# 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.

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