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Computational study on nitronium squarate - potential oxidizers for solid rocket propulsion?

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Abstract: The enthalpies of formation for solid ionic nitronium squarate, $[NO_2]_2[C_4O_4]$, and covalent squaric acid dinitrate ester, $O_2N\text{-}C_4O_4\text{-}NO_2$, were calculated using the complete basis set (CBS-4M) method of Petersson and coworkers in order to obtain very accurate energies. The covalent form ($O_2N\text{-}C_4O_4\text{-}NO_2$) was identified as the more stable isomer. The combustion parameters with respect to possible use as ingredients in solid rocket motors for both stable species were calculated using the EXPLO5 code. The performance of an aluminized formulation with covalently bound dinitrate ester ($O_2N\text{-}C_4O_4\text{-}NO_2$) was shown to be comparable to that of ammonium perchlorate/aluminum. This makes squaric acid dinitrate ester a potentially interesting perchlorate-free and environmentally benign oxidizer for solid rocket propulsion.

Key Words: Ammonium perchlorate, combustion, nitronium, squaric acid, oxidizers, specific impulse, rocket propellants

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