SCIENCE AND EDUCATION

ISSN 2181-0842 VOLUME 2, ISSUE 12

DECEMBER 2021

Pektin monomerining ba'zi geometrik va energetik parametrlarini Avagadro dasturida o'rganish

Zarifa Yangiboy qizi Samandarova
Muzaffar Turobjon o'g'li Shokirov
Hamza Sayidmurodovich Toshov
O'zbekiston milliy universiteti

Annotatsiya: Ushbu izlanishimizda Avagadro dasturi yordamida pektin monomerining ayrim geometrik va energetik parametrlarini empirik hisoblash usullarida o'rganish natijalari keltirilgan.

Kalit so'zlar: Pektin, Avagadro dasturi, potensial energiya qiymati, empirik hisoblash usuli, molekulyar mexanika, parametrlar.

Study of some geometric and energy parameters of pectin monomer in Avagadro program

Zarifa Yangiboy qizi Samandarova
Muzaffar Turobjon oglu Shokirov
Hamza Sayidmurodovich Toshov
National University of Uzbekistan

Abstract: In this study, the results of the study of some geometric and energy parameters of pectin monomer by empirical calculations using the Avagadro program are presented.

Keywords: Pectin, Avagadro program, potential energy value, empirical calculation method, molecular mechanics, parameters.

Kirish

Kompyuter kimyosi - kimyoning informatsion texnologiyalarsiz tasavvur qilish qiyin bo'lgan sohasidir [1-2]. Ushbu fan kvant-kimyoviy hisoblashlar bilan cheklanib qolmasdan o'z ichiga empirik usullarda birikmalarning turli xil fizik-kimyoviy xarakteristikalar hisobi, moddalar reaktsion qobiliyatini baholash va biologik faolliklarini ifodalovchi matematik modellar tuzish, hamda dinamik jarayonlarni modellash kabi izlanishlarni qamrab olmoqda. Uning yuzaga kelishiga kvant mexanikasi va kvant-kimyo fanlaridagi yutuqlar bevosita sababchi bo'lgan. [3-5]

Olingan natijalar tahlili

Pektin monomerining ba'zi geometrik va energiya parametrlari empirik hisoblash usullari bilan o'rganildi. Hisoblash jarayoni Avagadro dasturining Chemical, MMFF94, MMFF94S va UFF molekulyar mexanikasi usullarida olib borildi [6-7]. Olingan natijalar quyidagi jadvallarda keltirilgan (1-2 jadval):

Jadval-1

Pektin monomerining Avagadro dasturi yordamida olingan hosil bo'lish issiqlik energilari

Chemical	MMFF94	MMFF94S	UFF
196.013 kj/mol	729.191 kj/mol	728.484 kj/mol	538.142 kj/mol

Optimizatsiya qilish natijalari ko'rsatdiki, pektin monomerining hosil bo'lishining issiqlik energiyasi MMFF94 usulida maksimal qiymatga ega bo'ldi, Chemical usulida esa minimal qiymatni ko'rsatdi.

Jadval-2

Pektin monomerining Avagadro dasturi yordamida olingan real bog' uzunliklari (A^o)

T/r	Bog'lar	Chemical	MMFF94	MMFF94S	UFF
1	C1-C2	1.5511	1.5437	1.5437	1.5523
2	C1-O4	1.4486	1.4329	1.4328	1.4280
3	C1-C20	1.5082	1.5309	1.5310	1.5101
4	C1-H27	1.1004	1.0977	1.0977	1.1156
5	C2-C3	1.5417	1.5361	1.5359	1.5432
6	C2-O18	1.4363	1.4435	1.4435	1.4057
7	C2-H28	1.1008	1.0967	1.0968	1.1153
8	C6-C3	1.5404	15236	1.5234	1.5436
9	C3-O14	1.4329	1.4380	1.4380	1.4077
10	C3-H29	1.1008	1.0964	1.0963	1.1158
11	O4-C5	1.4411	1.4244	1.4243	1.4225
12	C5-C6	1.5408	1.5421	1.5420	1.5429
13	C5-O7	1.4551	1.4430	1.4426	1.4359
14	C5-H30	1.0989	1.0973	1.0972	1.1190
15	C6-O15	1.4317	1.4367	1.4367	1.4050
16	C6-H31	1.1008	1.0957	1.0957	1.1144
17	O7-C8	1.4468	1.4385	1.4384	1.4286
18	C8-C9	1.5529	1.5449	1.5444	1.5410
19	C8-C10	1.5557	1.5515	1.5513	1.5759
20	C8-H32	1.0996	1.0986	1.0986	1.1169
21	C9-C11	1.5514	1.5458	1.5458	1.5622
22	C9-O16	1.4336	1.4411	1.4408	1.4114
23	C9-H33	1.1001	1.0947	1.0948	1.1119
24	C10-O13	1.4317	1.4338	1.4339	1.4298
25	C10-C21	1.5037	1.5356	1.5358	1.5072
26	C10-H34	1.1014	1.0978	1.0978	1.1128
27	C11-C12	1.5377	1.5360	1.5366	1.5508

28	C11-O17	1.4307	1.4302	1.4301	1.4046
29	C11-H35	1.1013	1.0975	1.0975	1.1152
30	C12-O13	1.4291	1.4131	1.4133	1.4091
31	C12-O19	1.4311	1.4208	1.4209	1.4028
32	C12-H36	1.1010	1.0964	1.0964	1.1164
33	O14-H37	0.9502	0.9813	0.9812	0.9929
34	O15-H38	0.9501	0.9777	0.9785	0.9929
35	O16-H39	0.9501	0.9753	0.9755	0.9906
36	O17-H40	0.9512	0.9759	0.9760	0.9939
37	O18-H41	0.9485	0.9805	0.9805	0.9926
38	O19-H42	0.9512	0.9729	0.9729	0.9936
39	O24-C20	1.2207	1.2193	1.2192	1.2220
40	O25-C20	1.3324	1.3568	1.3567	1.3520
41	C21-O22	1.2226	1.2253	1.2240	1.2222
42	C21-O23	1.3422	1.3643	1.3643	1.3621
43	O23-C26	1.4383	1.4291	1.4297	1.3804
44	O25-H43	0.9509	0.9842	0.9843	0.9677
45	C26-H44	1.0986	1.0937	1.0935	1.1097
46	C26-H45	1.0997	1.0939	1.0938	1.1094
47	C26-H46	1.1012	1.0937	1.0937	1.1107

Moddadagi kimyoviy bog'lanishlarning uzunligi nazariy MM usuli bilan o'rganilganda, 4 ta empirik usulda sezilarli farqlar topilmaganligini ko'rish mumkin.

Tajriba qism

Pektin monomerining ba'zi geometrik va energetik parametrlari empirik hisoblash usullari bilan o'rganildi. Hisoblash jarayoni Avagadro dasturining Chemical, MMFF94, MMFF94s va UFF kabi molekulyar mexanika usullarida bajarildi.

Xulosa

Pektin monomerining hosil bo'lish issiqlik energiyalari hisoblanganda eng minimal qiymat Chemical usulida kuzatildi. Bog'lar orasidagi masofalarda esa 4 ta usulda optimizatsiya qilinganda deyarli katta farqlar kuzatilmadi. Bog'lar uzunligi ideal bog'lar uzunligidan katta farq qilmasligi MM usulning aniqligi yuqoriligidan dalolat beradi.

Foydalanilgan adabiyotlar

1. Eshimbetov A.G., Khaitbaev A.Kh., Toshov Kh.S., Inderpreet Kaur.A theoretical study an influence of oxygen group elements to rotational barrier of 2-(2'-pyridyl)-1,3,4-oxa(thia, selena and tellura) diazoles. Bull. NUUz: Math& Nat.Sc.>Vol.2(2019)>Iss. 4. P.256

2. Хаитбаев А.Х., Х.С.Тошов, Хушваков Ж.Т. Квантово-химическое исследование некоторых Шифф-оснований. Начный журнал «Austria-science» № 6. 2017 год. Ст. 48-51.

3. Kh.S.Toshov, Khaitbayev Kh.A.,Yuldashev Sh. I. Quantum-chemical study of geometric and energy characteristics of some bases of shiffgossipol. Progress in Chemical and Biochemical Research. 2019, №2, p.01-05.

4. Khaitbayev Kh.A., Yashinov A.Sh., Toshov H.S., Eshimbetov A.G. Structure and state of azomethine derivative gossypol with benzidine. Acta NUUZ. №3/1. 2014 y. Pp. 207-21.

5. Д.Н.Далимов, А.Х.Хаитбаев, Х.С.Тошов. Синтез, состав и некоторые физико-химические свойства супрамолекулярных комплексов глицирризиновой кислоты. Ўзбекистон кимё журнали. 2018 йил -№6. Б.3-10.

6. Ешимбетов А.Г. Хаитбаев А.Х., Ҳ.С.Тошов, Турғунбоев Ш, Бекназаров Ж. Госсипол айрим Шифф асосларининг геометрик ва энергетик характеристикаларини ярим эмпирик усулда ўрганиш. ФарДУ – Илмий хабарлар. №3. 2017 й. 27-31 бетлар.

7. А.Х.Хаитбаев, Ш.М.Хакбердиев, Х.С.Тошов. Моделирование реакции конденсации госсипола с о-толуидином. VI Международной научно-практической конференции «GLOBAL SCIENCE AND INNOVATIONS 2019: CENTRAL ASIA». VI ТОМ. Нур-Султан. (Казахстан). 9-13 май. 2019 г. Ст. 257-259.

References

1. Eshimbetov AG, Khaitbaev A.Kh., Toshov Kh.S., Inderpreet Kaur.A theoretical study an influence of oxygen group elements to rotational barrier of 2- (2'-pyridyl) -1,3,4-oxa (thia, selena and tellura) diazoles. Bull. NUUz: Math & Nat.Sc.> Vol.2 (2019)> Iss. 4.P.256

2. Khaitbaev A.Kh., Kh.S.Toshov, Khushvagov Zh.T. Quantum-chemical investigation of some Schiff bases. The initial journal "Austria-science" No. 6. 2017. Art. 48-51.

3. Kh.S.Toshov, Khaitbayev Kh.A., Yuldashev Sh. I. Quantum-chemical study of geometric and energy characteristics of some bases of shiffgossipol. Progress in Chemical and Biochemical Research. 2019, No. 2, p.01-05.

4. Khaitbayev Kh.A., Yashinov A.Sh., Toshov H.S., Eshimbetov A.G. Structure and state of azomethine derivative gossypol with benzidine. Acta NUUZ. No. 3/1. 2014 y. Pp. 207-21.

5. D.N.Dalimov, A.Kh. Khaitbaev, Kh.S.Toshov. Synthesis, composition and some physicochemical properties of supramolecular complexes of glycyrrhizic acid. Ўzbekiston kimyo magazines. 2018 yil -№6. B.3-10.

6. Yeshimbetov A.G. Khaitbaev A.Kh., O.S.Toshov, Turgunboyev Sh, Beknazarov J. FarDU - Ilmiy khabarlar. No. 3. 2017 th. 27-31 betlar.

7. A.Kh.Khaitbaev, Sh.M. Khakberdiev, Kh.S.Toshov. Modeling the condensation reaction of gossypol with o-toluidine. VI International Scientific and Practical Conference "GLOBAL SCIENCE AND INNOVATIONS 2019: CENTRAL ASIA". VI VOL. Nur-Sultan. (Kazakhstan). May 9-13. 2019 Art. 257-259.