2,4-Dihydroxy-3-[4-oxo-3-methyl-but-2E-en-1-yl]-acetophenon (**28**). Farbloses Öl, IR: CHO 1700; Ph CO 1630 cm^{-1}. MS: M^+ *m/e* 234.089 (10%) (ber. für $C_{13}H_{14}O_4$ 234.089). 5 mg **28** in 1 ml MeOH versetzte man mit 5 mg Na BH_4. Nach 3 min zersetzte man mit verd. H_2SO_4 und reinigte durch DC (Ether–Petrol 3:1). Man erhielt 3 mg **29**, ^{1}H-NMR: s. Tabelle 1.

Pardalianchol (**33**), Farbloses Öl, IR: OH 3570 cm^{-1}. MS: M^+ *m/e* 220.183 (6%) (ber. für $C_{15}H_{24}O$ 220.183); – $^{\cdot}$Me 205(1); – H_2O 202(1); – C_5H_9O 147(100).

$$[\alpha]^{\gamma}_{24^\circ} = \frac{589 \quad 578 \quad 546 \quad 436 \text{ nm}}{-71.9 \quad -74.9 \quad -85.6 \quad -149.5} \quad (c = 0.95).$$

5 mg **33** acetylierte man mit Ac_2O unter Zusatz von 4-Pyrrolidinopyridin [11] (12 hr RT). Nach DC (Ether–Petrol 1:10) erhielt man 5 mg **34**, farbloses Öl, MS M^+ *m/e* 262(2%); – AcOH 202(1); 202 – $^{\cdot}$Me 187(1.6); $C_{11}H_{15}^+$ 147 (100).

5 mg **33** in 1 ml CH_2Cl_2 rührte man 12 hr mit 20 mg Pyridinchlorochromat. Nach DC (Ether–Petrol 1:3) erhielt man 2 mg **36**, farbloses Öl, IR: CO 1730 cm^{-1}. MS: M^+ *m/e* 218(22%); $C_{11}H_{15}^+$ 147(60); $C_8H_{12}^+$ 108 (100). 20 mg **33** in 1 ml Benzol erwärmte man unter Zusatz von 0.05 ml Pyridin 1 hr mit 50 mg 3.5-Dinitrobenzoylchlorid auf 70°. Nach üblicher Aufarbeitung und DC (Ether–Petrol 1:3) erhielt man 15 mg **35**, farblose Kristalle aus MeOH, Schmp. 128° (^{1}H-NMR s. Tabelle 2).

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ISOINTERMEDEOL, A NEW SESQUITERPENE ALCOHOL FROM *CYMBOPOGON FLEXUOSUS*

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Key Word Index—*Cymbopogon flexuosus*; Gramineae; essential oil; a new sesquiterpene alcohol; isointermedeol.

INTRODUCTION

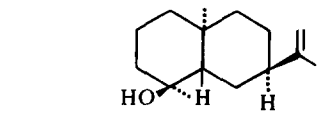
The essential oils of the genus *Cymbopogon* are a rich source of monoterpenoids. During screening of the 52 varieties and geographical races (including the same species collected from different areas of India), a number of important and new oils have been discovered [1–3]. A few new oils have been found to be rich in sesquiterpenoids, which is of rare occurrence in this genus. The essential oil of *C. flexuosus* (RRL-4)* contains *ca* 60% sesquiterpenes. A new sesquiterpene alcohol named isointermedeol has been isolated from this oil and a tentative structure has been assigned on the basis of ^{1}H NMR, ^{13}C NMR, IR and MS.

RESULTS AND DISCUSSION

The volatile oil of *C. flexuosus* was examined by using a Reoplex-400 column. The GC showed about 45 peaks and some of the identified components were α-pinene (0.10); β-pinene (1.01); Δ^3-carene (0.10); myrcene (0.66); limonene (0.84); ocimene (0.09); β-phellendrene (5.78); α-terpinene (0.18); *p*-cymene (0.18); terpinolene (0.07); methyl heptenone (0.41); citronellal (1.2); δ-elemene (0.66); geranyl acetate (0.20); β-elemene (2.36) β-caryophyllene (3.72); β-selinene (3.84); γ-elemene (0.05); geraniol (0.46); α-bisabolene (0.08); β-bisabolene (0.13); α-curcumene (0.11); δ-cadinene (0.05); γ-cadinene (1.18); methyl eugenol (0.92); elemol (0.49); β-caryophyllene oxide (0.48); eugenol (0.12); β-eudesmol (4.0); new sesquiterpene alcohol (50.56); elemicin (7.22); farnesol (0.97) and juniper camphor (9.23%).

The volatile oil of *C. flexuosus* on repeated chromatography over Si gel gave an oily fraction which solidified on cooling. Further purification with petrol gave a low melting solid, isointermedeol, which showed a single spot on TLC. It was analysed for $C_{15}H_{26}O$; M^+ 222, mp 40–41°; $[\alpha]_D$ +2° (*c*, 3.3; MeOH). IR gave bands at 3400, 1650, 930, 908 and 805 cm^{-1}. MS gave fragments at *m/e* 41 (77.1); 43 (100); 55 (44.5); 67 (43.3); 70 (40.0); 81 (22.8); 91 (22.8); 93 (23.0); 107 (19.5); 109 (17.2); 123

* Serial number assigned to the plots of *Cymbopogon* species grown and adapted under the conditions of the campus laboratory.



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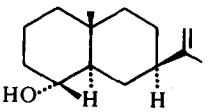

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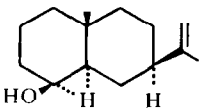

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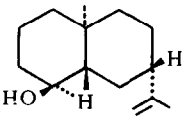

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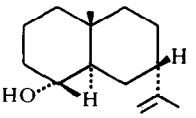

5

(17.8); 125 (16.0); 133 (8.7); 135 (11.9); 161 (17.4); 189 (22.9); 204 (23.0) and 222 (21.1%).

The ^{1}H NMR spectra were obtained in $CDCl_3$ and C_5D_5N. All the data suggested that isointermedeol contained a selinene type of skeleton. A survey of the literature showed three closely related structures, **1–3** [4–9], which could be assigned to the present compound. However, isointermedeol gave different physical constants as well as different spectral data to those of **1–3**. Compound **3** (neointermedeol), is totally different from the present compound as it has a C-10 Me and a C-4 OH on the same side of the ring system, which gave rise to a 1:3-interaction. No such interaction was seen in the new compound when pyridine was used as the solvent for ^{1}H NMR spectroscopy. Also, the C-10 Me in this case appeared at δ 0.92 in $CDCl_3$ and δ 0.93 in C_5D_5N.

The remaining two structures, **1** and **2**, differ in the position of the olefinic protons which appeared at δ 4.84 (CCl_4) for **1** and δ 4.65 for **2** whereas the signal for isointermedeol appeared at δ 4.97. The position of other signals for C-10, C-4 and C-11 Me of **1** and **2** is nearly the same as that of isointermedeol. Comparative ^{1}H NMR is given in Table 1.

From the above discussion, structures **1–3** are ruled out and an alternative structure **4** or **5** can be assigned. ^{13}C NMR (noise decoupled and off resonance decoupled) supported structure **5**. Since C-5 was downfield at 49.236, H-5 should have the α-configuration. This simultaneously assigns the configurations at C-10 (Me) and C-4 (—OH) which are *trans* to each other. Other ^{13}C NMR spectral values which are consistent with structure **5** are C-1, 41.405; C-2, 20.156; C-3, 43.590; C-4, 72.125; C-5, 49.236; C-6, 22.827; C-7, 39.401; C-8, 23.556; C-9, 40.373; C-10, 35.334; C-11, 146.982; C-12, 110.858; C-13, 22.827; C-14, 22.341; C-15, 18.546.

Table 1. ^{1}H NMR chemical shifts of **1**, **2** and **4**

	1*	2*	4 or 5†	4 or 5‡
C-10 Me	0.93*s*	0.90*s*	0.92*s*	0.93*s*
C-4 Me	1.01*s*	1.07*s*	1.08*s*	1.25*s*
C-11 Me	1.74*s*	1.75*s*	1.76*s*	1.78*s*
$=CH_2$	4.84*s*	4.65*m*	4.97*s*	5.03*d*

* In CCl_4.
† In $CDCl_3$.
‡ In C_5D_5N.

EXPERIMENTAL

The volatile oil was isolated by hydrodistillation. GLC was performed on a 6 m Reoplex-400 column, N_2 carrier gas flow rate 45 ml/min temp. 90° for 5 min and raising to 150°. The compounds on the chromatogram were identified by using reference samples. Some of the compounds were further confirmed by isolation and determination of IR spectra.

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