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Structure of Tris(5-acetyl-3-thienyl)methane–*n*-Hexane (3/1) Inclusion Compound

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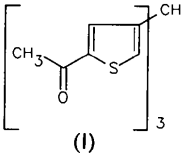
Abstract. $3C_{19}H_{16}O_3S_3.C_6H_{14}$, $M_r = 1251.7$, triclinic, $P\bar{1}$, $a = 20.604$ (5), $b = 12.694$ (5), $c = 12.647$ (5) Å, $\alpha = 93.64$ (5), $\beta = 105.69$ (5), $\gamma = 85.89$ (5)°, $V = 3173$ (1) Å^3, $Z = 2$, $D_x = 1.31$ Mg m^{-3}, λ(Mo $K\alpha$) = 0.7107 Å, $\mu = 0.353$ mm^{-1}, $F(000) = 1312$, $T = 298$ K, final $wR = 0.061$, $R = 0.100$ for 6841 observed reflections with $F > \sigma(F_o)$ and 723 variable parameters. The structure consists of three tris(5-acetyl-3-thienyl)methane host molecules and one *n*-hexane guest molecule. The *n*-hexane molecules fill the channels formed by two acetylthienyl groups from each host. The remaining group links the host molecules into parallel stacks with alternating orientation.

Experimental. The host molecule (I), tris(5-acetyl-3-thienyl)methane (TATM), is formed by the reaction of chloroform and 2-acetylthiophene (Yakubov, Sudarushkin, Belenkii & Gold'farb, 1973) and crystallization with many solvents yields 2/1 solute/solvent complexes (Bin Din & Meth-Cohn, 1977). Crystallization of TATM with *n*-hexane gave yellowish crystals with approximate dimensions 0.3 × 0.3 × 0.3 mm; m.p. 379–383 K. A Philips PW 1100



(I)

diffractometer was used for data collection with graphite-monochromated Mo radiation. The unit cell was determined and optimized from 25 reflections in the range $24 \le 2\theta \le 30°$. 8955 reflections for $6 \le 2\theta \le 56°$ in the range $-22 \le h \le 22$, $-13 \le k \le 13$, $0 \le l \le 13$ were measured using $\omega/2\theta$ scans, scan speed 0.0384° s^{-1} and scan width 1.6°. 8346 reflections were unique ($R_{int} = 0.0416$) and 6841 reflections were considered observed with $F > \sigma(F_o)$. Crystal stability was tested by measuring three standard reflections every hour (no decay). No absorption corrections were applied; Lorentz–polarization corrections were made.

The structure was solved with *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), and refined by blocked-full-matrix least

Table 1. *Fractional coordinates* (× 10^4) *and isotropic/equivalent isotropic thermal factors* (Å^2 × 10^3)

Hexane atoms C(58)—C(63) were refined isotropically. Equivalent isotropic thermal parameters for anisotropically refined atoms are given by $U_{eq} = (1/3)\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	*y*	*z*	U_{iso}/U_{eq}
C(1)	7700 (3)	4614 (4)	5932 (4)	42 (1)
S(1)	9211 (1)	2724 (1)	7706 (1)	62 (1)
C(2)	8799 (3)	3893 (5)	7227 (5)	54 (1)
C(3)	8182 (3)	3755 (4)	6515 (4)	41 (4)
C(4)	8035 (3)	2675 (4)	6362 (5)	47 (1)
C(5)	8549 (3)	2021 (5)	6948 (5)	51 (1)
C(6)	8597 (4)	864 (5)	7013 (6)	63 (2)
O(1)	9103 (3)	425 (3)	7589 (4)	82 (1)
C(7)	8008 (3)	261 (5)	6341 (6)	85 (2)
S(2)	7692 (1)	4882 (2)	2780 (1)	80 (1)
C(8)	7401 (3)	4606 (5)	3855 (5)	62 (2)
C(9)	7844 (3)	4833 (4)	4845 (5)	48 (1)
C(10)	8449 (3)	5244 (4)	4717 (5)	48 (1)
C(11)	8429 (3)	5329 (4)	3648 (5)	55 (1)
C(12)	8923 (4)	5723 (5)	3159 (6)	73 (2)
O(2)	8806 (3)	5776 (4)	2162 (4)	101 (1)
C(13)	9583 (3)	6040 (5)	3874 (6)	79 (2)
S(3)	7541 (1)	7517 (1)	7371 (1)	60 (1)
C(14)	7670 (3)	6612 (4)	6378 (5)	49 (1)
C(15)	7666 (3)	5591 (5)	6654 (5)	40 (1)
C(16)	7566 (3)	5555 (5)	7698 (5)	48 (1)
C(17)	7487 (3)	6545 (5)	8207 (5)	47 (1)
C(18)	7366 (3)	6795 (5)	9291 (5)	52 (1)
O(3)	7284 (2)	7710 (3)	9588 (3)	69 (1)
C(19)	7296 (3)	5894 (5)	9962 (5)	78 (2)
C(20)	9163 (3)	9217 (4)	10837 (4)	49 (1)
S(4)	9320 (1)	6302 (1)	9458 (1)	57 (1)
C(21)	9188 (3)	7233 (4)	10440 (5)	51 (1)
C(22)	9206 (3)	8227 (4)	10131 (5)	44 (1)
C(23)	9310 (3)	8261 (5)	9087 (5)	48 (1)
C(24)	9393 (3)	7272 (5)	8610 (5)	47 (1)
C(25)	9506 (3)	6980 (5)	7536 (5)	56 (1)
O(4)	9563 (2)	6063 (3)	7243 (3)	74 (1)
C(26)	9532 (4)	7836 (5)	6798 (5)	95 (2)
S(5)	7600 (1)	10997 (1)	9009 (1)	67 (1)
C(27)	8047 (3)	9881 (5)	9518 (5)	60 (1)
C(28)	8657 (3)	10065 (5)	10218 (5)	48 (1)
C(29)	8766 (3)	11149 (5)	10341 (5)	51 (1)
C(30)	8231 (3)	11754 (5)	9727 (5)	53 (1)
C(31)	8147 (4)	12903 (6)	9618 (6)	68 (2)
O(5)	7658 (3)	13302 (3)	8988 (4)	88 (1)
C(32)	8710 (3)	13578 (5)	10321 (6)	87 (2)
S(6)	9105 (1)	8989 (2)	13982 (1)	79 (1)
C(33)	9424 (3)	9244 (5)	12908 (5)	64 (2)
C(34)	9002 (3)	9020 (4)	11911 (5)	51 (1)
C(35)	8384 (3)	8639 (4)	12001 (5)	55 (1)
C(36)	8356 (3)	8559 (5)	13088 (5)	60 (2)
C(37)	7834 (4)	8203 (5)	13517 (6)	72 (2)
O(6)	7924 (3)	8203 (4)	14512 (4)	106 (1)
C(38)	7203 (4)	7844 (6)	12728 (6)	96 (2)
C(39)	4348 (3)	2883 (4)	2347 (5)	50 (1)
S(7)	4126 (1)	4408 (1)	5146 (1)	60 (1)
C(40)	4275 (3)	3346 (5)	4336 (5)	54 (1)
C(41)	4276 (3)	3641 (5)	3299 (5)	48 (1)
C(42)	4153 (3)	4746 (4)	3194 (5)	46 (1)
C(43)	4068 (3)	5273 (5)	4132 (5)	47 (1)
C(44)	3919 (3)	6387 (5)	4304 (5)	56 (1)
O(7)	3818 (2)	6728 (3)	5176 (3)	69 (1)
C(45)	3878 (3)	7114 (5)	3398 (5)	77 (2)
S(8)	5852 (1)	3971 (2)	1325 (2)	81 (1)
C(46)	5441 (3)	3671 (5)	2260 (5)	66 (2)
C(47)	4841 (3)	3242 (5)	1768 (5)	51 (1)

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Table 1 (*cont.*)

	x	*y*	*z*	U_{iso}/U_{eq}
C(48)	4706 (3)	3153 (5)	616 (5)	54 (1)
C(49)	5215 (4)	3512 (5)	263 (5)	63 (2)
C(50)	5272 (4)	3599 (6)	−869 (6)	81 (2)
O(8)	5746 (3)	4000 (4)	−1042 (4)	112 (2)
C(51)	4714 (4)	3186 (6)	−1784 (5)	112 (2)
S(9)	4378 (1)	−258 (1)	2566 (2)	80 (1)
C(52)	4068 (3)	962 (5)	2162 (5)	64 (2)
C(53)	4491 (3)	1725 (5)	2632 (5)	50 (1)
C(54)	5096 (3)	1326 (5)	3371 (5)	54 (1)
C(55)	5096 (3)	247 (5)	3411 (5)	57 (1)
C(56)	5621 (4)	−481 (6)	4059 (6)	75 (2)
O(9)	5527 (3)	−1428 (4)	3990 (4)	102 (1)
C(57)	6257 (3)	−68 (5)	4787 (5)	85 (2)
C(58)	8563 (6)	2051 (9)	3562 (9)	226 (2)
C(59)	7873 (6)	1677 (10)	3232 (11)	226 (2)
C(60)	7448 (7)	1433 (10)	2238 (10)	226 (2)
C(61)	6833 (7)	1056 (10)	2114 (10)	226 (2)
C(62)	6437 (7)	747 (10)	1104 (11)	226 (2)
C(63)	5840 (6)	243 (9)	831 (9)	226 (2)

Table 2. *Bond lengths* (Å) *and valence angles* (°)

C(1)—C(3)	1.506 (7)	C(1)—C(9)	1.528 (9)
C(1)—C(15)	1.502 (8)	S(1)—C(2)	1.716 (6)
S(1)—C(5)	1.713 (6)	C(2)—C(3)	1.359 (7)
C(3)—C(4)	1.416 (8)	C(4)—C(5)	1.375 (8)
C(5)—C(6)	1.471 (9)	C(6)—O(1)	1.218 (8)
C(6)—C(7)	1.508 (9)	S(2)—C(8)	1.692 (7)
S(2)—C(11)	1.725 (6)	C(8)—C(9)	1.362 (8)
C(9)—C(10)	1.438 (10)	C(10)—C(11)	1.353 (9)
C(11)—C(12)	1.457 (12)	C(12)—O(2)	1.223 (9)
C(12)—C(13)	1.482 (10)	S(3)—C(14)	1.709 (6)
S(3)—C(17)	1.703 (6)	C(14)—C(15)	1.364 (8)
C(15)—C(16)	1.395 (9)	C(16)—C(17)	1.394 (8)
C(17)—C(18)	1.469 (9)	C(18)—O(3)	1.213 (8)
C(18)—C(19)	1.504 (9)	C(20)—C(22)	1.507 (8)
C(20)—C(28)	1.537 (8)	C(20)—C(34)	1.521 (9)
S(4)—C(21)	1.722 (6)	S(4)—C(24)	1.723 (7)
C(21)—C(22)	1.351 (8)	C(22)—C(23)	1.396 (9)
C(23)—C(24)	1.379 (8)	C(24)—C(25)	1.460 (9)
C(25)—O(4)	1.207 (8)	C(25)—C(26)	1.489 (10)
S(5)—C(27)	1.697 (6)	S(5)—C(30)	1.693 (6)
C(27)—C(28)	1.355 (8)	C(28)—C(29)	1.402 (8)
C(29)—C(30)	1.379 (8)	C(30)—C(31)	1.467 (9)
C(31)—O(5)	1.205 (8)	C(31)—C(32)	1.535 (9)
S(6)—C(33)	1.717 (8)	S(6)—C(36)	1.748 (6)
C(33)—C(34)	1.350 (8)	C(34)—C(35)	1.431 (10)
C(35)—C(36)	1.402 (10)	C(36)—C(37)	1.439 (12)
C(37)—O(6)	1.221 (9)	C(37)—C(38)	1.489 (10)
C(39)—C(41)	1.525 (8)	C(39)—C(47)	1.513 (10)
C(39)—C(53)	1.525 (8)	S(7)—C(40)	1.702 (6)
S(7)—C(43)	1.715 (6)	C(40)—C(41)	1.387 (9)
C(41)—C(42)	1.415 (8)	C(42)—C(43)	1.371 (8)
C(43)—C(44)	1.441 (9)	C(44)—O(7)	1.224 (8)
C(44)—C(45)	1.497 (10)	S(8)—C(46)	1.704 (8)
S(8)—C(49)	1.709 (6)	C(46)—C(47)	1.359 (9)
C(47)—C(48)	1.406 (8)	C(48)—C(49)	1.361 (11)
C(49)—C(50)	1.479 (11)	C(50)—O(8)	1.209 (11)
C(50)—C(51)	1.493 (10)	S(9)—C(52)	1.688 (6)
S(9)—C(55)	1.714 (6)	C(52)—C(53)	1.349 (9)
C(53)—C(54)	1.422 (8)	C(54)—C(55)	1.374 (9)
C(55)—C(56)	1.472 (9)	C(56)—O(9)	1.224 (9)
C(56)—C(57)	1.493 (10)	C(58)—C(59)	1.47 (2)
C(59)—C(60)	1.36 (2)	C(60)—C(61)	1.35 (2)
C(61)—C(62)	1.37 (2)	C(62)—C(63)	1.38 (2)

C(3)—C(1)—C(9)	111.0 (5)	C(3)—C(1)—C(15)	112.9 (4)
C(9)—C(1)—C(15)	113.4 (5)	C(2)—S(1)—C(5)	91.2 (3)
S(1)—C(2)—C(3)	112.8 (4)	C(1)—C(3)—C(2)	126.1 (5)
C(1)—C(3)—C(4)	122.3 (5)	C(2)—C(3)—C(4)	111.6 (5)
C(3)—C(4)—C(5)	112.9 (5)	S(1)—C(5)—C(4)	111.5 (4)
S(1)—C(5)—C(6)	118.6 (4)	C(4)—C(5)—C(6)	129.9 (5)
C(5)—C(6)—O(1)	120.0 (6)	C(5)—C(6)—C(7)	117.7 (5)
O(1)—C(6)—C(7)	122.3 (6)	C(8)—S(2)—C(11)	91.7 (3)
S(2)—C(8)—C(9)	112.7 (5)	C(1)—C(9)—C(8)	122.0 (6)
C(1)—C(9)—C(10)	126.2 (5)	C(8)—C(9)—C(10)	111.7 (6)
C(9)—C(10)—C(11)	112.1 (5)	S(2)—C(11)—C(10)	111.8 (5)
S(2)—C(11)—C(12)	118.2 (5)	C(10)—C(11)—C(12)	130.0 (6)
C(11)—C(12)—O(2)	120.9 (7)	C(11)—C(12)—C(13)	119.7 (6)
O(2)—C(12)—C(13)	119.4 (8)	C(14)—S(3)—C(17)	91.8 (3)
S(3)—C(14)—C(15)	113.2 (5)	C(1)—C(15)—C(14)	126.8 (5)
C(1)—C(15)—C(16)	122.3 (5)	C(14)—C(15)—C(16)	110.7 (5)
C(15)—C(16)—C(17)	114.2 (5)	S(3)—C(17)—C(16)	110.1 (5)

Table 2 (*cont.*)

S(3)—C(17)—C(18)	121.4 (4)	C(16)—C(17)—C(18)	128.6 (6)
C(17)—C(18)—O(3)	119.6 (6)	C(17)—C(18)—C(19)	118.3 (5)
O(3)—C(18)—C(19)	121.9 (6)	C(22)—C(20)—C(28)	112.3 (4)
C(22)—C(20)—C(34)	113.6 (5)	C(28)—C(20)—C(34)	109.6 (5)
C(21)—S(4)—C(24)	91.4 (3)	S(4)—C(21)—C(22)	111.7 (5)
C(20)—C(22)—C(21)	125.1 (6)	C(20)—C(22)—C(23)	121.7 (5)
C(21)—C(22)—C(23)	113.2 (5)	C(22)—C(23)—C(24)	113.0 (5)
S(4)—C(24)—C(23)	110.6 (5)	S(4)—C(24)—C(25)	120.0 (4)
C(23)—C(24)—C(25)	129.4 (6)	C(24)—C(25)—O(4)	120.5 (6)
C(24)—C(25)—C(26)	118.8 (5)	O(4)—C(25)—C(26)	120.7 (6)
C(27)—S(5)—C(30)	91.2 (3)	S(5)—C(27)—C(28)	113.5 (5)
C(20)—C(28)—C(27)	125.4 (5)	C(20)—C(28)—C(29)	123.5 (5)
C(27)—C(28)—C(29)	111.1 (5)	C(28)—C(29)—C(30)	112.7 (5)
S(5)—C(30)—C(29)	111.6 (4)	S(5)—C(30)—C(31)	118.7 (4)
C(29)—C(30)—C(31)	129.8 (6)	C(30)—C(31)—O(5)	121.1 (6)
C(30)—C(31)—C(32)	117.7 (5)	O(5)—C(31)—C(32)	121.2 (6)
C(33)—S(6)—C(36)	92.1 (3)	S(6)—C(33)—C(34)	113.5 (6)
C(20)—C(34)—C(33)	123.1 (6)	C(20)—C(34)—C(35)	125.2 (5)
C(33)—C(34)—C(35)	111.6 (6)	C(34)—C(35)—C(36)	113.8 (5)
S(6)—C(36)—C(35)	109.0 (5)	S(6)—C(36)—C(37)	120.3 (5)
C(35)—C(36)—C(37)	130.6 (6)	C(36)—C(37)—O(6)	119.0 (7)
C(36)—C(37)—C(38)	118.6 (7)	O(6)—C(37)—C(38)	122.4 (8)
C(41)—C(39)—C(47)	112.4 (5)	C(41)—C(39)—C(53)	114.9 (5)
C(47)—C(39)—C(53)	111.6 (5)	C(40)—S(7)—C(43)	92.6 (3)
S(7)—C(40)—C(41)	111.6 (4)	C(39)—C(41)—C(40)	125.4 (5)
C(39)—C(41)—C(42)	122.9 (5)	C(40)—C(41)—C(42)	111.5 (5)
C(41)—C(42)—C(43)	113.4 (6)	S(7)—C(43)—C(42)	110.8 (4)
S(7)—C(43)—C(44)	121.0 (5)	C(42)—C(43)—C(44)	128.1 (6)
C(43)—C(44)—O(7)	120.1 (6)	C(43)—C(44)—C(45)	119.2 (6)
O(7)—C(44)—C(45)	120.7 (6)	C(46)—S(8)—C(49)	91.2 (3)
S(8)—C(46)—C(47)	111.9 (5)	C(39)—C(47)—C(46)	126.1 (5)
C(39)—C(47)—C(48)	121.1 (5)	C(46)—C(47)—C(48)	112.8 (6)
C(47)—C(48)—C(49)	111.8 (5)	S(8)—C(49)—C(48)	112.3 (5)
S(8)—C(49)—C(50)	117.8 (6)	C(48)—C(49)—C(50)	129.9 (6)
C(49)—C(50)—O(8)	121.3 (6)	C(49)—C(50)—C(51)	117.0 (7)
O(8)—C(50)—C(51)	121.7 (7)	C(52)—S(9)—C(55)	91.2 (3)
S(9)—C(52)—C(53)	112.9 (4)	C(39)—C(53)—C(52)	123.1 (5)
C(39)—C(53)—C(54)	123.9 (5)	C(52)—C(53)—C(54)	112.9 (5)
C(53)—C(54)—C(55)	110.6 (5)	S(9)—C(55)—C(54)	112.4 (4)
S(9)—C(55)—C(56)	119.0 (5)	C(54)—C(55)—C(56)	128.6 (6)
C(55)—C(56)—O(9)	119.1 (6)	C(55)—C(56)—C(57)	120.2 (6)
O(9)—C(56)—C(57)	120.7 (6)	C(58)—C(59)—C(60)	132.5 (14)
C(59)—C(60)—C(61)	123.3 (14)	C(60)—C(61)—C(62)	121.7 (14)
C(61)—C(62)—C(63)	129.8 (14)		

squares on F with *SHELX*76 (Sheldrick, 1976); $\sigma^{-2}(F)$ weights. All TATM non-H atoms were refined anisotropically, all H atoms isotropically in calculated positions (C—H = 1.08 Å, H—C—H = 109.4°) with a common thermal parameter U_{iso}(H) = 0.135 (5) Å^2. Hexane atoms were also treated isotropically with U_{iso} = 0.226 (2) Å^2. 723 variables were refined; $\sum w|\Delta F|^2$ was minimized. Final $wR = 0.061$, $R = 0.100$ (no obvious reason could be found for this fairly high value); $(\Delta/\sigma)_{max} < 1$; $(\Delta\rho)_{max} = 0.60$, $(\Delta\rho)_{min} = -0.45$ e Å^{-3}. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). Table 1 gives the atom coordinates and thermal parameters. Bond lengths and angles are given in Table 2. Fig. 1 shows the molecular structure and atom-numbering scheme, drawn by *ORTEP* (Johnson, 1965), and Fig. 2 shows the molecular packing.*

* Lists of structure factors, bond lengths and angles involving H atoms, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55203 (26 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AL0531]

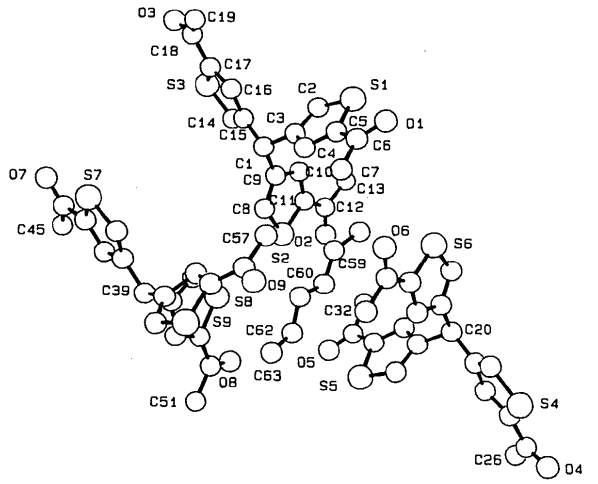

Fig. 1. Perspective drawing showing the numbering scheme.

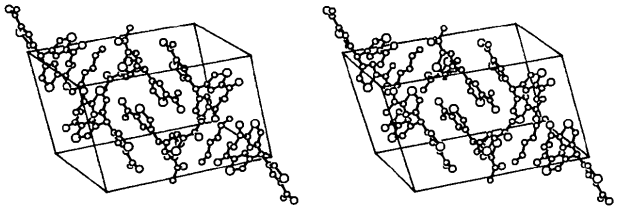

Fig. 2. Stereopair of the unit cell showing the packing.

Related literature. Related compounds are clathrates of TATM with ethyl acetate (van Rooyen & Roos, 1991*a*), benzene (van Rooyen & Roos, 1991*b*) and ethanol (Dillen & Roos, 1992). In contrast to the title compound, they crystallize in a ratio of 2/1.

The authors wish to thank Dr Meth-Cohn for supplying the title compound.

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N,N-Diethyl-6-(hydroxyimino)-α-methyl-1-cyclohexene-1-acetamide

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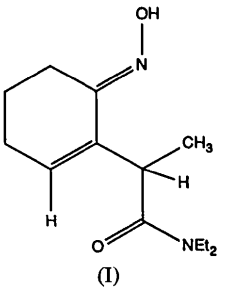
Abstract. $C_{13}H_{22}N_2O_2$, $M_r = 238.3$, monoclinic, $P2_1/c$, $a = 6.228$ (3), $b = 20.315$ (8), $c = 11.104$ (6) Å, $\beta = 103.87$ (5)°, $V = 1364$ (2) Å^3, $Z = 4$, $D_X = 1.16$ g cm^{-3}, λ(Mo $K\alpha$) = 0.7107 Å, $\mu = 0.73$ cm^{-1}, $F(000) = 520$, $T = 293$ K, final $R = 0.059$ for 1524 observed reflections. In the crystal structure disorder was found for one of the cyclohexene C atoms and in one of the ethyl groups. Molecules are connected by O—H···O hydrogen bonds.

Experimental. The title compound (I) was prepared by the reaction of the cyclic nitrone *N,N*-diethyl-8-methyl-7-azabicyclo[4.2.0]oct-6-ene-8-carboxamide 7-oxide with potassium *tert*-butoxide (van Eijk, Reinhoudt, Harkema & van Hummel, 1986) in THF under reflux. The crystal structure was solved to determine the conformation of the reaction product.



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