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trans,trans-Tricyclo[7.3.1.$0^{5,13}$]tridec-1-en-3-one

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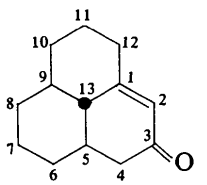
Abstract. $C_{13}H_{18}O$, $M_r = 190{\cdot}3$, monoclinic, $P2_1/c$, $a = 5{\cdot}61$ (1), $b = 11{\cdot}39$ (1), $c = 16{\cdot}84$ (2) Å, $\beta = 98{\cdot}90$ (2)° (from diffractometer measurements, Mo $K\bar{\alpha}$ radiation), $V = 1063{\cdot}3$ Å^3, $Z = 4$, $D_c = 1{\cdot}19$ Mg m^{-3}, $F(000) = 416$, $\mu = 0{\cdot}039$ mm^{-1}, approximate crystal dimensions $0{\cdot}45 \times 0{\cdot}1 \times 0{\cdot}1$ mm. The geometry of the ring fusion is *trans,trans*.

Introduction. The title compound (I) was recrystallized from a THF/petrol mixture.



(I)

Systematic absences (from precession photographs) *h*0*l*, *l* odd, and 0*k*0, *k* odd, indicated space group $P2_1/c$. Data were collected for 0–4*kl* with $\theta_{max} = 22{\cdot}5°$ on a Stoe STADI-2 two-circle diffractometer with graphite-monochromated Mo $K\bar{\alpha}$ radiation. This gave 1032 data of which 523 unique reflexions with $I > 3\sigma(I)$ were used in subsequent calculations. Lorentz and polarization corrections (but none for extinction or absorption) were applied, and the data scaled by a Wilson plot. The structure was solved by direct methods with *SHELX* 76 (Sheldrick, 1976), which was used for all calculations. Complex neutral atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Weighted full-matrix least-squares refinement (including isotropic H atoms) converged at $R = 0{\cdot}060$ for 523 observed reflexions ($R = \sum||F_o| - |F_c||/\sum|F_o|$); $R_w = 0{\cdot}050$ [$R_w = \sum(|F_o| - |F_c||w^{1/2})/\sum(|F_o|w^{1/2})$, $w = 3{\cdot}93/[\sigma^2(F_o) + 0{\cdot}00009F_o^2]$]. In the final cycle all shifts in parameters

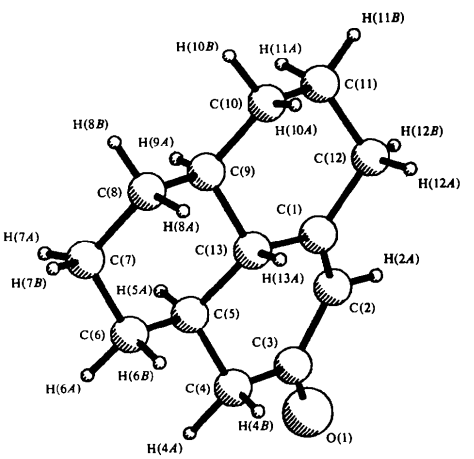


Fig. 1. General view of the molecule.

Table 1. *Fractional atomic coordinates* ($\times 10^4$) *with e.s.d.'s in parentheses*

	x	*y*	*z*
C(1)	4642 (19)	3883 (6)	6104 (5)
C(2)	2850 (20)	4080 (7)	5502 (5)
C(3)	2706 (20)	3505 (7)	4723 (5)
C(4)	4663 (24)	2667 (10)	4614 (6)
C(5)	5738 (21)	2067 (7)	5392 (5)
C(6)	7715 (23)	1210 (10)	5311 (6)
C(7)	8687 (32)	600 (11)	6100 (7)
C(8)	9427 (25)	1476 (9)	6788 (6)
C(9)	7336 (24)	2317 (8)	6861 (5)
C(10)	7908 (30)	3178 (11)	7552 (6)
C(11)	5772 (24)	3938 (10)	7619 (5)
C(12)	4991 (27)	4635 (8)	6859 (5)
C(13)	6531 (22)	2953 (8)	6057 (4)
O(1)	1032 (13)	3705 (5)	4176 (3)
H(2*A*)	1678 (104)	4688 (45)	5546 (28)
H(4*A*)	3702 (151)	2062 (61)	4144 (44)
H(4*B*)	5968 (140)	3014 (52)	4430 (37)
H(5*A*)	4312 (144)	1661 (47)	5552 (36)
H(6*A*)	7258 (121)	611 (50)	4879 (35)
H(6*B*)	8760 (178)	1619 (71)	5080 (47)
H(7*A*)	7245 (212)	46 (80)	6085 (60)
H(7*B*)	10251 (146)	144 (59)	6096 (39)
H(8*A*)	10823 (170)	1969 (54)	6692 (42)
H(8*B*)	9826 (106)	1024 (45)	7302 (31)
H(9*A*)	5898 (151)	1892 (51)	6922 (39)
H(10*A*)	9345 (172)	3589 (68)	7603 (47)
H(10*B*)	8638 (140)	2655 (59)	8070 (40)
H(11*A*)	4345 (160)	3420 (60)	7740 (42)
H(11*B*)	5712 (135)	4416 (52)	8104 (39)
H(12*A*)	6403 (139)	5177 (56)	6816 (38)
H(12*B*)	3411 (167)	4985 (61)	6896 (46)
H(13*A*)	8022 (147)	3346 (52)	6046 (39)

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Table 2. *Bond distances* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

C(1)–C(2)	1·332 (9)	C(5)–C(13)	1·522 (9)	C(2)–H(2*A*)	0·966 (54)	C(8)–H(8*B*)	1·002 (52)
C(1)–C(12)	1·520 (10)	C(6)–C(7)	1·524 (13)	C(4)–H(4*A*)	1·123 (77)	C(9)–H(9*A*)	0·959 (75)
C(1)–C(13)	1·509 (11)	C(7)–C(8)	1·536 (13)	C(4)–H(4*B*)	0·927 (72)	C(10)–H(10*A*)	0·924 (87)
C(2)–C(3)	1·457 (9)	C(8)–C(9)	1·534 (11)	C(5)–H(5*A*)	0·996 (72)	C(10)–H(10*B*)	1·083 (67)
C(3)–C(4)	1·487 (11)	C(9)–C(10)	1·519 (13)	C(6)–H(6*A*)	1·001 (57)	C(11)–H(11*A*)	1·040 (85)
C(3)–O(1)	1·230 (8)	C(9)–C(13)	1·540 (10)	C(6)–H(6*B*)	0·885 (92)	C(11)–H(11*B*)	0·987 (63)
C(4)–C(5)	1·518 (11)	C(10)–C(11)	1·497 (12)	C(7)–H(7*A*)	1·024 (109)	C(12)–H(12*A*)	1·015 (72)
C(5)–C(6)	1·500 (11)	C(11)–C(12)	1·512 (11)	C(7)–H(7*B*)	1·020 (77)	C(12)–H(12*B*)	0·983 (86)
				C(8)–H(8*A*)	0·997 (86)	C(13)–H(13*A*)	0·951 (75)

C(12)–C(1)–C(2)	121·7 (9)	H(2*A*)–C(2)–C(1)	120·4 (31)	H(8*B*)–C(8)–C(9)	108·8 (34)
C(13)–C(1)–C(2)	122·1 (8)	H(2*A*)–C(2)–C(3)	116·5 (31)	H(8*B*)–C(8)–H(8*A*)	110·7 (54)
C(13)–C(1)–C(12)	116·0 (9)	H(4*A*)–C(4)–C(3)	101·4 (42)	H(9*A*)–C(9)–C(8)	111·0 (42)
C(3)–C(2)–C(1)	122·7 (10)	H(4*A*)–C(4)–C(5)	114·6 (34)	H(9*A*)–C(9)–C(10)	109·0 (43)
C(4)–C(3)–C(2)	117·4 (9)	H(4*B*)–C(4)–C(3)	113·8 (42)	H(9*A*)–C(9)–C(13)	101·2 (41)
O(1)–C(3)–C(2)	121·4 (10)	H(4*B*)–C(4)–C(5)	104·6 (41)	H(10*A*)–C(10)–C(9)	118·4 (54)
O(1)–C(3)–C(4)	121·2 (8)	H(4*B*)–C(4)–H(4*A*)	110·1 (57)	H(10*A*)–C(10)–C(11)	113·4 (55)
C(5)–C(4)–C(3)	112·6 (9)	H(5*A*)–C(5)–C(4)	102·3 (37)	H(10*B*)–C(10)–C(9)	105·8 (36)
C(6)–C(5)–C(4)	114·5 (9)	H(5*A*)–C(5)–C(6)	111·0 (37)	H(10*B*)–C(10)–C(11)	117·8 (41)
C(13)–C(5)–C(4)	111·6 (7)	H(5*A*)–C(5)–C(13)	105·4 (36)	H(10*B*)–C(10)–H(10*A*)	89·3 (61)
C(13)–C(5)–C(6)	111·3 (9)	H(6*A*)–C(6)–C(5)	113·6 (40)	H(11*A*)–C(11)–C(10)	109·6 (41)
C(7)–C(6)–C(5)	112·7 (9)	H(6*A*)–C(6)–C(7)	109·9 (34)	H(11*A*)–C(11)–C(12)	109·5 (39)
C(8)–C(7)–C(6)	112·4 (10)	H(6*B*)–C(6)–C(5)	104·3 (57)	H(11*B*)–C(11)–C(10)	120·7 (44)
C(9)–C(8)–C(7)	110·2 (10)	H(6*B*)–C(6)–C(7)	116·8 (56)	H(11*B*)–C(11)–C(12)	111·7 (36)
C(10)–C(9)–C(8)	113·0 (10)	H(6*B*)–C(6)–H(6*A*)	98·8 (61)	H(11*B*)–C(11)–H(11*A*)	91·4 (56)
C(13)–C(9)–C(8)	110·3 (8)	H(7*A*)–C(7)–C(6)	94·8 (61)	H(12*A*)–C(12)–C(1)	106·6 (39)
C(13)–C(9)–C(10)	111·7 (8)	H(7*A*)–C(7)–C(8)	122·7 (59)	H(12*A*)–C(12)–C(11)	104·6 (40)
C(11)–C(10)–C(9)	110·7 (11)	H(7*B*)–C(7)–C(6)	114·7 (39)	H(12*B*)–C(12)–C(1)	106·4 (45)
C(12)–C(11)–C(10)	111·8 (10)	H(7*B*)–C(7)–C(8)	101·7 (41)	H(12*B*)–C(12)–C(11)	107·7 (48)
C(11)–C(12)–C(1)	113·3 (9)	H(7*B*)–C(7)–H(7*A*)	111·2 (61)	H(12*B*)–C(12)–H(12*A*)	118·6 (59)
C(5)–C(13)–C(1)	112·1 (8)	H(8*A*)–C(8)–C(7)	111·8 (43)	H(13*A*)–C(13)–C(1)	107·3 (38)
C(9)–C(13)–C(1)	113·3 (8)	H(8*A*)–C(8)–C(9)	106·9 (42)	H(13*A*)–C(13)–C(5)	117·1 (42)
C(9)–C(13)–C(5)	110·3 (7)	H(8*B*)–C(8)–C(7)	108·5 (28)	H(13*A*)–C(13)–C(9)	95·7 (41)

were less than their e.s.d.'s. Positional parameters are given in Table 1, bond distances and angles in Table 2.*

Discussion. The compound (Fig. 1) is an intermediate in the synthesis of a series of substituted *trans,trans*-tricyclo[7.3.1.0^{5,13}]tridecanes (Maskill, 1978), and structure analysis has confirmed the geometry of ring fusion.

* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33938 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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