Theoretical Study for the Determination the Octane Number of Gasoline Derivatives

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Abstract

In this study, some physical properties affecting the octane Number of gasoline derivatives were calculated using AM1 semi-experimental methods, including steric energy, heat formation, van der Waals strength, energy of the highest occupied molecular orbital energy (EHOMO), the lowest unoccupied molecular orbital energy (ELUMO), and hardness values using chemical software. Thus, the statistical analysis was carried out using the SPSS program between the calculated variables and the values of the practical octane number. The most important variables were found to have an effect on octane number values (high energy, steric energy, empty energy level, heat formation and spatial impedance) Was obtained in 0.974. The relative error was 7.34 and there was a good match between the values of the practical octane number the calculated from this study.

Keywords: Octane number, AM1method, Chemoffice.

دراسة نظرية لحساب العدد الاوكتاني لعدد من مشتقات الكازولين

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ألخلاصة

في هذه الدراسة تم حساب بعض الخصائص الفيزيائية التي تؤثر على العدد الاوكتاني باستخدام الطرق شبه التجريبية ومنها طريقة التقريب. والمتضمنة (طاقة الاعاقة، حرارة التكوين، قوى فاندرفالز، طاقة اعلى مستوي طاقي مشغول، واوطأ مستوي طاقي فارغ، قيم الصلابة) باستخدام البرامج الكيميائية، تم استخدام التحليل الاحصائي المتعدد لايجاد العلاقة بين المتغيرات المحسوبة والقيم العملية للعدد الاوكتاني ومن ثم حساب العدد الاوكتاني نظريا. وقد وجد ان المتغيرات الاكثر تاثير على قيم العدد الاوكتاني كانت (طاقة الاعاقة، الطاقة الكلية، اوطأ مستوي طاقي فارغ، اعلى مستوي طاقي مشغول). ومن خلال قيم معامل الارتباط الجيدة النسبي 7.34 نلاحظ وجود علاقة جيدة بين القيم العملية للعدد الاوكتاني ومقدار الخطأ 0.971 والمتغيرات المحسوبة من هذه الدراسة.

ألكلمات المفتاحية: العدد الاوكتاني، الطرق شبه التجريبية، حسابات نظرية.

Introduction

In the testn method used to determine antiknock [1] properties of gasolines, coparisions, are made with blends of two pure hydrocarbons, n-heptane and "iso-octane" (2,2,4-trimithylpentane). Iso-ocquit low (with an octane number of 0) in its resistance to knocking [2]. Isoaraffins have higher octane number than the corresponding normal isomers, and the octane number increases as the degree of branching of the chain is increased. aromatics usually have quite high-octane numbers [3].

Computational Chemistry

Theoretical chemistry is one of the branches of physical chemistry, which deals with the study of synthetic bodies and the physical and chemical properties of all compounds [4]. These calculations are based on the use of Schrodinger equation and its approximations in the creation of these variables (electronic density, double-clutch and force of van der Waals, the good methods used to calculate such variables because they do not need a long period of time not rely on the practical results stored in the program [5]. space disruptive energy and energy

variables like HOMO and LUMO values. HOMO represents the least energy to remove electrons from the orbital outside the compound to the oxidizing state [6, 7]. LUMO is the least possible energy needed to acquire an electron into the outer orbital and the compound changes to a reduced state called electronic affinity. [8, 9] Some other variables such as hardness (η) [10], electronic chemical potential (μ) [11], and the global electrophilicity index (W) [12] are calculated from these energy variables with the help of following relationships.

$\mu = (EHOMO + ELUMO)/2$ …....(1)

$\eta = (EHOMO – ELUMO)/2$ …....(2)

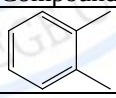
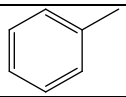
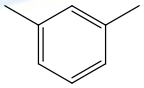
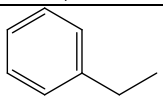
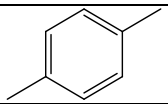
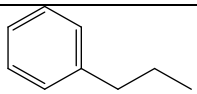
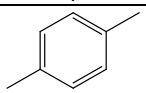
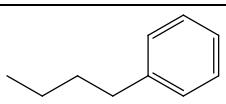
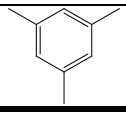
$W = (\mu 2/2\ \eta)$ …..……..... (3)

Theoretical Calculations

The default calculations in this study were completed using the AM1 method and according to the following steps [13]

1. Drawing the molecule using the Chem Draw program.
2. Configure the molecule using Clean Up.
3. The process of reducing the energy to obtain the best stable body space.
4. Variables were calculated according to AM1 method.
5. Multiple statistical analysis was performed on these variables with octane number values.

Table 1. Names of gasoline derivatives and their structure.

No.	Compound	Name	No.	Compound	Name
1.		Benzene	**6.**		O-xylene
2.		Toluen	**7.**		M -xylene
3.		Ethylbenzene	**8.**		P-xylene
4.		Propylbenzene	**9.**		Cumene
5.		Butylbenzene	**10.**		Mesitylene

Results and discussion

Theoretical calculations of some physical variables

Table 2: Parameters suggested to calculate the octane numbers of gasoline derivatives.

No.	SE. kcal/mol	1,4VDW	Stretch-Bend	Heat of Formation Kcal/Mol	Total energy Kcal/Mol
1.	-0.5738	5.2594	-0.0000	22.0222	-19609.0136
2.	-0.5680l	5.9152	-0.0019	14.4246	-23203.3557
3.	1.4687	6.7878	0.0453	8.9881	-26795.5367
4.	2.2019	7.4978	0.0660	2.3573	-30388.912
5.	2.8201	8.1948	0.0834	4.4506	-33982.4644
6.	0.7791	6.7208	-0.0022	8.0346	-26796.4902
7.	-0.5851	6.5428	-0.038	6.8721	-26797.6526
8.	-0.5809	6.5549	-0.0015	6.8226	-26797.7022
9.	1.80661	7.7203	0.0459	4.7201	-30386.5493
10.	--0.5145	7.1712	--0.0018	0.6319-	-30391.9012

We note from the above table that there is a difference in the values of the spatial impedance energy due to the difference of the stereotypes of the compounds under study with a convergence of the values of the total energies of these compounds. The power of van der Waals interactions (VDW 1-4). It was calculated as a model to describe the effect of the substituted groups difference of the structural bodies as well as in the values of the total energies of the compound and this is a proof of the effect of these variables at the expense of the octane number.

Table 3: theoretical calculation of Energy variables of gasoline derivatives.

No.	HOMO (ev)	LUMO (ev)	(Ƞ) (ev)	N (ev)	W(ev)
1.	-15.966	-1.703	7.1315	0.27737	-0.09644
2.	-15.118	-1.696	6.711	0.27720	-0.09583
3.	-14.965	-1.685	6.64	0.27702	-0.09561
4.	-15.075	-1.680	6.699	0.27640	-0.09577
5.	-15.087	-1.679	6.704	0.21600	-0.07384
6.	-14.674	-1.507	6.5835	0.22010	-0.12566
7.	-14.674	-1.507	6.5835	0.27379	-0.10343
8.	-14.385	-1.693	5.4995	0.27450	-0.10149
9.	-14.811	-1.674	6.5685	0.27706	-0.10161
10.	-14.737	-1.003	6.867	0.27309	-0.09435

Table 3 represents the values of energy variables calculated using semi-experimental methods including a method through which it can be observed a strong relationship among the variables. This confirms its effect in calculating the octane number of derivatives of gasoline [14, 15]. After calculating all the variables that are expected to affect the calculation of the octane count of the gasoline derivatives, the statistical analysis was performed to find the best of these variables.

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	970[a]	940	892	7.34164

a. Predictors: (Constant), SB, HOMO, LUMO, HF

ANOVA[a]

Model		Sum of Squares	df	Mean Square	F	.Sig
1	Regression	4229.344	4	1057.336	19.617	003[b].
	Residual	269.499	5	53.900		
	Total	4498.843	9			

a. Dependent Variable: octane number.

b. Predictors: (Constant), SB, HOMO, LUMO, HF

Coefficients[a]

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.
		B	Std. Error	Beta		
1	(Constant)	1080.119	206.527		5.230	003.
	Lumo	108.644	25.305	1.055	4.293	008.
	Homo	54.384	12.671	1.036	4.292	008.
	HF	3.453	1.242	1.153	2.781	039
	SB	376.431	236.532	568.	1.591	172.

a. The Dependent Variable: octane number.

Table 4: Observed and calculated octane number of the gasoline derivative under study

No.	ON. calculated	ON. Observed [2]
1.	102	99
2.	122	124
3.	130	124
4.	110	127
5.	92	98
6.	145	140
7.	140	145
8.	136	146
9.	126	132
10.	166	171

Note from the above table that there is a significant correlation between the values of practical and calculated octane number theoretically with a few differences in some compounds and this is evidence of the role of the variables proposed in the SABB octane number of derivatives of gasoline [16]. This study opens wide doors in the field of green software chemistry.

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