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## Phosphorus, Sulfur, and Silicon and the Related Elements

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Krystian Pluta

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## 3,3'-Diquinolinylnyl Sulfides. The Conformations and $^1\text{H}$ and $^{13}\text{C}$ NMR Spectroscopic Effects

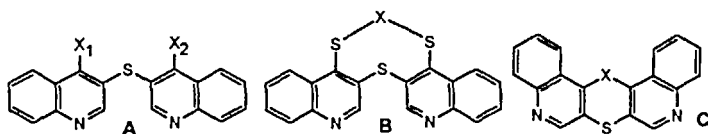
KRYSTIAN PLUTA

Department of Organic Chemistry, Silesian School of Medicine, ul. Jagiellońska 4,  
 41-200 Sosnowiec, Poland

Non-typical NMR effects in 3,3'-diquinolinylnyl sulfides and the chemical shift – conformation dependences are discussed.

**Keywords:** diquinolinylnyl sulfides; conformations;  $^1\text{H}$  and  $^{13}\text{C}$  NMR

We have studied NMR effects (ortho, meta and peri) in disubstituted 3,3'-diquinolinylnyl sulfides **A**, **B** and **C**, where a rotation around the central C-S-C bridge is permitted, restricted or hindered.

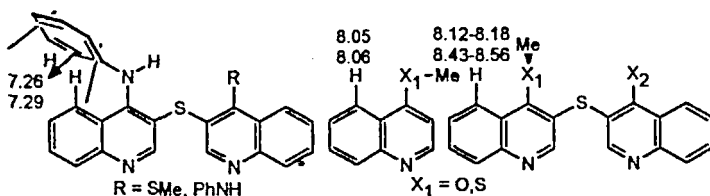


The peri effects calculated in relation to unsubstituted 3,3'-diquinolinylnyl sulfide ( $\delta_{\text{H},s} = 7.70$  ppm) are as follows:

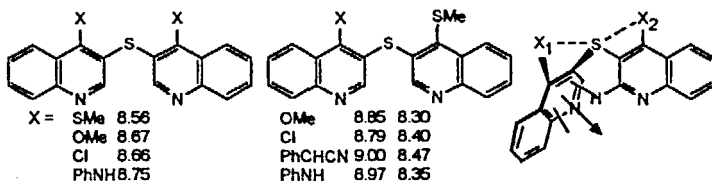
$\text{StBu} > \text{SEt} > \text{Sallyl} > \text{SMe} > \text{SCH}_2\text{Ph} > \text{SeCH}_2\text{Ph} > \text{SPh} > \text{Cl} > \text{PhCHCN}, \text{OMe}$   
 +0.98 0.89 0.86 0.73-0.86 0.76 0.73 0.72 0.52-0.55 0.47 0.42-0.48

The peri effect of the phenylamino group (-0.41-0.44 ppm) is unexpectedly contrary to the rest of the substituents and is a result of the ring current effect of the phenyl group. The peri effect of the methoxy and methylthio groups is different than in monosubstituted quinolines and is attributed to

a rotation around the C<sub>4</sub>-X bond. The perpendicular orientations of these groups were confirmed by X-ray analyses<sup>[1-3]</sup>.



The crucial element determining the H-2 and H-2' proton shifts is a rotation of the sulfide bridge. The X-ray analyses showed the H-2' atom to be under an influence of the ring current of the left quinoline ring<sup>[1-3]</sup>.



Whereas the H-5 protons are deshielded, the carbons connected with them are shielded in opposite way up to 10 ppm.

As well as the C-4a, C-5 and methyl carbon signals in methylthio- and methoxydiquinolyl sulfides depend on conformations of the methylthio and methoxy groups. These carbons are deshielded up to 6 ppm in comparison with the carbons found in 3-unsubstituted quinolines.

X-ray examinations showed the same conformations in the solid state as in CDCl<sub>3</sub> and revealed the donor-acceptor interactions of the heteroatoms.

## References

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- [3] K. Pluta, K. Suwińska, *J. Chem. Cryst.*, **27**, 465 (1997).