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SPATIAL STRUCTURE OF ISOEPOXYESTAFIATIN

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The spatial structure of the sesquiterpene lactone isoexpoxyestafiatin has been established by the x-ray method as 1,10β;3,4α-diepoxy-5,7α,6βH-11(13)en-6,12-olide.

The isolation of the sesquiterpene lactone isoepoxyestafiatin (**1**) from the epigeal part of *Artemisia filatovii* has been reported previously [1]. In order to establish its spatial structure, we have subjected it to an x-ray structural investigation.

The structure of the (**1**) molecule is shown in Fig. 1. The bond lengths and valence angles in (**1**) are the usual ones [2]. The five- and seven-membered carbocycles, and also the seven-membered and lactone rings, are linked in the *trans*- manner (torsion angle O4C1C5H5 = −161°).

The epoxy groups at the C1 and C10 and at the C3 and C4 atoms have β- and α- orientations, respectively. The conformation of the five-membered carbocycle is that of a 1β-envelope ($\Delta C_S^1 = 4.1°$) and the seven-membered ring assumes the conformation of an almost ideal 7α,1,10β-chair ($\Delta C_S^7 = 1.5°$, $\Sigma_2/(\Sigma_2 + \Sigma_S) = 0.95$). The torsion angles in the five- and seven-membered carbocycles differ from the corresponding ones in the structure of arborescin [3], which has the same conformation of these rings, by an average of 6°. The lactone ring assumes the conformation of a 6β,7α-half-chair ($\Delta C_{12}^2 = 3.9°$).

EXPERIMENTAL

The cell parameters and the intensities of 2108 independent reflections were measured on a Siemens P3/PC automatic four-circle diffractometer with monochromatized Mo-K_α radiation, $\theta/2\theta$ scanning, $2\theta < 60°$. Crystals rhombic, $a = 6.323(4)$, $b = 13.606(8)$, $c = 15.044(7)$ Å, $V = 1292.9$ Å^3, $d_{calc} = 1.347$ g/cm^3, $Z = 4$ ($C_{16}H_{18}O_4$), sp.gr, $P2_12_12_1$.

TABLE 1. Coordinates of the Atoms (× 10^4; for H, × 10^3) of the Structure of (**1**)

Atom	x	y	z	Atom	x	y	z
O1	7836(4)	9030(2)	10282(2)	H2a	1194(7)	1245(4)	985(3)
O2	5449(5)	7830(2)	10426(2)	H2b	1369(7)	1179(3)	928(3)
O3	11339(6)	11317(2)	11180(2)	H3	1426(7)	1111(3)	1071(3)
O4	11744(4)	10613(2)	8413(2)	H5	847(5)	1085(2)	1010(2)
C1	10849(6)	11141(2)	9168(2)	H6	985(6)	923(3)	922(3)
C2	12485(8)	11766(3)	9660(3)	H7	601(7)	1021(3)	912(3)
C3	12936(7)	11207(3)	10498(3)	H8a	641(8)	991(3)	759(3)
C4	11356(6)	10435(3)	10632(2)	H8b	887(8)	964(3)	772(3)
C5	9706(6)	10525(2)	9885(2)	H9a	833(7)	1113(3)	722(3)
C6	8773(6)	9571(2)	9532(2)	H9b	680(7)	1141(3)	802(3)
C7	6934(6)	9697(3)	8885(3)	H13a	425(7)	848(3)	795(3)
C8	7534(9)	9956(3)	7933(3)	H13b	383(9)	763(4)	873(3)
C9	8144(8)	11040(3)	7824(3)	H14a	1260(9)	1246(3)	803(4)
C10	10160(6)	11378(2)	8251(3)	H14b	1122(9)	1229(4)	711(4)
C11	5739(6)	8755(2)	9036(3)	H14c	998(7)	1279(3)	782(3)
C12	6254(6)	8452(2)	9962(3)	H15a	1205(6)	909(3)	1071(3)
C13	4447(8)	8266(4)	8514(4)	H15b	1298(9)	960(4)	1147(4)
C14	11000(9)	12302(3)	7809(3)	H15c	1054(7)	933(3)	1148(3)
C15	11792(8)	9502(4)	11127(3)				

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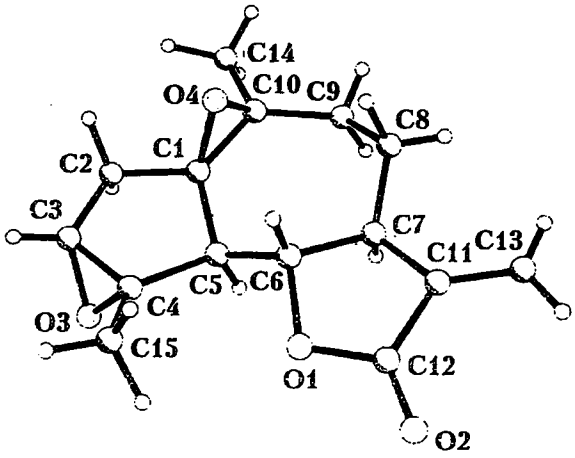

Fig. 1. Structure of the isoepoxyestafiatin molecule.

In the calculations we used 1624 reflections with $I > 3\sigma$. The structure was interpreted by the direct method and was refined by full-matrix MLS in the anisotropic approximation for the nonhydrogen atoms. The hydrogen atoms were revealed in a difference synthesis and their positions were refined isotropically. The final discrepancy factors were R = 0.065 and R_w = 0.065. The coordinates of the atoms are given in Table 1. All the calculations were performed on an IBM PC/AT computer by means of the Siemens SHELXTL program package (PC version).

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