

Abstract Submitted  
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**Computation of Atomic Solvent Accessible Surface Areas and Gradients for the Calculation of Solvation Energy and Forces on Molecules** MICHELLE HUMMEL, Department of Mathematics, University of New Mexico, CHRISTOPHER FENNEL, Department of Chemistry, Oklahoma State University, EVANGELOS COUTSIAS, Department of Applied Mathematics and Laufer Center, Stony Brook University, KENNETH DILL, Department of Chemistry and Laufer Center, Stony Brook University, EMILIANO BRINI, Laufer Center, Stony Brook University — Many models for the calculation of solvation energy and forces on a molecule involve atomic solvent accessible surface areas and their gradients. We present analytical formulas for such areas and gradients which utilize the Delaunay tetrahedrization of a molecule and its subset called the  $\alpha$ -complex. These formulas have been implemented in a fast computer program in conjunction with a solvation approach called *Semi Explicit Assembly (SEA)*, and has shown to produce quick and physically accurate results.

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