Tetrasiklinning ba’zi geometrik va energetik parametrlarini empirik usulda o’rganish

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Annotatsiya: Maqolada ayrim empirik usullar yordamida tetrasiklinning ayrim geometrik va energetik parametrlarini nazariy o’rganish natijalari keltirilgan. Bunda Avogadro dasturidan foydalanilgan va unda mavjud bo’lgan emprik usullar yordamida umumiy energiyani hamda uning tarkibiy qismlarini topish, real va ideal bog’lar orasidagi farqlarni o’rganilgan.

Kalit so’zlar: empirik usul, molekulyar mexanika, geometrik parametr, energetik parametr, hosil bo’lish issiqlik energiyasi, ideal bog’ uzunligi

Empirical study of some geometric and energy parameters of tetracycline

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Abstract: The article presents the results of the theoretical study of some geometrical and energetic parameters of tetracycline using some empirical methods. Avogadro’s program was used and the empirical methods available in it were used to find the total energy and its components, and the differences between real and ideal gardens were studied.

Keywords: empirical method, molecular mechanics, geometric parameter, energy parameter, thermal energy of formation, ideal bond length

Kirish

Tetrasiklin - Tetracyclinum 4-dimetilamino-1,4,4a,5,5a,6,11,12a oktagidro-3,6,10,12,12a - pentaoksi-6- metil-1,11 -diketonaftatsen-2-karboksamid. Hidsiz, achchiq ta’mli, sariq kristall kukun. Yoruglik ta’sirida qorayib qoladi. Suvda juda kam, 95% li spirtda esa qiyin eriydi.

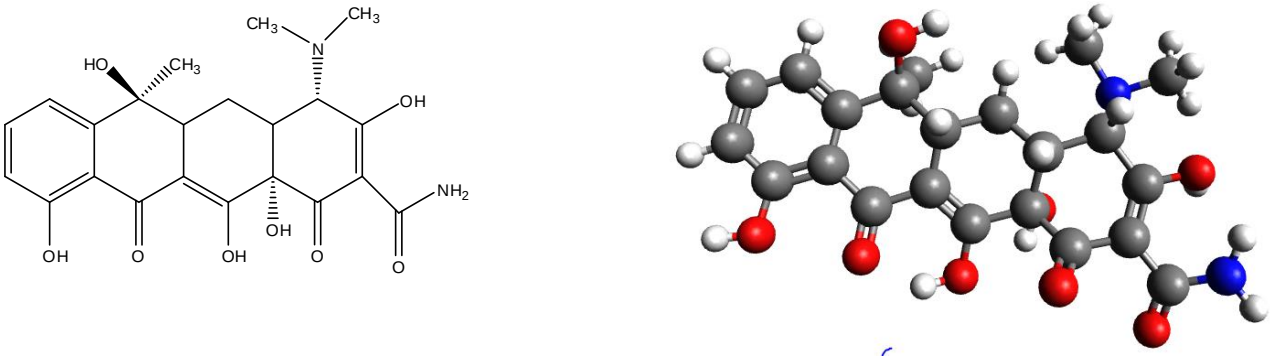
Tetrasiklin konsentrlangan sulfat kislota ta’sirida binafsha rang beradi. U rang 20-25 tomchi suv ta’sirida to’q-sariq, temir (III) xlorid eritmasi ta’sirida esa jigarrang yoki qizil-jigarrangga o’tadi. Oksitetrasiklin sulfat kislota ta’sirida qizil rangli

birikma hosil qiladi. Yangi tetratsiklin hosilalari tekshirilmoqda.

Tetratsiklinlar 1940-yillarda kashf etilgan va gramm-musbat va gramm-manfiy bakteriyalar, xlamidiyalar, mikoplazmalar, rikketsiyalar va protozoa parazitlari kabi mikroorganizmlarning keng doirasiga qarshi faollik ko'rsatdi. Ular arzon antibiotiklar bo'lib, ular odamlar va hayvonlarning infektsiyalarining profilaktikasi va davolashda, shuningdek, o'sish stimulyatorlari sifatida hayvonlarning ozuqasida subterapevtik darajada keng qo'llaniladi. Hozirgi vaqtda tetratsiklinga chidamlilik ko'payib borayotgan patogen, opportunistik va kommensal bakteriyalarda uchraydi. Tetratsiklinga chidamli patogenlarning mavjudligi kasallikni davolashda ushbu agentlardan foydalanishni cheklaydi. Tetratsiklin qarshiligi ko'pincha tetratsiklinlarning energiyaga bog'liq oqimini yoki bakterial ribosomalarni tetratsiklinlar ta'siridan himoya qiluvchi oqsilni kodlaydigan yangi genlarni olish bilan bog'liq. Agar biz ushbu toifadagi keng spektrli mikroblarga qarshi vositalardan hozirgi asr davomida foydalanishni davom ettirmoqchi bo'lsak, tetratsiklinlarni inson va hayvonlar salomatligi, shuningdek oziq-ovqat ishlab chiqarishda qo'llashni o'zgartirish kerak [1-3].

Olingan natijalar tahlili

Tetrasiklinning 2D va 3D holatdagi ko'rinishi 1-rasm:



1-rasm. Tetrasiklinning 2D va 3D holatdagi ko'rinishi

Tetrasiklinning ba'zi geometrik va energetik parametrlarini eksperimental o'rganish uchun Avogadro dasturidan foydalandik. Natijalar Chemical, MMFF94, MMFF94s, UFF metodlarida olindi. Har bir metodda qadamlar soni va energiya maksimal qiymatlarda olindi va optimizatsiya natijalari quyidagi jadvallarda keltirildi [4-6] (1-2 jadval):

1-Jadval

Tetrasiklinning umumiy energiyasi va uning tarkibiy qismlari

T/R	Chemical	MMFF94	MMFF94S	UFF
BOND STRUCTING ENERGY	4,006 kJ/mol	9,64551 kJ/mol	9,62043 kJ/mol	70,548 kJ/mol
ANGLE BENDING ENERGY	38,713 kJ/mol	20,72919 kJ/mol	19,79924 kJ/mol	90,943 kJ/mol
TORSIONAL ENERGY	46,120 kJ/mol	10,40052 kJ/mol	9,92520 kJ/mol	215,131 kJ/mol
VANDER VAALS ENERGY	3,238 kJ/mol	70,90517 kJ/mol	70,50084 kJ/mol	251,975 kJ/mol

ELECTROSTATIC ENERGY	8,731 kJ/mol	3,88874 kJ/mol	6.30449 kJ/mol	-
STRETCH BENDING ENERGY	-	2,02643 kJ/mol	2,00986 kJ/mol	-
OUT OF PLANT BENDING	-	-0,33239 kJ/mol	0,41027 kJ/mol	8,680 kJ/mol
TOTAL ENERGY	100,809 kJ/mol	117,26316 kJ/mol	118,57034 kJ/mol	637,27710 kJ/mol

Hisoblash natijalari shuni ko'rsatadiki, Tetrasiklinning hosil bo'lish issiqlik energiyasi *UUF* metodida muqobillashtirilganda maksimal qiymatga ega bo'ladi va *Chemical* metodida muqobillashtirganimizda esa minimal qiymatga ega bo'ldi. Demak, Tetrasiklin moddasi uchun energetik parametr hisoblashda empirik hisoblash usullaridan *Chemical* metodi samarali.

2-Jadval

Tetrasiklinning Avagadro dasturi yordamida olingan real bog' uzunliklari(A^0)

T/r	Bog'lar	Chemical	MMFF94	MMFF94S	UFF
1.	C_1-C_2	1,3951	1,3926	1,3920	1,3904
2.	C_6-C_1	1,3954	1,3952	1,3957	1,4017
3.	C_1-H_{33}	1,3968	1,4038	1,4037	1,4198
4.	C_2-C_3	1,3972	1,4102	1,4105	1,4183
5.	C_2-H_{34}	1,3958	1,4073	1,4070	1,4103
6.	C_3-C_4	1,3952	1,3941	1,3942	1,3915
7.	C_3-O_{19}	1,5107	1,4897	1,4904	1,4952
8.	C_4-C_5	1,4686	1,4998	1,5001	1,5024
9.	C_4-C_7	1,4954	1,5126	1,5118	1,5260
10.	C_5-C_6	1,5416	1,5573	1,5566	1,5677
11.	C_{10}-C_5	1,5296	1,5237	1,5234	1,5263
12.	C_6-H_{35}	1,3347	1,3515	1,3520	1,3797
13.	C_7-C_8	1,5180	1,5170	1,5212	1,5377
14.	C_7-O_{26}	0,8250	1,5415	1,5411	1,5397
15.	C_8-C_9	1,5550	1,5346	1,5343	1,5171
16.	C_8-C_{11}	1,5476	1,5482	1,5465	1,5447
17.	C_9-C_{10}	1,5078	1,5397	1,5474	1,5257
18.	C_{14}-C_9	1,4710	1,4904	1,4943	1,4996
19.	C_9-H_{36}	1,3273	1,3531	1,3521	1,3765
20.	C_{10}-C_{24}	1,4925	1,5427	1,5322	1,5414
21.	C_{10}-O_{30}	1,5721	1,5630	1,5568	1,5691
22.	C_{11}-C_{12}	1,3902	1,3661	1,3661	1,3506
23.	C_{11}-O_{20}	1,3344	1,3885	1,3890	1,3598
24.	C_{12}-C_{13}	1,3304	1,3925	1,3929	1,3565
25.	C_{12}-C_{15}	1,4723	1,4780	1,4774	1,5107
26.	C_{12}-O_{25}	1,3451	1,3662	1,3639	1,3576
27.	C_{13}-C_{14}	1,5404	1,5376	1,5376	1,5530
28.	C_{18}-C_{13}	1,4301	1,4254	1,4233	1,4086
29.	C_{13}-H_{37}	1,2201	1,2277	1,2277	1,2201
30.	C_{14}-H_{38}	1,2200	1,2292	1,2298	1,2234
31.	C_{14}-H_{39}	1,2200	1,2223	1,2222	1,2221
32.	C_{15}-C_{16}	1,4813	1,4826	1,4823	1,5060
33.	C_{15}-O_{27}	1,4303	1,4346	1,4351	1,4131
34.	C_{16}-C_{17}	1,4813	1,4643	1,4648	1,4277
35.	C_{16}-C_{22}	1,4771	1,4603	1,4630	1,4770

36.	C_{17}-C_{18}	1,0843	1,0875	1,0875	1,0825
37.	C_{17}-O_{21}	1,0843	1,0860	1,0861	1,0829
38.	C_{18}-N_{29}	1,0839	1,0890	1,0892	1,0826
39.	C_{18}-H_{40}	1,1007	1,1023	1,1022	1,1143
40.	O_{19}-H_{41}	1,1010	1,1052	1,1048	1,1174
41.	O_{20}-H_{42}	1,0973	1,0947	1,0953	1,1064
42.	O_{21}-H_{43}	1,1000	1,0964	1,0967	1,1098
43.	C_{22}-N_{23}	1,1007	1,1019	1,1019	1,1145
44.	C_{22}-O_{28}	0,9495	0,9702	0,9702	0,9681
45.	N_{23}-H_{44}	0,9467	0,9872	0,9869	0,9617
46.	N_{23}-H_{45}	0,9484	0,9767	0,9758	0,9643
47.	C_{24}-H_{46}	1,0005	1,0133	1,0119	1,0272
48.	C_{24}-H_{47}	1,0002	1,0140	1,0128	1,0313
49.	C_{24}-H_{48}	1,0997	1,0946	1,0946	1,1118
50.	O_{25}-H_{49}	1,0984	1,0946	1,0947	1,1070
51.	N_{29}-C_{31}	1,1001	1,0973	1,0972	1,1114
52.	N_{29}-C_{32}	0,9504	0,9801	0,9795	0,9937
53.	O_{30}-H_{50}	0,9496	0,9730	0,9729	0,9925
54.	C_{31}-H_{51}	1,1000	1,0960	1,0960	1,1034
55.	C_{31}-H_{52}	1,1004	1,0962	1,0961	1,1118
56.	C_{31}-H_{53}	1,0995	1,0934	1,0953	1,1119
57.	C_{32}-H_{54}	1,0995	1,0909	1,0902	1,1098
58.	C_{32}-H_{55}	1,1001	1,0944	1,0956	1,1122
59.	C_{32}-H_{56}	1,1000	1,0967	1,0964	1,1114

Tetrasiklinning real bog’ uzunliklari nazariy MM usuli bilan o’rganilib ideal bog’ uzunliklariga solishtirilganida empirik metodida ahamiyatli farqlar kuzatilmadi.

Tajriba qism

Tetrasiklinning 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 MMFF94s usulida kuzatildi. Bog’lar orasidagi masofalarda esa 4 ta usulda optimizatsiya qilinganda *Chemical* usulida real va ideal bog’lar orasidagi farq eng kam (0,1693 %) kuzatildi. Demak tetrasiklinni empirik usulda o’rganganimizda *Chemical* metodi samarali hisoblanadi.

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