Analysis of the Quadrupole Coupling Constants and Mössbauer Isomeric Shifts in Halogen Compounds Within the Gaussian98 Code

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Z. Naturforsch. **55 a,** 271–275 (2000); received September 11, 1999

Presented at the XVth International Symposium on Nuclear Quadrupole Interactions, Leipzig, Germany, July 25 - 30, 1999.

A comparison of the experimental and calculated nuclear quadrupole coupling constants of diatomic halogen, interhalogen, trihalide ions and complexes of pyridine is a good test of reliability of semiempirical and non-empirical theories as well as their usefulness in the interpretation of quadrupole coupling data from the qualitative and quantitative point of view. Therefore, a practical way of gaining insight into the bonding properties and electronic structure of such systems consists of combining semiempirical MO calculations with experimental data to derive reliable information. In the present work we report the results of ab initio studies of several iodine containing molecules and ions using the calculated NQCC as a test of the quality of the wavefunctions. To demonstrate the quality of our calculations, we compare the calculated halogen-halogen bond length and QCC with the corresponding experimental values for the compounds studied. With a few exceptions, the overall agreement with experiment is most satisfactory. The results on dipole moments and energy levels are also in a good agreement with the experimental data, however these quantities were measured only in the few cases.

Key words: DFT; QCC; Isomeric Mössbauer Shifts; Halogen Compounds.