BENZALDEGID VA UNING para-R-ALMASHGAN HOSILALARINI 3-XLOR-3-METILBUTIN-1 BILAN ETINILLASH ASOSIDA AROMATIK ATSETILEN SPIRTLARI SINTEZI

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Annotatsiya: 3-xlor-3-metilbutin-1 ning ilk bor CsF/TBACl/TGF katalitik sistemasida benzaldegid va uning ayrim gomologlari bilan reaksiyalari o‘rganilgan. Yangi avlod aromatik atsetilen spirtlarini sintez qilish usuli ishlab chiqilgan. Benzaldegid hosilalari molekulasidagi o‘rinbosarlar tabiatining reaksiya borishi va mahsulot unumiga ta’siri tahlil qilingan. Aldegidlarni alkinillash jarayonining eng muqobil sharoiti topilgan, reaksiyasi mexanizmi taklif qilingan. Sintez qilingan birikmalar identifikatsiyalangan.

Kalit so‘zlar: 3-xlor-3-metilbutin-1, benzaldegid va uning para-R-almashgan hosilalari, katalizator tabiati, aromatik atsetilen spirtlari, mahsulot unumi.

Аннотация: Впервые изучены реакции 3-хлор-3-метилбутина-1 с бензальдегидом и некоторыми его гомологами в каталитической системе CsF/TBACl/ТГФ. Разработан метод синтеза нового поколения ароматических ацетиленовых спиртов. Проанализировано влияние природы заместителей в молекуле производных бензальдегида на ход реакции и выход продуктов. Найдены наиболее оптимальные условия проведения процесса алкинилирования альдегидов и предложен механизм реакции. Идентифицированы синтезированные соединения.

Ключевые слова: 3-хлор-3-метилбутин-1, бензальдегид и его пара-R-замещенные производные, природа катализатора, ароматические ацетиленовые спирты, выход продуктов.

Abstract: The reactions of 3-chloro-3-methylbutyne-1 with benzaldehyde and some of its homologues in the CsF/TBACl/THF catalytic system have been studied for the first time. A method for synthesizing a new generation of aromatic

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acetylenic alcohols has been developed. The influence of the nature of substituents in the benzaldehyde derivative molecule on the reaction course and product yield has been analyzed. The most optimal conditions for carrying out the aldehyde alkynylation process have been found and a reaction mechanism has been proposed. The synthesized compounds have been identified.

Key words: 3-chloro-3-methylbutyn-1, benzaldehyde and its p-R-substituted derivatives, nature of catalyst, aromatic acetylenic alcohols, product yield.

Kirish

Hozirgi vaqtda jahonda farmatsevtika, to‘qimachilik, mashinasozlik va lok-bo‘yoq sanoatida keng masshtabda qo‘llaniladigan organik preparatlarga bo‘lgan qiziqish tobora kuchayib bormoqda. Natijada yuqori ehtiyojga ega organik moddalar va materiallar ishlab chiqarish yildan yilga ortib bormoqda, bu esa nozik organik sintez asosida yangi avlod organik moddalar olish, ularning qo‘llanish sohasini keng ko‘lamda o‘rganishni taqozo qilmoqda. Jumladan yuqori faollikga ega bo‘lgan aromatik atsetilen spirtlarini olishning yangi usullarini topish, fizik-kimyoviy xususiyatlarini tadqiq qilish hamda maqsadli qo‘llanish sohalarini aniqlash dolzarb hisoblanadi. Ayniqsa atsetilen spirtlarini neft-gaz, kimyo, rezina-texnika, lok-bo‘yoq va metallurgiya sanoatida yuqori sifatli preparatlar sifatida foydalanish muhim ahamiyat kasb etadi.

ADABIYOTLAR TAHLILI

Atsetilen spirtlari molekulasida bifunksional sintonlar, jumladan alkin va gidroksil guruhlari mavjudligi ularga muhim sintetik xom ashyo sifatida qarashga imkon beradi. So‘nggi yillarda atsetilen spirtlarini trasformatsiyalash asosida qimmatli organik preparatlar ishlab chiqarish jadallik bilan rivojlanmoqda [1]. Molekulasida aril-alkil, aril-aril yoki alkil-alkil o‘rinbosarlar saqlagan ketonlarni xona haroratida tetragidrofuran eritmasida aril va geterilalkinlar bilan katalitik reaksiyalari tetrabutilammoniy ftorid ishtirokida o‘rganilgan va propargil spirtlari sintez qilingan [2, 3]. Katalizator $Zn(OTf)_2$ va N-metilefedrin ishtirokida toluol eritmasida terminal atsetilen uglevodorodlari va aldegidlarning enantioselektiv nukleofil birikish reaksiyalari bo‘yicha 99% unumgacha atsetilen spirtlari sintez qilingan [4].

$Pd((R)\text{-}DTBM\text{-}SEGphos)Cl_2$ dan katalizator sifatida foydalanib ayrim alkinlar va atsetilenidlarni assimetrik karboksillanish reaksiyasi orqali optik faol ko‘p qirrali sintetik transformatsiyali atsetilen spirtlari olingan. Tadqiqot natijalari asosida eng yuqori unum bilan 2-feniloktin-3-ol-2 sintez qilingan [5]. Titan va BINOL hosilalari asosida tayyorlangan katalitik sistemaga promotor rux alkilatlarini kuchaytiruvchi agent sifatida qo‘shish orqali dixlormetan eritmasida aromatik aldegidlarni terminal alkinlar bilan reaksiyalari olib borilgan. Jarayonda

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titan hosilalari reaksiyaning bosqichma-bosqich borishini nazorat qilgan va yuqori unum bilan atsetilen spirtlarini sintez qilish uchun BINOL va rux tuzlarining katalitik faolligini reaksiyaning ohirigacha samarali ishlashini ta'minlagan [6].

Yangi polimer Zn (salen) kompleksi yordamida aldegidlar va ketonlarga fenilasetilenning enantioselektiv qo'shilishi natijasida yuqori rentabellikda, ya'ni 96% unumgacha ikkilamchi, 79% unumgacha uchlamchi atsetilen spirtlari olingan. Tadqiqot obyekti sifatida benzaldegid, *o*-metilbenzaldegid, *o*-metoksibenzaldegid, *m*-metoksibenzaldegid, *p*-metilbenzaldegid, 1-naftaldegid, izovalerianaldegid, siklogeksakarbaldegid, atsetofenon, *o*-metilatsetofenon, *o*-bromoatsetofenon, *p*-metilatsetofenon, *p*-metoksiatsetofenon, *p*-ftoratsetofenon, 10-naftilatsetofenon va 3-metilbutanon-2 lar olingan va ularni fenilatsetilen yordamida alkinillash reaksiya olib borilgan [7]. N-geterosiklik karbendan katalizator sifatida foydalanib karbonil birikmalarini triftorometillanish reaksiyasi o'rganilgan. Reaksiya xona haroratida, 45 daqiqa davomida dixlormetan eritmasida olib borilgan. Keyinchalik ushbu reaksiyalarni tetragidrofuran eritmasida olib borilgan va nisbatan yuqori unum bilan atsetilen spirtlari olingan. Bundan tashqari ushbu reaksiya natijalariga ko'ra alkinillanuvchi reagent sifatida olingan ketonlarga nisbatan aldegidlarda mahsulot unumining yuqori chiqishi isbotlangan [8].

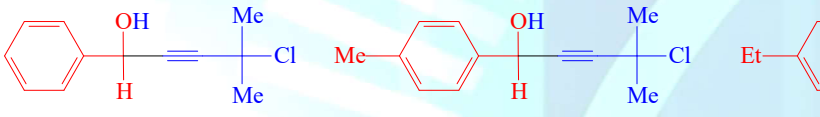
TADQIQOT METODOLOGIYASI.

Aromatik atsetilen spirtlarini sintez qilish reaksiyasi hajmi 50 ml bo'lgan flakonda amalga oshirildi. Reaksiyani olib borishda dastlab flakonda katalizator sifatida olingan 0,34 mmol (0,052 g) seziy ftorid hamda promotor sifatida olingan 0,18 mmol (0,052 g) tetrabutilammoniy xloridning 2,5 ml (0,03 mol) tetragidrofurandagi suspenziyasi tayyorlab olindi. So'ngra ushbu suspenziyaga dastlab 2,5 mmol (0,265 g) benzaldegid so'ngra 2,5 mmol (0,256 g) 3-xlor-3-metilbutin-1 dozator (VITLAB) yordamida solindi va aralashma 120 daqiqa davomida -15 ºC haroratda aralashtirildi. Bunda harorat -30 ºC da quruq muz (CO_2) va etanol yordamida ushlab turiladi, polimerlanishga qarshi gidroxinon qo'shiladi. Keyin 3 ml dixlormetan bilan suyultirildi va mahsulotni ajratib olish uchun dietilefir (3×5 ml) yordamida ekstraksiyalanib, suv (3×5 ml) bilan yuvildi. Organik qatlam $CaCl_2$ yordamida quritildi va erituvchilar rotorli bug'latgich (Heidolph) yordamida haydab olindi. Organik qatlam tarkibidan mahsulotni tozalab olish uchun silikagel 60 kolonkali xromatografiyada elyuentlardan (geksan/EtOAc 20:1) o'tkaziladi. Natijada 4-xlor-4-metil-1-fenilpentin-2-ol-1 (1) 87,1% unum bilan (0,181 mg) (R_f=18/40, sariq rangli suyuqlik) ajratib olindi.

Ushbu usul bo'yicha 3-xlor-3-metilbutin-1 ning 4-metilbenzaldegid, 4-etilbenzaldegid, 4-uchlamchibutilbenzaldegid, 4-ftorbenzaldegid, 4-xlorbenzaldegid, 4-(dimetilamino)benzaldegid, 4-(butoksi)benzaldegid va 4-

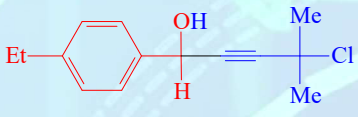
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(tioetil)benzaldegid bilan reaksiyalari bo‘yicha 0,198 mg (89,0%) 4-xlor-4-metil-1-(p-tolil)pentin-2-ol-1 (**2**, R_f=20/40, sariq rangli suyuqlik), 0,208 mg (88,1%) 4-xlor-1-(4-etilfenil)-4-metilpentin-2-ol-1 (**3**, R_f=17/40, sariq rangli suyuqlik), 0,225 mg (85,2%) 1-(4-(tret-butil)fenil)-4-xloro-4-metilpentin-2-ol-1 (**4**, R_f=16/40, sariq rangli suyuqlik), 0,211 mg (93%) 4-xlor-1-(4-ftorfenil)-4-metilpentin-2-ol-1 (**5**, R_f=15/40, sariq rangli suyuqlik), 0,220 mg (90%) 4-xlor-1-(4-xlorfenil)-4-metilpentin-2-ol-1 (**6**, R_f=17/40, sariq rangli suyuqlik), 0,225 mg (89%) 4-xlor-1-(4-(dimetilamino)fenil)-4-metilpentin-2-ol-1 (**7**, R_f=16/40, sariq rangli suyuqlik), 0,242 mg (86%) 1-(4-butoksifenil)-4-xlor-4-metilpentin-2-ol-1 (**8**, R_f=14/40, sariq rangli suyuqlik) va 0,226 mg (84%) 4-xlor-1-(4-(etiltio)fenil)-4-metilpentin-2-ol-1 (**9**, R_f=17/38, sariq rangli suyuqlik) kabi aromatik atsetilen spirtlari sintez qilindi va ularning tuzilish formulalari quyidagicha taklif etildi.

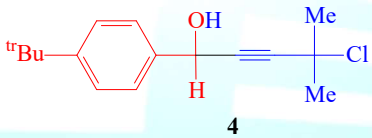


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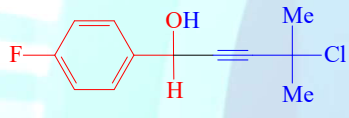
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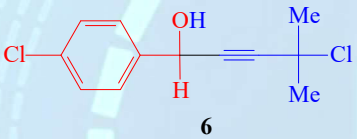
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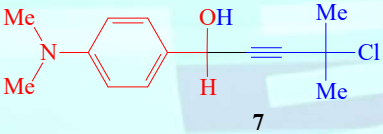
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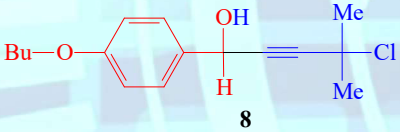
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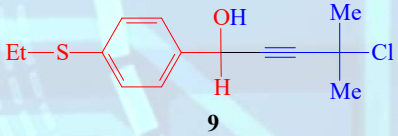
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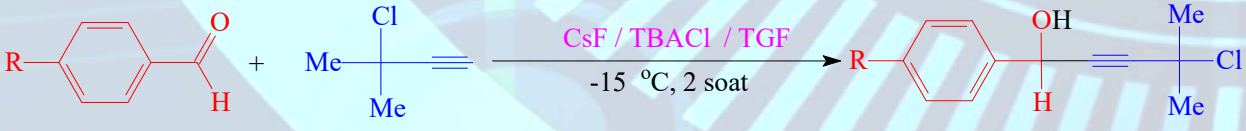
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9

MUHOKAMA VA NATIJALAR.

Tadqiqot ob’yekti bo‘lgan benzaldegid va uning quyidagi *para*-R-almashgan hosilalari 4-metilbenzaldegid, 4-etilbenzaldegid, 4-uchlamchibutilbenzaldegid, 4-ftorbenzaldegid, 4-xlorbenzaldegid, 4-(dimetilamino)benzaldegid, 4-(butoksi)benzaldegid va 4-(tioetil)benzaldegidni CsF/TBACl/TGF kompleks katalitik sistemasida 3-xlor-3-metilbutin-1 bilan alkinillash reaksiyalari ilk marta amalga oshirildi. Adabiyot manbalari asosida 3-xlor-3-metilbutin-1 ishtirokida tanlangan aldegidlarni alkinillash reaksiya sxemasi va mexanizmi quyidagicha taklif qilindi [9, 10].



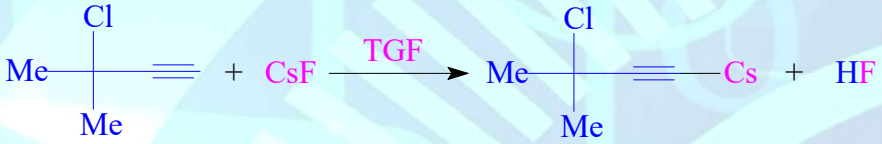
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R= –H (**1**), R= –Me (**2**), R= –Et (**3**), R= –^{tr}Bu (**4**), R= –F (**5**),

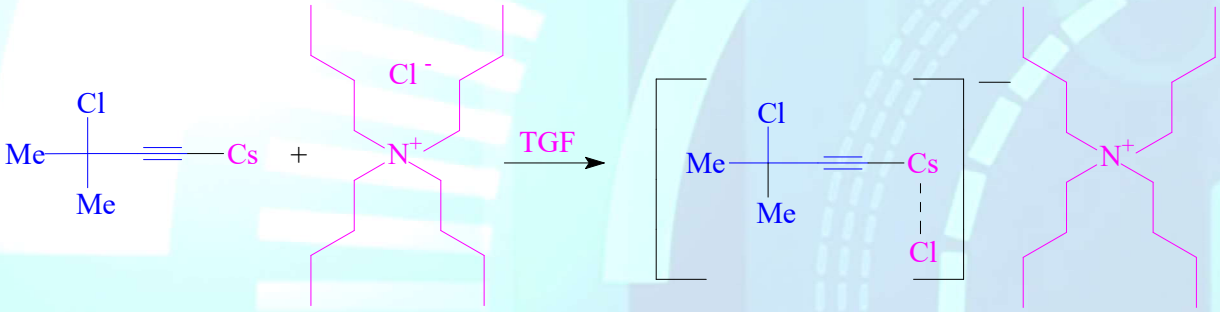
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R= –Cl (**6**), R= –N(Me)$_2$ (**7**), R= –OBu (**8**), R= –SEt (**9**)

Reaksiya mexanizmi. Tetragidrofuran eritmasida katalizator seziy ftorid kuchli ionlangan holatga o‘tishi natijasida faolligi yuqori bo‘lgan seziy kationiga yadroga kuchli tortilgan elektron bulutlardan hosil bo‘lgan, sp- gibridlangan alkin molekulasidagi C-H bog‘ining elektron buluti uglerod atomiga kuchli siljishi hisobiga harakatchan bo‘lib qolgan vodorod atomi o‘z o‘rnini berishi natijasida sistemada kuchsiz kislota xossasiga ega bo‘lgan seziy atsetilenidni hosil qiladi [11].

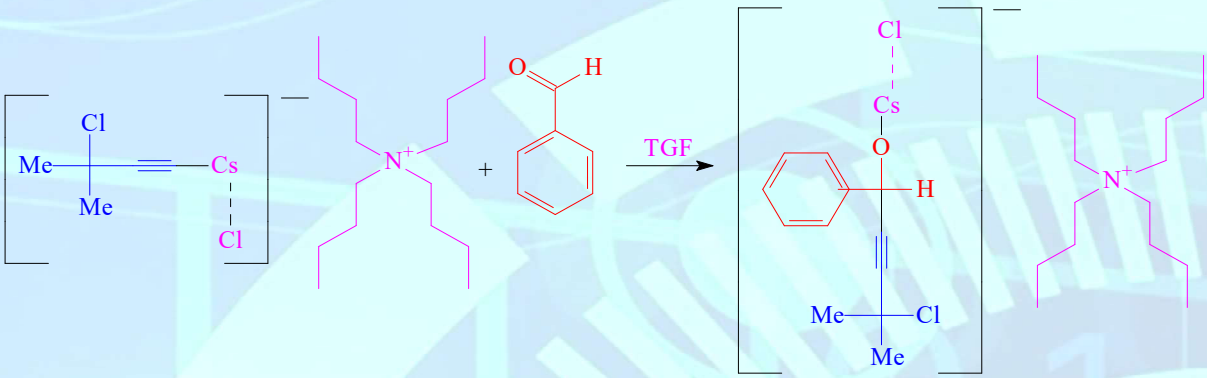


Reaksiyaning keyingi bosqichida atsetilenidlar sistemaga kuchli ishqoriy muhitni hosil qiluvchi promotor tetrabutilammoniy xlorid bilan ta’sirlashib, reaksiyani fazali o‘tish holatini oshiruvchi oraliq kompleks birikmaga aylanadi [12].

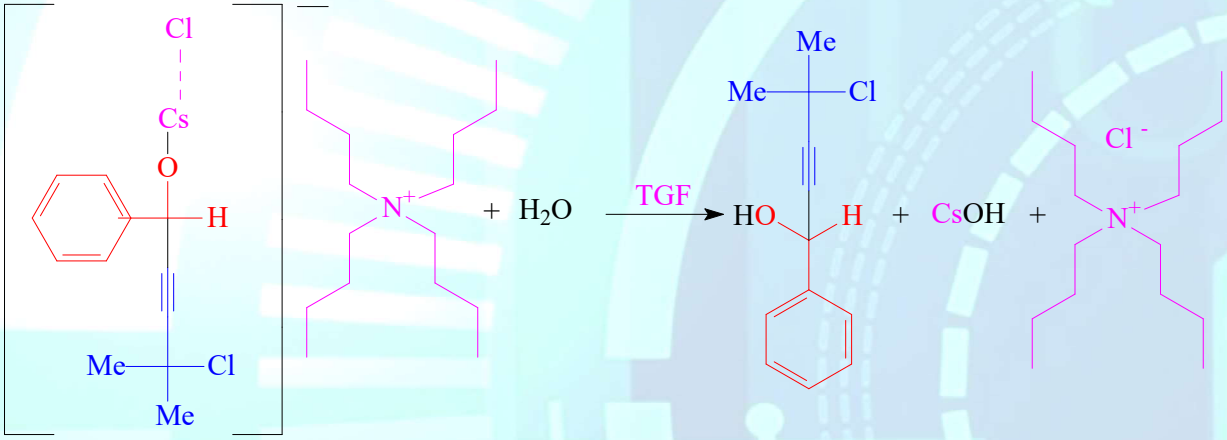


Aldegidlarni alkinillash jarayonining keyingi bosqichida sistemadagi kompleks birikma molekulasidagi seziyning elektron bulutini elektromanfiyligi yuqori xlor atomi o‘ziga kuchli tortishi kuzatilib, seziy va uchbog‘dagi sp gibridlangan uglerod orasidagi δ bog‘ning uzilishi osonlashadi, natijada katalizat tarkibida 3-xlor-3-metilbutin-1 nukleofilligi va miqdorining ortishiga olib keladi. Nukleofil reagent o‘z o‘rnida aldegidlar molekulasidagi elektron zichlik yuqori bo‘lgan kislorodga hujum qilib, karbonil guruhining π bog‘ining uzilishi, sp^2 gibridlangan uglerod sp^3 gibridlanishga o‘tishi natijasida aromatik atsetilen spirtlarining oraliq kompleks birikmalari, jumladan seziy alkogolyatning tetrabutilammoniy xloridini hosil qiladi. Tetragidrofuran eritmasida sistemada reaksion faolligi yuqori bo‘lgan barqaror karbkationlar hosil bo‘lishi, katalizat tarkibidagi katalizator va oraliq mahsulotlar bilan tezda birikib qo‘shimcha mahsulotlar miqdorini oshib ketishiga to‘sqinlik qilishi kuzatildi [13].

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Aromatik atsetilen spirtlarining oraliq kompleks birikmalari oson gidrolizga uchrab mos ravishdagi aromatik atsetilen spirtiga aylanadi. Sistemadagi ushbu kompleks birikma kuchli solvatlovchilik xususiyati yoki tetragidrofuranda oson erishi va gidrolizlanishi sababli o‘zida yuqori faollikni saqlaydi, bu esa mahsulot unumining oshishiga xizmat qiladi [14-15].



Alkogolyatlar molekulasidan chiqqan seziy qaytadan ham ishqor, ham atsetilenid hosil qiladi. Atsetilenidlar jarayon borishini, ishqor esa HF bilan birikib katalizatorning qayta tiklanishini ta’minlaydi [14-15].

$$CsOH + HF \xrightarrow{TGF} CsF + H_2O$$

Taqdim etilgan ushbu reaksiya mexanizmi adabiyot manbaalari asosida taklif sifatida kiritilmoqda, chunki jarayonlarda hosil bo‘lgan oraliq birikmalar ajratib olinmagan, ularning tarkibi, tuzilishi va xossalari o‘rganilmagan.

Yuqori unum bilan aromatik atsetilen spirtlarini sintez qilish maqsadida jarayonga turli omillar, jumladan harorat (-30 ÷ 30 ºC), reaksiya davomiyligi (30 ÷ 240 minut), erituvchi va katalizatorlar tabiati, boshlang‘ich moddalar mol miqdori ta’sirlari tizimli ravishda tahlil etildi. Jumladan alkinillash reaksiyalari -30 – 30 ºC intervallarda o‘rganilganda aromatik atsetilen spirtlari unumi -15 ºC da maksimum chiqishi kuzatildi. Reaksiya -30 ºC da olib borilganda CsF ning tetragidrofuranda qiyin erishi natijasida uning ionlangan holatga o‘tib atsetilenidlarni hosil qilishi uchun katalitik markazlarni yetarlicha faollashtira olmadi, reagent va substrat

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zarrachalari esa bir-biriga hujum qilish harakatining sekinligi, eski bog‘lar uzilib yangi bog‘lar hosil qilishi uchun yuqori enegrgiyaga ega bo‘lolmagan oraliq mahsulotlarning o‘tish holatga qiyin aylanishi natijasida reaksiya samaradorligi past chiqdi. Reaksiyalar 30 ºC haroratda olib borilganda sistemada polimerlanish va qo‘shimcha reaksiyalarning borishi hisobiga kutilgan mahsulot unumining kamayishi kuzatildi.

Tadqiqotlar 30-60 minut davomida olib borilganda boshlang‘ich reagentlar to‘liq katalitik faol holatda bo‘lmaganligi sababli sistemada aromatik atsetilen spirtlari unumi unchalik yuqori chiqmadi. Tanlangan aldegidlarni alkinillash reaksiyalari 180-240 daqiqa oraliqlarida olib borilganda aromatik atsetilen spirtlari unumdorligi pasayganligi kuzatildi. Chunki hosil bo‘lgan spirtlar sistemada qisman degidratlanishi, boshlang‘ich alkin bilan birikib qo‘shimcha mahsulot sifatida oddiy efirlar hosil qilishi, oksidlanib to‘yinmagan ketonlar hosil qilishi hamda alkinlarning dimerlanish va aldegidlarning kondensatsiyalanishga uchrashi aniqlandi. Bundan tashqari katalizat tarkibida katalizator va promotorlar ishlash samaradorligining pasayganligini ham aytish mumkin.

Aproton erituvchi tetragidrofuran eritmasida aldegidlarni alkinillash reaksiyalari rentabelligining yuqori bo‘lishini quyidagicha izohlash mumkin. Jumladan tetragidrofuran sistemada muhitning qutbliligini oshiradi, katalizat tarkibidagi kompleks birikmalar, atsetilenidlar va alkogolyatlar barqarorligini ta’minlaydi, boshlang‘ich moddalar faol markazlar hosil qilishini, reaksiya tezlik konstantasini oshiradi, reaksiya yo‘nalishini, ionlarning o‘zaro bir-biri bilan yangi bog‘lar hosil qilishi uchun qulay bo‘lgan yumshoq katalitik muhitning selektivligini ta’minladi.

Tadqiqot natijalari asosida jarayonning eng muqobil sharoiti topildi. Benzaldegid va uning para-R-almashgan hosilalarini alkinillash reaksiyalari -15 ºC haroratda, 2 soat davomida olib borilganda mahsulot unumining maksimum orqali o‘tishi kuzatildi. Jumladan **1**- 87%, **2**- 89%, **3**- 88,1%, **4**- 85,2%, **5**- 93%, **6**- 90%, **7**- 89%, **8**- 86%, ва **9**- 84% unumlar bilan sintez qilindi. Ushbu holatda alkin va aldegidlar mol miqdori o‘zaro ekvimolyar nisbatda, katalizator va promotorning miqdori esa reagent va substrat massasiga nisbatan 10:1 nisbatda olingan.

Sintez qilingan birikmalarning tozaligi xromatografik, tuzilishi spektroskopik usullarda o‘rganildi, tarkibi element analiz qilindi, aromatik atsetilen spirtlari molekulalarining fazoviy tuzilishi, molekulalarda zaryadlar va elektron zichlikning taqsimlanishi hamda kvant-kimyoviy ko‘rsatkichlari zamonaviy dasturlar asosida hisoblandi.

4-xlor-4-metil-1-fenilpentin-2-ol-1 (1). ^{1}H YaMR (400 MHz, xloroform-*d*) δ 7.35-7.23 (m, 5H), 5.65 (d, *J* = 1.1 Hz, 2H), 1.81 (s, 3H), 1.74 (s, 3H). ^{13}C YaMR

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(400 MHz, xloroform-*d*) δ 145.51, 139.28, 128.77, 126.69, 126.67, 124.33, 120.63, 116.61, 125.59, 88.21, 81.99, 65.91, 55.15.

4-xlor-4-metil-1-(*p*-tolil)pentin-2-ol-1 (2). ^{1}H YaMR (400 MHz, xloroform-*d*) δ 7.30 – 7.22 (m, 2H), 7.11 – 7.00 (m, 2H), 5.69 – 5.61 (m, 1H), 5.60 (d, *J* = 5.9 Hz, 1H), 2.31 – 2.21 (m, 3H), 1.77 (s, 3H), 1.72 (s, 3H).

4-xlor-1-(4-etilfenil)-4-metilpentin-2-ol-1 (3). ^{1}H YaMR (400 MHz, xloroform-*d*) δ 7.46 – 7.34 (m, 2H), 7.25 (dt, *J* = 7.5, 1.1 Hz, 2H), 5.81 – 5.66 (m, 2H), 2.74 (ddt, *J* = 9.1, 8.0, 1.1 Hz, 2H), 1.87 (d, *J* = 22.9 Hz, 6H), 1.29 (t, *J* = 8.0 Hz, 3H).

1-(4-(tret-butil)fenil)-4-xloro-4-metilpentin-2-ol-1 (4). ^{1}H YaMR (400 MHz, benzol-*d*) δ 7.56 – 7.32 (m, 4H), 5.84 (s, 2H), 1.92 (d, *J* = 24.9 Hz, 6H), 1.45 (s, 9H).

4-xlor-1-(4-ftorfenil)-4-metilpentin-2-ol-1 (5). ^{1}H YaMR (400 MHz, xloroform-*d*) δ 7.60 – 7.42 (m, 2H), 7.25 – 7.00 (m, 2H), 5.88 – 5.57 (m, 2H), 1.85 (d, *J* = 23.6 Hz, 6H).

4-xlor-1-(4-xlorfenil)-4-metilpentin-2-ol-1 (6). ^{1}H YaMR (400 MHz, xloroform-*d*) δ 7.35 – 7.31 (m, 2H), 7.28 – 7.21 (m, 2H), 5.69 – 5.54 (m, 2H), 1.69 (d, *J* = 21.4 Hz, 6H).

4-xlor-1-(4-(dimetilamino)fenil)-4-metilpentin-2-ol-1 (7). ^{1}H YaMR (400 MHz, xloroform-*d*) δ 7.30 – 7.18 (m, 2H), 6.85 – 6.69 (m, 2H), 5.67 (s, 2H), 2.93 (s, 6H), 1.75 (d, *J* = 22.5 Hz, 6H).

1-(4-butoksifenil)-4-xlor-4-metilpentin-2-ol-1 (8). ^{1}H YaMR (400 MHz, xloroform-*d*) δ 7.30 – 7.14 (m, 2H), 6.86 – 6.70 (m, 2H), 5.62 (k, *J* = 5.7 Hz, 2H), 3.99 – 3.72 (m, 2H), 1.83 – 1.57 (m, 8H), 1.46 – 1.22 (m, 2H), 0.87 (t, *J* = 8.0 Hz, 3H).

4-xlor-1-(4-(etiltio)fenil)-4-metilpentin-2-ol-1 (9). ^{1}H YaMR (400 MHz, xloroform-*d*) δ 7.41 – 7.29 (m, 2H), 7.30 – 7.20 (m, 2H), 5.77 – 5.61 (m, 2H), 2.98 – 2.74 (m, 2H), 1.80 (d, *J* = 21.8 Hz, 6H), 1.27 (t, *J* = 8.4 Hz, 3H).

Sintez qilingan birikmalarning tozaligi xromatografik, tuzilishi spektroskopik usullarda o‘rganildi, tarkibi element analiz qilindi, aromatik atsetilen spirtlari molekulalarining fazoviy tuzilishi, molekulalarda zaryadlar va elektron zichlikning taqsimlanishi hamda kvant-kimyoviy ko‘rsatkichlari zamonaviy dasturlar asosida hisoblandi.

1-jadval

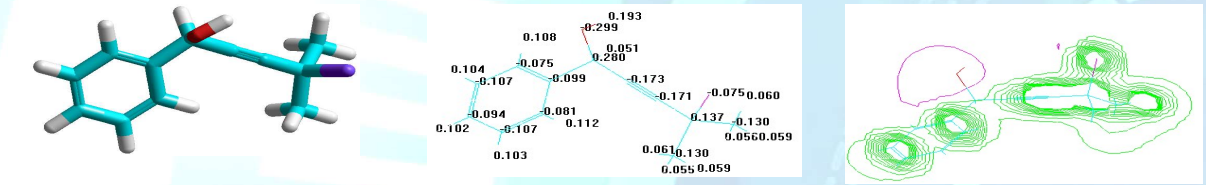
Sintez qilingan atsetilen spirtlarining kvant-kimyoviy hisoblashlari

Atsetilen spirtlari	Hosil bo‘lish issiqlik	Van-der-Vaals	Kulon energiyas	Torsion energiyasi, kkal/mol	Valent burchak	Bog‘ energiyasi, kkal/mol

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	energiyasi, kkal/mol	energiyasi, kkal/mol	i, kkal/mol		energiyasi, kkal/mol	
1	2,0078	5,7494	0,4776	-5,6501	0,4899	0,9410
2	-0,0406	3,9871	0,7111	-6,3945	0,5271	1,1285
3	0,8866	4,401	0,7116	-6,0426	0,613	1,2038
4	4,9546	6,6666	0,7084	-6,0367	1,448	2,1684
5	-0,0371	3,9906	0,7135	-6,3964	0,5275	1,1278
6	-0,0372	3,9937	0,7130	-6,3968	0,5279	1,1250
7	2,2640	5,1191	0,7074	-58710	0,8404	1,4681
8	1,6547	5,6084	0,7448	-7,7669	0,817	2,2513
9	6,6963	7,2266	0,7552	-5,6680	0,9194	3,4631

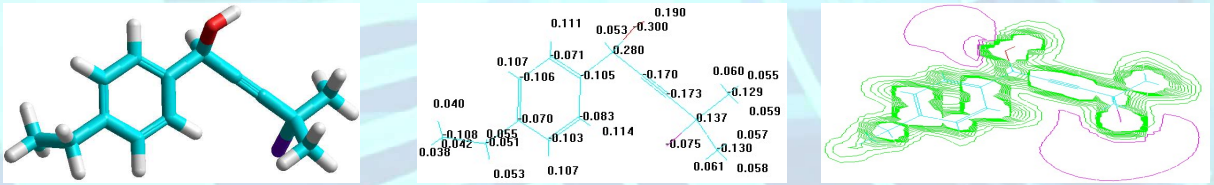
Sintez qilingan aromatik atsetilen spirtlari molekulalarining fazoviy tuzilishi, molekulalarda zaryadlar va elektron zichlikning taqsimlanishi hamda kvant-kimyoviy ko‘rsatkichlari zamonaviy dasturlar asosida hisoblandi.



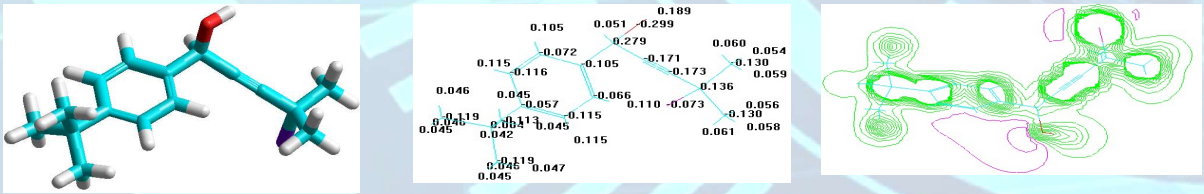
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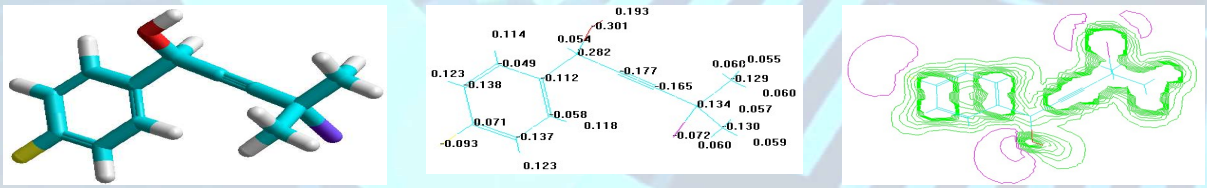
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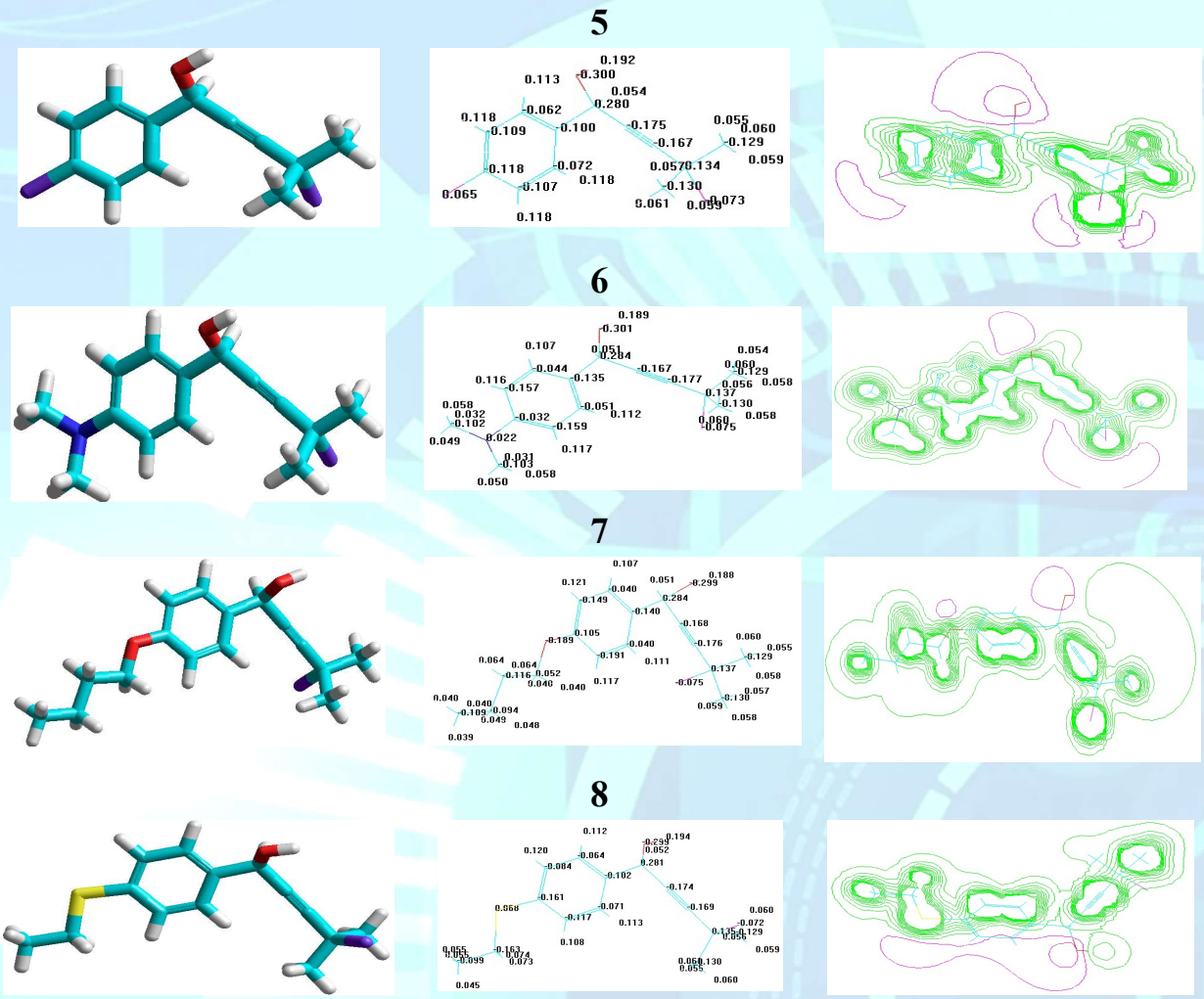
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4



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Molekulaning 3D fazoviy strurtura tuzilishi | Molekuladagi atomlar zaryadning qiymatlari | Molekulada elektron zichlikning taqsimlanishi

1-Rasm. Atsetilen spirtlarining ayrim fazoviy tuzilishlari

XULOSA VA TAKLIFLAR

Benzaldegid va uning molekulasida alkil, galogen, azot, kislorod va oltingugurt atomlari saqlagan para-R-almashgan hosilalarini yuqori asosli CsF/TBACl/TGF kompleks katalitik sistemasida 3-xlor-3-metilbutin-1 bilan enantioselektiv alkinillash reaksiyalari asosida yangi avlod aromatik atsetilen spirtlarini sintez qilish usuli topilgan.

Benzaldegid va uning para-R-almashgan hosilalari molekulasi tuzilishi, tarkibi va fazoviy joylashuvining mahsulot hosil bo‘lish va reaksiyaning borishiga ta’sirining samaradorligi ishlab chiqilgan.

Sintez qilingan aromatik atsetilen spirtlarining xususiy kattaliklari va fizik-kimyoviy xossalari zamonaviy tadqiqot usullari yordamida isbotlangan.

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