Public Abstract

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Graduation Term:FS 2016
Department:Chemistry
Degree:MA

Title:Mechanistic and Computational Studies of Ferroin, Organic Acids, and Bromine Oxides: Elucidating the Complex Electrochemical Dance in an Oscillating Reaction

Includes computationally derived data and literature reviews relating to autocatalytic or oscillating chemical reactions, specifically a ferroin-catalyzed Belousov-Zhabotinsky reaction. Mechanisms that cause the reaction to cycle from reactants to products and back are examined in terms of their viability and velocity. Physical mechanisms of electron transfer in ferroin and related transition-metal complexes are also examined, including references to similar phenomena in nature. The study concludes that bromine oxides with stoichiometric formulas Br2O, Br2O3, Br2O4 (BrO2), and Br2O5 likely play more significant roles in the reaction dynamics than previously postulated. Since halogen oxides are also known to cause ozone (O3) decomposition in the lower atmosphere, this natural cycle is also discussed. Specific reactions are proposed that may improve the experimental agreement of future models.