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Determination of the Torsional Potential Energy Surfaces of the Ortho- Meta-, and Para-Isomers of Dinitrobenzene PAUL SMITH, MARIO BORUNDA, Oklahoma State Univ — The three unique isomers of dinitrobenzene, the ortho-, meta-, and para-isomers, have widely varying steric hindrances and bond hybridizations. The steric effects and the hybridized bonds cause the molecular energy to be dependent on the rotation of the nitro groups. We have calculated the torsional potential energy surfaces of each of the three dinitrobenzene isomers using density functional theory, obtaining a 33x33 plot of the energy of each molecule as a function of the torsional angles of the C-N bonds. The accuracy of the method used is determined by comparsion with previous theoretical and experimental results. The potential energy surfaces provide valuable insight into the mechanics of conjugated molecules, and the method we present can be extended even to proteins, which have very complicated conformations and many conjugated bonds. This method makes the determination of the lowest energy conformations of complex molecules far more computationally accesible.

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