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

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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.