

Contribution ID: 85 Type: POSTER

## 14N NQR study of selected 1,4-benzoquinonedioximes

1,4-benzoquinonedioxime, 14N, NQR

## Please specify whether you would prefer an oral or poster contribution.

Poster

## **Summary**

1,4-benzoquinonedioximes are known for their use in industry and other applications[1]. They are effective non-sulfur vulcanizing agents for natural and synthetic elastomers. Additionally, their metal complexes have generated significant industrial and theoretical interest. This study examines the 14N NQR data for a series of 1,4-benzoquinone-dioximes: unsubstituted, mono-, di- and tri-methyl substituted. The results show that as more methyl substituents are added to the ring a shift in the NQR values are observed. Comparison of unsubstituted and tri-substituted benzoquinonedioximes (Table 1) shows that the quadrupole coupling constant ( $\boxtimes$ ) increases by about 1000 kHz and the asymmetry parameter ( $\boxtimes$ ) decreases from  $\boxtimes$  0.7 to 0.3. Ab-initio calculations show that for the unsubstituted compound hydrogen bonding between oxime groups and pi-ring stacking is possible which cannot be accommodated for in heavily methyl substituted dioximes and this is responsible for the differences in the NQR parameters.

Table 1: 14N NQR data for the 1,4-benzoquinonedioximes

Compound  $\boxtimes 0(kHz) \boxtimes -(kHz) \boxtimes +(kHz) \boxtimes (kHz) \boxtimes$ 

1,4-benzoquinone 1654 2673 4360 4689 0.706 dioxime 1654 2712 4360 4715 0.702

 $trimethyl\hbox{--}1,4\hbox{--}950\ 3750\ 4700\ 5633\ 0.337$ 

benzoquinonedioxime

Double resonance cross relaxation [2] was used to record the 14N NQR data. The ab-initio calculations were performed using GAMESS [3].

## References

- $[1] \ http://chemicalland 21.com/special tychem/perchem/p-QUINONE\% 20 DIOXIME. htm (last accessed 04-28-10) and the properties of the pr$
- [2] D. Stephenson and J. A. S. Smith, Proc R Soc Lond A 416, 149 (1988).
- [3] M. W. Schmidt et al., J. Comput. Chem. 14, 1347 (1993).

**Primary author:** Mrs SINGH, Nadia (The University of the West Indies, St. Augustine, Trinidad) **Co-author:** Dr STEPHENSON, David (The University of the West Indies, St. Augustine, Trinidad)

Presenter: Mrs SINGH, Nadia (The University of the West Indies, St. Augustine, Trinidad)

Track Classification: Biology, Chemistry, Medicine