

## **148b Extension of the Trappe-Ua Force Field to Thiols, Sulfides and Disulfides**

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The TraPPE-UA force field is extended to thiols, sulfides and disulfides by the introduction of pseudo-atoms for sulfur in each compound. In this force field, non-bonded interactions are given by Lennard-Jones 12-6 potentials combined with point charges. Partial charges were taken from the OPLS-UA force field, while parameters for the dispersion interactions were fit to reproduce liquid-vapor coexistence curves for selected model compounds. Grand canonical histogram-reweighting Monte Carlo simulations were performed to determine the liquid-vapor coexistence curves for methanethiol, pentanethiol, octanethiol, dimethyl sulfide, diethylsulfide, methylethylsulfide, dimethyl disulfide, and methyl ethyl disulfide. Overall, the agreement with experimental data excellent, and is a significant improvement over existing united-atom force fields.