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SPATIAL CONFIGURATION AND ELECTRONIC STRUCTURE OF GLYCYRRHYZINIC ACID WITH L-CARNITINE

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Abstract: *In recent years, our republic has been implementing consistent reforms in the rational use of natural resources of medicinal plants, their protection, the establishment of plantations for their cultivation and processing. Thus medicinal from plants one sweetie (Glycyrrhiza glabra L). In our republic wide widespread and industry in scale again worked from it dark extract, technical glycyrrhizin acid working is released. It is known him/her main impact provider from components one 18 β –H Glycyrrhizin acid is considered and his/her based on row complex medicine tools working removed in medicine wide is being used. Including to the virus against, liver to diseases Anti- allergic (hepatitis B, C) diseases and etc.*

Substances synthesis effective organization to do and targeted redirect for guess doer computer from programs use today's on the day advanced from methods This is one of them. ORCA (quantum chemical calculations methods for program package (computer) from programs used. Glycyrrhizin acid aromatic -nitro compounds, caffeine, biological active L- carnitine from supplements with supramolecular complex spatial structure and Gkni dimer and trimmers electronic structure and configuration analyses about information and results cited.

Keywords: *molecule, electron, GK, ORCA, atom, quantum chemistry, correlation, nuclei, L-carnitine, physical and chemical.*

Аннотация: *В последние годы в нашей республике проводятся последовательные реформы по рациональному использованию природных ресурсов, их охране, созданию и переработке плантаций лекарственных растений. Одним из таких лекарственных растений является солодка голая (Glycyrrhiza glabra L.). Он широко используется в нашей республике и*

перерабатывается в промышленных масштабах с получением густого экстракта — технической глицирризиновой кислоты. Известно, что одним из ее основных действующих компонентов является 18β–H-глицирризиновая кислота, на основе которой производится ряд комплексных препаратов, широко применяемых в медицине. В том числе противовирусные, заболевания печени (гепатит B, C), аллергические заболевания и т. д.

Использование предиктивных компьютерных программ для эффективной организации и целенаправленного синтеза веществ является одним из самых передовых методов на сегодняшний день. В данной работе использовались компьютерные программы ORCA (пакет программ для квантово-химических методов расчета). Представлены данные и результаты по пространственной структуре супрамолекулярного комплекса глицирризиновой кислоты с ароматическими нитросоединениями, кофеином и биологически активной добавкой L-карнитином, а также анализ электронной структуры и конфигурации димеров и тримеров Gkni.

Ключевые слова: *молекула, электрон, GK, ORCA, атом, квантовая химия, корреляция, ядра, L-карнитин, физико-химический.*

Anotatsiya: *Respublikamizda so‘ngi yillarda dorivor o‘simliklar tabiiy resurslardan oqilona foydalanish, ularni muhofaza qilish, yetishtiriladigan plantatsiyalar tashkil etish va qayta ishlash borasida izchil islohatlar amalga oshirilmoqda. Shunday dorivor o‘simliklardan biri shirinmiya o‘simligi (Glycyrrhiza glabra L). Respublikamizda keng tarqalgan va sanoat miqqiyosida qayta ishlanib undan quyuq ekstrakt, texnik glitsirrizin kislotasi ishlab chiqariladi. Ma’lumki uni asosiy ta’sir etuvchi komponentlaridan biri 18β–H Glitsirrizin kislota hisoblanadi va uning asosida qator kompleks dori vositalari ishlab chiqarilib tibbiyotda keng qo‘llanilmoqda. Jumladan virusga qarshi, jigar kasalliklariga qarshi (gepatit B, S) allergik kasalliklar va hokazo.*

Moddalar sintezini samarali tashkil qilish va maqsadli yo‘naltirish uchun taxmin qiluvchi kompyuter dasturlaridan foydalanish bugungi kunda ilg‘or metodlardan biridir. Ushbu ishda ORCA (kvantkimyoviy hisob-kitoblar metodlari uchun programma paketi) kompyuter dasturlaridan foydalanildi. Glitsirrizin kislotani aromatik-nitro birikmalar, kofein, biologik faol qo‘shimchalardan L-karnitin bilan supramolekulyar kompleksi fazoviy tuzilishi va Gkni dimer va trimerlarining elektron tuzilishi va konfiguratsiya tahlillari xaqida ma’lumotlar va natijalari keltirilgan.

Kalit so‘zlar: *molekula, elektron, GK, ORCA, atom, kvant-kimyo, korrelyatsiya, yadrolar, L-karnitin, fizik va kimyoviy.*

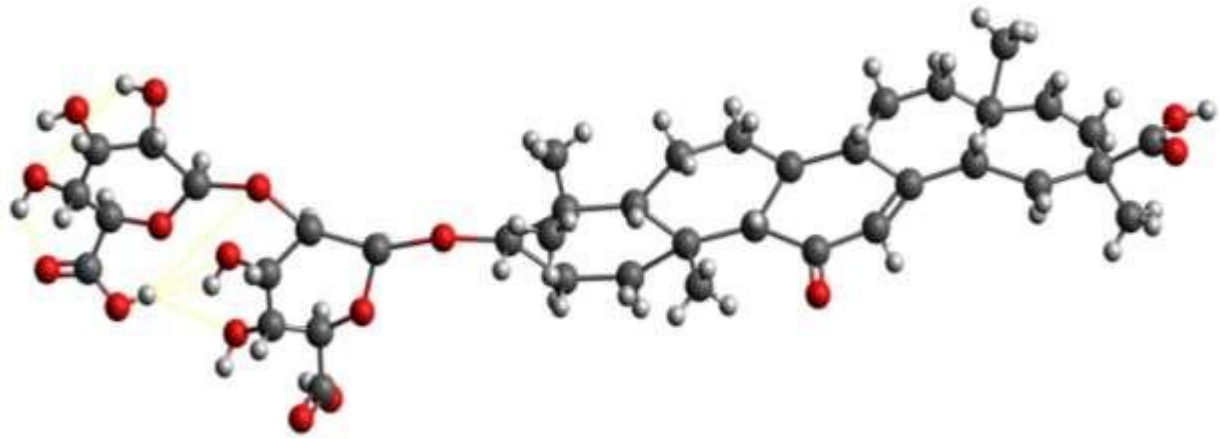
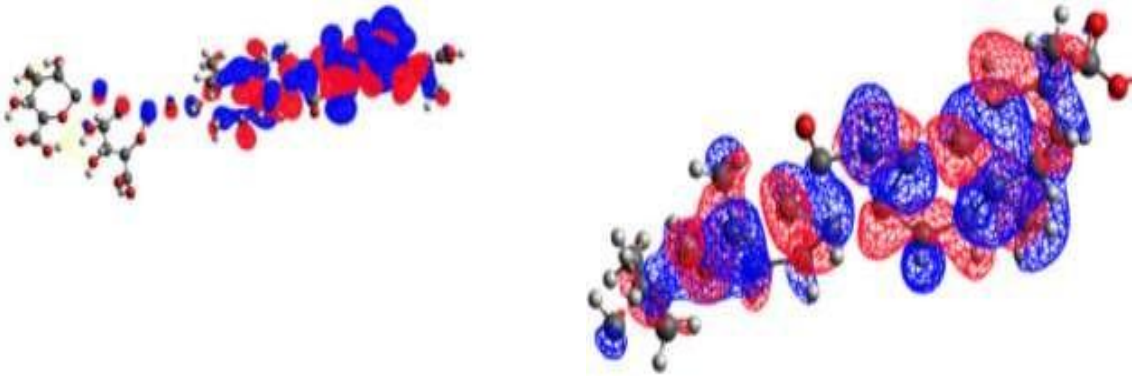


Figure 1. The spatial structure of glycyrrhizic acid

Contain three carboxyl, one carbonyl, and five hydroxyl groups, as shown in Figure 1. The molecule methyl groups branches with almost flat to form has.



a) b)

Figure 2. The most high located molecular in orbit electronic density distribution (different) colors electronic of the cloud wave function various to the stages suitable comes); complete picture; b) the most high- band molecular in orbit electronic cloudy molecule part of enlarged image.

From the picture visible it is clear that the most high- band molecular in orbit electronic density distribution mainly in the picture a- as shown molecule right half electronic from the cloud consists of, from this except for its electronegativity lower was in atoms located if, oxygen atoms and to the nucleus strong shooting because of deeper on the levels located to electrons has.

Table 1.

The most high busy molecular orbital and the most lower empty molecular orbital energy floors and to them the most close floors.

EUBMO -3	EYuBMO -2	EYuBMO -1	EYuBMO	EQBMO	EQBMO -1	EQBMO -2	EQBMO -3
-5,769	-5,675	-5,617	-5,198	-4,795	-4,632	-4,070	-3,725

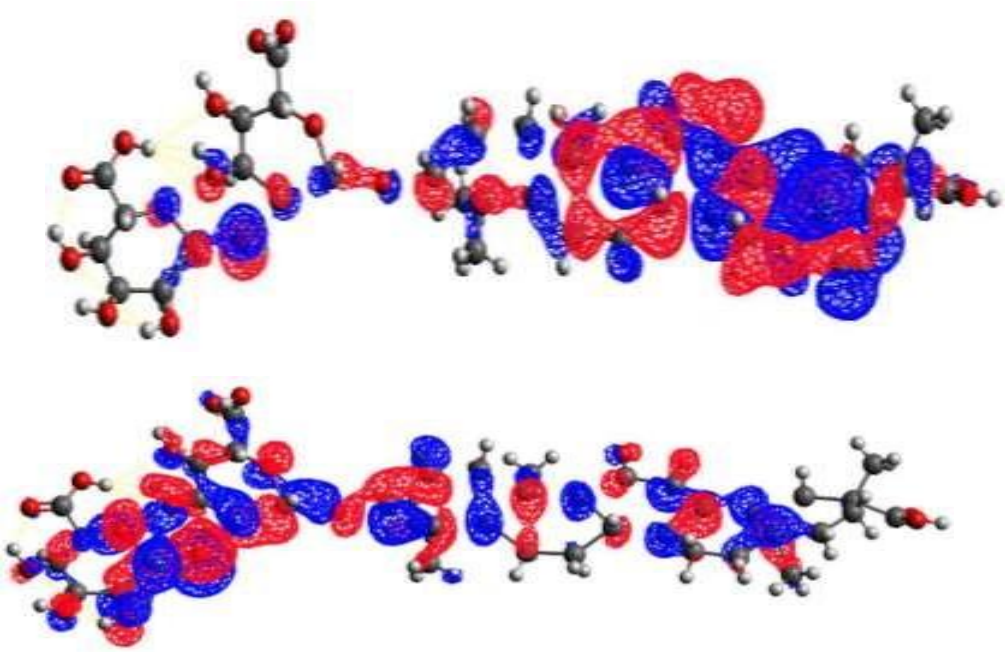


Figure 3. Electronics density distribution level a) most high busy molecular orbital -1 and b) the most high busy molecular orbital -2 atoms according to.

We also in the picture the most high busy molecular orbital and in the picture the most lower empty molecular to the orbital close energy on the floors electronic density distribution we will show you. This distributions energy level deepening with electronic distribution step by step shift shows, they chemical and physicochemical reactions in the process molecule excitable transition status in formation and new compounds, associations and conglomerates harvest in being also important role to play possible.

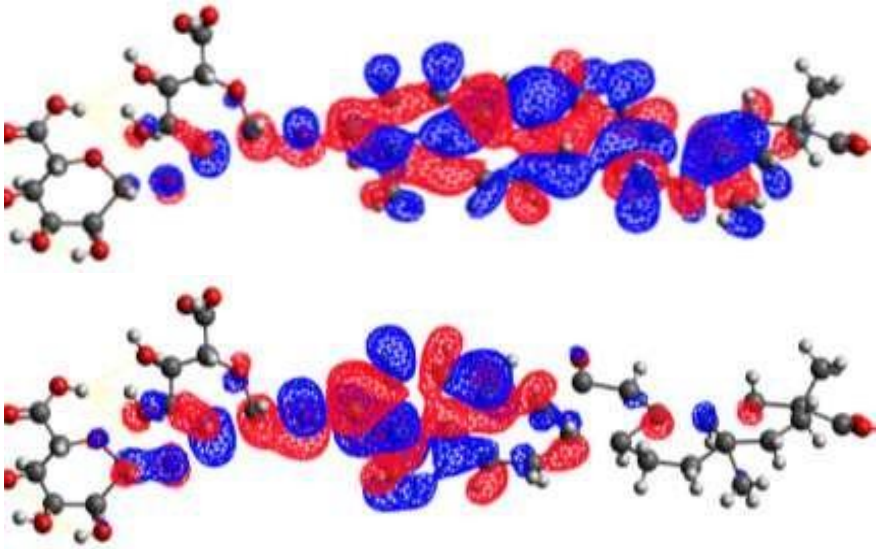


Figure 4. Electronics density distribution level a) most lower empty molecular orbital and b) in atoms the most lower empty molecular orbital-1.

We use L- carnitine also seeing we'll go out, he'll come later Glycyrrhizin acid with supramolecular complex harvest does. Connection Descartes coordinates in the application cited.

The most high busy molecular orbital electronic structure mainly carnitine in oxygens located if, the most lower empty molecular in orbit located electrons molecule other, opposite part occupies. From known It turns out that carnitine when excited electronic molecule central and opposite to the part will pass.

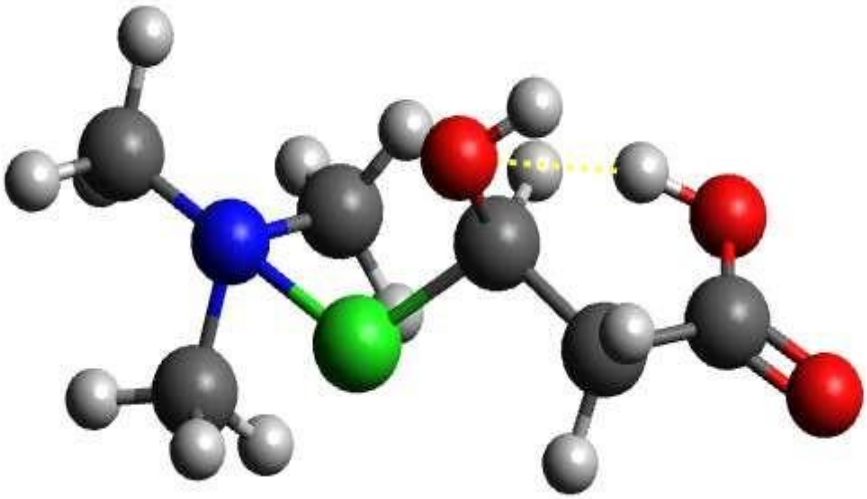
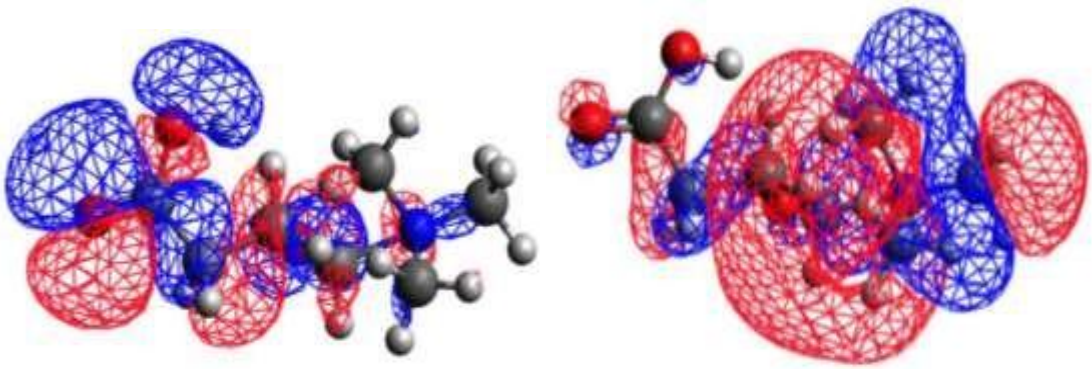


Figure 5. L- carnitine spatial structure.



a) b)

Figure 6. L- carnitine atoms according to a) the most high busy molecular orbital and b) the most lower empty in molecular orbital layers electronic density distribution.

Table 2.

L -Carnitine the most high busy molecular orbital and the most lower empty molecular orbital energy floors and to them the most close floors.

EYUBMO -3	EYUBMO -2	EYUBMO -1	EUBMO	ECBMO	ECBMO -1	ECBMO -2	ECBMO -3
-12,882	-11,937	-11,591	-10,264	-6,993	-3,771	-3,486	-3,055

Glycyrrhizin acid dimer and trimmer structure and electronic structure

Glycyrrhizin acid dimer to study, its the most simple association as, two acid molecule parallel to each other close in the distance located dimer elementary structure build with Later, the structure general energy minimize for to the complex molecular dynamics method and the most upright fall method to apply change through molecule step by step optimization done increased and this process one how many times repeated general of energy change in advance designated small from the value less it has been.

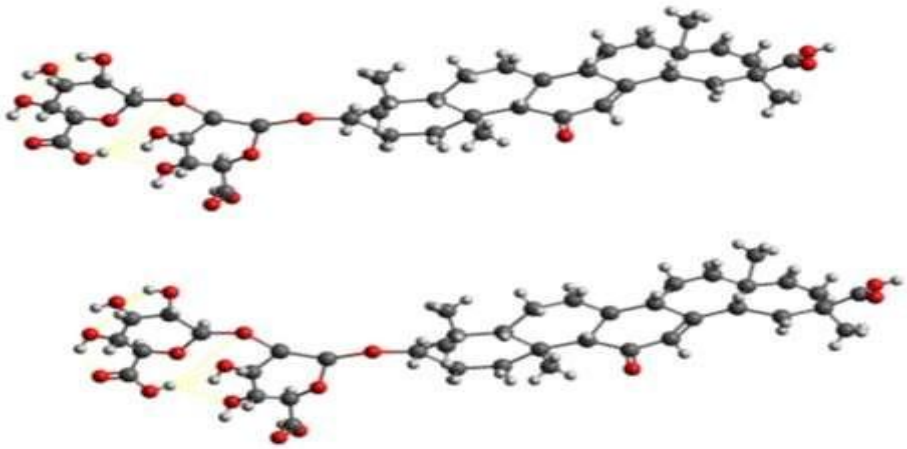


Figure 7. Two measurable molecule of the complex geometry optimization elementary point.

Table 3.

Glycyrrhizin acid dimer complete energy.

	Theoretical calculations	Experience results
Molecule	75042.5 eV	
Dimer	150085.159 eV	
Energy increase	0.159 eV	0.1736 Ev

In the literature given experimental from the point of view obtained $5.72*10^{-4}$J/mol Gibbs energy every one from 0.17 eV per particle right comes and complete not been hydrogen to the garden or one how many Van der Waals to the gardens right is coming.

Geometry optimization as a result we in the picture As shown, Glycyrrhizin acid dimer structure harvest we did, they each other with mutual connected to be, to be next door to the molecule more connection to the points has to be for every one molecule his/her own initial in the structure from bending passes. From the picture visible it is clear that the gardens one part hydrogen gardens on account of, second part, Van der Waals on principle mainly intermolecular shooting to the mechanism according to to the surface arrived.

Below cited in the picture in literature in the PM3 method presented calculated dimer harvest to be energy brought, our calculations 26.3 kcal/mol This is giving their as a result PM3 calculations in the literature are better head to the tail of the type connections showing if so, our accounts head per head connections shows.

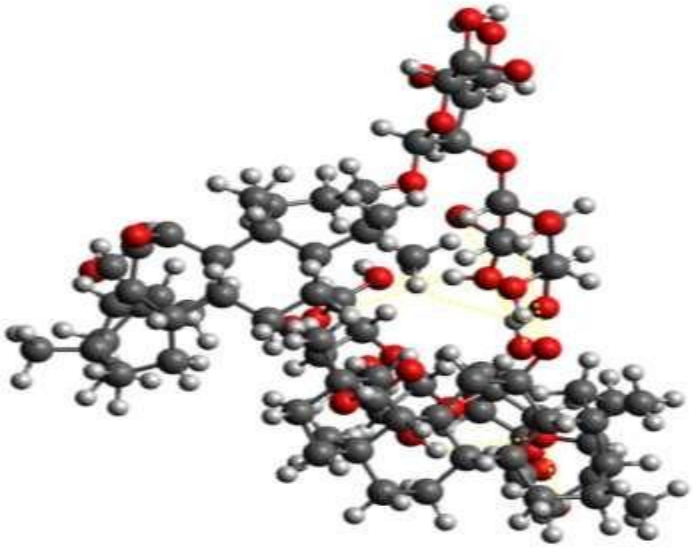
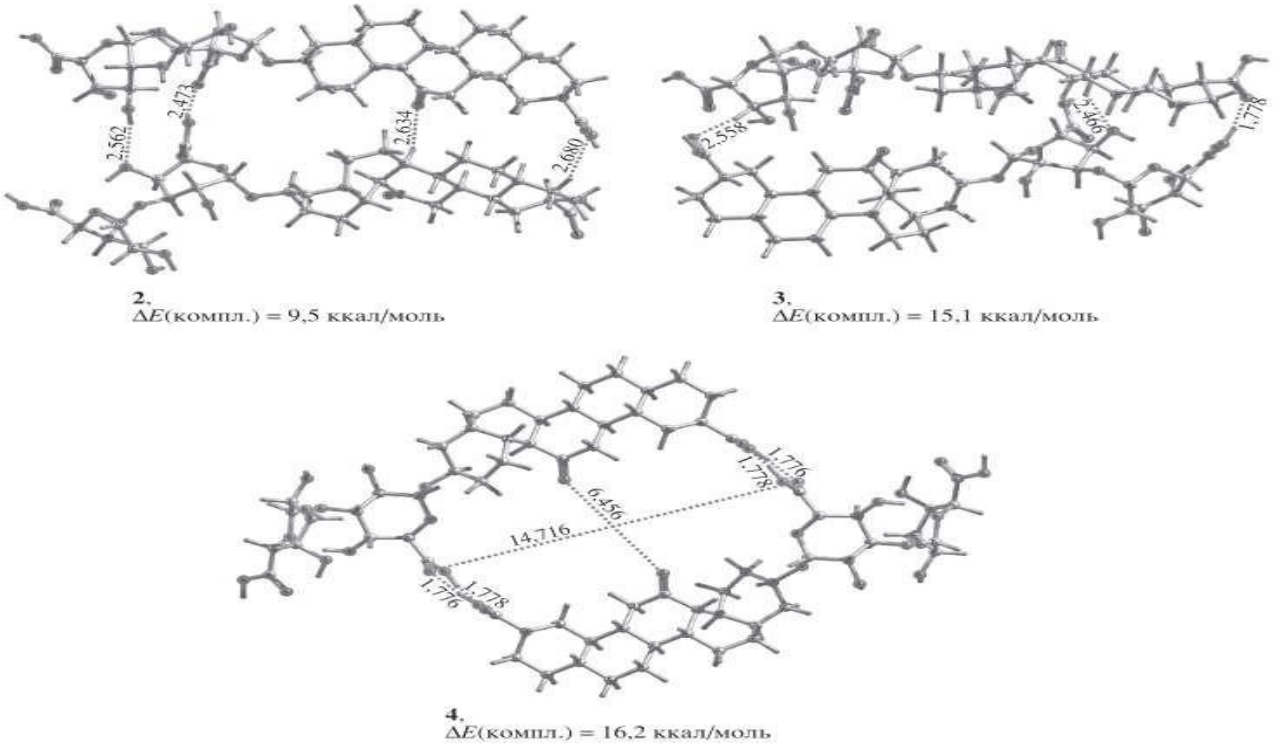


Figure 8. Two measurable molecule of the complex geometry optimization last point.



2.
ΔE(компл.) = 9,5 ккал/моль

3.
ΔE(компл.) = 15,1 ккал/моль

4.
ΔE(компл.) = 16,2 ккал/моль

In dimers the most big hole size 5.59 A is, inside the dimer of the void size 6.77 A organization will. In this Glycyrrhizin acid two on the edge atoms between distance from 36.6 A to 15.5 A decreased, that is one linear shaped molecule bending and deformation as a result his/her twice the size more than compacted.

Two measurable molecule of the complex geometry optimization last dimer formation at the point in being Glycyrrhizin acid molecules pieces location image, molecules various kind in colors painted, almost linear flat that Glycyrrhizin acid molecule association harvest in being bend, the molecule the most high- band molecular orbital electronic cloud bigger was in part gardens harvest Naturally, this without one molecule the most high- band molecular from orbital electrons other molecule the most lower empty molecular to the orbital passing, general molecular orbital product does.

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