Abstract Submitted
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Calculation of potential energy surfaces using explicitly correlated methods[1] GRANT HILL, KIRK A. PETERSON, Washington State University — Recent developments in explicitly correlated wavefunctions mean that highly accurate potential energy surfaces for small molecules can be obtained with a low computational cost. Key components of these composite surfaces will be presented, including extrapolation of explicitly correlated CCSD(T) correlation energies and correcting for core-valence correlation effects using F12 methods. Recent applications will be highlighted, including high-resolution spectroscopy of CCN, CCO^+ and COC^+.

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Grant Hill
Washington State University

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