EXPERIMENTAL STUDY OF SOME GEOMETRIC AND ENERGY PARAMETERS OF BETULIN

X.A. Xaitbayev
Supervisor: Professor of the National University of Uzbekistan
M.Z. Sulaymanova
1st year master's degree from the National University of Uzbekistan

Annotation: In this study, the results of the study of some geometric and energy parameters of betulin by empirical methods using the Avagadro program are presented.

Keywords: Molecular mechanics, real bond length, Chemical method, empirical method, geometric parameter, heat energy of formation.

BETULIN MODDASINING BA'ZI GEOMETRIK VA ENERGETIK PARAMETRLARINI EKSPERIMENTAL O'RGANISH

X.A. Xaitbayev
Ilmiy rahbar:O'zbekiston Milliy universiteti proffesori
M.Z. Sulaymanova
O'zbekiston Milliy universiteti1-kurs magistranti

Annotatsiya: Ushbu izlanishimizda Avagadro dasturi yordamida betulin moddasining ayrim geometrik va energetik parametrlarini empirik hisoblash usullari orqali o'rganish natijalari keltirilgan.

Kalit so'z: Molekulyar mexanika,real bog' uzunligi, Chemical metodi,empirik usul, geometrik parametr, hosil bo'lish issiqlik energiyasi.

Kirish

Molekulyar mexanika atom darajasidagi modellashtirish usulidir. Bu usulda birikmalar mikroskopik mexanik sistemalar deb qaraladi. Atomlar go'yoki o'zaro mexanik prujina orqali bog'langan va ularning fazoda joylashishi mexanik kuchlar (atom potensiallari) yordamida nazorat qilinadi.Molekulyar mexanika usullarining ko'pchiligi faqat organik birikmalarni hisoblashga mo'ljallangan. Ammo, UFF molekulyar mexanika usuli davriy sistemadagi qariyb barcha elementlarni hisoblash uchun mo'ljallangan. Molekulyar mexanika usullari kvant-kimyoviy usullar ichida nisbatan juda tezkor sanaladi. [1-2].

Olingan natijalar tahlili

Betulinning ba'zi geometrik va energetik parametrlarini eksperimental o'rganish uchun Avagadro dasturidan foydalandik. Ushbu dastur MM usulini o'rganishga juda qulay dastur hisoblanadi. Natijalar Chemical, MMFF94, MMFF94s, UFF metodlarida olindi. Har bir metodda olingan natijalari quyidagi jadvallarda keltirilgan (1-2 jadval):

1-Jadval

Betulinning Avagadro dasturi yordamida olingan hosil bo'lish issiqlik energiyalari

Chemical	MMFF94	MMFF94S	UFF
5305,6 kj/mol	1955,89 kj/mol	1955,89 kj/mol	4376,88 kj/mol

Hisoblash natijalari shuni ko'rsatadiki, betulinning hosil bo'lishi issiqlik energiyasi Chemical metodida optimizatsiya qilinganida maksimal qiymatga ega bo'ldi va MMFF94 va MMFF94s metodlarida optimizatsiya qilinganida esa bir xil minimal qiymatga ega bo'ldi. Demak, betulin moddasi uchun energetik parametr hisoblashda empirik hisoblash usullaridan MMFF94 va MMFF94s metodi samarali.

2-Jadval

Betulinning Avagadro dasturi yordamida olingan real bog' uzunliklari (Å)

T/r	Bog'lar	Chemical	MMFF94	MMFF94S	UFF
1.	C1-C2	1,585	1,514	1,527	1,544
2.	C2-C3	1,553	1,516	1,527	1,539
3.	C3-C4	1,580	1,551	1,554	1,556
4.	C4-C23	1,587	1,565	1,554	1,559
5.	C4-C24	1,573	1,552	1,547	1,551
6.	C4-C5	1,653	1,617	1,579	1,596
7.	C5-C10	1,632	1,587	1,567	1,582
8.	C10-C25	1,590	1,580	1,544	1,560
9.	C5-C6	1,550	1,562	1,536	1,548
10.	C6-C7	1,552	1,558	1,523	1,529
11.	C7-C8	1,591	1,549	1,560	1,569
12.	C8-C26	1,554	1,554	1,565	1,567
13.	C8-C9	1,618	1,581	1,591	1,614
14.	C9-C10	1,682	1,628	1,595	1,610
15.	C9-C11	1,574	1,553	1,531	1,544
16.	C11-C12	1,564	1,522	1,514	1,514
17.	C12-C13	1,549	1,516	1,538	1,548
18.	C13-C14	1,617	1,584	1,610	1,627
19.	C14-C27	1,586	1,580	1,573	1,576
20.	C14-C15	1,597	1,570	1,581	1,597
21.	C15-C16	1,563	1,525	1,531	1,546
22.	C16-C17	1,577	1,551	1,527	1,548
23.	C17-C18	1,635	1,582	1,551	1,551
24.	C13-C18	1,661	1,578	1,551	1,567
25.	C18-C19	1,625	1,555	1,557	1,560
26.	C19-C20	1,557	1,519	1,521	1,533
27.	C20-C29	1,354	1,353	1,345	1,347
28.	C20-C30	1,545	1,495	1,503	1,511
29.	C17-C22	1,592	1,538	1,539	1,544
30.	C17-C28	1,626	1,567	1,565	1,587
31.	C28-O32	1,459	1,422	1,422	1,402
32.	C3-O31	1,449	1,427	1,426	1,413
33.	C1-H33	1,130	1,098	1,096	1,109
34.	C1-H34	1,098	1,097	1,099	1,114
35.	C2-H35	1,098	1,095	1,095	1,112
36.	C2-H36	1,130	1,098	1,098	1,106
37.	C3-H37	1,100	1,098	1,098	1,117
38.	O31-H38	0,952	0,972	0,972	0,992
39.	C23-H39	1,098	1,094	1,095	1,093
40.	C23-H40	1,112	1,097	1,096	1,107
41.	C23-H41	1,100	1,096	1,096	1,112
42.	C24-H42	1,103	1,098	1,097	1,113
43.	C24-H43	1,102	1,092	1,090	1,109
44.	C24-H44	1,096	1,093	1,093	1,111
45.	C5-H45	1,097	1,101	1,103	1,113
46.	C25-H46	1,089	1,093	1,095	1,090

47.	C25-H47	1,103	1,095	1,089	1,107
48.	C25-H48	1,107	1,098	1,088	1,098
49.	C6-H49	1,102	1,100	1,095	1,093
50.	C6-H50	1,102	1,092	1,098	1,110
51.	C7-H51	1,095	1,096	1,091	1,093
52.	C7-H52	1,098	1,094	1,096	1,110
53.	C26-H53	1,099	1,095	1,094	1,105
54.	C26-H54	1,091	1,094	1,093	1,110
55.	C26-H55	1,103	1,070	1,096	1,108
56.	C9-H56	1,099	1,098	1,102	1,113
57.	C11-H57	1,098	1,096	1,092	1,107
58.	C11-H58	1,098	1,097	1,096	1,109
59.	C12-H59	1,088	1,093	1,090	1,094
60.	C12-H60	1,099	1,092	1,097	1,112
61.	C13-H61	1,101	1,099	1,098	1,110
62.	C27-H62	1,089	1,090	1,095	1,105
63.	C27-H63	1,106	1,095	1,096	1,106
64.	C27-H64	1,100	1,093	1,092	1,110
65.	C15-H65	1,095	1,093	1,098	1,105
66.	C15-H66	1,095	1,095	1,093	1,105
67.	C16-H67	1,105	1,098	1,097	1,113
68.	C16-H68	1,098	1,097	1,096	1,112
69.	C18-H69	1,098	1,087	1,103	1,119
70.	C28-H70	1,099	1,094	1,090	1,098
71.	C28-H71	1,110	1,095	1,096	1,116
72.	O32-H72	0,952	0,971	0,973	0,994
73.	C21-H73	1,106	1,096	1,095	1,111
74.	C21-H74	1,103	1,095	1,095	1,112
75.	C22-H75	1,113	1,095	1,098	1,113
76.	C22-H76	1,111	1,096	1,095	1,112
77.	C19-H77	1,101	1,105	1,098	1,102
78.	C29-H78	1,084	1,086	1,086	1,084
79.	C29-H79	1,068	1,085	1,087	1,086
80.	C30-H80	1,099	1,091	1,096	1,112
81.	C30-H81	1,104	1,097	1,096	1,111
82.	C30-H82	1,104	1,093	1,093	1,108

Betulinning ideal va real bog’ uzunliklari nazariy MM usuli bilan o’rganilganda empirik usulning 4 ta metodida sezilarli farqlar kuzatilmadi.

Tajriba qism

Betulin moddasining 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

Hosil bo’lish issiqlik energiyalari hisoblanganda eng minimal qiymat MMFF94 va MMFF94s 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 usulning aniqligi yuqoriligidan dalolat beradi.

Foydalanilgan adabiyotlar ro'yxati

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