Extraction of Dunham Coefficients from Murrell-Sorbie Parameters

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A set of relationships between parameters of the Dunham and Murrell-Sorbie potential energy function is developed. By employing Taylor series expansion and comparison of terms arranged in increasing order of bond length, a set of Dunham coefficients is obtained as functions of Murrell-Sorbie parameters. The conversion functions reveal the importance of factorials in extracting Dunham coefficients from Murrell-Sorbie parameters. Plots of both functions, based on parameters of the latter, reveal good correlation near the equilibrium bond length for a group of diatomic molecules. Potential function relations, such as that shown in this paper, are useful when the preferred/reliable data is based on a potential function different from that adopted in available computational software.