STATISTICAL ANALYSIS OF BODIPY DERIVATIVES ROTATIONAL ENERGY TRANSITIONS AND GEOMETRY

Rokas Garbačauskas, Stepas Toliautas

[1]Institute of Chemical Physics, Physics Faculty, Vilnius university, Lithuania
rokas.garbacauskas@ff.stud.vu.lt

Quantum chemistry modelling is a valuable tool for comparing, explaining and predicting various chemical phenomena. On the other hand, the results are very sensitive to chosen initial conditions and used parameter sets. The idea behind our research is to ride the wave of recent developments in data science and machine learning to cope with large amounts of synthesized molecular modelling data. The aforementioned techniques can be used to distill various degrees of freedom into compound class specific or general meta parameters that could help navigate the potential energy surfaces to find less local energy minima and/or help the current mainstream algorithms to converge faster. Our goal currently is the statistical analysis of a particular class of chemical compounds, namely boron-dipyrromethene (BODIPY) and its various derivatives, that are known for their usage as fluorescent dyes [1] and markers in biological research [2] or for viscosity measurements [3]. Our current focus of investigation is the creation of suitable tools for statistical analysis of Phenyl-BODIPY molecule and its rotational conformer models, generated with Gaussian software, geometry. The designed tools are still to be applied to a wider range of BODIPY derivatives.

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