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New Analytical Representation for Electronic Terms of Nuclear Schiff Moment

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The nuclear Schiff moment (NSM) is produced by a nuclear force that simultaneously violates charge conjugation (C) symmetry and spatial parity (P) inversion symmetry. The experimental detection of NSM is significant as CP violation is crucial for explaining the current matter-dominated universe. Measuring NSM in molecules necessitates precise experiments and theoretical calculations that incorporate both electronic and nuclear wavefunctions. Conventionally, electronic terms have been approximated using a first-order power series expansion of the electronic radial function; however, this may not be sufficiently accurate. In this study, we introduce a new accurate analytical expression for the electronic terms using Gaussian basis sets, which avoids any truncation of the power series. For the RaO molecule, a prime candidate for NSM observation, conventional methods overestimated the electronic terms by more than 50%, underscoring the significance of our analytical approach.

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