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1-Adamantyl propargyl ether

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.039
wR factor = 0.092
Data-to-parameter ratio = 14.2

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

1-Adamantyl propargyl ether, $C_{13}H_{18}O$, crystallizes in the 'extended' conformation with a close contact between the acetylenic H atom and the O atom of an adjacent molecule.

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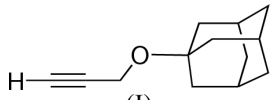
Comment

1-Adamantyl propargyl ether, (I), has been found to selectively inactivate the 2B5 form of rabbit cytochrome P-450 (Strobel *et al.*, 1999). In order to provide data for computer-modelling studies of the docking of (I) with the enzyme, the structure of (I) (Fig. 1) was determined. The compound crystallizes in the 'extended' conformation as the result of weak hydrogen bonding between the acetylenic H atom (H13 attached to C13) and the O atom of a neighboring molecule. This leads to the formation of spiral chains of molecules running parallel to the *a* axis. (Fig. 2 and Table 1).



(I)

Experimental

Compound (I) was prepared as reported in the literature (Strobel *et al.*, 1999) and recrystallized from a propan-2-ol/water mixture.

Crystal data

$C_{13}H_{18}O$
M_r = 190.27
Orthorhombic, $P2_12_12_1$
a = 7.4432 (2) Å
b = 10.9094 (2) Å
c = 13.2137 (4) Å
V = 1072.96 (5) Å^3
Z = 4
D_x = 1.178 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10416 reflections
θ = 2.5–30.0°
μ = 0.07 mm^{-1}
T = 120 (2) K
Block, colorless
0.23 × 0.18 × 0.17 mm

Data collection

Nonius KappaCCD diffractometer (with Oxford Cryosystems Cryostream cooler)
ω scans with κ offsets
Absorption correction: multi-scan (*HKL SCALEPAK*; Otwinowski & Minor, 1997)
T_{min} = 0.984, T_{max} = 0.988
10 416 measured reflections
1808 independent reflections
1579 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 30.0°
$h = -10 \rightarrow 10$
$k = -15 \rightarrow 15$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.092
S = 1.02
1808 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 0.2443P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

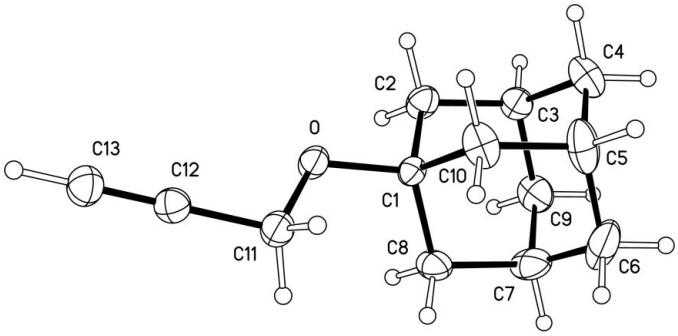


Figure 1
Perspective view of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by spheres of arbitrary radii.

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O^{i}	0.95	2.35	3.251 (2)	158

Symmetry code: (i) $\frac{1}{2}+x, \frac{3}{2}-y, 2-z$.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO* and *SCALEPAK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPAK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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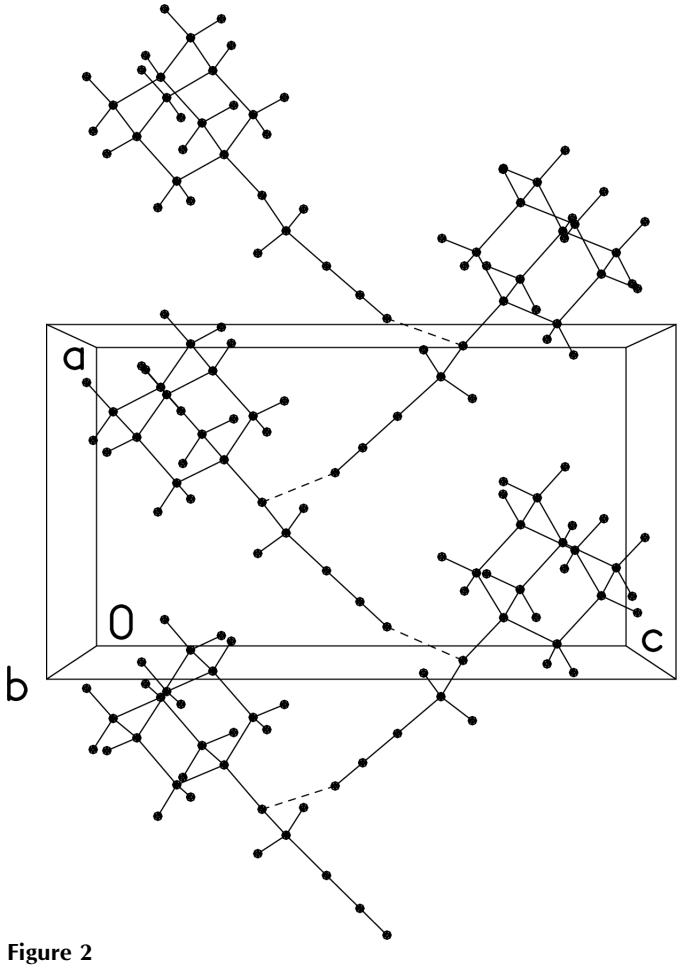

Figure 2
View of the hydrogen-bonding interaction in (I).

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