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CALCULATION OF ACIDITY CONSTANTS OF AZO DYES DERIVED 4-(PHENYLDIAZENYL)BENZENE-1,3-DIOL BY DFT METHOD

4-(PHENYLDİAZENİL)BENZEN-1,3-DİOLDEN TÜRETİLMİŞ AZO BOYARLARIN ASİTLIK SABİTLERİNİN DFT METODU İLE HESAPLANMASI

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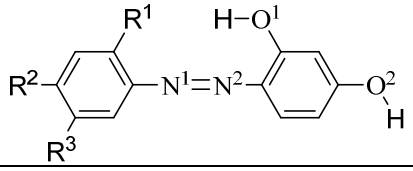
ABSTRACT

In this study, all acidity constants of six azo dyes derived from 4-(phenyldiazenyl)benzene-1,3-diol have been calculated by DFT method with Gaussian09 [1] program (B3LYP/6-311++G(d,p)) [2].The theoretical data has compared with those of experimental ones [3]. Then, proton gain and loose centers of these molecules have been determined. It has been indicated that first protonation is on N1 nitrogen with correlation constant R2=0,9996. First deprotonation is on the hydrogen binding O1 with the correlation constants (R2=0, 9957) and second deprotonation is on the hydrogen binding O1 and O2 with R2=0, 9715.

Table 1. IUPAC Nomenclature of the studied molecules.



Compound No	IUPAC Name	Substituents		
		R^1	R^2	R^3
1	4-(Phenyldiazenyl)benzene-1,3-diol	H	H	H
2	4-((2,4-Dihydroxyphenyl)diazenyl)benzenesulfonic acid	H	SO_3H	H
3	4-((2-Hydroxyphenyl)diazenyl)benzene-1,3-diol	OH	H	H
4	3-((2,4-Dihydroxyphenyl)diazenyl)-4-hydroxybenzenesulfonic acid	OH	H	SO_3H
5	4-((2-Chlorophenyl)diazenyl)benzene-1,3-diol	Cl	H	H
6	4-((2-Nitrophenyl)diazenyl)benzene-1,3-diol	NO_2	H	H

Dedication

This work is dedicated to the memory of our colleague Dear Prof. Dr. Cemil Öğretir, who passed away on January 19, 2011.

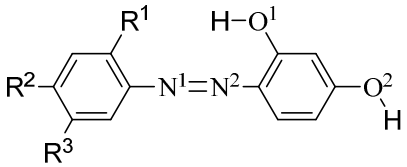
Keywords

Acidity constant, DFT, Azo dyes, theoretical calculation.

ÖZET

Bu çalışmada, 4-(phenyldiazenyl)benzene-1,3-diolden türetilmiş altı azo boyar maddenin asitlik sabitleri Gaussian09 [1] program (B3LYP/6-311++G(d,p)) (DFT metodu) ile hesaplanmıştır.[2]. Elde edilen teorik veriler deneysel verilerle kıyaslanmıştır [3].Daha sonra, bu moleküllerin proton alma ve verme merkezleri belirlenmiştir. İlk protonlanmanın N1 azotu üzerinde olduğu (R2=0,9996 korelasyon sabiti) gösterilmiştir. İlk deprotonlanma O1'e bağlı hidrojendendir (R^2=0, 9957) ve ikinci deprotonlanma ise O1 ve O2'ye bağlı olan hidrojendendir (R^2=0, 9715).

Tablo 1. Çalışılan bileşiklerin IUPAC isimlendirilmeleri.



Bileşik No	IUPAC Adı	Sübstitüentler		
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4	3-((2,4-Dihydroxyphenyl)diazenyl)-4-hydroxybenzenesulfonic acid	OH	H	SO_3H
5	4-((2-Chlorophenyl)diazenyl)benzene-1,3-diol	Cl	H	H
6	4-((2-Nitrophenyl)diazenyl)benzene-1,3-diol	NO_2	H	H

Anma

Bu çalışma, 19 Ocak 2011 tarihinde kaybettiğimiz çalışma arkadaşımız Sayın Prof. Dr. Cemil Öğretir'e adanmıştır.

Anahtar Kelimeler

Asitlik sabiti, DFT, azo boyar, teorik hesaplama.

Kaynaklar / References

[1] Gaussian 09. Revision B.01. Gaussian Inc. Wallingford. CT., 2009.
[2] B. Ghalami-Choobar, H. Dezhampanah, P. Nikparsa and A. Ghiami-Shomami, International Journal of Quantum Chemistry, 112, 2275–2280, 2012.
[3] H. Berber, C. Ogretir, E. C. S. Lekesiz and E. Ermis, J. Chem. Eng. Data, 53 (5), 1049-1055, 2008.