

# Graph generation for predictive chemistry

Laura Sheppardson  
The University of Mississippi

## **Abstract**

Graph theoretical methods have long been used to enumerate the isomers of organic compounds. There are few practical tools, however, for generating a listing of all isomers with a specific chemical formula. Those which have been developed are case specific. We will discuss a current project in collaboration with theoretical chemist G. Tchumper to develop such a generator. The graphs are to be used to guide searching of a potential energy hyper-surface, to produce ab initio predictions of chemical reactions.