104 (4)
C18	0.0220 (4)	0.0261 (4)	0.0193 (4)	0.0154 (3)	0.0094 (3)	0.0072 (3)

Geometric parameters (Å, °)

O1—C7	1.2342 (10)	C9—H9A	0.9300
O2—C3	1.3544 (11)	C10—C11	1.3983 (12)

O2—C16	1.4241 (12)	C10—C15	1.4083 (11)
O3—C4	1.3620 (10)	C11—C12	1.3902 (12)
O3—C17	1.4262 (12)	C11—H11A	0.9300
O4—C13	1.3657 (10)	C12—C13	1.3942 (12)
O4—C18	1.4278 (11)	C12—H12A	0.9300
C1—C6	1.3910 (12)	C13—C14	1.4010 (13)
C1—C2	1.3956 (13)	C14—C15	1.3828 (12)
C1—H1A	0.9300	C14—H14A	0.9300
C2—C3	1.3864 (12)	C15—H15A	0.9300
C2—H2A	0.9300	C16—H16A	0.9600
C3—C4	1.4167 (12)	C16—H16B	0.9600
C4—C5	1.3800 (13)	C16—H16D	0.9600
C5—C6	1.4098 (11)	C17—H17A	0.9600
C5—H5A	0.9300	C17—H17D	0.9600
C6—C7	1.4838 (12)	C17—H17B	0.9600
C7—C8	1.4779 (12)	C18—H18D	0.9600
C8—C9	1.3441 (13)	C18—H18A	0.9600
C8—H8A	0.9300	C18—H18B	0.9600
C9—C10	1.4628 (12)		
C3—O2—C16	117.14 (7)	C12—C11—C10	121.69 (7)
C4—O3—C17	117.36 (7)	C12—C11—H11A	119.2
C13—O4—C18	116.83 (7)	C10—C11—H11A	119.2
C6—C1—C2	120.19 (8)	C11—C12—C13	119.27 (8)
C6—C1—H1A	119.9	C11—C12—H12A	120.4
C2—C1—H1A	119.9	C13—C12—H12A	120.4
C3—C2—C1	120.51 (8)	O4—C13—C12	123.92 (8)
C3—C2—H2A	119.7	O4—C13—C14	116.08 (7)
C1—C2—H2A	119.7	C12—C13—C14	120.00 (8)
O2—C3—C2	124.98 (8)	C15—C14—C13	120.17 (8)
O2—C3—C4	115.27 (7)	C15—C14—H14A	119.9
C2—C3—C4	119.75 (8)	C13—C14—H14A	119.9
O3—C4—C5	126.05 (8)	C14—C15—C10	120.73 (8)
O3—C4—C3	114.64 (8)	C14—C15—H15A	119.6
C5—C4—C3	119.30 (7)	C10—C15—H15A	119.6
C4—C5—C6	120.97 (8)	O2—C16—H16A	109.5
C4—C5—H5A	119.5	O2—C16—H16B	109.5
C6—C5—H5A	119.5	H16A—C16—H16B	109.5
C1—C6—C5	119.19 (8)	O2—C16—H16D	109.5
C1—C6—C7	122.84 (7)	H16A—C16—H16D	109.5
C5—C6—C7	117.94 (7)	H16B—C16—H16D	109.5
O1—C7—C8	120.14 (8)	O3—C17—H17A	109.5
O1—C7—C6	120.16 (7)	O3—C17—H17D	109.5
C8—C7—C6	119.69 (7)	H17A—C17—H17D	109.5
C9—C8—C7	119.90 (8)	O3—C17—H17B	109.5
C9—C8—H8A	120.1	H17A—C17—H17B	109.5
C7—C8—H8A	120.1	H17D—C17—H17B	109.5
C8—C9—C10	127.71 (8)	O4—C18—H18D	109.5
C8—C9—H9A	116.1	O4—C18—H18A	109.5
C10—C9—H9A	116.1	H18D—C18—H18A	109.5

C11—C10—C15	118.12 (7)	O4—C18—H18B	109.5
C11—C10—C9	118.06 (7)	H18D—C18—H18B	109.5
C15—C10—C9	123.82 (8)	H18A—C18—H18B	109.5
C6—C1—C2—C3	0.48 (14)	C1—C6—C7—C8	−0.50 (13)
C16—O2—C3—C2	−3.87 (13)	C5—C6—C7—C8	−178.33 (8)
C16—O2—C3—C4	175.61 (8)	O1—C7—C8—C9	−9.03 (14)
C1—C2—C3—O2	176.43 (8)	C6—C7—C8—C9	169.93 (8)
C1—C2—C3—C4	−3.03 (13)	C7—C8—C9—C10	179.49 (8)
C17—O3—C4—C5	5.31 (13)	C8—C9—C10—C11	175.84 (9)
C17—O3—C4—C3	−174.36 (8)	C8—C9—C10—C15	−4.59 (15)
O2—C3—C4—O3	3.21 (11)	C15—C10—C11—C12	−0.60 (14)
C2—C3—C4—O3	−177.28 (8)	C9—C10—C11—C12	179.00 (8)
O2—C3—C4—C5	−176.47 (8)	C10—C11—C12—C13	−0.64 (14)
C2—C3—C4—C5	3.04 (13)	C18—O4—C13—C12	−0.56 (13)
O3—C4—C5—C6	179.83 (8)	C18—O4—C13—C14	−179.84 (8)
C3—C4—C5—C6	−0.53 (13)	C11—C12—C13—O4	−178.15 (8)
C2—C1—C6—C5	2.03 (13)	C11—C12—C13—C14	1.10 (14)
C2—C1—C6—C7	−175.77 (8)	O4—C13—C14—C15	178.99 (8)
C4—C5—C6—C1	−2.00 (13)	C12—C13—C14—C15	−0.31 (14)
C4—C5—C6—C7	175.91 (8)	C13—C14—C15—C10	−0.96 (14)
C1—C6—C7—O1	178.46 (8)	C11—C10—C15—C14	1.40 (13)
C5—C6—C7—O1	0.63 (13)	C9—C10—C15—C14	−178.17 (8)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9A···O1	0.93	2.42	2.775 (1)	102
C11—H11A···O1^{i}	0.93	2.34	3.245 (1)	165
C18—H18B···O1^{ii}	0.96	2.44	3.250 (2)	142
C5—H5A···Cg2^{iii}	0.93	3.30	3.604 (1)	102

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

Fig. 1

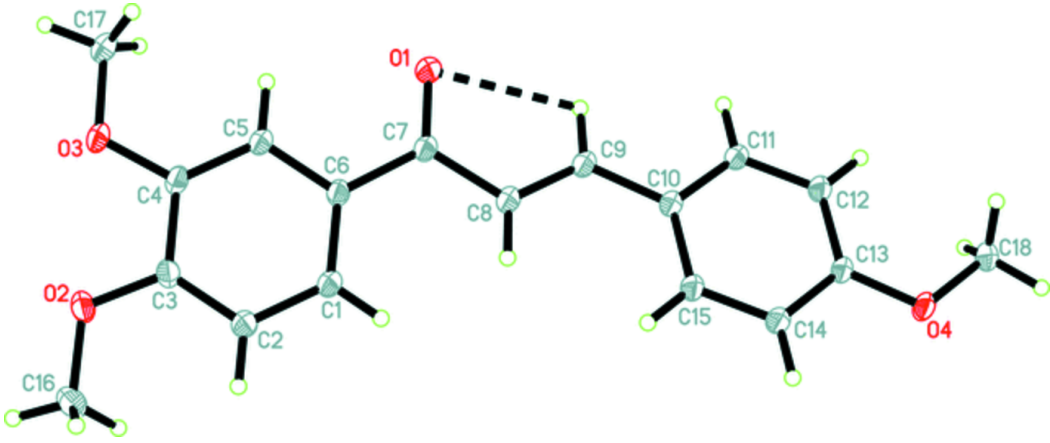
C17
O1
O3
C5
C7
C9
C11
C6
C4
C8
C10
C12
C13
C18
O2
C3
C1
C15
O4
C2
C14
C16

Fig. 2