

May 2022

SYNTHESIS OF AROMATIC ACETYLENE ALCOHOLS BASED ON BENZALDEHYDE AND ITS HALOGENATED PRODUCTS

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Recommended Citation

SAMATOV, Sanat; IKRAMOV, Abduvakhab; ABDURAKHMANOVA, Saida; ZIYADULLAYEV, Odiljon; and OTAMUKHAMEDOVA, Guzal (2022) "SYNTHESIS OF AROMATIC ACETYLENE ALCOHOLS BASED ON BENZALDEHYDE AND ITS HALOGENATED PRODUCTS," *CHEMISTRY AND CHEMICAL ENGINEERING*: Vol. 2022: No. 1, Article 7.

DOI: 10.34920/cce202217

Available at: <https://cce.researchcommons.org/journal/vol2022/iss1/7>

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Cover Page Footnote

The authors are thankful to Ministry of Higher and Secondary Specialized Education Republic of Uzbekistan and Tashkent Chemical-Technological Institute for their financial support. The authors are also thankful to the Chairman of the Department of Chemistry Chirchik State Pedagogical Institute for this technical supports.

SYNTHESIS OF AROMATIC ACETYLENE ALCOHOLS BASED ON BENZALDEHYDE AND ITS HALOGENATED PRODUCTS

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The aim of this study is to synthesize the corresponding aromatic acetylenic alcohols by alkylation with phenylacetylene in a complex catalytic system based on $Zn(OTf)_2$ and $TBAF \cdot 3H_2O$ for the first time with benzaldehyde and some of its halogen derivatives. The selectivity and stability of catalysts used for the yields of reactions for the synthesis of aromatic acetylene alcohols were analyzed. The effect of benzaldehyde and its halogenated derivatives on the product yield was analyzed. The nature, structure, isomerism, spatial structure and other properties influenced to this reactions were studied. Some features of reactions of synthesis of aromatic acetylene alcohols such as stages, activation energies, kinetics of chemical changes were determined, reaction mechanisms were proposed, the most optimal conditions for alkylation reactions were found. The synthesized aromatic acetylene alcohols were identified. Their several properties such as purity, composition, structure, specific and quantum chemical constants were proved using modern physicochemical research methods. A series of relative efficiencies of aromatic acetylene synthesis based on benzaldehyde and some of its derivatives in the selected catalytic system has been proposed.

Keywords: phenylacetylene, benzaldehyde and some of its derivatives, zinc trifluoromethanesulfonate, tetrabutylammonium fluoride, triethylamine, acetonitrile, aromatic acetylene alcohols, product yield

СИНТЕЗ АРОМАТИЧЕСКИХ АЦЕТИЛЕНОВЫХ СПИРТОВ НА ОСНОВЕ БЕНЗАЛЬДЕГИДА И ЕГО ГАЛОГЕНПРОИЗВОДНЫХ

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Целью настоящего исследования является синтез соответствующих ароматических ацетиленовых спиртов реакцией алкилирования фенилацетиленом в комплексной каталитической системе на основе $Zn(OTf)_2$ и $TBAF \cdot 3H_2O$ впервые с бензальдегидом и некоторыми его галогенпроизводными. Исследована селективность и стабильность катализаторов, использованных для эффективности реакции синтеза ароматических ацетиленовых спиртов. Анализировано действие природы, структуры, изомерии, пространственного строения и других свойств бензальдегида и его галогеновых производных на выход продуктов. Определена кинетика химических изменений, энергии активации, стадии реакций синтеза ароматических ацетиленов, предложены механизмы реакций, найдены наиболее оптимальные условия реакции алкилирования. Идентифицированы синтезированные ацетиленовые ароматические спирты и с помощью современных физико-химических методов исследования доказаны их чистота, строение, состав, собственные и квантово-химические константы. В выбранной каталитической системе предложен ряд относительной эффективности синтеза ароматических ацетиленовых спиртов на основе бензальдегида и его производных.

Ключевые слова: фенилацетилен, бензальдегид и его производные, трифторметилсульфонат цинка, фторид тетрабутиламмония, триэтиламин, ацетонитрил, ароматическое ацетиленовые спирты, выход продукта

BENZALDEGID VA UNING GALOGENLI XOSILALARI ASOSIDA AROMATIK ATSETILEN SPIRTRLARI SINTEZI

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Ushbu ilmiy tadqiqot ishidan maqsad ilk bor benzaldegid va uning ayrim galogenli hosilalarini $Zn(OTf)_2$ va $TBAF \cdot 3H_2O$ asosida tayyorlangan kompleks katalitik sistemada fenilatsetilen bilan alkinillash reaksiyasi bo'yicha mos ravishdagi aromatik atsetilen spirtrlarini sintez qilish. Aromatik atsetilen spirtrlarini sintez qilish reaksiyalarini samaradorligiga qo'llanilgan katalizatorlarning selektivligi va stabiligi tadqiq qilingan. Benzaldegid va uning galogenli hosilalarining tabiati, tuzilishi, izomeriyasi, fazoviy tuzilishi va boshqa xossalarning mahsulot hosil bo'lish unumiga ta'siri tahlil qilingan. Aromatik atsetilen spirtrlarini sintez qilish reaksiyalarining bosqichlari, faollanish energiyalari, kimyoviy o'zgarishlar kinetikasi aniqlangan, reaksiya mexanizmlari taklif etilgan, alkinillash reaksiyalarining eng muqobil sharoitlari topilgan. Sintez qilingan aromatik atsetilen spirtrlari identifikatsiyalangan, tozaligi, tarkibi, tuzilishi, xususiy va kvant-kimyoviy konstantalari zamonaviy fizik-kimyoviy tadqiqot usullari yordamida isbotlangan. Tanlangan katalitik sistemada benzaldegid va uning ayrim hosilalari asosida aromatik atsetilen spirtrlarini sintez qilishning nisbiy samaradorlik qatori tavsiya qilingan.

Kalit so'zlar: fenilatsetilen, benzaldegid va uning hosilalari, rux triflorometilsulfonat, tetrabutylammoniy florid, trietilamin, atsetonitril, aromatik atsetilen spirtrlari, mahsulot unumi

DOI: 10.34920/cee202217

Kirish

Molekulasida $C=O$ yoki $C=N$ guruhlari saqlagan elektrofil xossaga ega bo'lgan organik birikmalarga turli xil nukleofil reagentlarning birikishi natijasida biologik faol xossalarga ega bo'lgan, molekulasida $C-C$ bog'lanishning shakllan-

ishiga olib keladigan yangi organik birikmalarni yuqori unum bilan sintez qilish usullarini topish ilmiy jihatdan muhim bo'lgan vazifalardan biridir [1-3]. Siklogeksanalni [2,2] parasiklofan asosidagi ketimin ligandi yordamida ruhning alkil, alkenil, fenil hamda alkinil hosilalari ishtirokida

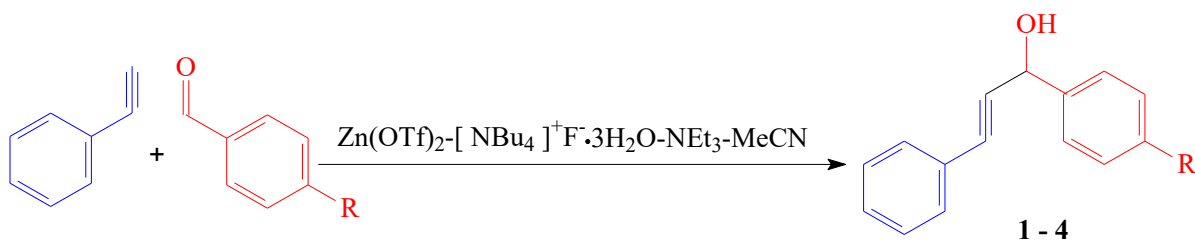
fenilatsetilen, trimetilsililatsetilen va geksin-1 lar bilan enantiosektiv alkinlash jarayoni orqali mos ravishda atsetilen spirtlari sintez qilingan. Ushbu jarayonda erituvchi sifatida geksan, toluol yoki tetragidrofurandan foydalanilgan. Olingan natijalarga ko'ra xona haroratida, 2 soat davomida toluol eritmasida katalizator sifatida [2,2] parasiklofan asosidagi ketimin ligandi (5 mol. %) va alkinilruh (0,5 ml 2M) qo'llanilganda 1-siklogeksil-3-fenilpropin-2-ol-1 (82%), 1-siklogeksil-3-(trimetilsilil)propin-2-ol-1 (52%) va 1-siklogeksilgeptin-2-ol-1 (56%) unum bilan sintez qilingan. Tanlangan rux hosilalari orasida atsetilen spirtlari hosil bo'lish samaradorligi alkinilruh<alkenilruh<fenilruh<alkinilruh qatori bo'yicha oshib borishi aniqlangan [4]. Karriera tomonidan alkinilruh va ularning hosilalarini superstioximetrik reagentlar tayyorlash orqali aldegidlar va alkinlarning o'zaro reaksiyalari o'rganilgan [37-40]. Mahsulot unumi va tozaligini oshirish maqsadida toluol, trietilamin va (+)-N-metilefidrindan foydalangan. Reaksiya 20-25 °C haroratda olib borilgan. Fenilatsetilen va 4-fenilbutin-1 ning benzaldegid, izobutanal, geksanal, 2-metilpentanal va 3-metilpentanal bilan reaksiyalar asosida yangi atsetilen spirtlari 82-94% unum bilan sintez qilingan [5]. Siklik aldegidlarning xrom yoki marganets metallari tuzlari yordamida Et₂O eritmasida, Et₃N ishtirokida -10 – 20 °C haroratda, 16-48 soat davomida terminal alkinlar galogenli hosilalari bilan kompleks katalitik sistema ishtirokida alkinlash reaksiyasi natijasida atsetilen spirtlari sintez qilingan. Jumladan, siklogeksanal-1 0 °C haroratda, 28 soatda 3-brompropin-1 bilan reaksiyaga kirishib, 90% unumda 4-siklogeksilbutin-1-ol-3 sintez qilingan. Ushbu usul bo'yicha atsetilen spirtlarini sintez qilishda aldol kondensatsiyalanishning kuchli ro'y berishi, sintez qilingan spirtlarning sistemada izolyatsiyaga uchrab qolishi, karbonil guruhning sterik to'siqqa va deaktivatsiyaga uchrashi kabi sub'ektiv holatlar kuzatilgan [6-8]. Bu₄NOH-H₂O-DMSO katalitik kompozitsiyasi ishtirokida ilk bor Ye.Yu. Shmidt ilmiy laboratoriyasida alifatik, siklik, atsiklik, aromatik va geteroaromatik aldegid va ketonlarning atsetilen bilan etinilash reaksiyasi o'rganilgan bo'lib, 64-93% unum bilan mos ravishdagi atsetilen spirtlari sintez qilingan. Jarayon uchun muqobil sharoit – reaksiya davomiyligi 1 soat, harorat 5 °C qilib tanlangan [9, 10].

Tadqiqot usullari

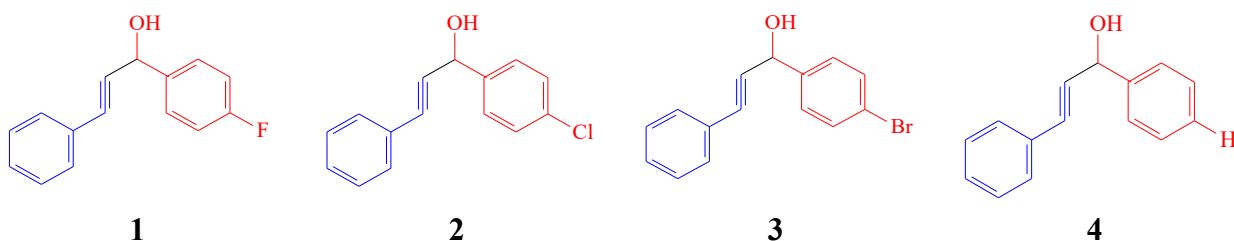
Atsetilen spirtlari sintezi hajmi 5000 ml sig'imga ega bo'lgan kimyoviy chidamli, termik bardoshli va mexanik mustahkam shaffof shishadan (BorSilicatum 3.3 markali) tayyorlangan besh og'izli ikki qavatli reaktor (AG!-5720-5000 markali) da amalga oshirildi. Ushbu reaktorga qaytarma sovutgich (Dimrota TS24/40.300 mm. markali), aralashtirgich (Eurostar 20/PTFE70.15.600/5000 markali), haroratni nazorat qilish uchun sensorli termodatchik (OD:φ8D:660 markali) va ikkita tomizgich voronka (RU-1000TW/375L markali) o'rnatiladi.

Dastlab reaktorda qalay triftoimetilsulfonat 10,4 g (0,025 mol), tetrabutylammoniyftorid trigidrat 7,8 g (0,025 mol) va 39 ml (0,75 mol) atsetonitril 60 minut davomida o'zaro aralashirilib suspenziya tayyorlanadi. Hosil bo'lgan suspenziyaga 30 minut davomida 7 ml trietilamindagi 11,2 ml fenilatsetilen (0,1 mol) va 7 ml trietilamindagi 5,35 ml (0,05 mol) 4-ftorbenzaldegidning eritmasi tomiziladi. Fenilatsetilen, 4-ftorbenzaldegid, sistemada hosil bo'ladigan 1-(4-ftorfenil)-3-fenilpropin-2-ol-1, oraliq va qo'shimcha moddalar polimerlanib ketmasligi uchun boshlang'ich reagentlarni sistemaga yuborishdan oldin reaktordagi triftoimetilsulfonat, tetrabutylammoniyftorid trigidrat va atsetonitril suspenziyasiga gidroxionon qo'shiladi. Yuqori unum bilan mahsulot olish uchun reaktordagi harorat suyuq azot yordamida doimiy nazorat qilinadi (sistemadagi harorat doimiy ravishda -10 °C haroratda bo'lishi kerak), substrat, reagent, katalizator va erituvchidan iborat komponentlar davriy ravishda bir maromda uzluksiz aralashirib turiladi. Fenilatsetilen va 4-ftorbenzaldegidning trietilamindagi eritmasi to'liq reaktorga berilgandan so'ng, yana 30 minut davomida -10 °C haroratda aralashirib turiladi. Hosil bo'lgan aralashma 360 minut davomida tindirilib, so'ngra dietilefir yordamida uch marta (3×25 ml) ekstraksiya qilinadi. Ekstraksiya qilingan organik qatlam dastlab erituvchilardan tozalanib, so'ngra vakuumda haydash orqali fraksiyalarga ajratib olinadi. Bunda 7,72 g 1-(4-ftorfenil)-3-fenilpropin-2-ol-1 (68%) unum bilan sintez qilindi. Ushbu usul bo'yicha 4-xlorbenzaldegid, 4-brombenzaldegid va benzaldegidni fenilatsetilen bilan etinilash reaksiyasi orqali 9,0 g 1-(4-xlorfenil)-3-fenilpropin-2-ol-1 (74%), 11,34 g 1-(4-bromfenil)-3-fenilpropin-2-ol-1 (79%) va 9,77 g 1,3-difenilpropin-2-ol-1 (96%), unum bilan sintez qilindi.

Jarayonning umumiy reaksiya sxemasi quyidagicha taklif etildi [11, 12].



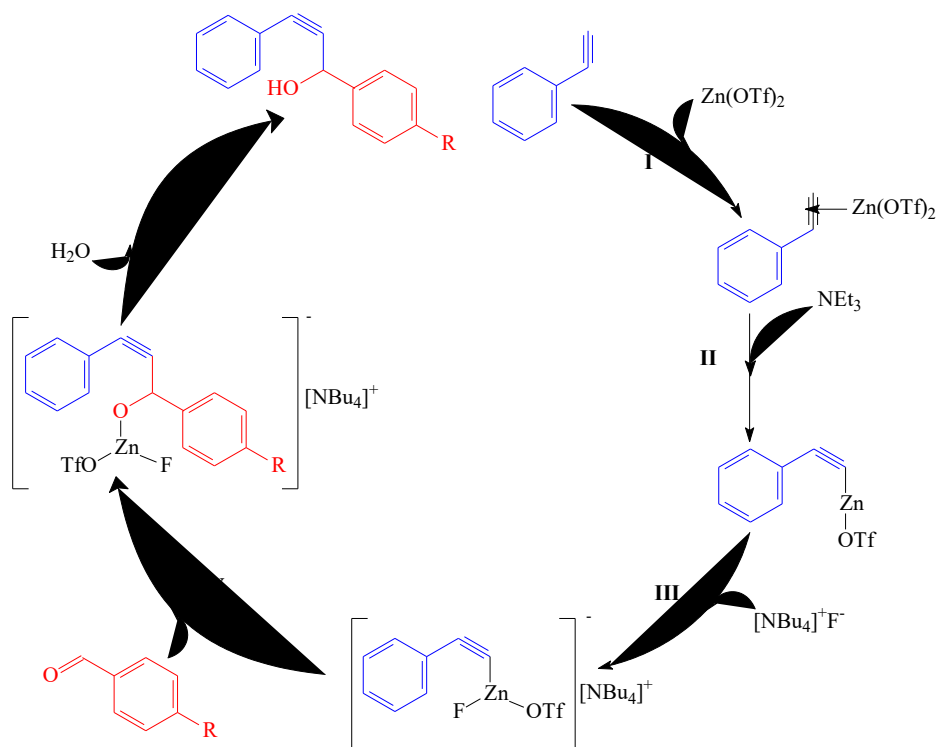
Sintez qilingan aromatik atsetilen spirlari.



Natijalar va muhokama

Reaksiya mexanizmi: Tanlangan aldegidlar-ni fenilatsetilen ishtirokida alkinillash reaksiyasi

mexanizmi adabiyot manbalarida keltirilgan ma'lumotlar asosida quyidagicha taklif etildi [13, 16].



Atsetilen spirlari sintez qilishda dastlab (I) katalizator rux triftoformetilsulfonat atsetonitril eritmasida fenilatsetilen molekulasidagi uchbog'ga oriyentatsion ta'sir etadi va natijada vodorod atomining harakatchanligini yanada oshirib, π -kompleks hosil qiladi [14, 17]. Sistemada hosil bo'lgan π -kompleks atsetonitril eritmasida trietilamin

yordamida deprotonlanishi (II) hisobiga barqaror nukleofil reagent feniletiniltriftoformetilsulfonat rux tuziga aylanadi [18]. Hosil bo'lgan oraliq birikma (nukleofil reagent) reaksiya muhitining ishqoriyiligi va molekular faolligini oshiruvchi tetrabu-tilammoniy ftorid bilan reaksiyaga kirishadi. Ushbu (III) jarayonda $[NBu_4]^+F^-$ feniletiniltrifto-

metilsulfonat rux tuzini fluor bilan faollashtirib $[\text{Ph}\equiv\text{ZnFOTf}][\text{NBu}_4]^+$ kompleksini hosil qiladi. $[\text{Ph}\equiv\text{ZnFOTf}][\text{NBu}_4]^+$ molekulasidagi triflat anioniga birikkan rux elektromanfiyligi yuqori bo'lgan fluor tomonga siljiydi. Natijada rux va sp gibridlangan uglerod orasidagi ion bog' oson uzilib erkin kationlar hosil bo'ladi, bu esa fenilatsetilenni aldegidlar bilan birikishini tezlashtiradi, ya'ni tanlangan aldegidlarning karbonil guruhidagi elektrofil xossaga ega bo'lgan uglerodga fenilatsetilen anionining nukleofil hujumini osonlashtiradi. Natijada IV bosqichda $[\text{Ph}\equiv\text{ZnFOTf}][\text{NBu}_4]^+$ aldegidning karbonil guruhiga ta'sir (hujum) qilib qo'shimcha mahsulot sifatida tetrabutylammoniyftoridning ligand hosilasiga aylanadi. Jarayonning oxirgi V bosqichida esa hosil bo'lgan qo'shimcha mahsulot suv ta'sirida gidrolizga uchrashi natijasida dastlab katalizatorlar $[\text{NBu}_4]^+\text{F}^-$ ni tiklaydi, so'ngra mos ravishdagi aromatik atsetilen spirti hamda ruxgidrosotriformetilsulfonatga aylanadi [19, 20]. Sistemadagi trietilaminning triformetilsulfonat tuzi ($\text{HN}^+\text{Et}_3\text{O}^-\text{Tf}$) ruxgidrosotriformetilsulfonat bilan ta'sirlashuvdan trietilamin, rux triformetilsulfonat va suvni hosil qiladi (ushbu holat keltirilmagan) [21-24]. Ushbu reaksiya mexanizmi adabiyot manbalari asosida taklif qilingan bo'lib, reaksiyaning xavfsizligi, mexanik tafsilotlari, assimetrik variantlari, jarayonni boshqarish va nazorat qilishning rentabel usullari hozirda o'rganilmoqda va kelgusida yakuniy xulosa to'g'risida ma'lumot berish rejalashtirilgan.

Aromatik atsetilen spirtlarini sintez qilish jarayoni va mahsulot unumiga turli omillar, jumladan erituvchilar tabiati, boshlang'ich moddalar va katalitik komponentlar miqdori, harorat va reaksiya davomiyligi ta'sirlari tizimli ravishda tahlil qilindi. 1-Jadvalda tanlangan aldegidlar bilan fenilatsetilenni reaksiyasiga reaksiya davomiyligi ta'siri natijalari keltirilgan. Bunda aldegidlarni

alkinlash reaksiyasi 1 soatdan 4 soatgacha bo'lgan vaqt davomida o'rganildi.

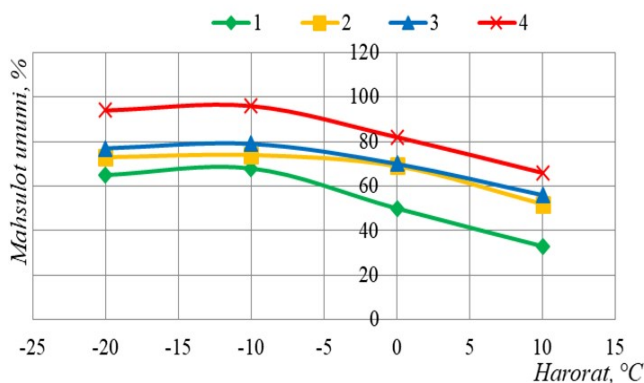
Olingan natijalarga ko'ra alkinlash jarayoni 1 soat davomida olib borilganda reagent va substart o'zaro to'liq reaksiyaga kirisha olmasligi natijasida aldegidlar proton (H^+) ta'sirida kondensatsiyaga uchrab qolishi yoki yenollanishi natijasida barqaror oraliq va qo'shimcha birikmalarni hosil bo'lishi kuzatildi. Jarayon 2 soat davomida olib borilganda atsetilen spirtlari eng yuqori unum bilan 1 – 68; 2 – 74; 3 – 79 va 4 – 96% hosil bo'ldi. Reaksiya davomiyligining yanada oshishi bilan mahsulot unumiga salbiy ta'sir etishi kuzatildi. Masalan reaksiya davomiyligini 2 soatdan 4 soatga oshirilganda sistemada hosil bo'lgan spirtlarning rux triformetilsulfonat bilan alkogolyatlar, fenilatsetilen bilan viniloksi efirlar hosil qilishi natijasida qo'shimcha mahsulotlar miqdorining ortishi, aromatik atsetilen spirtlari unumining esa keskin ravishda 1 – 38; 2 – 37; 3 – 34 va 4 – 31% gacha kamayishi aniqlandi.

Aromatik atsetilen spirtlari sinteziga harorat ta'siri o'rganildi. Alkinlash reaksiyalari $-25\div 15$ °C intervallarda olib borildi. Rasmdan ko'rinib turibdiki jarayon -10 °C haroratda olib borilganda reagent va substratning erituvchi molekularida harakat tezligi ortishi natijasida yuqori energiyaga ega faol molekular hosil bo'lishi hisobiga aromatik atsetilen spirtlari- 1 – 68; 2 – 74; 3 – 79 va 4 – 96% unumi eng yuqori chiqishi kuzatildi. Faol molekular bir-biri bilan to'qnashishi natijasida o'zaro nukleofil birikish reaksiyalari oson sodir bo'ladi. Natijada sistemada feniletiniltriformetilsulfonat rux tuzi hamda tetrabutylammoniyftoridning ligand hosilasining miqdori va faolligi ortib borib mahsulot unumining ortishiga xizmat qiladi. Bundan tashqari reaksiya -10 °C haroratda olib borilsa sistemadagi tuz molekulasidagi ion bog'lari oson uzilib erkin kationlar hosil bo'ladi, bu esa aldegidlar bilan birikishini tezlashtiradi.

1-Jadval

Mahsulot unumiga reaksiya davomiyligi ta'siri
(Harorat -10 °C, fenilatsetilen:aldegid miqdori 2:1 nisbatda, erituvchi MeCN)

Reaksiya davomiyligi, soat	Aromatik atsetilen spirtlari unumi, %			
	1	2	3	4
1	60	70	75	88
2	68	74	79	96
3	63	71	77	90
4	30	37	45	65



Mahsulot unumiga harorat ta'siri (Reaksiya davomiyligi 2 soat, fenilatsetilen:aldegid miqdori 2:1 nisbatda, erituvchi MeCN).

Reaksiya -20 yoki undan past bo'lganda sistemada tanlangan katalizatorlar hamda boshlang'ich moddalarning eritmada eruvchanligi past bo'lishi natijasida sistemada katalitik faol markazlarning kamligi, zarrachalarning o'zaro ta'sirlashuvi sekin borishi natijasida aromatik atsetilen spirtlari unumi nisbatan past chiqishi kuzatildi.

Harorat 10 °C gacha ko'tarilishi bilan aromatik atsetilen spirtlarining unumi keskin ravishda pasayganligi kuzatildi. Ya'ni jarayonda hosil bo'lgan spirtlarning qisman polimerlanishi, smolasimon va chiqindi mahsulotlarning paydo bo'lishi, katalizatorlar aldegidlar bilan reaksiyaga kirishib qo'shimcha mahsulotlar hosil bo'lishi, sistemada hosil bo'lgan aromatik atsetilen spirtlari boshlang'ich mahsulotlar bilan reaksiyaga kirishib, viniloksi efilari va atsetallarning hosil bo'lishi mahsulot unumining minimallashtirishga olib keldi.

Olib borilgan tadqiqot natijalariga asoslanib tanlangan aldegidlarni fenilatsetilen ishtirokida alkinillash jarayoni uchun eng muqobil sharoit topildi. Unga ko'ra harorat -10 °C, reaksiya davomiyligi 2 soat, katalitik sistema $Zn(OTf)_2 \cdot [NBu_4]^+ F^- \cdot 3H_2O : NEt_3$ komponentlari 1:1:4 mol nisbatda, boshlang'ich moddalar (fenilatsetilen:aldegid) esa 2:1 nisbatda, reagent va substrat massasiga nisbatan

erituvchi atsetonitril deyarli ikki karra ortiqcha miqdorda olingan holatda aromatik atsetilen spirtlari eng yuqori unum bilan sintez qilindi.

Fizik-kimyoviy tadqiqot natijalari

Sintez qilingan aromatik atsetilen spirtlari kvant-kimyoviy ko'rsatkichlari – molekulaning umumiy energiyasi, boshlang'ich energiyasi, issiqlik energiyasi, elektron energiyasi, yadro energiyasi, dipol momenti va kislorod atomi zaryadi Hyper Chem Activation 7,0 paketi STAT dasturining yarim empirik usuli bo'yicha aniqlandi (2-jadval). Sintez qilingan spirtlar molekulasidagi kislorod atomi o'zida yuqori energiyani saqlaganligi uchun mahsulot unumida ham maksimum orqali o'tish aniqlandi.

Sintez qilingan aromatik atsetilen spirtlarining tarkibi, tozaligi va tuzilishi zamonaviy fizik-kimyoviy tadqiqot usullari yordamida aniqlandi va tahlil qilindi.

1-(4-ftorfenil)-3-fenilpropin-2-ol-1 (1) – Rf (geksan-etilatsetat 10:1) = 0,33; mahsulot unumi 68%): 1H- YMR ($CDCl_3$): δ 7,64-7,59 (m, 2H); 7,49-7,47 (m, 2H); 7,34-7,30 (m, 3H); 7,13-7,06 (m, 2H); 5,66 (d, J=6,0 Hz, 1H); 2,33 (d, J=6,2 Hz, 1H). 13C- YMR ($CDCl_3$): δ 164,3; 136,6; 131,1; 128,5; 128,3; 128,1; 122,5; 115,6; 88,6; 86,8; 64,7.

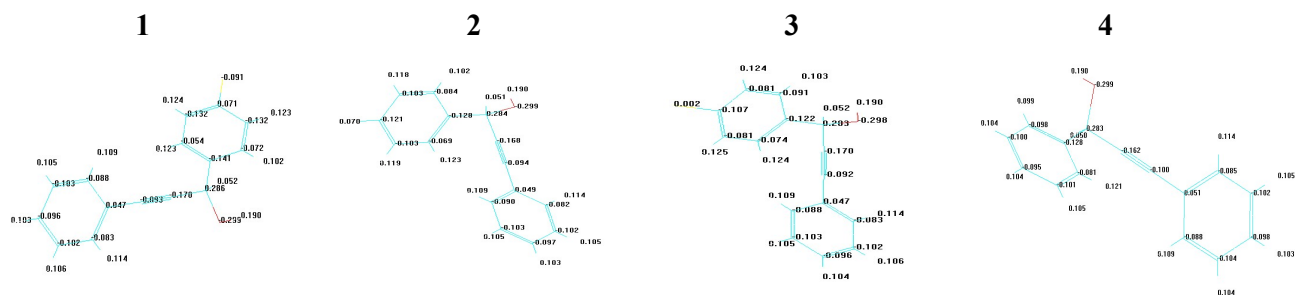
1-(4-xlorfenil)-3-fenilpropin-2-ol-1 (2) – Rf (geksan-etilatsetat 10:1) = 0,35; mahsulot unumi 74%): 1H- YMR ($CDCl_3$): δ 7,59-7,42 (m, 9H); 5,66 (s, 1H); 2,31 (br, 1H). 13C- YMR ($CDCl_3$): δ 139,1; 134,1; 131,6; 128,7; 128,5; 128,2; 128,0; 121,9; 88,2; 86,7; 64,3.

1-(4-bromfenil)-3-fenilpropin-2-ol-1 (3) – Rf (geksan-etilatsetat 10:1) = 0,39; mahsulot unumi 79%): 1H- YMR ($CDCl_3$): δ 7,85 (dd, J=1,7; 7,6 Hz, 1H); 7,60 (dd, J=1,3; 8,1 Hz, 1H); 7,51-7,26 (m, 7H); 6,03 (d, J=5,6 Hz, 1H); 2,55 (d, J=5,7; Hz, 1H). 13C- YMR ($CDCl_3$): δ 139,5; 132,6; 131,5; 129,8; 128,4; 128,1; 127,6; 122,8; 122,1; 87,8; 86,5; 64,4.

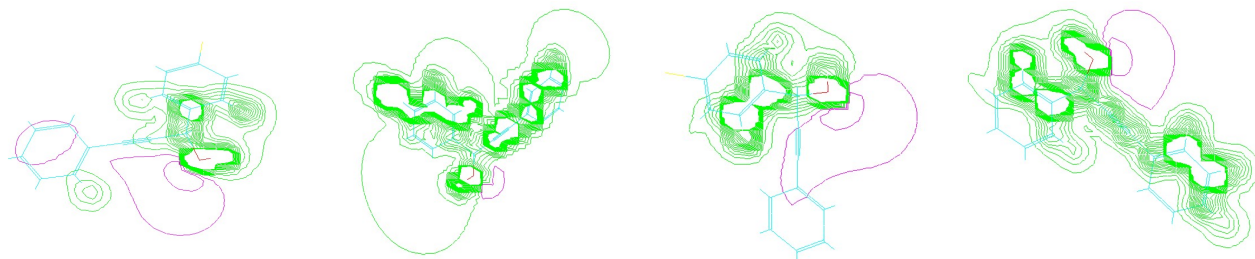
2-Jadval

Sintez qilingan birikmalarning kvant-kimyoviy hisoblashlari

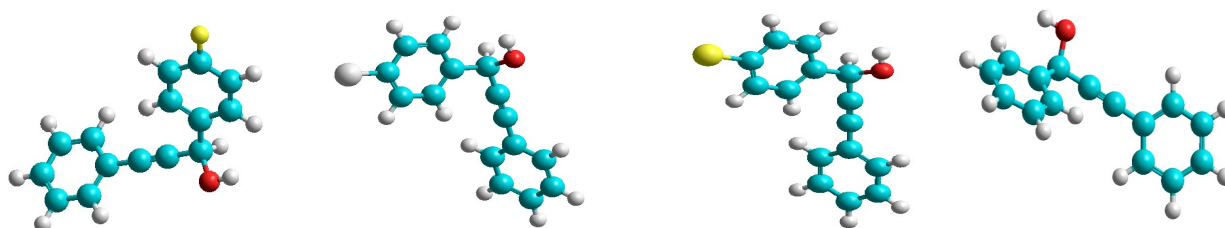
Birikmalar	Umumiy energiyasi kkal/mol	Hosil bo'lish energiyasi kkal/mol	Hosil bo'lish issiqligi, kkal/mol	Elektron energiyasi, eV	Yadro energiyasi, kkal/mol	Dipol momenti (D)	Kislorod atomining zaryadi
1	-61755,5	-3201,05	13,87	-347650,0	285894,56	1,042	-0,386
2	-58907,8	-3174,28	50,74	-342943,9	284036,03	0,9463	-0,352
3	-59752,3	-3157,54	65,22	-342899,8	283147,45	0,9206	-0,299
4	-51956,9	-3190,62	57,50	-307638,5	255681,59	1,497	-0,256



Molekuladagi atomlarning zaryad qiymatlari



Molekulalarda elektron zichliklarning taqsimlanishi



Molekulalarning 3D fazoviy struktura tuzilishi

1,3-difenilpropin-2-ol-1 (4) – Rf (geksan-etilatsetat 10:1) = 0,47; (mahsulot unumi 96%): 1H - YMR (CDCl₃): δ 7,81-7,74 (m, 2H); 7,62-7,58 (m, 2H); 7,56-7,49 (m, 6H); 5,88 (d, J=5,8 Hz, 1H), 2,44 (d, J=5,9 Hz, 1H). 13C- YMR (CDCl₃): δ 140,5; 131,6; 128,6; 128,4; 128,3; 128,2; 126,5; 122,4; 88,6; 86,7; 65,1.

Bundan tashqari sintez qilingan aromatik atsetilen spirtlarining molekularining fazoviy tuzilishi, molekularida zaryadlar va elektron zichlikning taqsimlanishi ASDFREE12 dasturi orqali o'rganildi.

Xulosa

Ilk bor Zn(OTf)₂:TBAF·3H₂O:NEt₃:MeCN kompleks katalitik sistemasida 4-ftorbenzaldegid, 4-xlorbenzaldegid, 4-brombenzaldegid va benzaldegidni fenilatsetilen ishtirokida alkinillash reaksiyasi orqali mos ravishdagi aromatik atsetilen spirtlari– 1-(4-ftorfenil)-3-fenilpropin-2-ol-1, 1-(4-xlorfenil)-3-fenilpropin-2-ol-1, 11,34 g 1-(4-bromfenil)-3-fenilpropin-2-ol-1 va 1,3-

difenilpropin-2-ol-1 larni sintez qilishning samarali usuli topildi.

Qo'llanilgan kompleks katalitik sistemaning aromatik atsetilen spirtlari sintezi va unumiga ta'sir qilish qonuniyati aniqlandi. Tanlangan katalizatorlarning selektivligi, samaradorligi va stabiligi ilmiy asoslangan.

Benzaldegid va uning gomologlari molekulasidagi galogenlarning mavjudligi, ularning tabiati va fazoviy ta'sir xossasiga ko'ra tanlangan aldegidlarning fenilatsetilen bilan ta'sirlashuvi quyidagi qator – 4-ftorbenzaldegid, 4-xlorbenzaldegid, 4-brombenzaldegid, benzaldegid qatori bo'yicha faollashib borishi anqlandi. Aromatik atsetilen spirtlarining hosil bo'lish samaradorlik qatori ishlab chiqildi.

Tadqiq qilingan reaksiyalarning kinetik parametrlari o'rganildi, reaksiya maxanzimlari taklif etildi, sintez qilingan birikmalarning xususiy kattaliklari aniqlandi, elektron tuzilishi, zaryadlarning molekular taqsimlanishi, kvant-kimyoviy va molekular-dinamik xususiyatlari o'rganildi.

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