

## II-1

### Problems of Compiling and Evaluating or What Is the Nuclear Moment?

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In the process of compiling a "best-value" list of nuclear magnetic moments with uncertainties of 0.01% or better, two kinds of problems arise. One is a fundamental problem associated with the measurement of a nuclear moment in the laboratory where the nucleus is part of an atom or molecule in some gas, liquid, or solid mixture. The second is the trivial one of the way experimenters write papers.

To dispatch the trivial one first, we want to know, for our compilations: 1) experimental conditions and environment of the nucleus; 2) Measured quantities, including units and signs (+, -,  $\pm$ ); 3) Assumptions made in applying theories and actual values of calibration standards, fundamental constants and corrections used for the calculation of the moments; and 4) A reasonable estimate of experimental uncertainties and probable errors. The omission of this information makes it impossible to consider many values if reevaluations are needed when theories, constants, or corrections change. In addition, a descriptive title and informative abstract can assure that the paper will not be missed.

To explore the fundamental problem, we can examine the magnetic moments for twenty nuclei which have been precisely measured by several different methods for the atom and molecule. We find that more than half of them show a magnetic moment discrepancy,  $D \equiv (\mu_{\text{molecule}} - \mu_{\text{atom}})/\mu_{\text{atom}} > +0.05\%$ . Where data exist for these nuclei, the chemical shifts observed in Nuclear Magnetic Resonance (NMR) are about this size or smaller.<sup>1)</sup> The remaining differences probably arise from the effect of configuration interactions and possible differences in the diamagnetic corrections,  $\sigma$ , for the different states as evidenced by some recent calculations of Feiock and Johnson.<sup>2)</sup>

To consider a few cases, let us look at  $^{207}\text{Pb}$ ,  $^{63}\text{Cu}$ , and  $^{135}\text{Ba}$ . For  $^{207}\text{Pb}$ ,  $D = (+1.98 \pm 0.01)\%$  using the Optical Pumping (OP) value<sup>3)</sup> for the  $^3\text{P}_0$  state and the NMR value<sup>4)</sup> for 1.0 molar  $\text{Pb}(\text{C}_2\text{H}_3\text{O}_2)_2 + 0.8$  molar  $\text{Mn}(\text{C}_2\text{H}_3\text{O}_2)_2$ . The calculated difference in the diamagnetic correction for these two states can

account for 0.4%.<sup>2)</sup> Calculations of Margerie<sup>5)</sup> show that the effect of configuration interactions on the Landé  $g$ -factor for the  $^3\text{P}_0$  state is  $\sim 1\%$ . He suggests that this may also be responsible for part of the Pb moment discrepancy.

The Atomic Beam value<sup>6)</sup> of the  $^{63}\text{Cu}$  moment and the average measured by NMR for  $\text{CuCl}$  and  $\text{CuCl}_2$ <sup>7)</sup> gives  $D = (+0.16 \pm 0.02)\%$ . The reported NMR values differ by 0.04%. Here the difference in  $\sigma$  cannot account for more than 0.007%. Recent measurements<sup>10)</sup> on some cuprous salt solutions would increase  $D$ , since they show chemical shifts as large as 0.088%. The large discrepancy may possibly be accounted for by some interference between the atomic energy levels used for the beam measurements.

$D = (+0.083 \pm 0.008)\%$  for  $^{135}\text{Ba}$  using the OP measurements<sup>8)</sup> on Ba vapor in the  $^1\text{S}_0$  state and the NMR measurements<sup>9)</sup> on  $\text{BaCl}_2$ . Here again the difference in  $\sigma$  cannot account for the observed discrepancy. Even larger discrepancies are observed between the NMR and  $^1\text{S}_0$ -state OP measurements for  $^{111,113}\text{Cd}$ ,  $^{171}\text{Yb}$  and  $^{199}\text{Hg}$ , while that for  $^{67}\text{Zn}$  is smaller.

In spite of the quoted uncertainties in the individual experimental values, there are only a few special nuclei for which it is possible to tabulate meaningful nuclear magnetic moments to accuracies of better than 0.1 to 1.0%.

#### References

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  - 10) R. W. Mebs, G. C. Carter, B. J. Evans and L. H. Bennett: Solid State Comm. **10** (1972) 769.
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