10-(Trifluoromethyl)-1,4,7-triazatricyclo[5,2,1,$0^{4,10}$]decane

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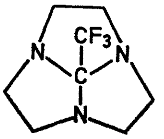
Summary The synthesis and proof of structure of the novel bridged heterocyclic system (I) are described.

Bridged polycyclic compounds have considerable chemical interest.[1a–f] Since the reported activity of adamant-1-ylamine hydrochloride as an antiviral agent, these compounds have also acquired pharmacological importance.[2a,b] Similar structures containing several hetero-atoms are not too common.

During an attempted synthesis of 2-trifluoromethyloxazoline by the pyrolysis of *N*-(2-hydroxyethyl)trifluoroacetamide[3] (easily prepared from ethyl trifluoroacetate and 2-aminoethanol[4]), we isolated a crystalline compound (I) that proved to be a novel heterocyclic ring system. When the hydroxyamide was heated at 220°, copious amounts of gas (CO_2, CHF_3, and H_2O) were evolved, and a colourless solid sublimed on the neck of the distilling flask (yield 29·5%). This product was recrystallized from MeOH and then from $CHCl_3$, m.p. 171—171·5°. It analysed for $C_8H_{12}F_3N_3$. A molecular weight determination showed it to be monomeric (*M* 210 osmotic, 207 mass spectral). The i.r. spectrum of (I) showed absorptions in the C–H stretching region (2975, 2950, 2020sh, 2890, and 2840 cm^{-1}) and three strong bands at 1173 cm^{-1} (C–F stretching) and 1164 and 1055 cm^{-1} (C–N stretching). No N–H stretching bands were visible. The n.m.r. spectrum of (I) ($CDCl_3$) showed only a symmetrical multiplet centred at δ 3·07 characteristic of an A_2B_2 or $AA'BB'$ splitting pattern. The decision between the two structures consistent with the above data, 1,1,1-tri(*N*-ethyleneimino)trifluoroethane and (I) was based on the mass spectral evidence. The molecular-ion peak (M^+) at *m/e* 207 (56%) confirmed the analytical and molecular weight data. The base peak at *m/e* 138 was due to loss of the $-CF_3$ group from the molecule. The peak at *m/e* 165 (38%) was due to the loss of $-N-CH_2\cdot CH_2-$ which could be observable in either of the two isomeric structures. However, the peak at *m/e* 151 (36%) and the complimentary peak at *m/e* 56 (70%) due to the loss of $-CH_2\cdot N\cdot CH_2\cdot CH_2-$ and also the peak at *m/e* 70 (40%) due to $-CH_2\cdot CH_2\cdot N\cdot CH_2\cdot CH_2-$, may be rationalized only on the basis of the tricyclodecane structure. A Courtauld model of (I) showed no undue strain.



(I)

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