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UNLOCKING MULTICENTER INTEGRALS: A SIMPLIFIED CARTESIAN APPROACH TO SPHERICAL HARMONICS

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ABSTRACT

This study introduces a systematic derivation of Cartesian expressions for both surface and regular solid spherical harmonics, leveraging the efficiency of binomial coefficients. While spherical harmonics are fundamental to representing atomic and molecular symmetries, their traditional forms often pose significant computational challenges in multi-center contexts. Our approach transforms these complex functions into a more manageable algebraic framework, facilitating the evaluation of multicenter molecular integrals over Slater-Type Orbitals.

The proposed formulations demonstrate their particular strength when dealing with high-order quantum numbers, where conventional numerical methods often encounter stability and speed issues. By reducing the reliance on intricate angular transformations, this Cartesian-based binomial logic provides a robust pathway for faster and more precise molecular simulations. We further discuss the computational advantages of these formulae, highlighting their potential to streamline large-scale quantum chemical calculations and improve the scalability of multicenter integration algorithms

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