**Executive summary of the work done**

**High precision second order Moller-Plosset Perturbation Theory and Density Functional Theory study of certain cycloaddition reactions**

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Nature of substituents influences the feasibility of reaction. Electron withdrawing or electron donating substituents on either diene or dienophile results in the decrease or increase in the feasibility of simple Diels Alder reaction involving 1,3-butadiene and ethene. In this paper the feasibility of several Diels Alder reactions having substituted diene and dienophile is calculated in terms of enthalpy of reaction. The way the substituents affect the rate of the reaction can be rationalized with the aid of the frontier molecular orbital theory. The pathway of reaction (normal or inverse electron demand) is predicted by means of HOMO-LUMO energy gap. Normal electron demand Diels Alder reactions are promoted by electron donating substituent on diene and electron withdrawing substituent on the dienophile. In contrast, inverse electron demand Diels Alder reactions are accelerated by electron withdrawing groups on diene and electron donating ones on dienophile. This study helps us to predict the feasibility and path way of certain normal and explosive Diels Alder reactions.

**Keywords:** DFT, Diels-Alder reaction, inverse electron demand Diels-Alder reaction, explosive reactions

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