N-VINYL-α-(TRIFLUOROACETYL)PYRROLES

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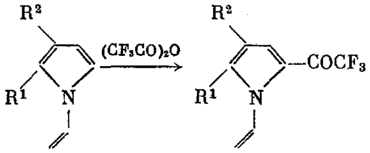
The course of the trifluoroacetylation of N-vinylpyrroles is difficult to predict from published results. The reactions of N-vinylindole (annelated pyrrole) imply that the site of attack by the electrophile in such systems may be the vinyl group rather than the heterocycle [1, 2]. This is consistent with the ease of electrophilic substitution of the N-vinyl hydrogen in the trifluoroacetylation of some N-vinyl heterocycles [3].

With the intention of synthesizing a new group of reactive pyrroles and of determining the position most sensitive to electrophilic attack in the N-vinylpyrrole system we have examined the trifluoroacetylation of N-vinylpyrroles (I)-(III). This reaction forms only the N-vinyl-α-(trifluoroacetyl)pyrroles (IV)-(VI). We did not detect any products of trifluoroacetylation of the N-vinyl group or of the β-position of the pyrrole ring



(I)—(III) (IV)—(VI)

$R^1{=}CH_3$, $R^2{=}H$ (I), (IV); $R^1{=}CH_3$, $R^2{=}CH_3$ (II), (V); $R^1 = R^2 = (CH_2)_4$ (III), (VI)

Results: compound no., yield, %; bp, °C (p, mm Hg); n_D^{20}; d_4^{20}; UV spectrum (hexane), λ_{max}, nm (log ε): (IV) 75, 73-74 (3); 1.5110; 1.2590; 200 (4.01), 266 (3.74), 310 (4.2); (V) 76; 92-93 (4); mp 37°C; 206 (3.84), 279 (3.72), 325 (4.01); (VI), 63; 122-123 (3) 1.5460; 1.2675; 208 (4.12), 282 (3.98), 328 (4.23). Elemental analyses (C, H, N, F) of compounds (IV)-(VI) corresponded to the empirical formulas. IR spectra of (IV)-(VI), cm^{-1}: 877-908 and 957-967 (C−H deformation modes in the N-vinyl group), 1642-1645 [ν(C=C)], as a shoulder on the very intense band at 1665-1670 [ν(C=O)]. The PMR spectrum of compound (IV) (100 MHz, 25°C, 20 vol.% CCl_4, internal standard TMS): 7.25 (H_α), 7.10 (H_4), 6.10 (H_3), 5.34 (trans-H_β); 5.14 (cis-H_β), 2.38 (CH_3) ppm; J, Hz: 8.5 (H_α-cis-H_β), 15.8 (H_α-trans-H_β), 0.7 (cis-H_β-trans-H_β), 0.4 (CH_3-H^3), 4.3 (H^3-H^4), 2.1 (H^4-CF_3). The splitting of the H^4 signals into quartets by coupling with CF_3 confirms the structure of (IV) and the assignment.

LITERATURE CITED

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