

## 6-[4-(2-Chloroethoxy)naphthyl]fulvene. Corrigendum

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In the paper by Li, Ma, Huang & Dong [*Acta Cryst.* (2005), **E61**, o3901–o3902], the correspondence author is incorrectly indicated. The correct correspondence author is given here, together with revised postal and e-mail addresses.

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## Key indicators

Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$   
 $R$  factor = 0.062  
 $wR$  factor = 0.145  
Data-to-parameter ratio = 17.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## 6-[4-(2-Chloroethoxy)naphthyl]fulvene

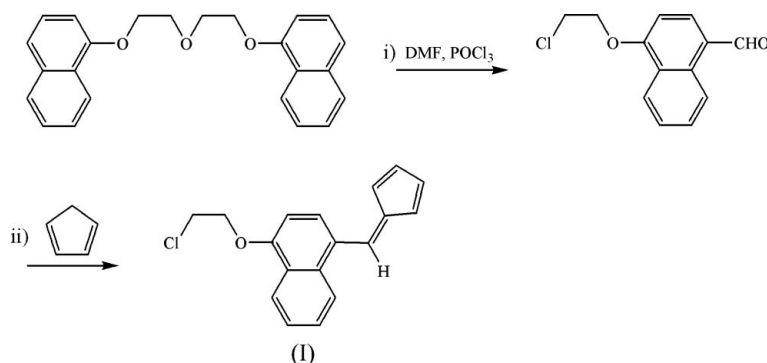
The title compound,  $\text{C}_{18}\text{H}_{15}\text{ClO}$ , has been synthesized by reacting cyclopentadiene with 4-(2-chloroethoxy)naphthaldehyde. The naphthalene and cyclopentadienyl rings make a dihedral angle of  $42.4 (1)^\circ$ .

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## Comment

Fulvene is widely used in organic synthesis because of its special structure and characteristic reactivity (Stone & Little, 1984). It is well known that fulvene is a good candidate for the synthesis of organometallic coordination polymers or supramolecular complexes (Wang *et al.*, 2003).

We prepared the title compound, (I), which is a new fulvene derivative (see scheme). Single-crystal analysis of (I) reveals that the asymmetric unit consists of one molecule (Fig. 1). The naphthalene and cyclopentadienyl rings make a dihedral angle of  $42.4 (1)^\circ$ . The dihedral angle between the plane defined by atoms O1/C11/C12 and the naphthalene ring plane is  $7.9 (2)^\circ$ . The largest dimension of the molecule, estimated as the  $\text{Cl1} \cdots \text{H3}$  separation, is  $12.65\text{ \AA}$  (H3 is bonded to C3). Other dimensions (Table 1) are as expected.

## Experimental

All organic solvents were of reagent grade and were used without further purification. Cyclopentadiene and 4-(2-chloroethoxy)naphthaldehyde were prepared according to the literature methods (Korach *et al.*, 1973; Wang *et al.*, 2003). A solution of tetrahydropyrrole (0.5 ml) in methanol (5 ml) was added to a solution of 4-(2-chloroethoxy)naphthaldehyde (0.75 g, 3.20 mmol) and cyclopentadiene (1.17 ml, 14 mmol) in  $\text{CH}_2\text{Cl}_2$  (10 ml). The mixture was stirred overnight at 298 K, and then acetic acid (0.42 ml) and water (5 ml) were added. The product was extracted with  $\text{CH}_2\text{Cl}_2$  and purified by column chromatography on silica gel using  $\text{CH}_2\text{Cl}_2$  as eluant to afford (I) as an orange solid (0.75 g, 83%). Single crystals of (I) were obtained by layering *n*-hexane on to a  $\text{CH}_2\text{Cl}_2$  solution of the crude reaction product. Single crystals were obtained after a period of one week at 298 K.

Crystal data

C<sub>18</sub>H<sub>15</sub>ClO  
*M<sub>r</sub>* = 282.75  
 Orthorhombic, *Pbca*  
*a* = 12.764 (9) Å  
*b* = 7.361 (5) Å  
*c* = 31.03 (2) Å  
*V* = 2915 (4) Å<sup>3</sup>  
*Z* = 8  
*D<sub>x</sub>* = 1.288 Mg m<sup>-3</sup>

Mo *K*α radiation  
 Cell parameters from 1401 reflections  
 $\theta = 3.1\text{--}20.1^\circ$   
 $\mu = 0.25\text{ mm}^{-1}$   
*T* = 298 (2) K  
 Needle, orange  
 0.40 × 0.12 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (*SADABS*; Bruker, 1999)  
*T<sub>min</sub>* = 0.905, *T<sub>max</sub>* = 0.982  
 16129 measured reflections

3175 independent reflections  
 1764 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.071  
 $\theta_{\text{max}} = 27.0^\circ$   
*h* = -15 → 16  
*k* = -9 → 8  
*l* = -39 → 39

Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.062  
*wR*(*F*<sup>2</sup>) = 0.145  
*S* = 1.02  
 3175 reflections  
 181 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2 + 0.0844P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.15\text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.17\text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

C1—C2	1.324 (3)	C10—O1	1.362 (3)
C3—C4	1.332 (4)	C11—O1	1.428 (3)
C5—C6	1.345 (3)	C11—C12	1.489 (3)
C6—C7	1.457 (3)	C12—C11	1.770 (3)
C5—C6—C7	127.5 (2)	C10—O1—C11	118.32 (19)

All H atoms were included in calculated positions and refined as riding on their carrier C atoms, with *U<sub>iso</sub>*(H) = 1.2*U<sub>eq</sub>*(C) and C—H

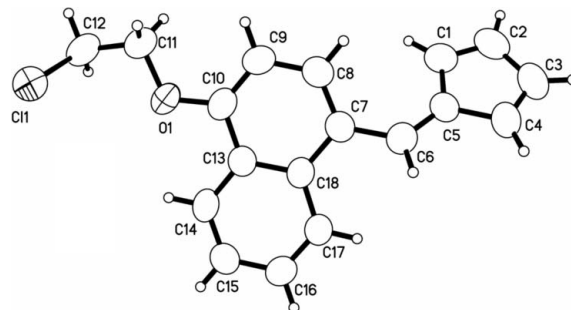


Figure 1

The structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

distances constrained to 0.93 (aromatic CH) or 0.97 Å (methylene CH<sub>2</sub>).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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