XVIII Simpósio Brasileiro de Química Teórica – SBQT 2015
Pirenópolis – GO, 22-25 Novembro de 2015

# The Nuclear Quadrupole Moment of Xenon

Guilherme Arantes Canella[a] (PG), Régis Tadeu Santiago[a] (PG), Roberto Luiz Andrade Haiduke[a] (PQ)

[a]*Departamento de Química e Física Molecular, Instituto de Química de São Carlos, Universidade de São Paulo.*
*guilherme.canella@usp.br.*

Keywords: Xenon, Nuclear Quadrupole Momment, Electric Field Gradient, Relativistic Basis Set.

## INTRODUCTION

Nuclear Quadrupole Moments (NQMs) have been systematically investigated in the last decades, since they are relevant to important spectroscopy techniques, *e.g.*, nuclear magnetic ressonance, Mössbauer espectroscopy, etc[1]. The molecular method is one of the treatments used to determine this property. In this method, the NQM can be calculated based on a simple relation between the Nuclear Quadrupole Coupling Constants (NQCCs) and Electric Field Gradients (EFGs)[2],

$$Q(X) = \frac{\nu_Q(X)}{0.2349647 q(X)}, \qquad (1)$$

where $Q(X)$, $\nu_Q(X)$ and $q(X)$ stand for the NQM (milibarns), NQCC (MHz) and EFG (a.u.) respectively.

Some years ago, Kellö *et al*. calculated the EFG and consequently determined the NQM, for the isotope $^{131}$Xe in the $XeH^+$ molecule. They found values of 13.8183 a.u. and -114 mb respectively[3]. Here, we calculated the EFG for xenon in $XeH^+$ by using a more advanced level of theory and a new relativistic basis set.

## METHODS

All EFG calculations have been performed with fully uncontracted basis sets for Xe (25s20p14d11f3g) and H (6s3p2d1f). We used a new relativistic prolapse-free basis set of quadrupole-$\zeta$ quality (RPF-4Z) for xenon and the cc-pVTZ basis set for hydrogen. Moreover, we employed the Dirac-Coulomb Hamiltonian (DC), with a Gaunt correction estimated at the Hartree-Fock level. Møller-Plesset Perturbation Theory with second-order approximation (MP2) and Coupled-Cluster Theory (CCSD, CCSD(T) and CCSD-T) were also used to achieve a reliable description of electron correlation effects. The chosen active space accounts for 26 electrons in the 4s, 4p, 4d, 5s and 5p shells of xenon. The calculations also were done within a four-component formalism.

## RESULTS AND DISCUSSION

As one can notice in Table (1), nice accordance with Kellö's results were obtained with DC+G-CCSD(T) and DC+G-CCSD-T treatments. This is surprising since they used Douglas-Kroll (DK) theory level (two-components).

Table 1: EFG and NQM for $^{131}$Xe in $XeH^+$ as given by different theoretical treatments.

| Method | EFG (a.u.) | NQM (mb) |
|---|---|---|
| DC-HF | 14.1081 | -111.8 |
| DG-HF | 14.0399 | -112.3 |
| DC-B3LYP | 14.1898 | -111.1 |
| DC+G-MP2 (full) | 13.4829 | -117.0 |
| DC+G-CCSD | 13.9070 | -113.4 |
| DC+G-CCSD(T) | 13.7595 | -114.6 |
| DC+G-CCSD-T | 13.7590 | -114.6 |

## CONCLUSIONS

The results show that a more advanced theory level along with a quadrupole-$\zeta$ quality basis set still provide NQM values in nice agreement with Kellö's results (deviations smaller than 1%).

## ACKNOWLEDGMENTS

The authors are grateful for the support from FAPESP (2010/18743-1 and 2014/23714-1), CNPQ and São Carlos Institute of Chemistry (USP).

[1] J.W. Zwanziger, *Computing Electric Field Gradient Tensors, in NMR of Quadrupolar Nuclei in Solid Materials*; R.E. Wasylishen, S.E. Ashbrook e S. Wimperis (Eds); Wiley: United Kingdom, (2012).

[2] R. T. Santiago and R. L. A. Haiduke, *Phys. Rev. A* 91, (2015), 042516.

[3] V. Kellö, P. Pyykkö, A. J. Sadlej, *Chem. Phys. Let.* 346, (2001), 155-159.