Symmetry-Adapted Polynomial Basis for Global Potential Energy Surfaces - Applications to XY4 Molecules

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Abstract

Potential energy surfaces (P.E.S.) inherit the symmetries of molecules, and are therefore invariant under the action of the permutation-translation-rotation-inversion group. One should therefore take advantage of this property, both theoretically and numerically.

The present work concentrates on the invariant theory issues and should be understood as the prolongation of the work of Schmelzer-Murrell and Collins-Parsons on the subject. We present a simplified technique to parametrize symmetry-adapted global P.E.S., together with algorithmic recipes that make the problem computationnally tractable. The method is illustrated in detail on XY_4-molecules for which a full description of the algebra of invariant polynomials under the full symmetry group of the molecule is given.