

Structure of 9-Acetoxy-10-(2-acetoxy-5-bromophenyl)anthracene

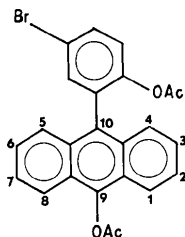
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Abstract. $C_{24}H_{17}BrO_4$, $M_r = 449.3$, triclinic, $P\bar{1}$, $a = 11.321(2)$, $b = 11.212(1)$, $c = 16.454(4)$ Å, $\alpha = 94.32(2)$, $\beta = 87.54(2)$, $\gamma = 81.83(2)^\circ$, $V = 2058.4(7)$ Å³, $Z = 4$, $D_m = 1.44$, $D_x = 1.45$ Mg m⁻³, m.p. = 436.0–437.1 K, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 1.96$ mm⁻¹, $F(000) = 912$, room temperature. Final $R = 0.050$ for 4874 observed reflections. The two crystallographically independent molecules in the asymmetric unit are stacked in two alternating columns along the a and b axes respectively. Br atoms lie on the puckered ribbons extending in the c direction. A short Br...Br intermolecular distance of 3.693 Å is observed.

Introduction. The structure of the title compound was determined as a part of investigations of 9-acetoxy-10-arylanthracenes, which all exhibit a marked fluorescence in organic solvents and are studied as active media for the dye lasers.



The crystals were kindly supplied by Professor J. Gronowska of the Organic Chemistry Department of our University. Synthesis and the electronic absorption and emission spectra of 9-acetoxy-10-(acetoxyhalophenyl)anthracenes have been reported by Dzieleńdzia (1982) and Gronowska, Dzieleńdzia & Heldt (1983).

Experimental. Greenish-yellow parallelepipedal crystals grown from acetic acid by slow evaporation; crystal system and approximate cell dimensions determined from Weissenberg photographs; crystal approx. 0.3 × 0.3 × 0.5 mm; density measured by flotation in aqueous KI solution; Syntex $P\bar{1}$ four-circle diffractometer, ω -scan mode, scan range 0.75°, scan rate varied from 2.0 to 24.0° min⁻¹, background radiation measured on each side of reflection center ($\Delta\omega = 1.0^\circ$) for one half of total scan time; three standard reflections

measured every 50 reflections displayed no significant variations in their intensities; max. $(\sin\theta)/\lambda = 0.6499$ Å⁻¹, $0 \leq h \leq 14$, $-14 \leq k \leq 14$, $-21 \leq l \leq 21$, 8091 unique reflections measured, 4882 classified as observed [$I > 3\sigma(I)$], Lp correction, absorption ignored. Structure solved by direct methods with *MULTAN78* (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), choice of space group $P\bar{1}$ justified by calculated E statistics and successful refinement; best set of phases allowed location of 46 of 58 non-H atoms, remainder found by weighted Fourier synthesis. Refinement by block-diagonal least-squares procedures with each molecule of asymmetric unit in single block (program *SHELX76*, Sheldrick, 1976), function minimized $\sum w(|F_o| - |F_c|)^2$, $w^{-1} = \sigma^2(F_o) + 0.0007F_o^2$, $\sigma(F_o)$ based on counting statistics; 19 H atoms found from difference Fourier map, positions of remaining H atoms calculated; methyl groups treated as rigid groups and allowed to rotate, with tetrahedral geometry and constrained C–H distances of 1.08 Å; eight very strong reflections, seriously affected by extinction, excluded from final stages of refinement; anisotropic temperature factors for non-H atoms and isotropic for H atoms, final $R = 0.050$, $wR = 0.058$; max. and mean Δ/σ in cycle 0.59 and 0.10; residual electron density in final ΔF synthesis within -0.55 and 0.54 e Å⁻³, highest peaks associated with Br atoms; atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Discussion. Final atomic parameters are given in Table 1.* The geometries of the two independent molecules in the asymmetric unit with the numbering scheme are shown in Fig. 1. The bond lengths and angles are listed in Table 2. According to the Cruickshank & Robertson (1953) test there are no significant differences between these values for molecules *A* and *B*. For a few of them the differences are 'possible' significant; more for angles than for bond lengths. A comparison of bond lengths

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, bond lengths and angles involving H atoms and some shorter intermolecular contact distances have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42287 (28 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

and angles for the anthracene moiety found here with those for 'average unsubstituted anthracene' assuming *mmm* symmetry (Harlow, Loghry, Williams & Simonsen, 1975) or with those for 9,10-dimethylantracene (Iball & Low, 1974) shows good agreement except for those associated with atom C(9), to which the acetoxy group is attached. This substituent causes the C(12)–C(9)–C(13) angle to increase by about 3° and the C(12)–C(9) and C(9)–C(13) bonds to contract by

Table 1. Fractional coordinates ($\times 10^4$, for Br $\times 10^5$) and equivalent isotropic thermal parameters for non-H atoms of the two molecules of the asymmetric unit with *e.s.d.*'s in parentheses

$$B_{eq} = \frac{1}{3} \pi^2 \sum_i U_{ij} a_i^* a_j^* a_i \cdot a_j \quad (\text{Hamilton, 1959}).$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{eq} (Å ²)
Molecule A				
Br	47338 (5)	−8189 (4)	34845 (3)	5.55 (3)
O(1)	3412 (2)	7110 (2)	5855 (2)	3.5 (1)
O(2)	1448 (3)	7552 (3)	5721 (2)	6.5 (2)
O(3)	845 (2)	2978 (2)	5060 (2)	3.9 (2)
O(4)	100 (3)	1797 (3)	5952 (2)	6.4 (2)
C(1)	2948 (4)	5443 (5)	6995 (3)	4.8 (3)
C(2)	2712 (5)	4632 (5)	7528 (3)	6.0 (3)
C(3)	2602 (5)	3433 (5)	7238 (3)	5.7 (3)
C(4)	2745 (4)	3077 (4)	6434 (3)	4.1 (2)
C(5)	3504 (4)	4085 (4)	3588 (2)	3.4 (2)
C(6)	3726 (4)	4911 (4)	3061 (3)	4.4 (3)
C(7)	3894 (4)	6094 (4)	3358 (3)	4.7 (3)
C(8)	3791 (4)	6410 (4)	4166 (3)	3.8 (2)
C(9)	3348 (3)	5896 (3)	5569 (2)	3.0 (2)
C(10)	3123 (3)	3543 (3)	5001 (2)	2.7 (2)
C(11)	3398 (3)	4367 (3)	4446 (2)	2.8 (2)
C(12)	3531 (3)	5575 (3)	4737 (2)	2.8 (2)
C(13)	3120 (3)	5106 (3)	6135 (2)	3.1 (2)
C(14)	3002 (3)	3888 (3)	5843 (2)	3.1 (2)
C(15)	2867 (3)	2318 (3)	4687 (2)	2.9 (2)
C(16)	1719 (3)	2039 (3)	4724 (2)	3.2 (2)
C(17)	1444 (4)	943 (4)	4409 (3)	4.1 (2)
C(18)	2340 (4)	92 (4)	4047 (3)	4.0 (2)
C(19)	3491 (4)	351 (3)	3997 (2)	3.4 (2)
C(20)	3767 (4)	1448 (3)	4314 (2)	3.3 (2)
C(21)	2353 (4)	7875 (4)	5902 (2)	3.8 (2)
C(22)	2526 (5)	9133 (4)	6187 (3)	5.3 (3)
C(23)	109 (4)	2768 (5)	5708 (3)	4.9 (3)
C(24)	−596 (5)	3939 (5)	6051 (4)	6.3 (3)
Molecule B				
Br	47097 (4)	85526 (5)	−20515 (3)	5.54 (3)
O(1)	−2934 (2)	8933 (2)	330 (2)	4.3 (2)
O(2)	−3071 (3)	6963 (3)	347 (3)	8.8 (3)
O(3)	1797 (2)	5796 (2)	80 (2)	4.6 (2)
O(4)	3074 (3)	5575 (3)	1092 (2)	7.3 (3)
C(1)	−1233 (5)	8846 (4)	1542 (3)	4.4 (3)
C(2)	−412 (5)	8819 (4)	2105 (3)	5.3 (3)
C(3)	818 (5)	8581 (4)	1877 (3)	5.2 (3)
C(4)	1184 (4)	8343 (4)	1076 (3)	4.2 (2)
C(5)	166 (4)	7784 (4)	−1824 (3)	4.0 (2)
C(6)	−661 (4)	7865 (4)	−2393 (3)	4.9 (3)
C(7)	−1874 (4)	8259 (4)	−2148 (3)	5.2 (3)
C(8)	−2234 (4)	8522 (4)	−1358 (3)	4.6 (3)
C(9)	−1695 (3)	8637 (3)	89 (3)	3.4 (2)
C(10)	714 (3)	8011 (3)	−371 (2)	3.1 (2)
C(11)	−129 (3)	8083 (3)	−971 (2)	3.4 (2)
C(12)	−1369 (3)	8433 (3)	−731 (2)	3.4 (2)
C(13)	−888 (4)	8611 (3)	697 (2)	3.3 (2)
C(14)	356 (3)	8322 (3)	453 (2)	3.2 (2)
C(15)	1997 (3)	7542 (3)	−608 (2)	3.0 (2)
C(16)	2545 (4)	6445 (3)	−360 (2)	3.5 (2)
C(17)	3712 (4)	5975 (4)	−588 (3)	3.9 (2)
C(18)	4382 (4)	6606 (4)	−1080 (3)	4.0 (2)
C(19)	3847 (4)	7691 (4)	−1330 (2)	3.6 (2)
C(20)	2679 (4)	8161 (4)	−1102 (2)	3.4 (2)
C(21)	−3544 (4)	7976 (5)	455 (3)	5.1 (3)
C(22)	−4805 (4)	8413 (6)	723 (4)	7.1 (4)
C(23)	2140 (5)	5425 (4)	821 (3)	5.5 (3)
C(24)	1145 (6)	4862 (6)	1208 (4)	8.9 (4)

about 0.02 Å. Bonds C(1)–C(2), C(3)–C(4), C(5)–C(6) and C(7)–C(8) have almost pure double-bond character.

The anthracene ring system is not strictly planar, which has been observed in other cases of non-centrosymmetrically substituted anthracene derivatives: 9-methylantracene (Cox & Sim, 1979), 10-methylantracene derivatives (Glusker & Zacharias, 1972; Stallings, Monti & Glusker, 1982) and 9-[[2-chloroethyl]thio]methylanthracene (Lewis, Carrell, Glusker & Sparks, 1976) but is slightly buckled as shown in Fig. 2(a). The r.m.s. deviations from the least-squares planes calculated using the coordinates of the 14 atoms of the anthracene ring system are 0.024 (A) and 0.049 Å (B) for the two molecules in the asymmetric unit. In both anthracene ring systems the central ring is bent along the C(9)–C(10) line. The outer rings are more planar and form dihedral angles of 2.6 and 5.3° for molecules A and B respectively. Additionally, the anthracene ring system is slightly twisted round its long axis (Fig. 2a), which was also observed in the cases mentioned above.

The bonds C(9)–O(1) and C(10)–C(15), connecting anthracene with its 9- and 10-substituents, are displaced from the least-squares plane of the anthracene moiety in an opposite direction to the central ring (Fig. 2a). Fig. 2(b) shows the values of these angle deviations.

The phenyl ring is planar (r.m.s. deviation 0.003 and 0.001 Å for molecules A and B respectively). The angles C(20)–C(15)–C(16), C(15)–C(16)–C(17) and C(18)–C(19)–C(20) and the distances C(15)–C(10), C(16)–O(3) and C(19)–Br of the phenyl ring are in very good agreement with values reported (in Tables 10 and 11) by Domenicano, Vaciago & Coulson (1975), where those values have been correlated with the electronegativity of C, O and Br elements, respectively. The least-squares plane of the phenyl ring forms a dihedral angle of 69.9 (A) and 64.8° (B) with the least-squares plane of the anthracene moiety.

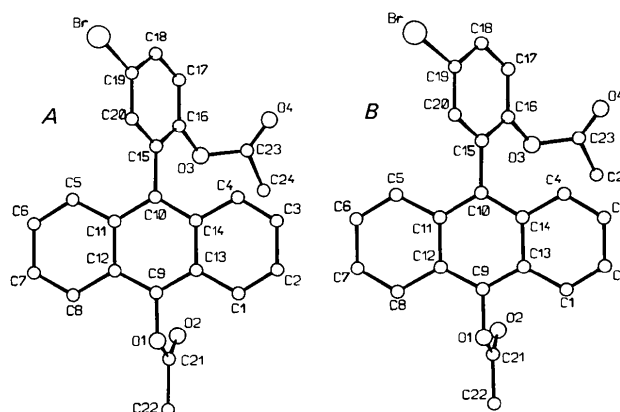


Fig. 1. The two independent molecules in the asymmetric unit with numbering scheme; H atoms have been omitted for clarity (PLUTO, Motherwell & Clegg, 1978).

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

	Molecule A	Molecule B		Molecule A	Molecule B		Molecule A	Molecule B
C(1)—C(2)	1.355 (8)	1.340 (8)	C(9)—C(13)	1.374 (6)	1.383 (6)	C(17)—C(18)	1.372 (6)	1.385 (7)
C(1)—C(13)	1.434 (6)	1.424 (6)	C(9)—O(1)	1.420 (4)	1.427 (5)	C(18)—C(19)	1.375 (6)	1.380 (6)
C(2)—C(3)	1.417 (8)	1.409 (8)	C(10)—C(11)	1.403 (5)	1.400 (6)	C(19)—C(20)	1.382 (5)	1.378 (5)
C(3)—C(4)	1.350 (6)	1.359 (7)	C(10)—C(14)	1.406 (5)	1.403 (5)	C(19)—Br	1.902 (4)	1.907 (4)
C(4)—C(14)	1.428 (6)	1.419 (6)	C(11)—C(12)	1.433 (5)	1.433 (5)	C(21)—O(1)	1.367 (5)	1.379 (6)
C(5)—C(11)	1.419 (5)	1.433 (6)	C(13)—C(14)	1.440 (5)	1.432 (5)	C(21)—O(2)	1.177 (6)	1.183 (6)
C(5)—C(6)	1.357 (6)	1.350 (7)	C(10)—C(15)	1.502 (5)	1.498 (5)	C(21)—C(22)	1.494 (6)	1.478 (7)
C(6)—C(7)	1.419 (7)	1.412 (7)	C(15)—C(16)	1.379 (6)	1.395 (5)	C(23)—O(3)	1.380 (6)	1.373 (6)
C(7)—C(8)	1.346 (7)	1.344 (7)	C(15)—C(20)	1.393 (5)	1.385 (6)	C(23)—O(4)	1.189 (7)	1.193 (7)
C(8)—C(12)	1.427 (6)	1.451 (6)	C(16)—C(17)	1.379 (6)	1.376 (6)	C(23)—C(24)	1.493 (7)	1.508 (9)
C(9)—C(12)	1.388 (5)	1.377 (6)	C(16)—O(3)	1.401 (4)	1.405 (5)			
C(2)—C(1)—C(13)	121.2 (5)	120.8 (5)	C(10)—C(11)—C(12)	119.9 (3)	119.3 (3)	C(17)—C(16)—O(3)	122.5 (4)	121.7 (4)
C(1)—C(2)—C(3)	120.1 (5)	121.0 (5)	C(8)—C(12)—C(9)	122.6 (3)	122.6 (4)	C(16)—C(17)—C(18)	119.2 (4)	119.5 (4)
C(2)—C(3)—C(4)	120.8 (5)	119.9 (5)	C(8)—C(12)—C(11)	119.4 (3)	119.0 (4)	C(17)—C(18)—C(19)	119.5 (4)	118.4 (4)
C(3)—C(4)—C(14)	121.7 (4)	121.7 (4)	C(9)—C(12)—C(11)	117.9 (3)	118.4 (4)	C(18)—C(19)—C(20)	121.3 (4)	122.0 (4)
C(6)—C(5)—C(11)	122.1 (4)	122.8 (4)	C(1)—C(13)—C(9)	123.6 (4)	123.4 (4)	C(18)—C(19)—Br	119.7 (3)	119.9 (3)
C(5)—C(6)—C(7)	120.5 (4)	119.5 (4)	C(1)—C(13)—C(14)	118.5 (4)	119.1 (4)	C(20)—C(19)—Br	119.0 (3)	118.0 (3)
C(6)—C(7)—C(8)	119.7 (5)	121.6 (5)	C(9)—C(13)—C(14)	117.9 (3)	117.6 (3)	C(15)—C(20)—C(19)	119.8 (4)	120.3 (4)
C(7)—C(8)—C(12)	121.3 (4)	120.2 (4)	C(4)—C(14)—C(10)	122.5 (4)	122.6 (4)	C(9)—O(1)—C(21)	115.4 (3)	116.5 (3)
C(12)—C(9)—C(13)	124.0 (3)	123.8 (4)	C(4)—C(14)—C(13)	117.7 (4)	117.4 (4)	C(1)—C(21)—O(2)	122.5 (4)	121.7 (4)
C(12)—C(9)—O(1)	118.2 (3)	118.5 (4)	C(10)—C(14)—C(13)	119.8 (4)	120.0 (4)	O(1)—C(21)—C(22)	111.0 (4)	110.7 (4)
C(13)—C(9)—O(1)	117.8 (3)	117.6 (3)	C(10)—C(15)—C(16)	120.9 (3)	121.3 (4)	O(2)—C(21)—C(22)	126.5 (4)	127.6 (5)
C(11)—C(10)—C(14)	120.3 (3)	120.5 (3)	C(10)—C(15)—C(20)	121.3 (3)	121.5 (3)	C(16)—O(3)—C(23)	118.9 (3)	118.7 (4)
C(11)—C(10)—C(15)	119.6 (3)	119.7 (3)	C(16)—C(15)—C(20)	117.8 (3)	117.2 (3)	O(3)—C(23)—O(4)	123.3 (4)	123.0 (5)
C(14)—C(10)—C(15)	119.9 (3)	119.8 (3)	C(15)—C(16)—C(17)	122.4 (3)	122.6 (4)	O(3)—C(23)—C(24)	109.1 (5)	108.7 (5)
C(5)—C(11)—C(10)	123.2 (3)	123.8 (4)	C(15)—C(16)—O(3)	115.0 (3)	115.5 (3)	O(4)—C(23)—C(24)	127.5 (5)	128.3 (5)
C(5)—C(11)—C(12)	116.9 (3)	116.8 (4)						

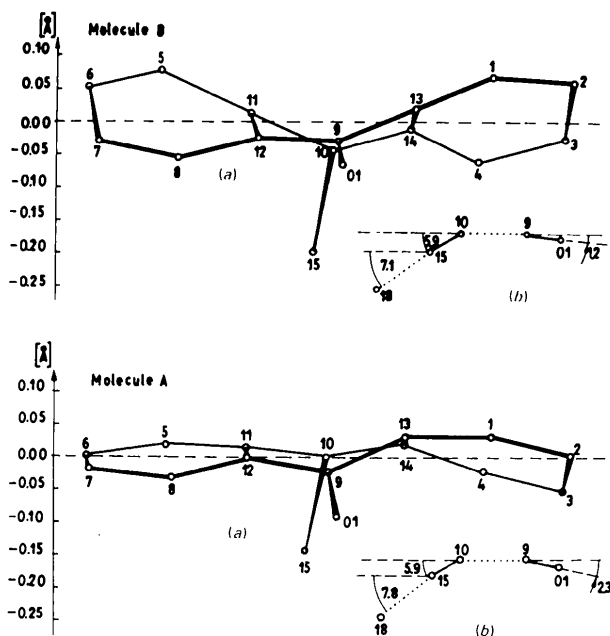


Fig. 2. (a) Distortions in the anthracene ring system in relation to its least-squares plane. The vertical scale is exaggerated ten times. (b) Angle deviations (°) of bonds C(10)—C(15) and C(9)—O(1) and the diagonal of the phenyl ring from the least-squares plane of anthracene. The angles are exaggerated five times.

All acetoxy groups are planar and their geometry is similar to those reported before (*e.g.* Foces-Foces, Cano & García-Blanco, 1980; Fortier & Ahmed, 1980). The acetoxy group connected with the phenyl ring forms a dihedral angle of 52.2 (A) and 52.9° (B)

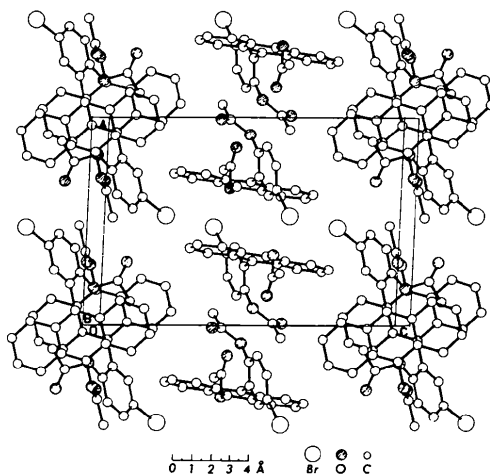


Fig. 3. The packing of molecules in the unit cell viewed along the *b* axis (PLUTO, Motherwell & Clegg, 1978).

with the ring. The acetoxy group bonded to C(9) is approximately perpendicular to the least-squares plane of the anthracene ring system; the dihedral angles are 89.7 and 86.3° for molecules A and B respectively. The arrangement of all discussed groups in relation to each other seems to minimize steric interactions. Molecules A and B have nearly the same conformation.

The molecular arrangement in the unit cell, viewed down the *b* axis, is shown in Fig. 3. The structure consists of the two alternating columns, formed by molecules A and B, extending along *a* and *b* crystallographic axes respectively. The A molecules related by centers of symmetry at $0, \frac{1}{2}, \frac{1}{2}$ and $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ are

stacked in the column with alternate interplanar distances of 3.558 and 7.233 Å between adjacent anthracene ring systems. The *B* molecules related by symmetry centers at 0, 0, 0 and 0, $\frac{1}{2}$, 0 form the other column with these distances of 3.822 and 7.324 Å respectively. These alternating short and long separations in each column result from the shape of the molecules.

The Br atoms lie on puckered ribbons extending in the *c* direction and passing through the centers of unit cells. The closest contact between Br atoms (of *A* and *B* molecules) is 3.693 (1) Å, which is 0.207 Å shorter than the expected van der Waals contact of 3.90 Å using Pauling's (1960) radius of 1.95 Å for Br. However, it is nearly twice the van der Waals radius using Bondi's (1964) corrected value of 1.85 Å. The other intermolecular distances are in the normally expected range for nonbonding contacts.

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Structure of 8-Methylguanosine Trihydrate

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Abstract. $C_{11}H_{15}N_5O_5 \cdot 3H_2O$, $M_r = 351.3$, orthorhombic, $C222_1$, $a = 8.464$ (1), $b = 30.848$ (4), $c = 12.233$ (1) Å, $V = 3194.0$ (7) Å³, $Z = 8$, $D_m = 1.459$ (3), $D_x = 1.462$ Mg m⁻³, $\lambda(\text{Cu } K\alpha) = 1.5418$ Å, $\mu = 1.09$ mm⁻¹, $F(000) = 1488$, $T = 295$ K, final $R = 0.053$ for 1448 unique reflections. The glycosidic torsion angle, $\chi = 52.7$ (5)°, is in the *syn* conformation. The ribose ring has a $C(2')$ -*endo* (²*E*) pucker and the

conformation around the $C(5')$ – $C(4')$ bond is *gauche-gauche* (g,g). An intramolecular hydrogen bond connects the $O(5')$ hydroxyl group with the $N(3)$ atom of the guanine base. The crystal structure is stabilized by intermolecular face-to-face base stackings and extensive hydrogen-bond networks involving guanine–guanine base-pairing.

Introduction. The glycosidic torsion angle defines the orientation of the base plane relative to the sugar moiety and it is one of the most important parameters for determining the molecular conformation of a

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