Abstract Submitted
for the DAMOP12 Meeting of
The American Physical Society

An integro-differential transform to analytically reduce H_2 molecular integrals JACK STRATON, Portland State University — Molecular integrals that have a coordinate dependence akin to the bonding H_2 wave function are often carried out one-by-one, using hyper-spherical coordinates [1], Jacobi coordinates or bond-length coordinates [2], or confocal ellipsoidal coordinates [3]. An alternative strategy is to extend the general result developed by the author [4] for evaluating integrals of any number of products of multicenter ground-state or excited [5] atomic wave functions, Coulomb or Yukawa potentials, and Coulomb-waves [6] to include the H_2 molecular wave function. Modifications for semi-infinite integrals that terminate on a surface such as a Scanning Tunneling Microscope sample are also discussed.

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Date submitted: 27 Jan 2012 Electronic form version 1.4