Making TraPPE Accessible:
A Searchable Online Database for Force Field Parameters

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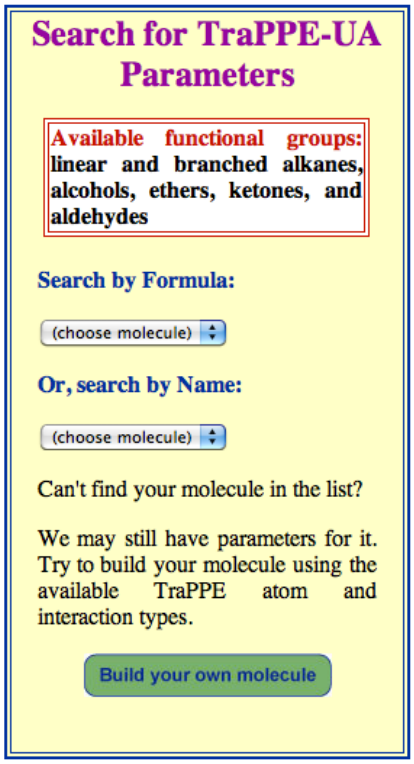
The Transferable Potentials for Phase Equilibria Force Field (TraPPE) has become an accurate method for describing molecular interactions for a wide variety of chemical systems in molecular mechanics simulations. Like most common force fields, TraPPE uses several functional forms and a vast collection of specific parameters to model a range of different molecule types. To date, the TraPPE force field spans all of the common functionalities of small organic molecules and includes united-atom, all-atom, polarizable, and most recently, coarse-grain models.



With the growing range and applicability of the TraPPE force field, an important goal for TraPPE developers is to encourage its broad use and accessibility. Given the myriad of parameters and different functional forms that make up TraPPE, finding the correct set of parameters for a given molecule, in a form that works with one's chosen simulation program, is far from straightforward. This greatly limits the extent to which novice simulators can successfully take advantage of the hallmark transferability of the TraPPE force field and exists as a potential barrier to widespread use, especially among non-expert users. To overcome these limitations, we present here ongoing work towards a web-based searchable parameter database and accompanying user interface for the TraPPE force field.

http://www.chem.umn.edu/groups/siepmann/trappe/intro.php