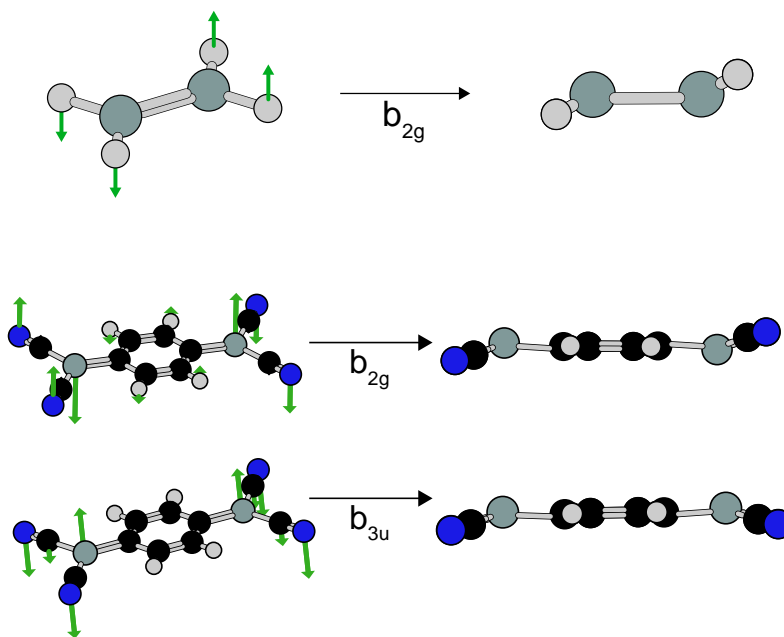


How Hartree-Fock Exchange Contributions Affect the Observation of Pseudo Jahn-Teller Effects in Conjugated Silicon Compounds

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Potential energy surfaces are a concept at the heart of computational chemistry. Previous studies have detailed the effect of both integration grid size and exact exchange on various properties including the nature of stationary points (i.e., transition structure v. minimum) on potential energy surfaces but none have addressed the root cause of such discrepancies. In this work we introduce a catastrophe theory approach to the problem and examine two contentious stationary points[1,2] belonging to planar disilene and 2Si TCNQ from the perspective of the pseudo Jahn-Teller effect (pJTE) using DFT methods. First the planar stationary points are characterized using a variety of model chemistries and integration grids. The effect of the amount of Hartree-Fock exchange is then studied and the usage of DFT for assessing pJTE parameters is explored.



[1] Maley, S. M.; Esau, C.; Mawhinney, R. C.; *Structural Chemistry* **30**, 289 (2019)

[2] Maley, S. M.; Mawhinney, R. C.; *Structural Chemistry* **30**, 1873 (2019)