Graph generation for predictive chemistry

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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.