Comparative Modeling of Improved Synthesis of Energetic Dinitro-Benzofuroxan (DNBF) Derivatives

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Abstract

Quantum chemical theoretical computation was performed on gaseous molecular reaction systems to simulate parallel synthesis of energetic primary explosive precursor 4,6-dinitro benzofuroxan (4,6-DNBF) and its isomeric derivatives. Related liquidus polarized continuum model (PCM) and Materials studio (MS/forcite) energies were collected via kinetic rate and thermodynamic equilibrium analyses, enabling comparison of and suggestions as to suitable reaction conditions (reaction temperature, reagent concentration, mixed acid ratio) together with feasible pathways to obtain a high production yield of the research target. In summary, at a low reaction temperature of 278K, 1.0 M 4-nitro benzofuroxan (or 5- , 6- nitro benzofuroxan) could be nitrated using concentrated nitric acid/sulfuric acid at a 1 to 2 volume ratio to efficiently and rapidly produce 4,6-dinitro benzofuroxan (or 5-, 6-dinitro benzofuroxan), in agreement with the experimental results reported in the literature.

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