

MP2 calculations of the effect of the π -conjugation on the electronic and nonlinear optical properties of para-nitroaniline (pNA) derivatives

Nuha Wazzan¹

¹King Abdulaziz University

May 11, 2020

Abstract

long-range charge transfer organic compounds are remarkable for having very large hyperpolarizabilities and thus improved nonlinear optical (NLO) properties. p-nitroaniline (pNA) is known as a prototypical NLO organic material. The question answered in this work is the NLO properties of pNA will be improved by introducing an extended π -conjugation chain between the phenyl ring and the two NH₂/NO₂ terminal? By means of sophisticated ab initio/MP2 calculations, new derivatives of pNA with an extended π -conjugation have been designed by introducing $-(CH=CH)_nNH_2$ or $-(CH=CH)_nNO_2$ ($n = 1-5$) chain into pNA. The results indicate that introducing such chains results in smaller energy gaps and transition energies, which lead to a significant improvement in the hyperpolarizability (β_0). The novel pNA derivatives exhibit larger β_0 amplitudes up to 4.67×10^4 au, which is 27-fold greater than that of pNA. Moreover, with increasing the β_0 amplitude, the $-(CH=CH)_nNO_2$ chain beats the $-(CH=CH)_nNH_2$ chain. It is hoped that this study can provide a help for designing higher performance NLO materials based on pNA.

Hosted file

PNA_NLO_MANUSCRIPT_IJQC.docx available at <https://authorea.com/users/320330/articles/450199-mp2-calculations-of-the-effect-of-the-%CF%80-conjugation-on-the-electronic-and-nonlinear-optical-properties-of-para-nitroaniline-pna-derivatives>