Journal of the Serbian Chemical Society
Version Electronic
JSCS-info@shd.org.rs • www.shd.org.rs/JSCS

J. Serb. Chem. Soc. *83* (12) 1339–1349 (2018)
JSCS–5155

UDC 519.177.004.14:536.77:547.395:
544.131
Original scientific paper

Application of spectral graph theory on the enthalpy change of formation of acyclic saturated ketones

ANA GLIGORIJEVIĆ, SVETLANA MARKOVIĆ*, IZUDIN REDŽEPOVIĆ
and BORIS FURTULA#

Faculty of Science, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Serbia

(Received 6 September, accepted 15 October 2018)

Abstract: The dependence of the enthalpy change of formation of saturated acyclic ketones on molecular structure (the number of carbon atoms, the position of the carbonyl group, and the branching of the molecules) was investigated. For this purpose, a simple computational model, the parameterization of which is based on spectral graph theory, was developed. It was found that the major part of the enthalpy change of formation is determined by molecular size, whereas the fine structure of the enthalpy change of formation is determined by the branching of the molecule and the position of the carbonyl group. The developed model proved itself very useful for such investigations. The model is simple and practical, and the agreement between the experimental and calculated enthalpy changes of formation is very good, with an average relative error of 0.7 %.

Keywords: modified adjacency matrix; spectral moments; parameterization; 8-parametric approximate formula; molecular structure.

INTRODUCTION

An important goal of theoretical chemists is to examine the dependence of various physicochemical features of molecules on their structure. For this purpose, the chemical graph theory is often applied.[1] According to the graph theory, molecules are represented with corresponding molecular graphs. A molecular graph G with n vertices and m edges can be represented with its adjacency matrix **A**, which reflects the adjacency of ordinarily non-hydrogen atoms (*i.e.*, the existence of chemical bonds). Namely, **A** is a square matrix of order n whose elements $a(i,j)$ take non-zero (usually unity) and zero values depending on whether the vertices i and j are adjacent or not. Eigenvalues of the adjacency matrix,

---

* Corresponding author. E-mail: mark@kg.ac.rs
# Serbian Chemical Society member.
https://doi.org/10.2298/JSC180906086G

$\lambda_1,\lambda_2,\dots,\lambda_n$, form the spectrum of the respective molecular graph. Then, the k^{th} spectral moment of G is defined as:

$$M_k(G)=\sum_{i=1}^{n}\lambda_i^k \tag{1}$$

It is well known that odd spectral moments are equal to zero in bipartite graphs. In addition, Eq. (2) holds for all **A** matrices, and Eq. (3) is valid in those cases where all edges are of weight 1:

$$M_0=n \tag{2}$$

$$M_2=2m \tag{3}$$

Spectral moments have found remarkable applications in the physical chemistry of solid state.[2–4] Namely, using a continued fraction technique, the normalized moments were employed to obtain the Hückel molecular orbital (HMO) density of states and other useful properties of solids. The applications of spectral moments in the theoretical chemistry of conjugated molecules are too numerous to be summarized here in due detail.[5–29] Explicit formulas, in terms of counts of simple structural properties, were designed for the first few spectral moments of various classes of molecular graphs.[7–9,12,17,18,22,24,26,27] A procedure based on energy partitioning *via* spectral moments was proposed for investigating the aromaticity of conjugated systems.[15,16] In a series of works, moments were used to estimate the HMO total π-electron energy and examine its dependence on molecular structure.[5,6,8–13,17,19,21,25,29] The spectral moments of polycyclic aromatic hydrocarbons (PAHs) from coal-tar pitch were used to examine the relationship between the rate of supercritical fluid extraction of PAHs and the corresponding topological invariants.[28] Contemporary applications of spectral moments have shifted towards biochemical systems and drug discovery.[30,31] This line of research has particularly flourished by the introduction of the so-called Estrada index, which is tightly connected to the concept of spectral moments of graphs.[32,33] The mathematical properties and structural dependence of spectral moments of graphs and the Estrada index and their modifications have also been heavily investigated.[34–37] The enthalpy change of formation (ΔH_f), an important physicochemical property of substances, was approximated in terms of spectral moments of phenylenes.[27] The goal of the present paper is to examine the dependence of ΔH_f of saturated acyclic ketones on molecular structure using the spectral graph theory. To accomplish this task, it is necessary to calculate the ΔH_f values for those ketones for which the experimental enthalpies are not available.

Accurate prediction of the enthalpy changes of formation of the gas-phase molecules was achieved *via* high-level quantum chemistry methods. As for ketones, the G2 *ab initio* approach was applied to calculate the enthalpy changes of formation of small molecules: cyclopropenone, cyclopropanone and acetone.[38]

Computationally less demanding, the combined HF/6-31G(d)-empirical scheme for calculating the ΔH_f values of carbonyl compounds was developed.[39] In addition, molecular mechanics MM3 and MM4 calculations of ΔH_f for about 50 open chain, ring and fused ring carbonyl compounds were performed.[40] The semi-empirical parametric method 5 (PM5) was successfully applied in the investigations of the dependence of ΔH_f of ketones on molecular structure (*i.e.*, the size of the molecule, the position of the carbonyl group, and the number of methyl substituents).[41] The results obtained there could serve for comparison to the findings of this work.

COMPUTATIONAL METHODOLOGY

To develop a computational model for examining the dependence of ΔH_f of ketones on their structure, the experimental gas-phase ΔH_f values for 27 saturated acyclic ketones were used (Table I).[42,43] This is exactly the same set of data that was used in the investigation of ΔH_f by means of the PM5 method.[41] It was supposed that ΔH_f of the examined ketones could be expressed as a linear combination of the corresponding spectral moments:

$$\Delta H_\mathrm{f} \approx a_0M_0 + a_2M_2 + a_4M_4 + a_6M_6 + a_8M_8 + \cdots + \text{const.} \tag{4}$$

The spectral moments and enthalpies of formation were calculated by means of in-house FORTRAN programs. For this purpose, three types of the adjacency matrix were used:

a. All matrix elements that correspond to chemical bonds were equal to unity, independently of the existence of a heteroatom;

b. The element of the adjacency matrix that corresponds to the C=O bond was given the weight of 2 (double bond). The elements that correspond to all other bonds were equal to unity;

c. The element of the adjacency matrix that corresponds to the C=O bond was given the weight of 1.24 (the C=O bond length in ketones usually amounts to 1.24 Å). The elements that correspond to all other bonds were equal to unity;

The so-constructed adjacency matrices were used to calculate the spectral moments (Eq. (1)) up to M_{20}, and their values were inserted in Eq. (4). The quality of the obtained approximations for ΔH_f was examined by comparison between the experimental and calculated ΔH_f values, where correlation coefficient (R) and average relative error (ARE) were used as descriptors. The results for 8-parametric formulas (4) are presented in Table II. It is apparent that case c) provides the best agreement between the experimental and calculated results for ΔH_f of ketones. The cases where the $a(i,j)$ element that corresponds to the C=O bond was given the weights of 1.1, 1.2, 1.3 and 1.4 were also examined but there was no improvement over the case c. Taking these facts into account, the adjacency matrix where the weight for the C=O bond was 1.24 was used for all further investigations.

It should be emphasized that in all three cases, a, b and c, Eq. (4), was constructed in a way that the number of summands was gradually increased, and the quality of each approximation was inspected. The results for case c (best approximation) are summarized in Table III. The increase of parameters in Eq. (4) necessarily improves the approximation, *i.e.*, decreases the average relative error and increases the correlation coefficient. With an increasing number of parameters, this improvement decreases, and for M_{14} and higher spectral moments, it becomes negligible. Using F statistics, the justification for introducing a new parameter in the model shown in Eq. (4) was tested. The F-test acknowledges the noticeable alteration in the variance of the model on the addition of a new parameter. Obtained results indicated that the 4-parametric model is sufficient for predicting the ΔH_f of ketones.

TABLE I. Molecular graphs and ΔH_f values for the set of ketones used for parameterization. The vertices and edges that correspond to the carbonyl groups are marked with different color

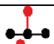
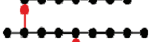
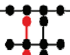
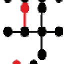
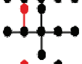
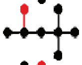
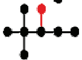
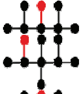
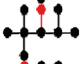
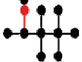
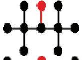
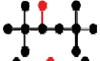
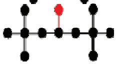
Ketone	Molecular graph	ΔH_f / kJ mol^{-1}	
		Exp.	Calcd.
2-propanone		–218.53	–218.75
2-butanone		–238.57	–236.80
2-pentanone		–259.03	–258.71
3-pentanone		–253.55	–255.33
2-hexanone		–279.78	–280.18
3-hexanone		–278.24	–277.23
4-heptanone		–298.32	–298.93
2-nonanone		–340.79	–343.12
5-nonanone		–344.93	–341.45
6-undecanone		–387.40	–386.33
2-dodecanone		–404.26	–406.39
3-methyl-2-butanone		–262.59	–264.10
3,3-dimethyl-2-butanone		–290.66	–294.32
3-methyl-2-pentanone		–284.09	–283.89
4-methyl-2-pentanone		–291.21	–288.74
2-methyl-3-pentanone		–286.19	–282.71
3,3-dimethyl-2-pentanone		–303.76	–309.97
4,4-dimethyl-2-pentanone		–320.49	–322.12
2,2-dimethyl-3-pentanone		–313.80	–311.30
2,4-dimethyl-3-pentanone		–311.29	–308.88
3,3,4-trimethyl-2-pentanone		–328.44	–330.53
2,2,4-trimethyl-3-pentanone		–338.32	–333.74
3,3,4,4-tetramethyl-2-pentanone		–347.69	–343.84
2,2,4,4-tetramethyl-3-pentanone		–345.81	–351.51
2,6-dimethyl-4-heptanone		–357.69	–357.51
2,2,5,5-tetramethyl-3-hexanone		–393.88	–389.03
2,2,6,6-tetramethyl-4-heptanone		–421.33	–421.53

TABLE II. Correlation coefficients (R) and average relative errors (ARE) for 8-parametric Eq. (4)

A matrix	R	ARE / %
Case a	0.990	1.38
Case b	0.996	1.09
Case c	0.998	0.69

TABLE III. Correlation coefficients (R) and average relative errors (ARE) for increasing number of parameters in Eq. (4). The results refer to the adjacency matrices whose elements that correspond to the C=O bonds are equal to 1.24

No. of parameters	R	ARE / %
2 (up to M_0)	0.983	2.11
3 (up to M_2)	0.985	2.03
4 (up to M_4)	0.990	1.49
5 (up to M_6)	0.996	1.00
6 (up to M_8)	0.998	0.79
7 (up to M_{10})	0.998	0.73
8 (up to M_{12})	0.998	0.69

However, such a model was not able to describe the dependence of ΔH_f of ketones on fine structural details. Additionally, the introduction of more than 4 parameters in the model still significantly lowered the average relative error of the estimate. Therefore, the results obtained by the F-test were ignored and it was decided that the optimal approximation for ΔH_f of ketones would be given with 8-parametric Eq. (5). This approximate formula reproduces ΔH_f of saturated ketones with satisfactory accuracy, resulting in ARE values of less than 1 %. Thus, it was used to calculate the ΔH_f of numerous unbranched and branched ketones. The results for the set of ketones used for parameterization are listed in Table I:

$$\begin{aligned}\Delta H_f \approx & -39.29136n + 17.68924M_2 - 2.65522M_4 - 1.74032M_6 + \\ & +1.08415M_8 - 0.23210M_{10} + 0.01749M_{12} - 117.23579 \ \left(\text{kJ mol}^{-1}\right)\end{aligned} \tag{5}$$

RESULTS AND DISCUSSION

The dependences of ΔH_f on the size of molecule n (number of carbon atoms), the position of carbonyl group c, and the branching of the molecule b (number of methyl substituents) were examined. For this purpose, Eq. (5) was used to calculate ΔH_f values for numerous ketones the experimental data of which are not available in the scientific literature. The results obtained are presented in Table IV. When the dependence of ΔH_f on a certain structural property was investigated, the other two were kept constant. It was expected that the influence of all structural features could be better analyzed in this manner because a weak influence of some structural property is protected from possible screening by a much stronger influence of another structural property.

The dependence of ΔH_f on molecular size was examined on the series of unbranched ketones listed in Tables I and IV. The maximum number of carbon atoms n was 17. In accordance with the experimental and theoretical findings,[41–43]

ΔH_f of ketones decreases with the increasing size of the molecules by approximately 21 kJ mol^{-1} per methylene group. The dependence of ΔH_f on n is linear (Fig. 1). The correlation coefficients for the homologous series of 2-, 3-, and 4-ketones amount to –0.99998, –0.9997, and –0.9997, respectively.

TABLE IV. Calculated enthalpies of formation for some ketones

Ketone	ΔH_f / kJ mol^{-1}	Ketone	ΔH_f / kJ mol^{-1}
2-heptanone	–301.35	3,4,4-trimethyl-2-hexanone	–353.36
3-heptanone	–298.49	3,3,5-trimethyl-2-hexanone	–357.89
3-nonanone	–340.39	3,3,4-trimethyl-2-hexanone	–347.46
4-nonanone	–339.89	7-methyl-3-octanone	–348.03
2-decanone	–364.83	6-methyl-3-octanone	–345.97
3-decanone	–361.44	5-methyl-3-octanone	–346.76
4-decanone	–361.24	4-methyl-3-octanone	–344.13
5-decanone	–362.33	2-methyl-3-octanone	–346.01
2-undecanone	–385.29	8,9-dimethyl-3-heptanone	–360.25
3-undecanone	–382.52	5,6-dimethyl-3-heptanone	–352.33
4-undecanone	–382.59	4,6-dimethyl-3-heptanone	–351.59
5-undecanone	–387.34	2,6-dimethyl-3-heptanone	–353.64
2-heptadecanone	–122.32	5,5-dimethyl-3-heptanone	–355.44
3-heptadecanone	–121.42	4,5-dimethyl-3-heptanone	–346.91
4-heptadecanone	–121.49	2,5-dimethyl-3-heptanone	–351.45
5-heptadecanone	–121.53	4,4-dimethyl-3-heptanone	–346.58
6-heptadecanone	–121.45	2,4-dimethyl-3-heptanone	–348.27
7-heptadecanone	–121.45	2,2-dimethyl-3-heptanone	–352.78
8-heptadecanone	–121.45	4,5,5-trimethyl-3-hexanone	–354.99
9-heptadecanone	–121.45	2,5,5-trimethyl-3-hexanone	–364.22
7-methyl-2-octanone	–351.12	4,4,5-trimethyl-3-hexanone	–345.41
6-methyl-2-octanone	–348.90	4,4,2-trimethyl-3-hexanone	–347.28
5-methyl-2-octanone	–349.41	2,2,5-trimethyl-3-hexanone	–359.44
4-methyl-2-octanone	–350.19	2,2,4-trimethyl-3-hexanone	–351.01
3-methyl-2-octanone	–347.04	2,4,5,5-tetramethyl-3-pentanone	–352.65
6,6-dimethyl-2-heptanone	–363.66	7-methyl-4-octanone	–348.80
5,6-dimethyl-2-heptanone	–355.45	6-methyl-4-octanone	–347.04
4,6-dimethyl-2-heptanone	–357.07	5-methyl-4-octanone	–344.42
3,6-dimethyl-2-heptanone	–354.73	3-methyl-4-octanone	–344.40
5,5-dimethyl-2-heptanone	–359.23	2-methyl-4-octanone	–349.58
4,5-dimethyl-2-heptanone	–353.78	6,6-dimethyl-4-heptanone	–360.65
3,5-dimethyl-2-heptanone	–352.49	5,6-dimethyl-4-heptanone	–349.64
4,4-dimethyl-2-heptanone	–359.67	3,6-dimethyl-4-heptanone	–351.91
3,4-dimethyl-2-heptanone	–351.44	2,6-dimethyl-4-heptanone	–357.51
3,4,5-trimethyl-2-hexanone	–355.57	5,5-dimethyl-4-heptanone	–346.54
4,5,5-trimethyl-2-hexanone	–364.45	3,5-dimethyl-4-heptanone	–345.74
3,5,5-trimethyl-2-hexanone	–365.78	2,5-dimethyl-4-heptanone	–351.91
4,4,5-trimethyl-2-hexanone	–361.41		

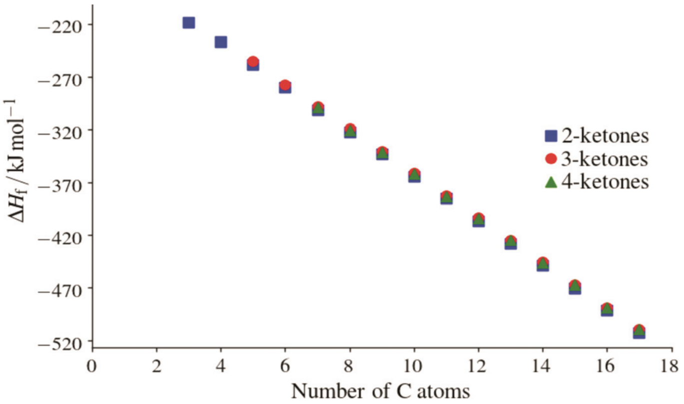


Fig. 1. Dependence of the enthalpy change of formation of ketones on molecular size.

The dependence of ΔH_f on the position of carbonyl group *c* was examined on the series of unbranched isomeric ketones where *n* ranges 7–11. The influence of *c* upon ΔH_f is illustrated in Fig. 2. Tables I and IV show that the influence of *c* is much smaller than that of *n*, and does not exceed 3–4 kJ mol^{-1}.

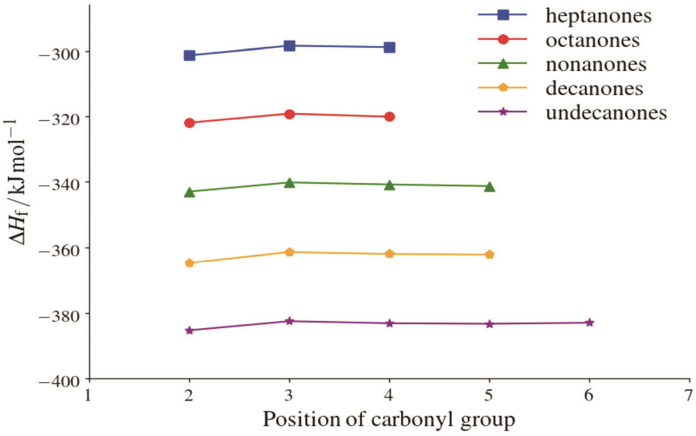


Fig. 2. Dependence of the enthalpy change of formation of ketones on the position of the carbonyl group.

In each examined series of isomeric ketones, the ΔH_f value of 3-ketone is larger than that of 2-ketone (Tables I and IV and Fig. 2). As the carbonyl group is further shifted toward the middle of a molecule, the enthalpy change of formation decreases. An interesting feature of Fig. 2 is that the ΔH_f values of 4- and 5-decanones, as well as of 4- and 5-undecanones, are mutually very similar. It could be assumed that larger ketones would also exhibit such behavior, implying that, in the cases where carbonyl group is sufficiently separated from the end and middle of the molecule, the enthalpy change of formation becomes independent of *c*. An attempt was made to examine this assumption in heptadecanones. However, Fig. 3 reveals that the last four ΔH_f values are identical. This occurrence is, certainly, a consequence of imperfection of the employed computational model, which does not distinguish among larger isomeric ketones. This limitation would be eliminated by increasing the number of parameters in Eq. (4), *i.e.*, by introducing higher spectral moments. However, such treatment would make the resulting approximate formula difficult to manage and impractical.

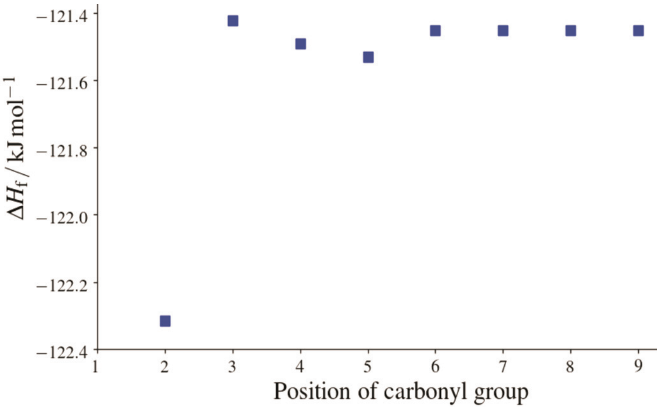


Fig. 3. Dependence of the enthalpy change of formation on the position of the carbonyl group in heptadecanones.

To investigate the dependence of ΔH_f on the branching of the molecule b, all unbranched and branched 2-, 3-, and 4-nonanones (b ranges 0–4) were constructed (each series consisting of 24 isomers), and their ΔH_f values calculated (Tables I and IV). Graphical depiction of the results obtained is given in Fig. 4 and in the Supplementary material to this paper.

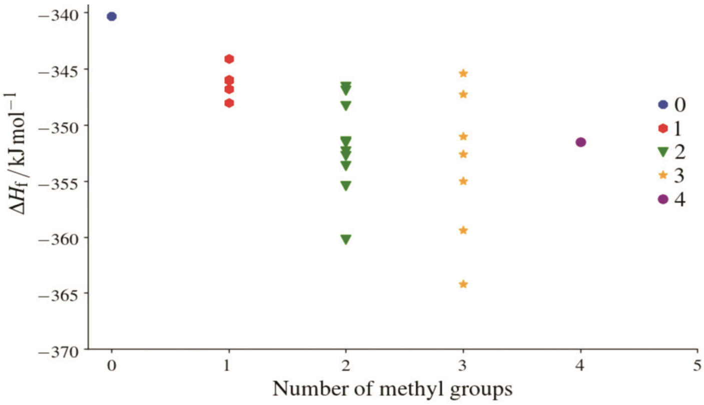


Fig. 4. Dependence of the enthalpy change of formation on the branching of the molecule in 3-nonanones.

The molecules 2-, 3-, and 4-nonanones show very similar dependence of ΔH_f on b. The larger b is, the wider is the range of ΔH_f values of isomeric ketones. ΔH_f generally decreases with increasing number of methyl substituents. The difference between an unbranched nonanone and the corresponding branched isomer of the lowest ΔH_f is around 20 kJ mol^{-1}. It could be concluded that the branching of a molecule strongly influences the enthalpy change of formation of ketones. The influence of this structural property is comparable to that of the molecular size. It could be supposed that the influence of branching could be even stronger in the case of larger molecules, where the isomers are more numerous, and b can take larger values.

CONCLUSIONS

There are two main conclusions regarding the dependence of ΔH_f of acyclic saturated ketones on molecular structure. Firstly, molecular size (presented as the number of carbon atoms) exerts the greatest influence on ΔH_f of ketones. Secondly, the influence of fine structural details, such as the position of the carbonyl group and the number of methyl substituents, is weaker. However, the impact of the latter structural property could be comparable to that of the molecular size, particularly when large ketones are in question.

The computational model based on the spectral graph theory was found to be useful for such investigations. Thus, the model is simple and practical. Furthermore, the agreement between the experimental and calculated enthalpies of formation of ketones is very good, with an average relative error of 0.7 %. A comparison of the findings of this work with those performed by means of the PM5 method[41] revealed that both investigations follow the same trends, and the differences are only quantitative.

The calculation of the enthalpies of formation of flexible compounds by means of semi-empirical methods (and all other quantum-mechanical methods) is complicated by the fact that a molecule of such compounds can adopt many conformers, where each conformer has its own enthalpy. Therefore, to determine the enthalpy of formation of a flexible molecule it is necessary to construct all its conformers, calculate the enthalpy of formation of every single conformer, and finally, calculate ΔH_f using the formula:[44]

$$\Delta H_\mathrm{f} = \sum_i N_i \left(\Delta H_\mathrm{f}\right)_i \tag{6}$$

where N_i represents the mole fraction of the i^th conformer and is given by the formula:

$$N_i + \sum_{j \neq i} \frac{N_i}{e^{\frac{(\Delta H_\mathrm{f})_j - (\Delta H_\mathrm{f})_i}{RT}}} = 1 \tag{7}$$

An advantage of the model used in this work is that it predicts a unique ΔH_f value for a certain compound, independently of the number of rotamers that the compound can adopt. Certainly, the model is also characterized with some shortcomings. Namely, it does not distinguish among the isomers of large ketones. Finally, Eq. (5) can only be applied to ketones. A new parameterization would be required for another class of compounds.

SUPPLEMENTARY MATERIAL

Additional data are available electronically at the pages of journal website: http:// //www.shd.org.rs/JSCS/, or from the corresponding author on request.

Acknowledgment. This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project Nos. 172016 and 174033).

ИЗВОД

ОДРЕЂИВАЊЕ ПРОМЕНЕ ЕНТАЛПИЈЕ ФОРМИРАЊА ЗАСИЋЕНИХ КЕТОНА ПРИМЕНОМ СПЕКТРАЛНЕ ТЕОРИЈЕ ГРАФОВА

АНА ГЛИГОРИЈЕВИЋ, СВЕТЛАНА МАРКОВИЋ, ИЗУДИН РЕЦЕПОВИЋ и БОРИС ФУРТУЛА

Природно–математички факултет, Универзитет у Крагујевцу, Радоја Домановића 12, 34000 Крагујевац

Испитана је зависност промене енталпије формирања засићених кетона од молекулске структуре (броја угљеникових атома, позиције карбонилне групе и гранања молекула). У ову сврху конструисан је једноставан компјутерски модел, чија је параметризација заснована на спектралној теорији графова. Нађено је да највећи део промене енталпије формирања зависи од величине молекула, а фини детаљи су одређени грањањем молекула и позицијом карбонилне групе. Развијени модел се показао као веома користан за оваква испитивања. Са једне стране модел је једноставан и практичан, а са друге слагање израчунатих промена енталпија формирања са експерименталним је веома добро, са просечном релативном грешком од 0,7 %.

(Примљено 6. септембра, прихваћено 15. октобра 2018)

REFERENCES

1. M. Randić, M. Novič, D. Plavšić, *Solved and unsolved problems of structural chemistry*, CRC Press, Boca Raton, FL, 2016
2. J. K. Burdett, S. Lee, *J. Am. Chem. Soc.* **107** (1985) 3050
3. J. K. Burdett, S. Lee, *J. Am. Chem. Soc.* **107** (1985) 3063
4. S. Lee, *Acc. Chem. Res.* **24** (1991) 249
5. G. G. Hall, *Proc. R. Soc. London* **229** (1955) 251
6. R. A. Marcus, *J. Chem. Phys.* **43** (1965) 2643
7. Y. Jiang, A. Tang, R. Hoffmann, *Theor. Chim. Acta* **66** (1984) 183
8. L. Türker, *MATCH Commun. Math. Chem.* **16** (1984) 83
9. J. Cioslowski, *Z. Naturforsch., A* **40** (1985) 1167
10. Y. S. Kiang, A. C. A. Tang, *Int. J. Quantum Chem.* **29** (1986) 229
11. J. Cioslowski, *MATCH Commun. Math. Chem.* **20** (1986) 95
12. G. G. Hall, *Theor. Chim. Acta* **70** (1986) 323
13. J. R. Dias, *J. Mol. Struct. (Theochem)* **149** (1987) 213
14. J. R. Dias, *Can. J. Chem.* **65** (1987) 734

15. Y. Jiang, H. Zhang, *Theor. Chim. Acta* **75** (1989) 279
16. Y. Jiang, H. Zhang, *Pure Appl. Chem.* **62** (1990) 451
17. I. Gutman, G. G. Hall, S. Marković, Z. Stanković, V. Radivojević, *Polycycl. Arom. Comp.* **2** (1991) 275
18. D. Babić, A. Graovac, I. Gutman, *Theor. Chim. Acta* **79** (1991) 403
19. S. Marković, I. Gutman, *J. Mol. Struct. (Theochem)* **235** (1991) 81
20. S. Marković, *Theor. Chim. Acta* **81** (1992) 237
21. I. Gutman, *Theor. Chim. Acta* **83** (1992) 313
22. Y. Jiang, X. Qian, Y. Shao, *Theor. Chim. Acta* **90** (1995) 135
23. I. Gutman, V. R. Rosenfeld, *Theor. Chim. Acta* **93** (1996) 191
24. S. Marković, A. Stajković, *Theor. Chim. Acta* **96** (1997) 256
25. I. Gutman, S. Marković, A. Vesović, E. Estrada, *J. Serb. Chem. Soc.* **63** (1998) 639
26. S. Marković, *J. Chem. Inf. Comput. Sci.* **39** (1999) 654
27. S. Marković, Z. Marković, R. I. McCrindle, *J. Chem. Inf. Comput. Sci.* **41** (2001) 112
28. S. Marković, Z. Marković, J. P. Engelbrecht, R. I. McCrindle, *J. Chem. Inf. Comput. Sci.* **42** (2002) 82
29. S. Marković, *Indian J. Chem., A* **42** (2003) 1304
30. U. Debnath, S. B. Katti, Y. S. Prabhakar, *Curr. Comput. Aided Drug Design* **9** (2013) 472
31. M. Mahani, S. Sheikhghomi, H. Sheikhghomi, J. Fasihi, *J. Struct. Chem.* **58** (2017) 344
32. E. Estrada, *Bioinformatics* **18** (2002) 697
33. E. Estrada, *Proteins: Struct. Function Bioinf.* **54** (2004) 727
34. R. Nasiri, H. R. Ellahi, A. Gholami, G. H. Fath-Tabar, A. R. Ashrafi, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 157
35. G. P. Clemente, A. Cornaro, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 673
36. B. Li, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 701
37. G. Lekishvili, *MATCH Commun. Math. Comput. Chem.* **75** (2016) 355
38. D. W. Rogers, F. J. McLafferty, A. V. Podosenin, *J. Org. Chem.* **63** (1998) 7319
39. L. R. Schmitz, I. Motoc, C. Bender, J. K. Labanowski, N. L. Allinger, *J. Phys. Org. Chem.* **5** (1992) 225
40. C. H. Langley, J. Lii, N. L. Allinger, *J. Comput. Chem.* **22** (2001) 1476
41. S. Marković, A. Despotović, D. Jovanović, I. Đurović, *Russ. J. Phys. Chem.* **83** (2009) 1430
42. J. D. Cox, G. Pilcher, *Thermochemistry of organic and organometallic compounds*, Acad. Press, London, 1970
43. J. D. Pedley, R. D. Naylor, S. P. Kirby, *Thermochemical data of organic compounds*, Chapman & Hall, London, 1986
44. W. J. Hehre, A. J. Shusterman, J. E. Nelson, *The molecular modeling workbook for organic chemistry*, Wavefunction, Irvine, CA, 1998.