

# An Online Database for TraPPE Force Field Parameters

Amara J. Sunnarborg, Andrew Bliss, Hudson Stern, Becky L. Eggimann  
Wheaton College, Wheaton, IL

The Transferable Potentials for Phase Equilibria Force Field (TraPPE) is used to describe interactions between molecules of interest in molecular mechanics simulations. The TraPPE force field aims to be accurate, computationally efficient, and applicable to a wide range of chemical compounds, state points and thermophysical properties. To date, the TraPPE force field spans most of the common functionalities of small organic molecules and includes united-atom, explicit hydrogen, polarizable, and most recently, coarse-grain versions.

The Siepmann Group Home People Research Publications Software TraPPE Teaching

## The Transferrable Potentials for Phase Equilibria Family of Force Fields

See the Complete List of TraPPE Publications

### Browse the TraPPE Gallery

**TraPPE-UA**  
Molecular Structures

**TraPPE Small Molecule**  
Phase Diagram

**TraPPE-EH**  
Phase Diagrams, Molecular Structures, Liquid Structures

**TraPPE-CG**  
Force Field Parameters

**TraPPE-pol**  
Force Field Parameters

### Search the Parameter Database

Complete parameters for the United Atom and Small Molecule development sets are available.

Search by Formula:  
(choose molecule) ↓

Or, Search by Name:  
(choose molecule) ↓

Can't find your molecule in the list?  
We may still have parameters for it. Try to build your molecule using the available TraPPE atom and interaction types.

**Build Your Own Molecule**

**Thanks to Our Supporters**  
This work is generously supported through continuing grants from the National Science Foundation - Chemical, Bioengineering, Environmental, and Transport Systems with additional support from Merck & Co., Inc., 3M Co., Procter and Gamble Co., and Abu Dhabi National Oil Co.

Chemical Theory Center | Chemistry Department | Chemical Engineering and Materials Science Department | Minnesota Supercomputing Institute | University of Minnesota

When new users wish to implement TraPPE models into their chosen simulation program, they face potentially prohibitive barriers to success: the TraPPE models are dispersed over dozens of separate publications and misinterpretations of the primary literature are common; the TraPPE force field makes specific choices for standard conventions that may require non-trivial code modifications for some simulation software. Therefore, an important goal for TraPPE developers is to encourage its broad use and accessibility. We present here the continuing development of a resource website and online searchable parameter database designed to provide new and experienced users with tools for successful implementation and validation of TraPPE. This work is done in collaboration with the Siepmann Group at the University of Minnesota.

<http://www.chem.umn.edu/groups/siepmann/trappe/>