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Outlier Detection in the Approximation of Tension Strain Energy of C_{44} Fullerenes: An Approach Based on Fragmental Matrix Property Indices and Non-Parametric Residual Analysis

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Abstract

The functional approximation of quantum mechanical properties over discrete isomer spaces frequently encounters outliers that distort predictive stability. This work proposes a mathematical methodology to isolate these anomalies in modeling the Tension Strain Energy (TSE) of the complete set of C_{44} fullerene isomers, utilizing operators based on Fragmental Matrix Property Indices (FMPI) [1].

Unlike classical filtering based on standardized residual distances, our approach treats outlier identification as a compliance problem of the error distribution within the approximation manifold. The impact of systematically eliminating specific isomers is critically evaluated through non-parametric tests based on the empirical distribution function of residuals [2]: Anderson-Darling (AD), Kolmogorov-Smirnov (KS), Cramér-von Mises (CM), Kuiper (KV), and Watson U^2 (WU). The underlying error dynamics are monitored computationally via structural tracking indicators (G0, G1, H1, WS, and SF).

Numerical precision and convergence difficulties in standard environments (Python) were resolved by developing a native computing engine in PHP, optimized for fit integrals on finite samples. The concerted use of AD and KV statistics successfully isolated isomers defying the linear approximation. For the TSE property, the most distant outlier exhibits C_1 symmetry, followed by specific structures belonging to the D_2, C_s, D_3, S_4, and T symmetry groups. The methodology provides an objective selection criterion aligned with numerical approximation theory, overcoming the limitations of subjective data trimming in structural modeling [3].

Keywords: Approximation theory, residual analysis, C_{44} fullerenes, non-parametric tests, fragmental matrix property indices (FMPI), PHP.

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