

INDEN MOLEKULASIDA ELEKTRON BULUTI VA ZARYAD TAQSIMOTI

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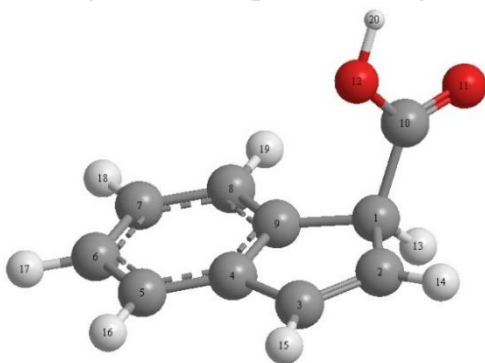
Annotatsiya: Ushbu maqolada inden-1 karbon kislotasining molekulyar tuzilishi, geometriyasi, atomlaridagi zaryad taqsimoti va boshqa kvant-kimyoviy xossalari yarim empirik usulda aniqlangan.

Kalit soʻzlar: inden-1 karbon kislota, kvant kimyosi, molekula, zaryad taqsimoti, elektron tuzilishi.

Hozirgi kunda kompyuter dasturlari asosida tadqiqot usullari ham kimyo fanida katta ahamiyat kasb etmoqda. Kvant-kimyoviy hisoblashlardan foydalanib kimyoviy reaksiya mexanizmlarini nazariy asoslash, birikmaning reaksion qobiliyatini baholash, uning geometrik va elektron tuzilishini o‘rganish mumkin. Shuningdek, moddalarning biologik faolligini bashorat qilishda ham kompyuter texnologiyalarining muqobili yo‘q, deyilsa, mubolag‘a bo‘lmaydi [1, 2, 3, 4, 5].

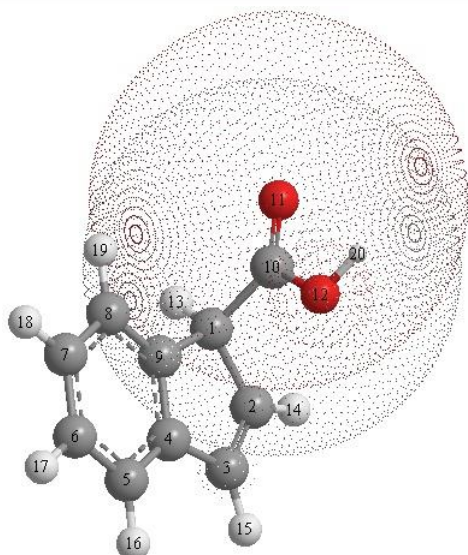
Ushbu tadqiqot ishida inden-1 karbon kislotasini kvant-kimyoviy o‘rganish va biologik faolligini baholash maqsad qilingan.

Kvant-kimyoviy hisoblash yarim empirik usulda bajarilgan. 1-rasmda inden molekulasining molekulyar-mexanik optimallashtirishdan so‘nggi 3d modeli tasvirlangan bo‘lib, unda atomlarning tartib sonlari ham ko‘rsatilgan. Rasmdan ko‘rinadiki, molekulada sterik o‘zgarishlar mavjud hamda karboksil guruhi inden tekisligiga nisbatan perpendikulyar tarzda joylashgan. Molekulaning bunday tuzilishi karboksil guruhidagi elektronlarning uglerod va kislorod atomlari bo‘ylab siljishini osonlashtiradi va umumiy zaryad zichligini (2-rasm) va elektrostatik potentsialini (3-rasm) shu guruhda taqsimlanishiga imkon yaratadi.

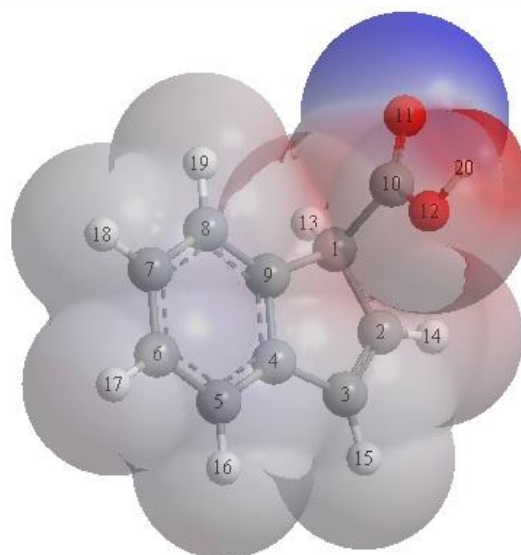


1-rasm. Molekulaning 3d tuzilishi.





2-rasm. Umumiy zaryad zichligining taqsimlanish diagrammasi.



3-rasm. Elektrostatik potentsialning molekulada taqsimlanish diagrammasi: ko‘k rangda musbat qiymatlar, qizil rangda manfiy qiymatlar tasvirlangan.

Molekulaning bog‘ uzunligi va valent burchaklari kabi geometrik ko‘rsatkichlarini tavsiflovchi hisoblash natijalari 1-jadvalda keltirildi.

1-jadval. Inden molekulasidagi hisoblangan bog‘ uzunliklari va valent burchaklar qiymati

Atomlar		Bog‘ uzunligi, Å	Atom	Bog‘ burchagi, grad.	Atom	Ikki tomonlama burchak, grad
4C						
9C	C(4)	1.3941				
1C	C(9)	1.5227	C(4)	109.1543		
8C	C(9)	1.3737	C(1)	129.8258	C(4)	120.9903
3C	C(4)	1.4784	C(9)	108.1452	C(1)	0.8818
5C	C(4)	1.3782	C(3)	131.2942	C(9)	120.5585
6C	C(5)	1.3888	C(4)	118.5612	C(3)	-179.4707
7C	C(8)	1.3914	C(9)	118.5459	C(1)	178.5070
2C	C(1)	1.5258	C(9)	101.6839	C(4)	-1.3584
10C	C(1)	1.5044	C(2)	111.8187	C(9)	111.3844
12O	C(10)	1.3506	C(1)	112.2719	C(2)	-55.9773
11O	C(10)	1.2038	C(1)	125.3525	O(12)	122.3755
14H	C(2)	1.0683	C(1)	122.1697	C(3)	126.6719

15H	C(3)	1.0692	C(2)	126.1202	C(4)	124.0304
16H	C(5)	1.0727	C(4)	120.9862	C(6)	120.4525
17H	C(6)	1.0721	C(5)	119.5943	C(7)	119.5988
18H	C(7)	1.0711	C(6)	119.8061	C(8)	119.6596
19H	C(8)	1.0724	C(7)	120.2932	C(9)	121.1607
13H	C(1)	1.0810	C(2)	112.2702	C(9)	112.2132
20H	O(12)	0.9689	C(10)	111.7573	C(1)	-178.1882

Molekuladagi atomlarning energetik ko'rsatkichlari zaryad birliklarida hisoblab topildi va 3-jadvalda keltirildi.

3-jadval. Inden molekulasida atomlaridagi hisoblangan zaryad qiymati

Atom	Zaryad qiymati, atom birligida	Atom	Zaryad qiymati, atom birligida
[C(1)]	-0.048	[O(11)]	-0.630
[C(2)]	0.006	[O(12)]	-0.178
[C(3)]	-0.099	[H(13)]	0.067
[C(4)]	0.027	[H(14)]	0.026
[C(5)]	-0.062	[H(15)]	0.029
[C(6)]	-0.054	[H(16)]	0.029
[C(7)]	-0.050	[H(17)]	0.029
[C(8)]	-0.069	[H(18)]	0.029
[C(9)]	0.084	[H(19)]	0.029
[C(10)]	0.628	[H(20)]	0.205

Tadqiqot natijalarini umumlashtirib, quyidagi xulosalar chiqarish mumkin. Kvant kimyosi usullaridan foydalanib, inden-1 karbon kislota molekulasining tuzilishi o'rganildi. Molekulyar yadro bir tekislik bilan ajralib turishi, karboksil guruhi qismida sterik buzilishlar mavjudligi aniqlandi. Natijada, umumiy zaryad zichligi va elektrostatik potentsialning turlicha taqsimlanishi kuzatildi. Bog' uzunligi, bog' burchaklari va atomlardagi zaryadlar hisoblash yo'li bilan aniqlandi.

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