

(1*RS*,4*RS*)-1-Methoxyspiro[bicyclo[2.2.2]oct-5-ene-2,2'-[1',3']dithiolane]. Corrigendum

Zeynep Gültekin,^a Harry Adams^b
 and Tuncer Hökelek^{c*}

^aZonguldak Karaelmas University, Department of Chemistry, 067100 Zonguldak, Turkey,

^bUniversity of Sheffield, Department of Chemistry, Sheffield S3 7HF, England, and ^cHacettepe University, Department of Physics, 06532 Beytepe Ankara, Turkey

Correspondence e-mail:
 merzifon@hacettepe.edu.tr

Key indicators

Single-crystal X-ray study
 T = 293 K
 Mean $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$
 R factor = 0.058
 wR factor = 0.144
 Data-to-parameter ratio = 14.9

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

In the paper by Gültekin, Adams & Hökelek [*Acta Cryst.* (2003), **E59**, o926–o928], the placement of H atoms bonded to C3, C4, C10 and C11 is wrong. C10=C11 is a double bond, but there are two H atoms on each C atom instead of one. On the other hand, C3–C4 is a single bond and there is one H atom on each C atom instead of two. The structure has now been re-refined with the correct assignment of H atoms and the structure is shown in Fig. 1.

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Experimental

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.144$
 $S = 1.02$
 1983 reflections
 133 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0805P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.30 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$

Table 1
 Selected geometric parameters (\AA , $^\circ$).

S1–C7	1.802 (5)	C2–C1	1.558 (5)
S1–C2	1.823 (4)	C2–C6	1.566 (5)
S2–C8	1.774 (7)	C4–C3	1.511 (7)
S2–C2	1.844 (4)	C4–C5	1.529 (7)
O1–C1	1.416 (4)	C5–C6	1.536 (8)
O1–C9	1.420 (5)	C7–C8	1.467 (9)
C1–C10	1.506 (6)	C11–C10	1.332 (7)
C1–C3	1.516 (6)	C11–C5	1.502 (7)
C7–S1–C2	97.3 (2)	C1–C2–S2	110.7 (3)
C8–S2–C2	99.3 (2)	C6–C2–S2	110.4 (3)
C1–O1–C9	116.2 (3)	S1–C2–S2	106.1 (2)
O1–C1–C10	114.9 (3)	C4–C3–C1	112.1 (3)
O1–C1–C3	112.7 (3)	C4–C5–C6	106.0 (4)
O1–C1–C2	106.6 (3)	C8–C7–S1	109.5 (4)
C3–C1–C2	107.1 (3)	C7–C8–S2	114.0 (4)
C1–C2–S1	113.8 (2)	C11–C10–C1	114.7 (4)
C6–C2–S1	108.4 (3)	C10–C11–C5	114.0 (4)
C7–S1–C2–S2	30.0 (3)	C9–O1–C1–C3	–70.9 (5)
C2–S1–C7–C8	–37.9 (5)	S1–C2–C1–O1	56.8 (4)
C2–S2–C8–C7	–9.2 (5)	S2–C2–C1–O1	–62.5 (3)
C8–S2–C2–S1	–15.6 (3)	S1–C7–C8–S2	31.2 (6)

Atoms H10 and H11 were located in a difference map and refined isotropically [C–H = 0.96 (2)–0.99 (2) \AA]. The other H atoms were positioned geometrically, with C–H = 0.96, 0.97 and 0.98 \AA for methyl, methylene and methine H atoms, respectively, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{carrier atom})$, where $x = 1.5$ for methyl H atoms and $x = 1.2$ for all others.

Data collection: XSCANS (Siemens, 1996); cell refinement: XSCANS; data reduction: SHELXTL (Bruker, 1997); program(s)

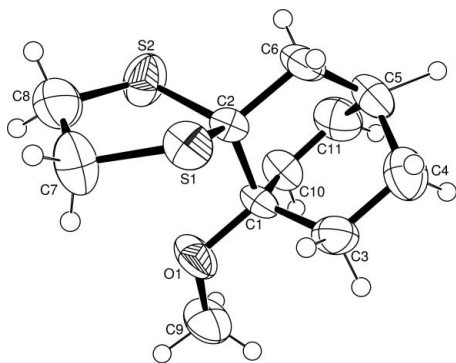


Figure 1

A view of the molecular structure, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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