O'ZBEKISTON RESPUBLIKASI
OLIY TA'LIM, FAN VA INNOVATSIYALAR VAZIRLIGI

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IQTIDORLI TALABALAR, MAGISTRANTLAR, TAYANCH DOKTORANTLAR VA DOKTORANTLARNING
“TAFAKKUR VA TALQIN”
MAVZUSIDAGI RESPUBLIKA MIQYOSIDAGI ILMIY-AMALIY ANJUMAN
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TAUTOMERIC FORMS OF TRIFLUOROACETYLACETONE.

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Annotatsiya: Trifluroasetilaseton 2 ta tautomer shaklga ega bo'lib, ular 1,1,1-trifloro-4-gidroksi-3-penten-2-on 95%. Triftoratsetilaseton rangsiz suyuqlik bo'lib, u asosan geterotsiklik birikmalarning prekursori sifatida ishlatiladi. Proton NMR spektroskopiyasi bo'yicha tahlilga ko'ra, birikma asosan (33 ° C da 95%, sof) enol sifatida mavjud.

Kalit so'zlar: trifluroasetilaseton,tautomer, spektroskopiya.

Аннотация: Трифторацетилацетон имеет 2 таутомерные формы, которые представляют собой 1,1,1-трифтор-4-гидрокси-3-пентен-2-он 95%. Трифторацетилацетон представляет собой бесцветную жидкость, которая в основном используется в качестве предшественника гетероциклических соединений. По данным анализа протонной ЯМР-спектроскопии, соединение существует преимущественно (95% при 33 °C, чистое) в виде енола.

Ключевые слова: трифторацетилацетон, таутомер, спектроскопия.

Annotation: Trifluoroacetylacetone has 2 tautomeric forms, which are 1,1,1-trifluoro-4-hydroxy-3-penten-2-one 95%. Trifluoroacetylacetone is a colorless liquid that is mainly used as a precursor of heterocyclic compounds. According to analysis by proton NMR spectroscopy, the compound exists mainly (95% at 33 °C, pure) as the enol.

Key words: trifluoroacetylaceton, tautomer, spectroscopy.

Molecular systems possessing internal hydrogen bonds draw close scientific attention, as understanding of the properties of this type of interaction is of crucial importance. Good candidates for the studies of internal hydrogen bonding are the small and medium size molecules, because it is possible to easily handle them during experiments and perform high level quantum chemistry calculations in reasonable amounts of time. The molecules possessing a pseudo ring structure where hydrogen bond "closes" this ring form a peculiar class of molecules where properties of hydrogen bond (H-bond) are strongly dependent on the delocalized π type electronic structure of the molecule. Such type of hydrogen bonding is often called Resonance Assisted Hydrogen Bonding (RAHB).[1,2] The smallest members of these molecular families are malonaldehyde and acetylacetone (acac), with symmetric substituents linked to the pseudo ring and widely investigated in previous matrix works,3–8 and the asymmetric acetylacetaldehyde. This type of molecules can exist in two tautomeric forms, namely enol and keto, the enol form being the most stable one due to the strong internal hydrogen bond. These molecules in enolic configuration possess double well potential function for the proton transfer from one oxygen to the other. The halogenated derivative of acetylacetone 1,1,1-

trifluoroacetylacetone (noted hereafter TFacac) presents an interesting case of the acetylacetone derivatives. Due to the modification, when all fluorine atoms are localized on one side of the molecule, the pseudo C_{2v} symmetry of acac is broken.
Consequently, the hydrogen transfer potential function becomes an asymmetric one, since it is more probable for the hydrogen atom to be localized in one of the two sides (see Figure 1b). This results in the possibility of coexistence of two enolic forms having different structure and stability: one isomer 1,1,1-trifluoro-4-hydroxy-3-penten-2-one (1) is the structure where perfluoromethyl (CF_3) group is on the same side of the molecule as -C=O group and another isomer is 5,5,5-trifluoro-4-hydroxy-3-penten-2-one (2) with CF_3 group on the same side of the molecule as -C-O-H group. As shown in Figure 1b, these structures are those of the chelated enol forms of 1 and 2 which will be noted as CCC(CO) and CCC(OH) respectively in this paper. The "CCC" notation is taken from previous works on β-dicarbonyl molecules where it depicts the chelated enol conformer with three "Cis" arrangements in the C-C-C-O-H chain of the molecule skeleton.[3]

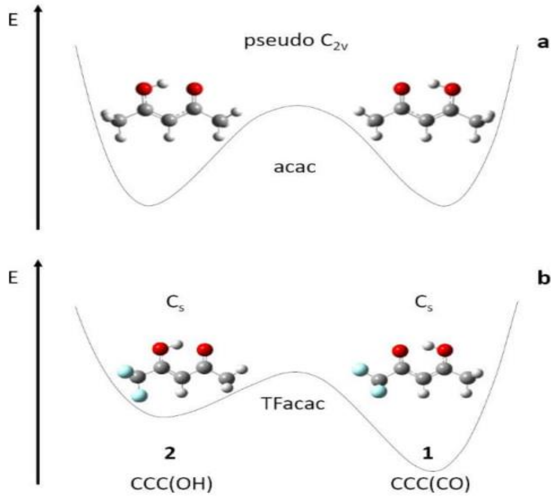
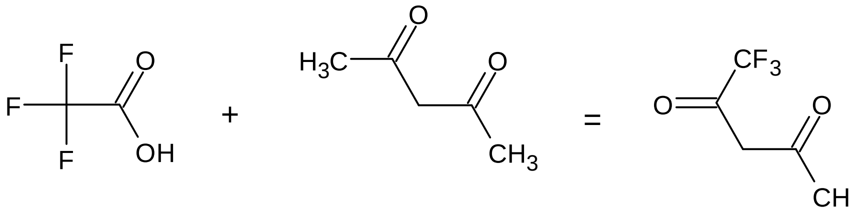
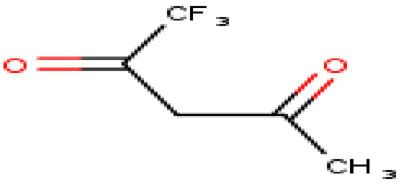


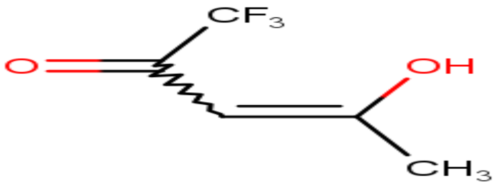
Figure 1: Potential functions (schematic) of hydrogen tunneling for (a) acetylacetone - acac - and (b) trifluoroacetylacetone - TFacac -. Fluorine atoms are represented in light blue. The chelated enol forms of 1 and 2 isomers of TFacac are shown in panel b and labelled CCC(CO) and CCC(OH) respectively. The labels indicate cis conformation in respect of rotation around three internal bonds in the O=C-C=C-O-H chain, and OH or CO group in the brackets indicating on which side of the molecule CF3 group resides.[4]



The formed ligand has 2 tautomeric forms, which are 1,1,1-trifluoro-4-hydroxy-3-penten-2-one 95%.Trifluoroacetylacetone is a colorless liquid, which is mainly used as a precursor of heterocyclic compounds. According to analysis by proton NMR spectroscopy, the compound exists mainly (95% at 33 °C, pure) as an enol. For comparison under the same conditions, the percentage of enol for acetylacetone and hexafluoroacetylacetone is 85 and 100%, respectively.



a)



b)

a) 1,1,1-trifluoro-4-hydroxy-3-penten-2-one (95%)
b) trifluoroacetylacetone(5%)

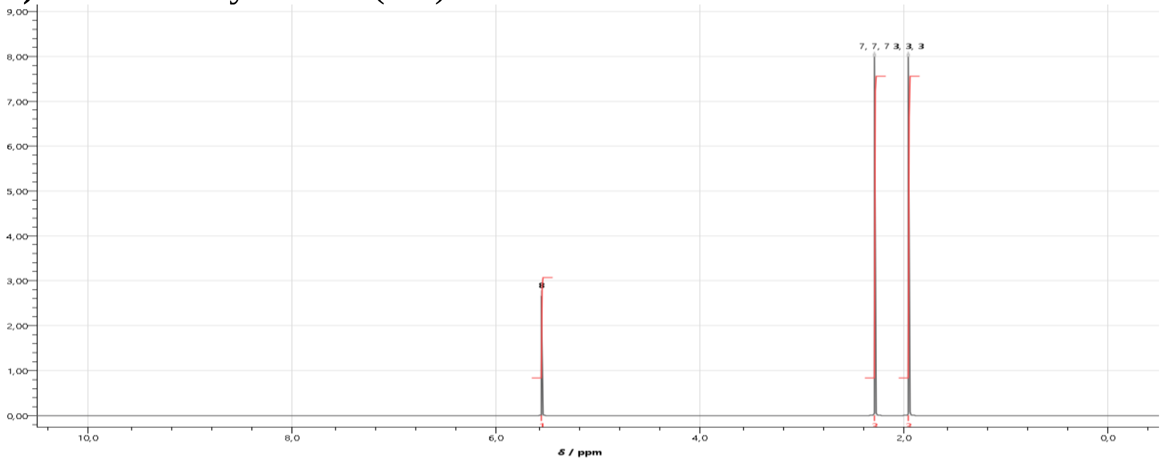
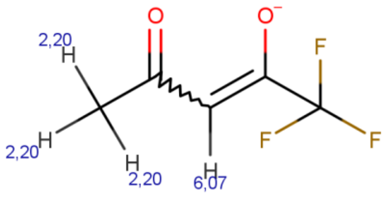
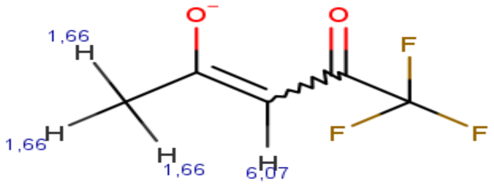


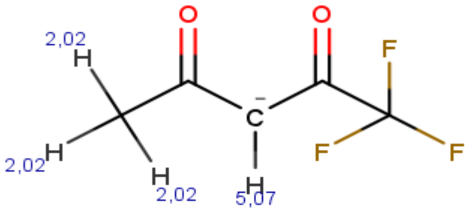
Figure2: NMR spectroscopy analysis of tautomeric state of 1,1,1-trifluoro-4-hydroxy-3-penten-2-one

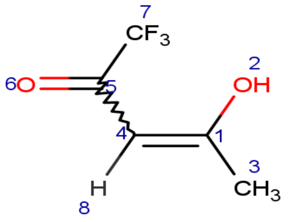
Figure 2 shows the NMR spectrum of 1,1,1-trifluoro-4-hydroxy-3-penten-2-one, and according to it, the hydrogen group in the 2 atomic position gave a signal at 12.38 ppm.

But if we take the pH value as 7.4, we have 4 tautomeric states. The NMR spectrum was obtained from each of them and analyzed.









The four tautomeric forms showed 4 different spectra. The main chemical shift occurred in the first tautomeric form at 6.07 ppm.

LITERATURE

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ARZON YO’L WEB ILOVASI

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BuxDU, Amaliy matematika va dasturlash
texnalogiyalari mutaxassisligi 2-bosqich magistranti

Annotatsiya. Maqolada uzoq masofaga qatnovlarda ishtirok etishda yo’l harakati qatnashuvchilari haydovchi va yo’lovchilarga online buyurtma berish, online marshrut yaratish va uni qabul qilish xizmatlarini bajaruvchi web ilovaning loyihasi haqida bo’ladi.

Abstract: The article is about the project of a web application that provides online ordering, online route creation and reception services to drivers and passengers participating in long-distance journeys.

Аннотация. В статье рассматривается проект веб-приложения, предоставляющего услуги онлайн-заказа, онлайн-формирования маршрутов и приема водителей и пассажиров, участвующих в дальних поездках.

Kalit so’zlar: API integratsiya, EJS, MySQL malumotlar ombori, Node.js dasturlash tili**,** algoritm, funksiya, Saqlangan protseduralar.

Hozirgi rivojlanib borayotgan zamonda taksi xizmatlarini ko’rsatuvchi ilovalarning soni kundan kunga oshib bormoqda, bular o’zlarining qulayliklari va o’zlarining alohida xususiyatlari bilan bir-biridan farqlanadi. Bu ilovalar foydalanuvchiga qulay user interfeys ta’minlab va haydovchi va yo’lovchilar orasidagi aloqani ta’minlab beruychi ko’prik vazifasini bajaradi [1].

Shunday ilovalardan biri Arzon yo’l web ilovasi bo’lib, bu dastur maqsadi hozirda mavjud taksi xizmatini ko’rsatuvchi ilovalardan tubdan farq qiladi va aynan bir shahar hududida emas, balki kattaroq hudud miqiyosida uzoqroq manzillarga