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# Large Scale Configuration Interaction Calculations of Linear Optical Absorption of Octacene and Nonacene

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**Abstract.** The technological importance of higher acenes has led to resurgence of interest in synthesizing higher acenes such as octacene, nonacene etc.[1] Recently, Tonshoff and Bettinger have synthesized octacene and nonacene [2]. Motivated by their work, we have performed large scale calculations of linear optical absorption of octacene and nonacene and compared the results with their experimental work. Methodology adopted in our work is based upon Pariser-Parr-Pople model (PPP) Hamiltonian, along with large-scale multi-reference singles-doubles configuration interaction (MRSDCI) approach.

**Keywords:** Octacene, Nonacene, Acenes, Linear Optical Absorption, Configuration Interaction
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## INTRODUCTION

Larger acenes have lot of technological importance [1] in opto-electronic applications. Recently efforts have been made to synthesize them. Using, low temperature matrix isolation techniques, Tonshoff and Bettinger have synthesized octacene and nonacene [2].

## THEORY

Octacene and Nonacene are shown in Fig. 1 and Fig. 2

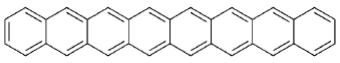

**FIGURE 1**. Octacene

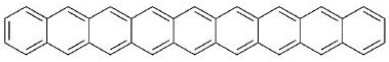

**FIGURE 2**. Nonacene

The correlated calculations are performed using the PPP model Hamiltonian as

$$H = \sum_{i,j,\sigma} t\left(c_{i\sigma}^{+}c_{j\sigma} + c_{j\sigma}^{+}c_{i\sigma}\right) + U\sum_{i} n_{i_\uparrow}n_{i_\downarrow} + \sum_{i<j} V_{i,j}\left(n_i - 1\right)\left(n_j - 1\right) \quad (1)$$

where $t = 2.4eV$ is nearest-neighbor hopping , $U$ and $V$ are on site and long range Coulomb interactions respectively

The Coulomb interactions are parametrized according to the Ohno relationship,[3]

$$V_{i,j} = \frac{U}{\kappa_{i,j}\sqrt{\left(1 + 0.6117\mathrm{R}_{i,j}^{2}\right)}} \quad (2)$$

where, $\kappa_{i,j}$ depicts the dielectric constant of the system which can simulate the effects of screening and $R_{i,j}$ is the distance in Å between $i^{th}$ and the $j^{th}$ carbon. We have performed calculations using "standard parameters(std)" [3] with $U$ =11.13eV and $\kappa_{i,j}$ =1 as well as "screened parameters(scr)" [4] with $U = 8$ eV and $\kappa_{i,j} = 2\left(i \neq j\right)$ and $\kappa_{i,i} = 1$. Using PPP model, optical absorption calculations of smaller acenes have been performed in our group [5-6].

## RESULTS AND DISCUSSION

We present large scale MRSDCI results of octacene and nonacene on linear optical absorption spectra, from lowest lowest singlet state $1^1A_g$ , and compare the results with the experimental spectrum [2]

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in Fig.[3] and Fig.[4] using screened and standard parameters respectively.

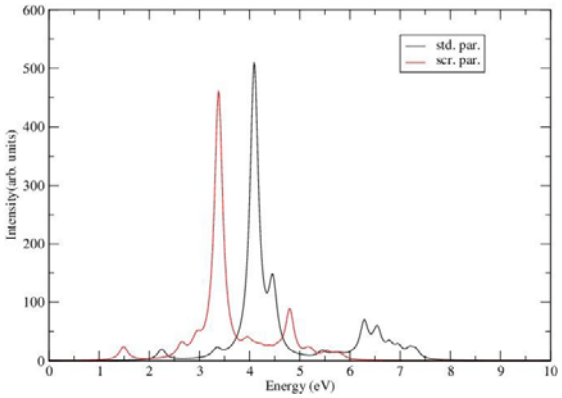


**FIGURE 3.** linear absorption spectra of octacene

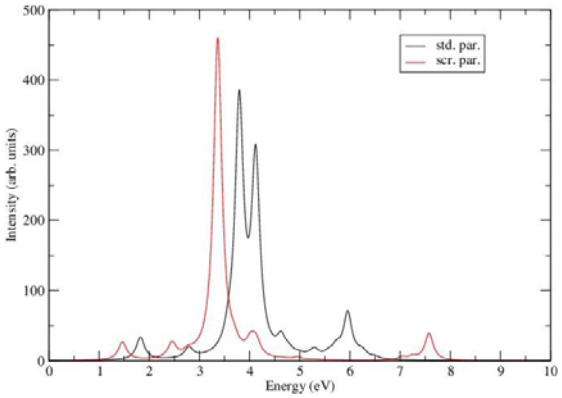


**FIGURE 4.** Linear absorption spectra of nonacene

Table. [1] presents the wavelengths of the most intense state of singlet linear absorption spectra of octacene and nonacene (std. and scr.) and the experimental spectra [2]. Our results are in good agreement with the experimental work.

## CONCLUSION

In this paper, we presented a MRSDCI method based correlated calculations of the singlet linear optical spectra of octacene and nonacene and compared the results with their experimental spectra. Based on the most intense absorption state, we found good agreement between them. Further work on other absorption states and the triplet excited state absorption spectra of higher acenes such as octacene nonacene and decacene is in progress[7].

**TABLE 1.** Energies (eV) of of most intense state of linear optical and experimental [2] absorption spectra of octacene and nonacene.

| spectra | octacene | nonacene |
|---|---|---|
| Std.par. | 4.09 | 3.79 |
| Scr. par. | 3.38 | 3.36 |
| Experimental | 3.78 | 3.66 |

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