Quadrupole Moment of ^{57}Fe^m

In a recent Letter,[1] a new first-principles calculation of the electric field gradient (EFG) at the iron nucleus in $FeCl_2$ and $FeBr_2$ molecules has been reported. From the calculated EFG's and measured quadrupole interaction energies for these molecules trapped in Ar and Xe, the authors[1] conclude that the quadrupole moment of the Mössbauer isomer in ^{57}Fe is $8.2(8)e$ fm^2, considerably smaller than the previously accepted value,[2] $21.1e$ fm^2. As this new work[1] is in disagreement with many other calculations and depends on cancellations of several large terms in the calculated gradient, it would be helpful to have a completely independent line of reasoning to predict the Mössbauer-level quadrupole moment and hence either support or contradict the EFG calculations of Ref. 1. Unfortunately, it is difficult to make any realistic prediction directly from shell-model calculations of ^{57}Fe because of the many configurations which enter into the low-spin ($J^\pi = \frac{3}{2}^-$) Mössbauer level.

We show in this Comment, on the other hand, that $Q(^{57}\mathrm{Fe}^m)$ can be predicted from shell-model calculations of a $J^\pi = 10^+$ isomeric state[3] in ^{54}Fe together with the result of a recent measurement[4] of the *relative* quadrupole moments of the ^{54}Fe and ^{57}Fe isomers.

A shell-model calculation[5] for ^{54}Fe has been made which included the $f_{7/2}$, $p_{3/2}$, and $f_{5/2}$ orbitals. Kuo-Brown matrix elements were used and the energies of the $p_{3/2}$ and $f_{5/2}$ orbitals were taken as 2.1 and 6.5 MeV, respectively. The wave function of the lowest ^{54}Fe $J^\pi = 10^+$ state was found to correspond predominantly (> 90%) to a $p_{3/2}$ neutron coupled to a $J^\pi = \frac{19}{2}^- (f_{7/2})^3$ core. Table I shows the calculated quadrupole moment and $E2$ and $E4$ decay transition strengths of ^{54}Fe^m, together with similar results for another recent calculation.[6] The excellent agreement obtained between the experimental transition strengths and the results of either calculation strongly supports the reliability of the calculations of $Q(^{54}\mathrm{Fe}^m)$.

With these calculated values of the ^{54}Fe^m quadrupole moment and the measured[4] ratio of moments $Q(^{54}\mathrm{Fe})/Q(^{57}\mathrm{Fe}^m) = 3.45(30)$, we deduce the values of the ^{57}Fe^m quadrupole moment shown in Table I. We conclude that shell-model calculations for ^{54}Fe^m together with the measurement of Ref. 4 strongly favor the ^{57}Fe^m quadrupole moment value deduced by Duff, Mishra, and Das[1] and contradict earlier EFG calculations[2] which implied $Q(^{57}\mathrm{Fe}^m)$ over twice as large.

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TABLE I. Properties of ^{54}Fe^m and ^{57}Fe^m.

	Theory[a]	Theory[b]	Experiment
$[B(E2)(10^+ \rightarrow 8^+)]^{1/2}$, e fm^2	4.5	4.9	4.61(5)[c]
$Q[^{54}\mathrm{Fe}(10^+)]$, e fm^2	24	29	
$Q[^{57}\mathrm{Fe}(3/2^+)]$, e fm^2	7.0[d]	8.5[d]	
$[B(E4)(10^+ \rightarrow 6^+)]^{1/2}$, e fm^4	63	43	45(5)[c]

[a] Ref. 5, using $e_p = 1.3(1)e$, $e_n = 0.6(1)e$ [see E. Dafni, H. E. Mahnke, J. W. Noé, M. H. Rafailovich, and G. D. Sprouse, Phys. Rev. C 23, 1612 (1981)].

[b] Ref. 6, using $e_p = 1.5e$, $e_n = 0.5e$.

[c] Ref. 3.

[d] Derived from the ratio of quadrupole interaction frequencies for ^{54}Fe and ^{57}Fe in Zn given in Ref. 4.

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