Phytochemistry, 1978, Vol. 17, p 2045. © Pergamon Press Ltd. Printed in England. 0031-9422/78/1101-2045 $02.00/0

CAJAFLAVANONE: A NEW FLAVANONE FROM *CAJANUS CAJAN*

S. Bhanumati†, S. C. Chhabra†, S. R. Gupta*† and V. Krishnamoorthy‡

†Department of Chemistry, University of Delhi, Delhi-110007, India; ‡Sri Venkateshwara College, Dhaula Kuan, Delhi-110023, India

(*Received* 4 *April* 1978)

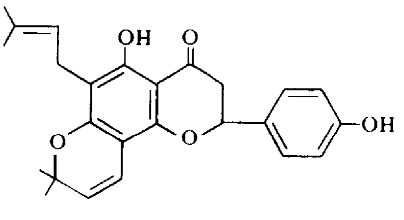
Key Word Index—*Cajanus cajan*; Leguminosae; pigeon pea; cajaflavanone; 5,4′-dihydroxy-6-(3‴-methyl-2‴-butenyl)-2″,2″-dimethyl pyrano-[5″,6″:7,8]-flavanone.

A number of isoflavones and an isoflavanone have been reported from the fungus infected roots of *Cajanus* [1]. Cajanone, an isoflavanone which inhibits the growth of *Fusarium oxysporum* has also been isolated recently [2]. During the course of our investigation of the root bark of *C. cajan*, a new flavanone, cajaflavanone (**1**) has been isolated from the C_6H_6 soluble portion using column chromatography and preparative TLC. Cajaflavanone (M^+ 406, $C_{25}H_{26}O_5$), a minor phenolic component (0.01 %) was separated as straw yellow needles, mp 129–30°, $[\alpha]_D^{25}$ −66.6 (*c* 1.05 in $CHCl_3$). It gave a dark green colour with alcoholic $FeCl_3$, a positive Shinoda and $NaBH_4$/HCl tests. IR(KBr) showed strong absorption at 1613 cm^{-1} (chelated CO group) and 3246 cm^{-1} (OH).

The PMR (60 MHz, $CDCl_3$, δ) showed one 2,2-dimethylchromene group [6.51 (1H) *d*, $J = 12$ Hz, H_α; 5.39 (1H) *d*, $J = 12$ Hz, H_β; 1.41 (6H, *s*, 2× Me], one γ,γ-dimethylallyl group [5.18 (1H) *t*, $J = 7$ Hz, —CH═; 3.12 (2H) *d*, $J = 7$ Hz, —CH_2—Q; 1.61 (6H) *s*, 2× Me]. Further there were two *ortho* coupled doublets centred at δ 7.19 and 6.74 integrating for four protons of an A_2B_2 system of a *para* disubstituted benzene ring. The singlets at δ 11.99 and 6.4, each integrating for one proton which disappeared on addition of D_2O, were attributed to the hydroxyls at C-5 and C-4′ positions. Multiplets centred at δ 5.24 and 2.83 for one and two protons, respectively of an ABX system, were assigned to the protons at C-2 and C-3 of a flavanone [3].

The base peak at M-15 and fragments at M-43 and M-55 confirmed the presence of a dimethylchromene and a dimethylallyl group [4]. The retro Diels–Alder fragments in the MS at *m/e* 271(28) and *m/e* 120(12) could be rationalized only if the non-chelated OH and the dimethylallyl sidechain were assigned to B and A rings, respectively. Therefore, the hydroxyl group must be at 4′ and the γ,γ-dimethylallyl group at C-6 or C-8 positions [3].

Treatment of (**1**) with HCOOH gave a compound which did not respond to Fe^{3+} reaction, indicating that the dimethylallyl group is at C-6. The UV absorption (λ_{max}^{MeOH} (log ε) nm: 225(4.11), 275(4.03), 300(3.84), 345(3.21), 360(3.39), 380(3.39)) and the bathochromic shift of the longer wavelength band with $AlCl_3$ (275, 300, 315, 335, 355, 390 nm) and NaOMe (275, 300, 315, 360, 385 nm) confirmed the presence of hydroxyls at C-5 and C-4′, respectively. A negative Gibb's test indicated that the position *para* to the OH is blocked. Hence **1** is 5,4′-dihydroxy-6-(3‴-methyl-2‴-butenyl)-2″,2″-dimethyl pyrano-[5″,6″:7,8]-flavanone. Cajaflavanone was identical (co TLC, IR) with a synthetic sample, obtained as an isomer during the synthesis of lupinifolin [5], thus confirming the proposed structure. This is the first report of the isolation of a flavanone in the genus *Cajanus*.



Cajaflavanone (**1**)

REFERENCES

1. Ingham, J. L. (1976) *Z. Naturforsch. Teil C* **31**, 504.
2. Preston, N. W. (1977) *Phytochemistry* **16**, 143.
3. Smalberger, T. M., Vleggaar, R. and Weber, J. C. (1974) *Tetrahedron* **30**, 3927.
4. Ramà Rao, A. V., Rathi, S. S. and Venkataraman, K. (1972) *Indian J. Chem.* **10**, 989.
5. Nagar, A., Gujral, V. K. and Gupta, S. R. (1978) *Tetrahedron Letters* **23**, 2031.

---

*To whom correspondence should be addressed.