Evaluation of the ^{57m}Fe Quadrupole Moment from Hartree-Fock Calculations*

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Two theoretical evaluations of ^{57m}Fe quadrupole moment (Q), based on different formalisms, namely the Hartree-Fock theory and the Linearized Augmented Plane Wave method have yielded results differing by a factor of two. In both cases, Q was obtained from experimental quadrupole interaction frequencies through investigation of the Electric Field Gradients at the nuclear site of the ^{57m}Fe probe. It is the purpose of the present work to reexamine the earlier Hartree-Fock approach. In particular, the earlier model is extended through a more realistic description of the environment of ^{57m}Fe in the respective experiments, as well as through inclusion of electron correlation effects.

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