DFT and TD-DFT investigations of diazensulfonate dye sensitizers for solar cells: Effects of hydroxyphenyl, methoxyphenyl and methylthiophenyl substituents on the dye

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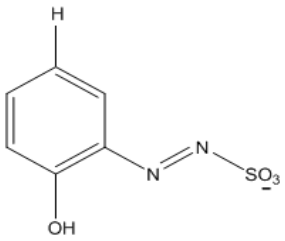
Abstract:

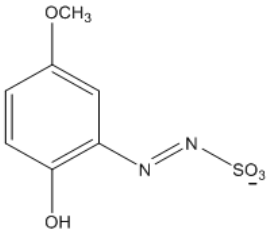
In this study, the influence of substitution on dye including (E)-2-(2-hydroxyphenyl) diazenesulfonate, (E)-2-(2-hydroxy-5-methoxyphenyl) diazenesulfonate and (E)-2-(2-hydroxy-5-(methylthio) phenyl) diazenesulfonate were investigated. The microscopic properties of molecules such as electron wave functions and molecular properties depend on the nature of solvent .The solvent effects change in both the geometries and the absorption spectra, so these effects have been investigated on diazensulfonate dye. Finally, the UV-Vis spectra of dyes have been study in different solvents.

Introduction:

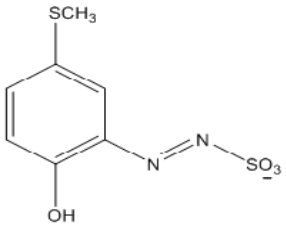
Solar energy is the greatest source for production renewable energy carriers on the earth. First, Gratzel et al. were produced dye sensitized solar cell (DSSC) with energy conversion efficiency of about 7% in 1991 and 10% in 1993 [1]. Organic and inorganic dyes anchored to semiconductor nanoparticles, have been found important applications as photosensitizes for solar cells and other optoelectronic systems [2]. As the name implies, azo dyes are compounds that contain azo groups (-N = N-) linked to methane or aromatic sp2- hybridized C- atoms. Di-azo dyes are divided two groups of mono-azo and di-azo. The synthesis of azo dyes is considered economically. The color potential of diazo dyes are included the color range from very greenish yellow to reddish yellow and orange and red [3].



Hydrogen substituent



Methoxy substituent



Methylthio substituent

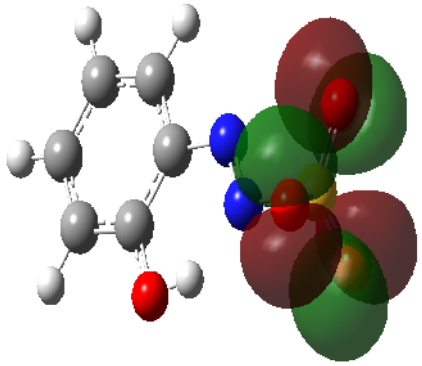
Figure1: schematics of diazensulfonate

Computational Details:

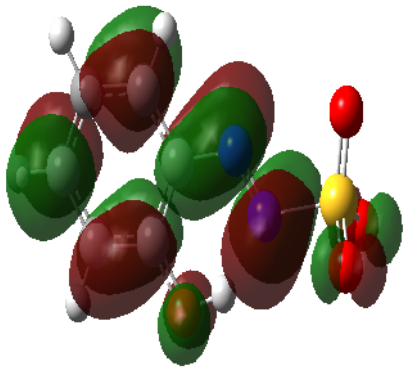
Calculations were done using software Gaussian 98. Dye molecules (Figure 1) were optimized by DFT/6-31G (d, p) method in gas phase. Dyes were optimized in Chloroform, Ethanol and THF solvents by using CPCM model and DFT/6-31G (d, p) method. The UV-Vis spectra of dyes were computed by using the TD-DFT/6-31G (d, p) method in gas phase and Chloroform, Ethanol and THF solvents.

Results and Discussion:

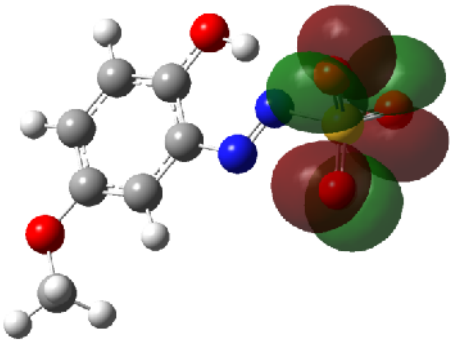
Different functional groups effects were studied in the ability of diazensulfonate dye to absorption sunlight. Photo physical and photo electrical properties of dye depends on the substitution of dyes. The electron donor substituent (SCH_3) in compare to substituent (OCH_3) transfers HOMO and LUMO energy levels to lower energy level. Therefore OCH_3 substituent has better red shift than SCH_3 substituent. Then (E)-2-(2-hydroxy-5-methoxyphenyl) diazenesulfonate dye has physical and photo electrochemical properties better than other dyes. HOMO and LUMO orbitals for these dyes in gas phase have been shown in Figure 2.



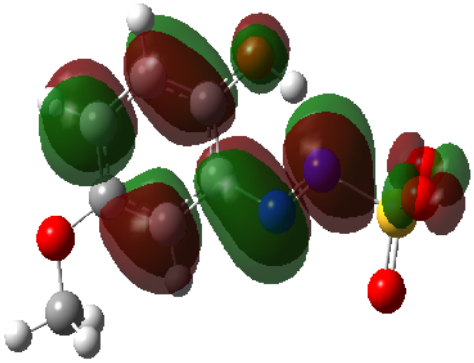
H-HOMO



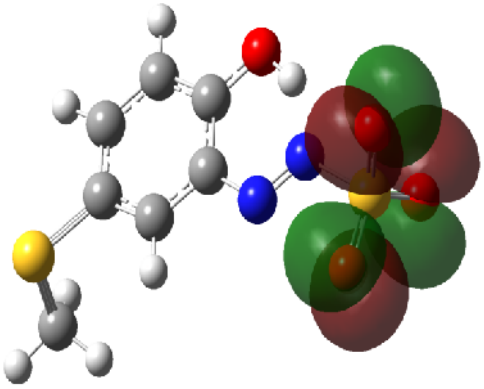
H-LUMO



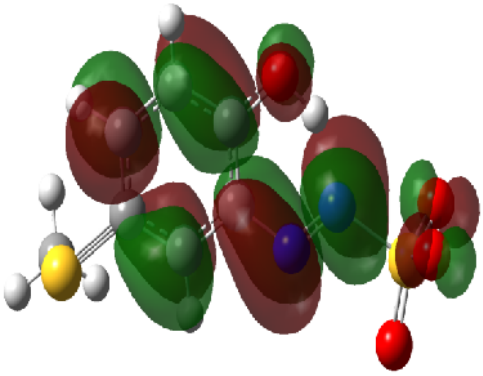
OCH_3-HOMO



OCH_3-LUMO



SCH_3-HOMO



SCH_3-LUMO

Figure2: HOMO and LUMO orbitals for dyes in gas phase

Table1: UV-Vis spectra of azobenzen

Dye	Phase	UV-Vis(nm)	Oscillator strength	E(g) / (ev)
Methoxy substituent	**Gas**	341.08	0.1519	3.6200
	Chloroform	383.99	0.1308	3.7248
	THF	389.99	0.1225	3.6698
	Ethanol	398.27	0.1129	3.5969
Methylthio substituent	**Gas**	314.88	0.1862	3.6693
	Chloroform	336.40	0.1391	4.1711
	THF	342.25	0.1001	4.1898
	Ethanol	357.49	0.0591	4.0486
Hydrogen substituent	**Gas**	314.18	0.1964	3.7340
	Chloroform	336.93	0.1437	4.1887
	THF	340.36	0.1313	4.2075
	Ethanol	345.42	0.1174	4.1506

Reference:

[1] K. Bouzek and etal; “Heat losses in Gratzel solar cells”; Solar Energy Materials & Solar Cells; 57, 359-371, 1999.

[2] E. Galoppini; “Linkers for anchoring sensitizers to semiconductor nanoparticles”; Coordination Chemistry Reviews 248, 1283–1297, 2004

[3] W. Herbst, K. HungerJohn; “Industrial Organic Pigments”; Wiley & Sons, Apr 21, 2006 - 678 pages