

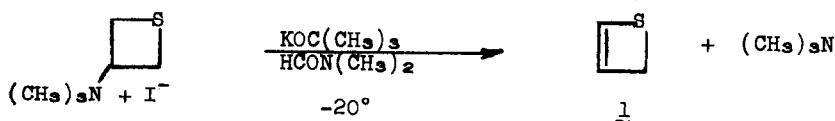
THIETE (THIACYCLOBUTENE)[★]

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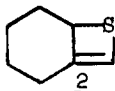
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Thiete (thiacyclobutene) 1, hitherto unknown, has been isolated in 20-30% yield by elimination of trimethylamine from trimethyl- β -thietanyl ammonium iodide. Only one other aliphatic thiete, 7-thiabicyclo[4.2.0]-1(8)octene, 2,



is known (1). Two thietes in which the double bond is part of a fused, aromatic ring have been prepared (2). Derivatives of thiacyclobutane which have an exocyclic double bond have been reported (3).

Thiete is of interest because it may form an anion isoelectronic with the anion of cyclopentadiene as has been discussed previously (4). Preliminary

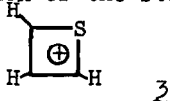


results indicate thiete is not greatly acidic, but no information concerning the thermodynamic stability or the reactivity of thiete anion has been obtained. Work is in progress on this aspect.

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Thiete itself appears to be more stable than the bicyclic compound 2; the latter decomposes vigorously when warmed to room temperature while thiete appears to be stable for up to one hour. The analysis for carbon and hydrogen indicated the presence of about 1.2% of water, probably the result of handling the cold thiete in a humid atmosphere. Anal. Calcd. for C_3H_4S : C, 49.95; H, 5.59. Found: C, 49.45, 49.29; H, 6.05, 6.08.

The mass spectrum of thiete showed fragments at m/e 72 (parent ion), 71 (base peak), 58 (C_2H_2S), 46 (CH_2S), 45 (CHS) and 39 (C_3H_3). The base peak is consistent with the formation of the stable cation $C_3H_3S^+$, 3.



The fragments at m/e 58 and 39 may have structures 4 and 5 respectively.



The proton nmr spectrum (at 60 mc) of thiete showed absorption at 6.50 δ (doublet, 1 H), 5.60 δ (multiplet, probably a sextet, 1 H) and 3.80 δ (doublet, 2 H). The ultraviolet spectrum in 2,2,4-trimethylpentane showed absorption at 215 ($\epsilon \sim 1920$), 236 ($\epsilon \sim 3000$) and 285 $m\mu$ ($\epsilon \sim 50$). An infrared spectrum of thiete (neat) showed absorption at 3100(w), 3040(w), 2924(m), 2785(w), 1670(m), 1540(m), 1400(m), 1250(s), 1137(m), 1030(m), 1017(m), 965(m), 900(m), 818(s), and 650(s) cm^{-1} .

References

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