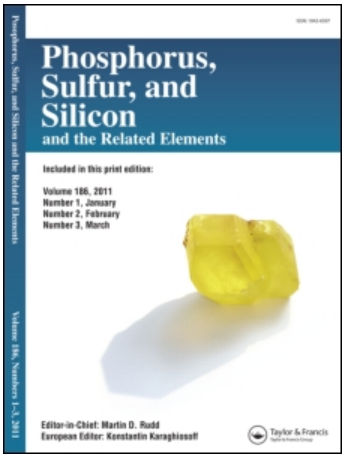


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# THE STRUCTURE OF 1,6,6Aλ⁴-TRITHIAPENTALENE AND OXYGEN ANALOGUES STUDIED BY MEANS OF NMR SPECTROSCOPY IN AN ISOTROPIC AND AN ANISOTROPIC PHASE

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**To cite this Article** Pedersen, Carl Th. and Jacobsen, Jens Peter(1979) 'THE STRUCTURE OF 1,6,6Aλ⁴-TRITHIAPENTALENE AND OXYGEN ANALOGUES STUDIED BY MEANS OF NMR SPECTROSCOPY IN AN ISOTROPIC AND AN ANISOTROPIC PHASE', Phosphorus, Sulfur, and Silicon and the Related Elements, 6: 1, 237
**To link to this Article: DOI:** 10.1080/03086647908080392
**URL:** http://dx.doi.org/10.1080/03086647908080392

*Phosphorus and Sulfur*
1979, Vol. 6, p. 237



# THE STRUCTURE OF 1,6,6a$\lambda^4$-TRITHIAPENTALENE AND OXYGEN ANALOGUES STUDIED BY MEANS OF NMR SPECTROSCOPY IN AN ISOTROPIC AND AN ANISOTROPIC PHASE.

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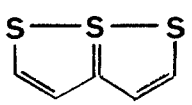
The NMR spectra of 1 and 2 have been recorded in both an isotro-



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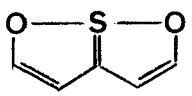

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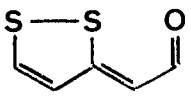
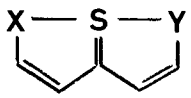


3

pic ($CDCl_3$) phase and an anisotropic phase (N-(4'-ethoxybenxylidene)-4-butylaniline (EBBA) and 3 in an isotropic phase. The structure of the compounds may be described by the following formulae, where 4 - 6 can be resonance forms of the same molecule or



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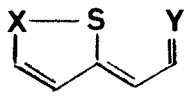

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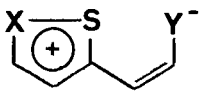

6

be different valence tautomers. If structure 4 is correct the compounds should be found to possess $C_{2v}$ symmetry for X = Y, whereas 5 and 6 have only $C_s$ symmetry. For 1 and 2 data from both isotropic 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 spectra 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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[1] T. Pedersen, S. V. Skaarup and C. Th. Pedersen
Acta Chem. Scand. B31 (1977) 711.