UDK: 678.043.53 (661.718.5)

NATRIY METASILIKAT VA PARADIXLORBENZOL REAKSIYASIDA UNUM VA POLIMERLANISH DARAJASIGA TA‘SIR ETUVCHI OMILLAR

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Annotatsiya. Ushbu ishda natriy metasilikat (Na_2SiO_3) va paradixlorbenzol ($C_6H_4Cl_2$) o‘rtasidagi nukleofil aromatik o‘rin almashish (SNAr) reaksiyasining kinetik xususiyatlari batafsil o‘rganilgan. Reaksiya tezligi va mahsulot hosil bo‘lishiga ta‘sir qiluvchi asosiy omillar – harorat, katalizator konsentratsiyasi, erituvchi turi va reaksiya vaqti – tajribalar asosida baholanib, ularning unum va polimerlanish darajasiga ta‘siri tahlil qilingan. Tajribalar natijasida reaksiya ikkinchi tartibli kinetikaga mos kelishi, faollashish energiyasi (Ea) 85-95 kJ/mol oralig‘ida bo‘lishi va optimal sharoitlarda unum 75-85% gacha yetishi aniqlangan.

Kalit so‘zlar: SNAr reaksiyasi, kinetika, natriy metasilikat, paradixlorbenzol, reaksiya tezligi, polimerlanish darajasi, faollashish energiyasi.

Abstract. In this work, the kinetic properties of the nucleophilic aromatic substitution (SNAr) reaction between sodium metasilicate (Na2SiO3) and paradichlorobenzene (C6H4Cl2) were studied in detail. The main factors affecting the reaction rate and product formation - temperature, catalyst concentration, solvent type and reaction time - were evaluated experimentally, and their effects on the yield and degree of polymerization were analyzed. The experiments showed

that the reaction follows second-order kinetics, the activation energy (Ea) is in the range of 85-95 kJ/mol, and the yield reaches 75-85% under optimal conditions.
Keywords: SNAr reaction, kinetics, sodium metasilicate, paradichlorobenzene, reaction rate, degree of polymerization, activation energy.
Аннотация. В данной работе подробно изучены кинетические свойства реакции нуклеофильного ароматического замещения (SNAr) между метасиликатом натрия (Na2SiO3) и парадихлорбензолом (C6H4Cl2). Экспериментально оценены основные факторы, влияющие на скорость реакции и образование продуктов: температура, концентрация катализатора, тип растворителя и время реакции, а также проанализировано их влияние на выход и степень полимеризации. Эксперименты показали, что реакция протекает по закону второго порядка, энергия активации (Ea) находится в диапазоне 85–95 кДж/моль, а выход достигает 75–85% в оптимальных условиях.
Ключевые слова: реакция SNAr, кинетика, метасиликат натрия, парадихлорбензол, скорость реакции, степень полимеризации, энергия активации.

1.Kirish.

Nukleofil aromatik o‘rin almashish (SNAr) reaksiyalari organik sintezda, xususan, yuqori samarali polimer materiallar hosil qilishda muhim rol o‘ynaydi. Ushbu reaksiyalar Meisenheimer kompleksi hosil bo‘lishi orqali ikki bosqichli mexanizm bo‘yicha kechadi, bunda nukleofilning qo‘shilishi tezlikni belgilovchi bosqich hisoblanadi [1, 2]. Kremniyorganik polimerlar sintezi kontekstida SNAr reaksiyalari noorganik silikatlarni organik birikmalar bilan bog‘lash imkonini beradi, natijada yuqori termik barqarorlikka ega materiallar olinadi, ular qurilish sohalarda qo‘llaniladi [3, 4]. Biroq, an’anaviy organosilanlar (masalan, tetraetoksisilan) o‘rniga arzon natriy metasilikatni ishlatish eruvchanlik va reaktivlik muammolarini keltirib chiqaradi, bu esa kinetik tadqiqotlarni talab qiladi [5, 6].

Natriy metasilikat va paradixlorbenzol o‘rtasidagi SNAr reaksiyasi kremniyorganik polimerlar hosil qilish uchun istiqbolli bo‘lib, lekin uning kinetik parametri (tezlik konstantasi, faollashish energiyasi) batafsil o‘rganilmagan. Ushbu reaksiyada harorat, katalizator (masalan, CuI) va erituvchi (DMF yoki DMSO) kabi omillar reaksiya yo‘nalishini va mahsulot sifatini belgilaydi [7, 8]. Tadqiqot maqsadi – ushbu omillarni tajribaviy baholash orqali reaksiya kinetikasini modellashtirish, unum va polimerlanish darajasiga ta‘sirini aniqlash. Bu nafaqat ilmiy, balki sanoat jarayonlarini yaxshilash uchun ham ahamiyatli, chunki optimal kinetik sharoitlar energiya sarfini kamaytiradi va ekologik toza sintezni ta’minlaydi [9, 10].

ISSN 3030-3907

Ushbu tadqiqotda natriy metasilikat va paradixlorbenzol o‘rtasidagi SNAr reaksiyasi asosida issiqlikka chidamli kremniyorganik oligomerlar sintez jarayoniga turli omillarning ta’siri o‘rganildi.

2. Materiallar va usullar

2.1. Materiallar. Tadqiqotda 99% tozalikdagi natriy metasilikat (Na_2SiO_3, <50 μm o‘lchamda maydalangan), paradixlorbenzol ($C_6H_4Cl_2$, 99% sof), dimetilformamid (DMF) va dimetilsulfoksid (DMSO) erituvchilari, shuningdek, mis(I) yodid (CuI, 0.1-1.0%) katalizatori ishlatildi. Qo‘shimcha monomer sifatida etilenglikol (HO-CH_2CH_2-OH, 0.05 mol) qo‘shildi. Barcha reagentlar qo‘shimcha tozalashsiz qo‘llanildi.

2.2. Usullar. Reaksiya 100 ml avtoklavda molyar nisbat 1:1 ($C_6H_4Cl_2$:Na_2SiO_3) da, 140-180°C harorat oralig‘ida, 3-7 atm bosim ostida o‘tkazildi. Eruvchanlikni oshirish uchun erituvchiga 5-10% suv qo‘shildi. Kinetikani o‘rganish uchun reaksiya turli vaqt davomiyligida olib borildi: tezlik konstantasi (k) va unum titrimetrik usullar orqali aniqlandi. Faollashish energiyasi Arrhenius tenglamasi ($k = Ae^{\frac{-E_a}{RT}}$) bo‘yicha hisoblandi. Tajribalar turli harorat (140, 160, 180°C), katalizator miqdori (0.1, 0.5, 1.0%), erituvchi turi (DMF, DMSO, DMF + suv) va vaqt (2-8 soat) davomiyligi bilan o‘tkazildi.

3. Natijalar

SNAr reaksiyasining kinetikasi tajribalar orqali o‘rganilganda, uning ikkinchi tartibli bo‘lishi (tezlik = k [$C_6H_4Cl_2$] [Na_2SiO_3]) tasdiqlandi. Harorat oshishi reaksiya tezligi oshdi: 140°C da unum 45-55%, 160°C da 65-75%, 180°C da 80-90% ga yetdi. Faollashish energiyasi Ea = 85-95 kJ/mol deb topildi.

Katalizator (CuI) miqdorining ta‘siri: unum 0.1% da 35-45%, 0.5% da 65-75%, 1.0% da 80-90% ni tashkil qildi. Katalizatorning qimmatligini hisobga olmaganda eng maqbul miqdor 1.0%. Erituvchi turi bo‘yicha DMSO DMF ga nisbatan 1.5-2 barobar tezlikni ta’minladi, suv qo‘shilishi eruvchanlikni yaxshilagani bilan gidroliz xavfini oshirdi.

Vaqtga bog‘liqlik: Dastlabki 4 soatda unum tez o‘sib 75% ga yetdi, keyin sekinlashdi. Polimerlanish darajasi (DP) omillarga bog‘liq bo‘lib, optimal sharoitlarda 250-450 oralig‘ida bo‘ldi.

1-jadval 1.

Omillarning unum va polimerlanish darajasiga ta‘siri

Omil	Qiymati	Unum (%)	DP
Harorat	140°C	45-55	100-200
	160°C	65-75	200-300
	180°C	80-90	300-450
Katalizator (CuI)	0.1%	35-45	100-150

ISSN 3030-3907

	0.5%	65-75	200-350
	1.0%	80-90	300-450
Erituvchi	DMF	55-65	150-250
	DMSO	75-85	250-400
	DMF + 10% suv	70-80	200-350
Vaqt	2 soat	40-50	100-200
	4 soat	70-80	250-350
	8 soat	80-90	300-450

4. Muhokama

Olingan natijalar SNAr reaksiyalarining umumiy kinetikasiga mos keladi: qo‘shilish bosqichi harorat va katalizatorga sezgir [11, 12]. DMSO ning yuqori dielektrik o‘tkazuvchanligi ionlanishni yaxshilaydi, natriy metasilikatni faollashtirib, eruvchanlik muammosini bartaraf qiladi [13]. Polimerlanish darajasining oshishi etilenglikolning kondensatsiya rolida ekanligini ko‘rsatadi, ammo yuqori haroratda yon jarayonlar polimerlanish darajasini cheklaydi [14]. Ushbu kinetik model boshqa aromatik galogenidlar bilan solishtirganda yuqori samaradorlikni ko‘rsatadi, lekin erituvchisiz sharoitlarni o‘rganish zarur [15]. Natijalar digalogenli organik birikmalar asosida kremniyorganik birikmalar sintezlarni optimallashtirishda amaliy ahamiyatga ega.

5. Xulosa

Natriy metasilikat va paradixlorbenzol o‘rtasidagi SNAr reaksiyasining kinetik o‘rganishi harorat, katalizator, erituvchi va vaqtning unum va polimerlanish darajasiga sezilarli ta‘sirini ko‘rsatdi. Optimal sharoitlar (170°C, 0.5-1% CuI, DMSO, 4-6 soat) reaksiya tezligini oshirib, yuqori sifatli kremniyorganik oligomerlar olishni ta’minlaydi. Ushbu natijalar ekologik toza sintez usullarini rivojlantirishga hissa qo‘shadi va kelgusida sanoat jarayonlarini modellashtirishda qo‘llanilishi mumkin.

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ISSN 3030-3907