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Quadrupole moments from measurements in condensed matter: The "missing link"cases Cd, Sn, Pb

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In order to determine reliable values for nuclear quadrupole moments (Q) from experiments accurate theoretical calculations of the electric-field gradients (EFG) acting at the nuclear site are needed. Though considerable progress in calculating the EFG in condensed matter has been made with density-functional methods (DFT), it has been become more and more evident over the years that this technique has some intrinsic deficiencies obtaining precision absolute EFG numbers. Many-electron theory, on the other hand, in principle does not suffer from such shortcomings. Calculations in atoms or simple molecules are therefore now considered to produce the most reliable EFG values.
Thus, experimental PAC measurements at ISOLDE for free molecules have recently solved this "missing link" gap for Cd isotopes. Similar experiments for Pb are planned. For the case of the119Sn Mössbauer state, however, such measurements would present extreme technical difficulties. Therefore, only data for simple molecules embedded in inert solids are available. Computing the EFG shift between free and embedded molecules with DFT techniques, of the order of 2-5%, has here also produced a reliable value for Q, much different from the presently accepted number.

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