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The quadrupole moments of Zn and Cd isotopes - an update

Precise nuclear quadrupole moments (Q) are a prerequisite for any quantitative analysis of measured quadrupole coupling constants. While historically good precision of calculated electric field gradient (EFG) values for normalization could only be achieved for atoms, the progress of calculations for molecules and solids in recent times has opened up a new possibility. Thus in many cases now values for Q have been obtained in this way [1]. Here we have used the full-potential linearized augmented plane waves (FLAPW) method to obtain updated values of Q for the Zn and Cd isotopes. The most reliable results come from the calculations in the hexagonal metals. Here accurate lattice constants at 4K have been determined and precise values for the coupling constants are known. For error analysis numerous calculations were made using different density functionals and computational parameters. In particular a very dense mesh of k-points in the Brillouin zone was needed. The final results (absolute values) are: Q (67Zn, g. st.) = 0.145 (3) b, Q (111*Cd, 5/2+) = 0.764 (15) b. Calculations of the EFG in various other compounds, mostly halides, give results in agreements with these values, of less precision, however. To check the procedures employed the EFG in several simple gallium and indium halides was calculated. The resultant quadrupole moments agree within 1% with the precisely known values. Using the experimentally determined ratios of Q, generally known with high accuracy, the moments of the other Zn and Cd isotopes can be obtained. In the case of Cd the trends of coupling constants from optical spectroscopy and perturbed angular distribution measurements must be considered for this purpose.

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Poster

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