Quadrupole Coupling Constants and Mössbauer Isomeric Shifts in Antimony Compounds within Gaussian 98

O. Kh. Poleshchuk[a] and J. N. Latosińska

Institute of Physics, Adam Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland
[a] *Permanent address:* Tomsk Pedagogical University, Komsomolskii 75, 634041 Tomks, Russia

Reprint requests to Dr. J. N. L.; Fax: +48-61-8257758; E-mail: jolanala@amu.edu.pl

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The electron density and quadrupole coupling constants of molecules containing Sb are analysed. The NQCC for antimony, calculated using the extended basis 6-311G** are much lower than the experimental data, while the use of the small 3-21G* basis led to NQCC closer to the experimental ones.

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