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# Dimerization of Cyclopentadiene via Diels–Alder Reaction Documented by Refrachor (*F*)

**Sanjeev Rachuru[1], V. Jagannadham[2,*]**

[1]Department of Chemistry, St. Ann's College for Women, Mehdipatnam Hyderabad, Telangana-500028
[2]Department of Chemistry, Osmania University, Hyderabad-500007, India
*Corresponding author: jagannadham1950@yahoo.com

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**Abstract** Cyclopentadiene is a five membered cyclic organic compound with molecular formula C5H6 abbreviated as CpH. The p*Ka* of CpH is 15. It is probably known world strongest carbon acid after Fluoradene (p$K_a$ is 11.0 in DMSO, ref. 17) with only carbon-hydrogen framework without any hetero atoms. It is highly reactive diene, and dienophile can undergo dimerization via Diels–Alder Reaction to dicyclopentadiene (DCPD). In the present work we have tried to characterize the percentage mole fraction of the dimerization product by a physical constant Refrachor (*F*).

***Keywords:*** *Cyclopentadiene, Refrachor, Diels–Alder Reaction, Dimerization*

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## 1. Introduction

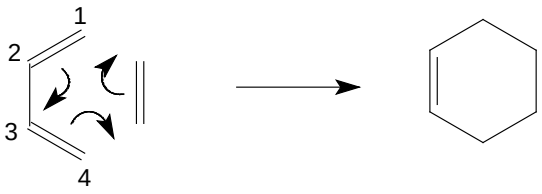
Cyclopentadiene (CPD) is a liquid at room temperature. Cyclopentadiene is both a diene and a dienophile, can undergo dimerization to form dicyclopentadiene. The rate constant for the dimerization of cyclopentadiene to endo-DCPD at 25 °C has been reported to be $8.3 \times 10^{-7}$ $M^{-1}s^{-1}$ with a half-life of ~28 h [1,2]. Dimerization is temperature dependent [3]. In a kinetic model between 40 and 120 °C [4], it was shown that ≥ 99 mol% of endo-DCPD was the primary reaction product. Diels–Alder Reaction of CPD is well described computationally [5]. This reaction is also called as [4+2] cycloaddition reaction with Woodward–Hoffmann symbol [$_{\pi}4_s$ + $_{\pi}2_s$]. In the present work we have given a trail to show that dimerization process is the prime reaction path at room temperature using a physical constant Refrachor (***F***).

## 2. Methods

All chemical structures were drawn using ChemDraw software.

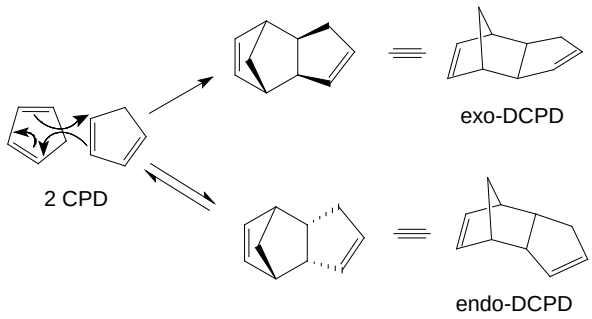
## 3. Discussion

The simplest example of Diels–Alder Reaction is the reaction between 1,3-butadiene (a diene) and ethylene (a dienophile) and the scheme is shown below (scheme 1).




Scheme 1

Scheme 2 depicts the dimerization of cyclopentadiene (CPD) to dicyclopentadiene (DCPD) at 120 °C via a Diels–Alder reaction to give ≥ 99% kinetically favored endo-isomer and ≤ 1% thermodynamically favored exo-isomer [6].




Scheme 2

In the present work we have studied the dimerization of cyclopentadiene (CPD) to dicyclopentadiene (DCPD) using Refrachor (***F***). In order to see the dimerization of cyclopentadiene (CPD) to dicyclopentadiene (DCPD), first observed Parachor ($P_{obsd}$) is calculated using equation

1 suggested by Sugden [7] and observed Refrachor ($\boldsymbol{F}_{obsd}$) is calculated using the equation 2 suggested by Tuli and Joshi [8,9].

$$P_{obsd} = \gamma^{\frac{1}{4}} \frac{M}{\rho_L} \quad (1)$$

$$\boldsymbol{F}_{obsd} = - P_{obsd} \log ( n_D^{20} - 1) \quad (2)$$

Therefore, using equation 1 the Parachor of cyclopentadiene is calculated by substituting its molar mass (M), the surface tension ($\gamma$) and the density ($\rho_L$). All these values are observed quantities. The molar mass (M) of cyclopentadiene is 66.1. Surface tension [10], refractive index [11] and density [12] of cyclopentadiene are 28.4 dynes/cm, 1.44 and 0.802 gm/mL respectively. Therefore, Parachor (P) is an observed quantity now termed as $P_{obsd}$. Substituting $P_{obsd}$ and refractive index $\left(n_D^{20}\right)$ [11] in equation 2, Refrachor ($\boldsymbol{F}_{obsd}$) is calculated.

$$P_{obsd} = (28.4)^{\frac{1}{4}} \frac{66.1}{0.802} = 190.26$$

$$\mathbf{P_{obsd}^{cyclopentadiene}} = 190.26$$

and

$$F_{obsd}^{cyclopentadiene} = - 190.26 \log (1.44 - 1)$$

$$\boldsymbol{F_{obsd}^{cyclopentadiene}} = \mathbf{67.84}$$

In table 1 the data of bond Parachors ($\boldsymbol{P}$) and bond refraction coefficients $\left(\mathbf{Mn_D^{20}}\right)$ summarized are from reference [13].

**Table 1. Selected and required bond Parachors, and bond-refraction coefficients (at 20°C) are from table 51 of reference 13**

| Sl. No | Bond | Bond Parachor (**P**) | Bond-refraction coefficients ($\mathbf{Mn_D^{20}}$) |
|---|---|---|---|
| 1 | C–H | 17.85 | 3.87 |
| 2 | C–C | 4.30 | 12.86 |
| 3 | C=C | 28.5 | 9.39 |

Now the Refrachor of both cyclopentadiene and dicyclopentadiene are to be calculated from the bond Parachors (P) and bond refractive coefficients ($\mathbf{M}\, n_D^{20}$) taking from table 1.

Cyclopentadiene has 6 C–H bonds, 3 C–C bonds and 2 C=C bonds. Therefore,

$P_{(cyclopentadiene)} = (6 \times P_{C-H}) + (3 \times P_{C-C}) + (2 \times P_{C=C}) = (6 \times 17.85) + (3 \times 4.30) + (2 \times 28.5) = 177.0$, taking bond Parachor values from table 1.

$$\mathbf{P_{cal}^{cyclopentadiene}} = \mathbf{177.0}$$

$(M\, n_D^{20})_{(cyclopentadiene)} = (6 \times (M\, n_D^{20})_{C-H}) + (3 \times (M\, n_D^{20})_{C-C}) + (2 \times (M\, n_D^{20})_{C=C}) = (6 \times 3.87) + (3 \times 12.86) + (2 \times 9.39) = 80.58$, bond refraction coefficients $(M\, n_D^{20})$ are from table 1.

$$(M\, \mathbf{n_D^{20}})_{(cyclopentadiene)} = \mathbf{80.58}$$

Therefore

$$\left(n_D^{20}\right)_{(cyclopentadiene)} = \frac{\left(Mn_D^{20}\right)_{(cyclopentadiene)}}{M} = \frac{80.58}{66.1} = 1.219$$

$$\left(\mathbf{n_D^{20}}\right)_{(cyclopentadiene)} = \mathbf{1.219}$$

Using the relation between Refrachor ($\boldsymbol{F}$) and Parachor (P) [8,9]

$F = - P \log (n_D^{20} - 1)$

$F = - 177.0 \times \log (1.219 - 1)$

$F = -177.0 \times \log (0.219)$

$F = -177.0 \times (- 0.66) = 116.82$

$$\boldsymbol{F_{cal}^{(cyclopentadiene)}} = \mathbf{116.82}$$

Dicyclopentadiene has 12 C–H bonds, 10 C–C bonds and 2 C=C bonds. Therefore,

$P_{(dicyclopentadiene)} = (12 \times P_{C-H}) + (10 \times P_{C-C}) + (2 \times P_{C=C}) = (12 \times 17.85) + (10 \times 4.30) + (2 \times 28.25) = 314.2$, taking bond Parachor values from table 1.

$$\mathbf{P_{cal}^{dicyclopentadiene}} = \mathbf{314.2}$$

$(M\, n_D^{20})_{(dicyclopentadiene)} = (12 \times (M\, n_D^{20})_{C-H}) + (10 \times (M\, n_D^{20})_{C-C}) + (2 \times (M\, n_D^{20})_{C=C}) = (12 \times 3.87) + (10 \times 12.86) + (2 \times 9.39) = 193.82$, bond refraction coefficients $(M\, n_D^{20})$ are from table 1.

$$(M\, \mathbf{n_D^{20}})_{(dicyclopentadiene)} = \mathbf{193.82}$$

Therefore

$$\left(n_D^{20}\right)_{dicyclopentadiene} = \frac{\left(Mn_D^{20}\right)_{dicyclopentadiene}}{M} = \frac{193.82}{132.2} = 1.466$$

$$\left(n_D^{20}\right)_{dicyclopentadiene} = 1.466$$

Using the relation between Refrachor ($\boldsymbol{F}$) and Parachor (P) [8,9]

$F = - P \log ( n_D^{20} - 1)$

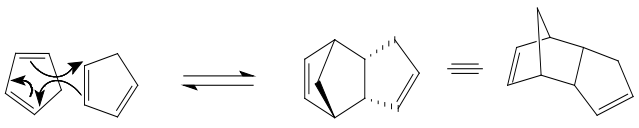
$F = - 314.2 \times \log (1.466 - 1)$

$F = - 314.2 \times \log (0.466)$

$F = - 314.2 \times (- 0.3316) = 104.19$

$$\boldsymbol{F_{cal}^{dicyclopentadiene}} = \mathbf{104.19}$$

Taking the equilibrium between cyclopentadiene and dicyclopentadiene



2 CPD

$2 \times (1 - x)$/mol. $L^{-1}$

x/mol.$L^{-1}$

endo-DCPD

According **to** mixture law as it was applied by Tuli [8,9] to find out keto-enol tautomeric composition in acetylacetone, if 'x' be the molar fraction of dicyclopentadiene present in the equilibrium mixture, and that of cyclopentadiene be $2 \times (1 - x)$:

$$2\times F_{\text{obsd}}^{\text{cyclopentadiene}} = 2\times F_{\text{calc}}^{\text{cyclopentadiene}}(1-\text{x}) + F_{\text{calc}}^{\text{dicyclopentadiene}}(x)$$

$2 \times 67.84 = [(1 - x) \times 233.64] + (x \times 104.19)$

$135.68 - 233.64 = - x \times (233.64 - 104.19)$

Therefore

$$\text{x} = \frac{97.96}{129.45} = 0.7567$$

Therefore, molar percentage of dicyclopentadiene is $0.7567 \times 100 = 75.7$. Our value of 75.7% of DCPD is less than the values of ≥ 99% reported earlier [4,6]. These higher values are between the temperature range 40 to 120°C. But our value obtained by Refrachor is at room temperature. Therefore, it is quite encouraging and reasonable that we got a less value of 75.7% using Refrachor (***F***).

## 4. Conclusions

As a continuation of our earlier work on Refrachor [14,15,16], we have demonstrated that the dimerization process of cyclopentadiene to dicyclopentadiene via Diels-Alder reaction is 76%.

## Conflict of Interest

The authors don't have any conflict of interest.

## Competing Interest

We don't have any kind of such thing.

## Dual Publication

We don't have any.

## Third Party Material

We don't have any third-party material.

## Funding

We did not receive any funding from any financial source.

## Author Contribution Declaration

Both of us the authors contributed equally.

## Data Availability Statement

The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

## Clinical Studies

Our manuscript is not for clinical studies.

## Ethics and Consent to Participate Declarations, Consent to Publish Declaration

We agree with all these.

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