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THE STRUCTURE OF 1,6,6 λ^4 -TRITHIAPENTALENE AND OXYGEN ANALOGUES STUDIED BY MEANS OF NMR SPECTROSCOPY IN AN ISOTROPIC AND AN ANISOTROPIC PHASE

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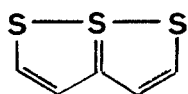
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THE STRUCTURE OF 1,6,6aλ⁴-TRITHIAPENTALENE AND OXYGEN ANALOGUES STUDIED BY MEANS OF NMR SPECTROSCOPY IN AN ISOTROPIC AND AN ANISOTROPIC PHASE.

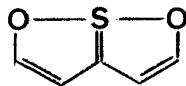
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Denmark

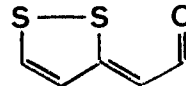
The NMR spectra of 1 and 2 have been recorded in both an isotro-



1

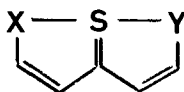


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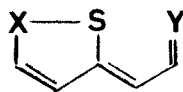


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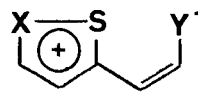
pic (CDCl₃) phase and an anisotropic phase (N-(4'-ethoxybenxyl-
idene)-4-butyraniline (EBBA) and 3 in an isotropic phase. The
structure of the compounds may be described by the following for-
mulae, where 4 - 6 can be resonance forms of the same molecule or



4



5



6

be different valence tautomers. If structure 4 is correct the
compounds should be found to possess C_{2v} symmetry for X = Y, whe-
reas 5 and 6 have only C_s symmetry. For 1 and 2 data from both i-
sotropic and anisotropic experiments are in accordance with C_{2v}
symmetry, this is for 2 supported by a microwave study (ref. 1).
From the dipole-dipole coupling constants obtained from the spec-
tra in EBBA it has been possible to evaluate relative structural
parameters for the two compounds 1 and 2, which seem to have a
slightly different geometry. The data from an isotropic phase for
3 are in agreement with a structure which is in between 5 and 6.

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