

# **Ab initio Study of Diels-Alder Reaction between Cyclic Dienes and Olefin**

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## **Author's contribution**

The sole author designed, analysed, interpreted and prepared the manuscript.

## **Article Information**

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## **ABSTRACT**

Theoretical modeling of organic synthesis is a powerful tool and leads to further insight into chemical systems. Computational chemistry allows obtaining the potential energy surface that experimentally cannot be observed, in addition to transition state calculations, which lead to better understanding the reactivity of an organic synthesis work. The Diels-Alder (DA) reaction of cyclopentadiene **1** and N-phenylmaleimide **2** has been studied at the MP2/6-311++G(d,p) level of theory. This DA reaction occurs through a one-step mechanism. It was expected that this reaction undergoes two regio-isomeric reaction paths passing through two different transition states to form two different products **3** and **4**. The reaction paths are irreversible due to the exothermic character of -41.24 and -41.73 kcal.mol<sup>-1</sup>. This DA reaction are exergonic with reactions Gibbs free energies between -27.26 and -27.74 kcal.mol<sup>-1</sup>. Analysis of the CDFT indices predict the global electronic flux from the strong nucleophilic cyclopentadiene **1** to the electrophilic N-phenylmaleimide **2**.

**Keywords:** MP2; cycloaddition; diels-alder reaction; conceptual DFT.

## **1. INTRODUCTION**

Computational studies on cycloaddition reactions, in recent years, have been the subject

of a number of researches due to their wide applications on synthetic organic compounds [1-6]. Among cycloadditions, Diels-Alder reaction (DA) represent versatile process for the

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synthesis of a system with six membered ring and a large variety of cyclic compounds can be synthesized relying on the choice of the diene and the alkenes derivative [7-10]. The DA reaction of cyclic compounds as a diene to alkenes has been widely used during recent two decades as a key step for the construction of various compounds that are of great interest in pharmaceutical and medicinal chemistry [11-14].

In the past few years, the advent of computational chemistry has gradually attracted theoretical chemists to analyze the reactivity and selectivity of organic molecules. A new theoretical outlook for organic reactions was proposed by Domingo in 2016 named the molecular electron density theory (MEDT) after interpretation of a vast array of organic reactivity, majority of them dedicated to Diels-Alder and [3+2] cycloaddition (32CA) reactions [15-17]. This theory analyzes the changes in electron density to study the molecular reactivity and has been successfully applied for several 32CA reactions since last four years [18-27].

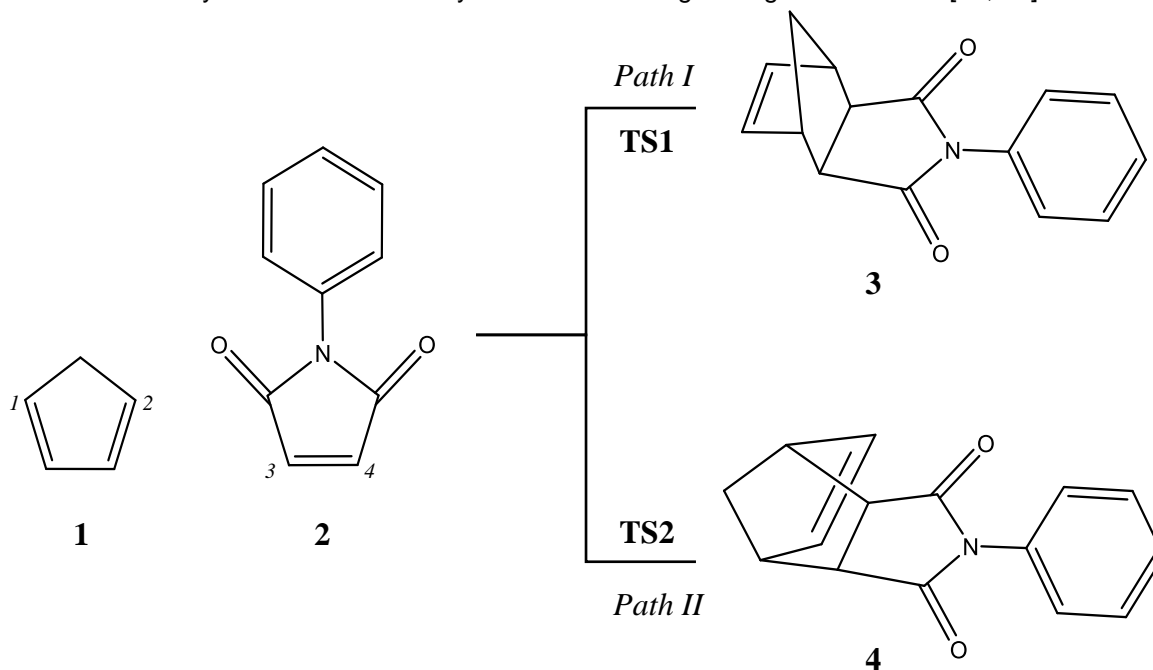
In this work, MP2 is used throughout in combination with the 6-311++G(d,p) basis set for the synthesis of six membered cyclic compounds from DA reaction of cyclopentadiene **1** with N-phenylmaleimide **2** (Scheme 1). Herein, we studied the analysis of the reactivity indices

derived from conceptual DFT for the reagents, the thermodynamic parameters of the DA of the both reactants, and local electrophilicity/nucleophilicity descriptors such as the Parr functions for understanding the bonding changes.

## 2. COMPUTATIONAL METHODS

All calculations were done using the Gaussian 16 package under Linux operation system [28]. MP2 method has been proven to be a suitable method for the study of DA reactions and is employed in this study [29-31]. MP2 is used throughout in combination with the 6-311++G(d,p) basis set [32, 33]. Geometry optimization were performed in default settings on geometry convergence, integration grid and electron density (SCF) convergence.

Computations consist on geometry optimizations followed by frequency calculations to ensure of that a transition state has only one imaginary frequency and that a local minimum has no imaginary frequencies (all positive frequencies). Intrinsic reaction coordinate (IRC) computations were carried out to verify that the minimum energy reaction pathway via a transition state connects with the corresponding reactants and products using the second order González–Schlegel integration method [34, 35].



**Scheme 1. The DA reaction of cyclopentadiene 1 with N-phenylmaleimide 2**

All energies and thermodynamic parameters reported in this paper were obtained from the frequency calculations at the same level of theory. The enthalpies, Gibbs free energies and entropies in gas phase were deduced with the standard statistical thermodynamics at 298.15 K and 1 atm.

The chemical hardness ( $\eta$ ) and the electronic chemical potential ( $\mu$ ) quantities may be approached in terms of the one electron energies of Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO),  $\epsilon_{HOMO}$  and  $\epsilon_{LUMO}$ , as in Equation 1 and 2, respectively [36, 37]. The global electrophilicity index ( $\omega$ ) is calculated using Equation 3 [38]. The relative nucleophilicity index (N) is obtained based on the energies of HOMO within the scheme of Kohn-Sham [39]. This quantity can be defined as in Equation 4. As reference, we chose TCE (tetracyanoethylene) due to its lowest HOMO energy [40].

$$H = (E_{LUMO} - E_{HOMO}) \quad (1)$$

$$\mu = \frac{E_{HOMO} + E_{LUMO}}{2} \quad (2)$$

$$\omega = \frac{\mu^2}{2\eta} \quad (3)$$

$$N = E_{HOMO(Nu)} - E_{HOMO(TCE)} \quad (4)$$

The electrophilic  $P_k^+$  and nucleophilic  $P_k^-$  Parr functions [41], which allow for the characterisation of the electrophilic and nucleophilic centers of a molecule, were obtained through the analysis of the Mulliken atomic spin density of the radical cation and the radical anion of cyclopentadiene **1** and N-phenylmaleimide **2**, by single-point energy calculations from the optimised neutral geometries.

In chemistry and physics, the branching ratio is the ratio of the rate constant for a particular product of a reaction to the rate constant for the

total set of possible products. For example, in nuclear physics, the branching ratio for a decay process is the ratio of the number of particles which decay via a specific decay mode with respect to the total number of particles which decay via all decay modes. It is also equal to the ratio of the partial decay constant to the overall decay constant [42].

$$BR_{Product\ 1} = \frac{K_1}{K_1 + K_2}$$

$$BR_{Product\ 2} = \frac{K_2}{K_2 + K_1}$$

### 3. RESULTS AND DISCUSSION

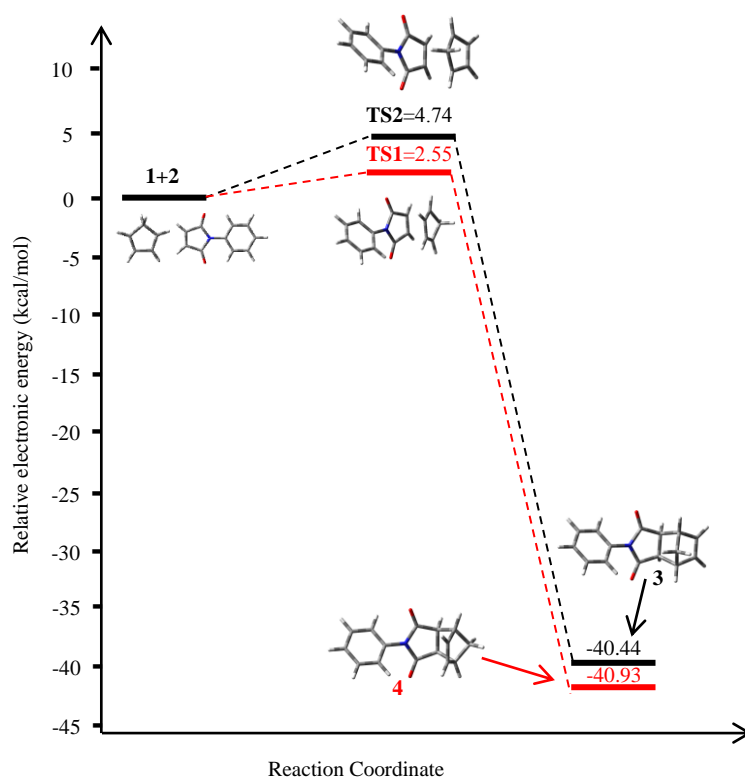
#### 3.1 Analysis of the Reaction Paths

Due to the molecular symmetry of the reactants, cyclopentadiene **1** and N-phenylmaleimide **2**, in the double bound sides, two reaction paths, namely path I and path II, are feasible for these DA reactions (see Scheme 1). The search for the stationary points involved in the reaction paths associated with these DA reactions allowed characterizing the reactants, **1** and **2**, two TSs for the DA reaction, TS1, and TS2, and the corresponding products **3** and **4**, respectively. The relative energies and thermodynamic data of the TSs and cycloadducts are given in Table 1.

The activation enthalpies associated with these DA reactions are 4.94 and 2.78 kcal.mol<sup>-1</sup> for TS1 and TS2, respectively, at MP2/6-311++G(d,p) level of theory. However, this value increases by about 4 and 2 kcal.mol<sup>-1</sup> using DFT method at B3LYP/6-311++G(d,p) and M06-2X/6-311++G(d,p), respectively, the reactions are exothermic between 41.24 and 41.73 kcal.mol<sup>-1</sup> using MP2, while these values decreased to about 24.04 and 25.57 kcal.mol<sup>-1</sup> using B3LYP-D3, and 33.54 and 34.51 kcal.mol<sup>-1</sup> using M06-2X.

**Table 1. Relative energies, enthalpies and Gibbs free energies, in kcal.mol<sup>-1</sup>, computed at different levels of theories of the stationary points involved in the DA reactions of cyclopentadiene **1** and N-phenylmaleimide **2**.**

	MP2			B3LYP-D3			M06-2X		
	$\Delta E$	$\Delta H$	$\Delta G$	$\Delta E$	$\Delta H$	$\Delta G$	$\Delta E$	$\Delta H$	$\Delta G$
<b>3</b>	-40.44	-41.24	-27.26	-23.41	-24.04	-10.35	-32.88	-33.54	-19.78
<b>4</b>	-40.93	-41.73	-27.74	-24.95	-25.57	-11.98	-33.56	-34.21	-20.23
<b>TS1</b>	4.74	4.94	9.81	8.55	8.43	20.92	6.84	6.69	19.32
<b>TS2</b>	2.55	2.78	8.15	6.36	6.24	18.94	3.90	3.71	16.52



**Fig. 1.** MP2/6-311++G(d,p) potential energy surface of the DA reaction of cyclopentadiene **1** and N-phenylmaleimide **2**. Relative energies are in unit kcal/mol

Products branching ratios (BR) were estimated for the DA reaction to obtain the product percent yield. The BR for path II of the DA reaction has the higher percent yield of 51% than the other path, 49%.

Analysis of the thermodynamic parameters allows establishing some appealing conclusions: (i) The DA reaction between cyclopentadiene **1** and N-phenylmaleimide **2** leading the formation of cycloadduct **4** presents the lower activation enthalpy than cycloadducts **3** at all levels of theory. (ii) The activation enthalpy for this DA reaction that corresponds to the formation of cycloadduct **4** is lowered by about 41.73, 25.57 and 34.21 kcal mol<sup>-1</sup> MP2/6-311++G(d,p), B3LYP-D3/6-311++G(d,p) and M06-2X/6-311++G(d,p). (iii) The exothermic character of the DA reaction that leads to the formation of product **3** and **4** makes the reaction irreversible. (iv) These DA reactions are exergonic with reactions Gibbs free energies of -27.26 for path I and -27.74 kcal.mol<sup>-1</sup> MP2/6-311++G(d,p).

The MP2/6-311++G(d,p) optimized geometries of the TSs are given in Fig. 2. The distances between C1 and C3, and C2 and C4 interacting centres at TS1 are: 2.23 and 2.23 Å, and 2.20

and 2.21 Å at TS2, respectively. The TSs geometries show similar trend and minimal changes at B3LYP/6-311++G(d,p) and M06-2X/6-311++G(d,p) levels of theory.

These geometrical parameters indicate that the TS1 is found to be a synchronous attack, while TS2 with the lower activation energy shows low asynchronicity processes. The analysis of the geometrical parameters indicates that at both transition states, the formation of the C1–C3 and C2–C4 single bond has not yet begun.

### 3.2 Analysis of the CDFT Indices of Cyclopentadiene **1** and N-phenylmaleimide

The CDFT indices can be used to gain a basic understanding of organic molecule reactivity. Since the electrophilicity and nucleophilicity scales were computed at the B3LYP/6-31G(d) computational level, so similar level of theory were used to calculate the CDFT indices. The electronic chemical potential,  $\mu$ , chemical hardness,  $\eta$ , electrophilicity,  $\omega$ , and nucleophilicity,  $N$ , in the ground state of cyclopentadiene **1** and N-phenylmaleimide **2** are mentioned in Table 2.

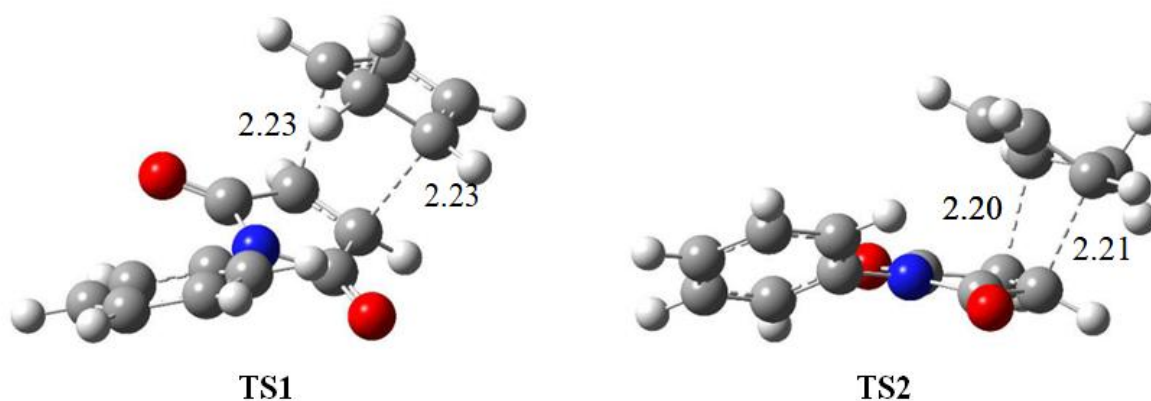


Fig. 2. MP2/6-311++G(d,p) optimized geometries of the transition states involved in the DA reaction of cyclopentadiene **1** and N-phenylmaleimide **2**. Bond lengths are given in Angstroms.

Table 2. The chemical hardness  $\eta$ , electronic chemical potential  $\mu$ , global nucleophilicity  $N$  and global electrophilicity  $\omega$ , in eV, of cyclopentadiene **1** and N-phenylmaleimide **2** at the B3LYP/6-31G(d) level of theory.

Reactant	$\eta$	$\mu$	$\omega$	$N$
<b>1</b>	3.07	-4.22	2.90	3.73
<b>2</b>	3.49	-4.56	2.98	3.19

The electronic chemical potential  $\mu$  of cyclopentadiene **1**,  $\mu = -4.22$  eV, is higher than that of N-phenylmaleimide **2**, which is  $-4.56$  eV thereby indicating that the global electron density transfer will take place from cyclopentadiene **1** towards electron poor N-phenylmaleimide **2**. The nucleophilicity  $N$  indices of cyclopentadiene **1** and N-phenylmaleimide **2** are 3.73 and 3.19 eV, respectively, being classified as strong nucleophiles within the corresponding scales. The electrophilicity  $\omega$  of cyclopentadiene **1** and N-phenylmaleimide **2** is 2.90 and 2.98 eV, respectively, being classified as a marginal electrophile.

In addition to the global indices, local electrophilicity/nucleophilicity descriptors such as the Parr functions are extensively used to explore the local reactivity and site selectivity, especially in cycloaddition reactions. The Parr electrophilic  $P_{K^+}$  and Parr nucleophilic  $P_{K^-}$  functions at the atoms of cyclopentadiene **1** and N-phenylmaleimide **2** are given in Table 3. An analysis of Parr functions found that the carbon atom C1 and C2 are the most electrophilic center with,  $P_{K^+}=0.422$ . However, the nucleophilic  $P_{K^-}$  Parr functions at the C3 and C4 are the most nucleophilic center in N-phenylmaleimide **2** with a value,  $P_{K^-}=0.32$ , while C1 and C2 are the most

nucleophilic center with a value,  $P_{K^-}=0.503$  for cyclopentadiene **1**.

Table 3. The Parr electrophilic  $P_{K^+}$  and Parr nucleophilic  $P_{K^-}$  functions at the atoms of cyclopentadiene **1** and N-phenylmaleimide **2** at B3LYP/6-31G(d) level of theory

Reactant	Site	$P_{K^-}$	$P_{K^+}$
<b>1</b>	C1	0.503	0.422
	C2	0.503	0.422
<b>2</b>	C3	0.321	0.227
	C4	0.321	0.227

The HOMO and LUMO energies in electron volt (eV) at MP2/6-311++G(d,p) level of theory are computed for all possible products, as shown in Table 4. It is worth to realize that the energy gap for cycloadduct **4** is higher than the cycloadducts **3** which indicates the stability of the cycloadduct **4**.

Table 4. HOMO energies ( $E_{HOMO}$ ), LUMO energies ( $E_{LUMO}$ ), and energy gap ( $E_{Gap}$ ), in eV unit, for cycloadducts at MP2/6-311++G(d,p) level of theory

Product	$E_{HOMO}$	$E_{LUMO}$	$E_{Gap}$
<b>3</b>	6.48	0.67	5.80
<b>4</b>	6.45	0.59	5.86

#### 4. CONCLUSION

The DA reaction between cyclopentadiene **1** with N-phenylmaleimide **2** has been investigated at MP2/6-311++G(d,p) level of theory. The reaction can undergo two regio-isomeric reaction paths to form two different products. The reaction mechanisms are reported and the potential

energy surfaces are plotted with respect to the energies of the stationary points. The global electronic flux from the cyclopentadiene **1** to N-phenylmaleimide **2** is predicted, owing to the high electronic chemical potential and strong nucleophilicity of the cyclopentadiene **1** relative to the N-phenylmaleimide **2**, which is confirmed from the GEDT calculations at the located transition states. This DA reactions is exergonic with negative free energy of reaction. The product **4** shows higher thermodynamic stability relative to the product **3**. The product **4** obtained from the path I DA reaction is thermodynamically more stable compared to that generated from the path II DA reaction.

### COMPETING INTERESTS

Author has declared that no competing interests exist.

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