A Force Field with Complete Coverage

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To solve the common “missing parameter” problem in force field applications, we have developed a unique force field database that promises complete coverage of rational molecules using empirical functions. This approach is based on the following techniques: 1) precise definition of atom types, 2) rational transfer of parameters, 3) automatic fit of ab initio data, and 4) empirical optimization of LJ parameters. The force field database has been parameterized to cover common synthetic polymers, proteins, drug molecules, ions, metals and transition metals. Unprecedented coverage has been achieved; for example, all (about 55K) drug-like and building-block molecules in the Maybridge® database have been parameterized. New parameters can be readily added into the force field database as long as the representing molecules can be calculated using ab initio methods. We will explain the techniques and present the validation results of the proposed force field in this presentation.