INVESTIGATION OF THE POTENTIAL ENERGY SURFACE FOR THE CCO + N₂ REACTION

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ABSTRACT

The potential energy surface of the CCO + N₂ reaction was investigated using theoretical methods at the CBS-QB3 level of theory. Three different product channels were found for the reaction. The enthalpies of reaction for these three product channels were used to estimate a value for \( \Delta H_f^\circ \) (CCO) of 372 ± 5 kJ/mol. Results of this investigation help to answer questions about prompt NOₓ formation via the CCO radical.