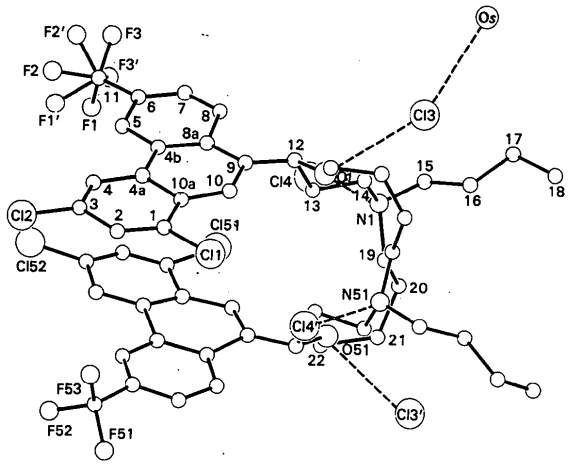

Fig. 2. Diagram of the two halofantrine conformers. The numbering scheme is indicated for the C atoms of one halofantrine conformer, for the heteroatoms of both halofantrine conformers, for the Cl atoms of the hydrochloride salt, and for a solvent atom (symbolized Os) not present at full weight. The numbering of the atoms in molecule (II) differs from the numbering of the atoms in molecule (I) by the addition of 50. Hydrogen bonds are depicted by dashed lines. The size of the circles was arbitrarily chosen to correspond approximately to the atomic weight of the atom.

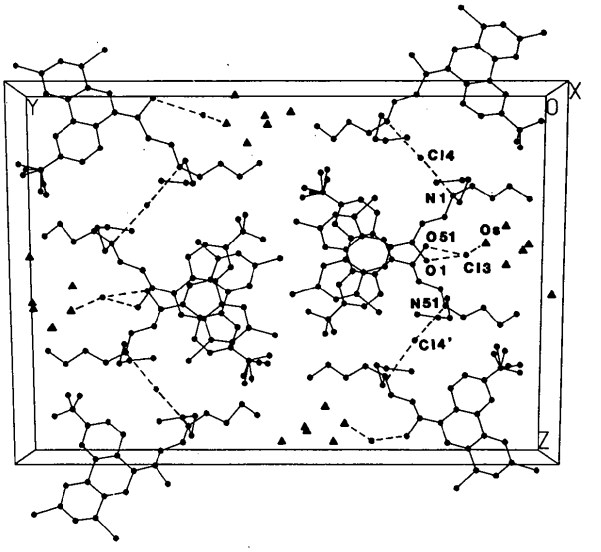

Fig. 3. View of halofantrine hydrochloride down the *a* axis. The packing diagram illustrates the stacking of the two halofantrine conformers such that a pseudo twofold axis, parallel to the *y* direction, passes between the stacked ring systems of molecules (I) and (II) (see near center of diagram). The isolated circles represent Cl atoms from the hydrochloride salt. The triangles represent disordered solvent molecules. Hydrogen bonds are depicted by dashed lines.

length of the H atoms attached to the C atoms was kept fixed at 0·96 Å throughout the refinement procedure. The atomic numbering scheme is shown in Fig. 2, molecular packing in Fig. 3.

Related literature. Halofantrine has demonstrated significant antimalarial activity against multi-drug-resistant malaria especially West African isolates of *Plasmodium falciparum* (Oduola, Milhous, Salako, Walker & Desjardins, 1987) and in humans against endemic *P. falciparum* malaria at the Thai–Kampuchean border (Boudreau *et al.*, 1988).

References

BOUDREAU, E. F., PANG, L. W., DIXON, K. E., WEBSTER, H. K., PAVANAND, K., TOSINGHA, L., SOMUTSAKORN, P. & CANFIELD, C. J. (1988). *Bull. WHO*, **66**, 227–235.

KARLE, J. & KARLE, I. L. (1966). *Acta Cryst.* **21**, 849–859.

ODUOLA, A. M. J., MILHOUS, W. K., SALAKO, L. A., WALKER, O. & DESJARDINS, R. E. (1987). *Lancet* II, pp. 1304–1305.

SHELDRICK, G. M. (1980). *SHELXTL. An Integrated System for Solving, Refining and Displaying Crystal Structures from Diffraction Data.* Univ. of Göttingen, Federal Republic of Germany.

Acta Cryst. (1989). C**45**, 1250–1251

Structure of Dimethyl 7,8-Benzobicyclo[2.2.2]octa-2,5,7-triene-2,3-dicarboxylate

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Abstract. $C_{16}H_{14}O_4$, $M_r = 270{\cdot}29$, tetragonal, $I\bar{4}$, $a = 18{\cdot}572$ (4), $c = 7{\cdot}957$ (7) Å, $V = 2744$ (2) Å^3, $Z = 8$, $D_x = 1{\cdot}31$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}9$ cm^{-1}, $F(000) = 1136$, $T = 295$ K, $R = 0{\cdot}034$ for 608 reflections. The molecule contains a benzobicyclooctatriene ring system with an average C=C–C angle of 113·3 (5)° and other dimensions close to normal values. One methoxycarbonyl group makes an angle of 8·3° with the plane of the C(2)=C(3) double bond, and is thus conjugated, with C–C = 1·473 (8) Å; the other methoxycarbonyl group is not conjugated, angle 87·1° and C–C = 1·498 (9) Å.

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Table 1. *Positional and equivalent isotropic thermal parameters* (Å^2), *with e.s.d.'s in parentheses*

$B_{eq} = (8\pi^2/3)(U_{11} + U_{22} + U_{33})$.

	x	y	z	B_{eq}
O(1)	0·06068 (21)	0·08976 (23)	0·1741 (7)	4·6 (2)
O(2)	0·09357 (22)	0·1079 (3)	0·4380 (7)	4·5 (2)
O(3)	0·27400 (22)	0·24877 (23)	0·1713 (8)	5·8 (3)
O(4)	0·1567 (3)	0·23364 (22)	0·2115 (7)	5·6 (3)
C(1)	0·2133 (3)	0·0047 (3)	0·2364 (9)	3·7 (3)
C(2)	0·1835 (3)	0·0822 (3)	0·2348 (8)	3·5 (3)
C(3)	0·2320 (3)	0·1318 (3)	0·1926 (9)	3·4 (3)
C(4)	0·3060 (3)	0·0992 (3)	0·1532 (10)	4·3 (3)
C(5)	0·2939 (4)	0·0420 (4)	0·0190 (10)	5·3 (4)
C(6)	0·2459 (4)	−0·0065 (4)	0·0629 (11)	5·1 (4)
C(7)	0·2757 (3)	0·0071 (3)	0·3562 (9)	3·1 (3)
C(8)	0·3264 (3)	0·0577 (3)	0·3098 (10)	3·9 (3)
C(9)	0·3881 (3)	0·0658 (4)	0·4057 (12)	5·0 (4)
C(10)	0·3977 (4)	0·0232 (5)	0·5474 (13)	5·9 (5)
C(11)	0·3469 (5)	−0·0269 (4)	0·5902 (11)	5·5 (4)
C(12)	0·2852 (3)	−0·0349 (3)	0·4961 (10)	4·1 (3)
C(13)	0·1085 (3)	0·0961 (3)	0·2962 (10)	3·3 (3)
C(14)	−0·0139 (3)	0·1000 (4)	0·2222 (11)	5·7 (4)
C(15)	0·2159 (3)	0·2095 (3)	0·1917 (10)	4·0 (3)
C(16)	0·2640 (4)	0·3260 (4)	0·1768 (16)	7·4 (5)

Experimental. Colorless [001] prisms, m.p. 379 K, {100}, {110}, developed, 0·22 × 0·22 × 0·38 mm, Rigaku AFC-6 diffractometer, graphite monochromator, lattice parameters from 24 reflections with $2\theta = 15$–$20°$. Intensities for $\theta \leq 25°$, hkl: 0 to 22, 0 to 22, 0 to 9, ω–2θ scan, ω-scan width $(0{\cdot}94 + 0{\cdot}30\tan\theta)°$ at 32° min^{-1} with up to nine scans, background measurement for 50% of scan time, standard reflections showed negligible variations in intensity, Lp but no absorption corrections, 1304 independent reflections measured, 608 with $I \geq 3\sigma(I)$, where $\sigma^2(I) = S + 4(B_1 + B_2) + (0{\cdot}05I)^2$, S = scan, B_1 and B_2 = background counts. Structure by direct methods, refined by full-matrix least squares on F, H atoms in calculated positions, extinction correction, $w = 1/\sigma^2(F)$, scattering factors from *International Tables for X-ray Crystallography* (1974), *TEXRAY* and *TEXSAN* programs (Molecular Structure Corporation, 1985), final $R = 0{\cdot}034$, $wR = 0{\cdot}041$ for 608 reflections, $S = 1{\cdot}10$, 182 parameters, $R = 0{\cdot}162$ for all 1304 reflections, $\Delta/\sigma = 0{\cdot}008$ (maximum), maximum final difference density $\pm 0{\cdot}12$ e Å^{-3}. Atomic parameters are in Table 1, bond lengths and angles in Table 2, and a view of the molecule in Fig. 1.*

Related literature. The structure was determined in an extension of studies of the di-π-methane reaction in the solid state (Scheffer, Trotter, Garcia-Garibay & Wireko, 1988).

*Lists of anisotropic thermal parameters, hydrogen positions, torsion angles, and structure factors, and stereo diagrams have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51780 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

O(1)–C(13)	1·321 (8)	C(3)–C(15)	1·473 (8)
O(1)–C(14)	1·449 (7)	C(3)–C(4)	1·535 (8)
O(2)–C(13)	1·182 (8)	C(4)–C(8)	1·51 (1)
O(3)–C(15)	1·314 (7)	C(4)–C(5)	1·52 (1)
O(3)–C(16)	1·446 (8)	C(5)–C(6)	1·31 (1)
O(4)–C(15)	1·198 (7)	C(7)–C(12)	1·370 (9)
C(1)–C(7)	1·501 (8)	C(7)–C(8)	1·382 (8)
C(1)–C(6)	1·52 (1)	C(8)–C(9)	1·39 (1)
C(1)–C(2)	1·542 (8)	C(9)–C(10)	1·39 (1)
C(2)–C(3)	1·331 (8)	C(10)–C(11)	1·37 (1)
C(2)–C(13)	1·498 (9)	C(11)–C(12)	1·38 (1)

C(13)–O(1)–C(14)	115·9 (6)	C(12)–C(7)–C(8)	121·1 (6)
C(15)–O(3)–C(16)	116·2 (5)	C(12)–C(7)–C(1)	126·8 (6)
C(7)–C(1)–C(6)	105·9 (5)	C(8)–C(7)–C(1)	112·1 (6)
C(7)–C(1)–C(2)	104·8 (5)	C(7)–C(8)–C(9)	119·4 (7)
C(6)–C(1)–C(2)	105·2 (6)	C(7)–C(8)–C(4)	113·3 (6)
C(3)–C(2)–C(13)	126·3 (5)	C(9)–C(8)–C(4)	127·3 (7)
C(3)–C(2)–C(1)	113·9 (5)	C(8)–C(9)–C(10)	119·4 (7)
C(13)–C(2)–C(1)	119·5 (5)	C(11)–C(10)–C(9)	120·1 (7)
C(2)–C(3)–C(15)	122·8 (5)	C(10)–C(11)–C(12)	120·8 (8)
C(2)–C(3)–C(4)	112·6 (5)	C(7)–C(12)–C(11)	119·1 (7)
C(15)–C(3)–C(4)	124·5 (5)	O(2)–C(13)–O(1)	124·1 (6)
C(8)–C(4)–C(5)	105·1 (5)	O(2)–C(13)–C(2)	124·1 (6)
C(8)–C(4)–C(3)	104·9 (6)	O(1)–C(13)–C(2)	111·7 (6)
C(5)–C(4)–C(3)	106·6 (6)	O(4)–C(15)–O(3)	124·2 (6)
C(6)–C(5)–C(4)	113·1 (7)	O(4)–C(15)–C(3)	123·6 (5)
C(5)–C(6)–C(1)	114·7 (6)	O(3)–C(15)–C(3)	112·2 (5)

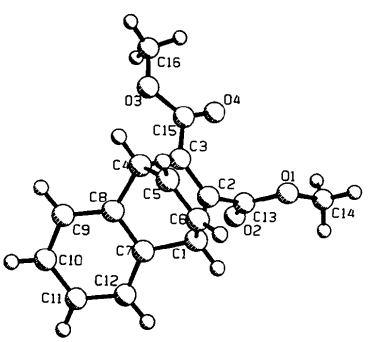

Fig. 1. View of the molecule.

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References

International Tables for X-ray Crystallography (1974). Vol. IV, pp. 99–102. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Molecular Structure Corporation (1985). *TEXSAN. TEXRAY Structure Analysis Package.* MSC, 3200A Research Forest Drive, The Woodlands, TX 77381, USA.

SCHEFFER, J. R., TROTTER, J., GARCIA-GARIBAY, M. & WIREKO, F. (1988). *Mol. Cryst. Liq. Cryst.* **156**, 63–84.