Density Functional Theory Investigation on the Mechanism of Chemiluminescent Decomposition in Monofluoro 1, 2-Dioxetane (Mfd)

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Abstract: Mechanism of chemiluminescent decomposition in Monofluoro substituted 1, 2-dioxetane, (MFD) is investigated at B3LYP/6-31+G* level using the Gaussian 09 program. The energetics of the decomposition reaction via transition states/intermediates in the lowest singlet and triplet states are studied by complete optimization with frequency analysis. The present study reveals that the decomposition of the chemiluminescent decomposition follows a biradical mechanism. The reaction proceeds via a triplet biradical intermediate. The formation of 1TS1 from S0 is the rate determining step. The results are in agreement with the earlier experimental and theoretical studies.

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