

## Atsetilasetoanilid hosilalari va ular asosidagi Ni(II) va Cu(II) kompleks birikmalarining sintezi, tuzilishi va xossalari.

**Rakhmatova R.S**

*Bukhara State University 1st stage graduate student*

**Mail:** [r.s.rahmatova@buxdu.uz](mailto:r.s.rahmatova@buxdu.uz)

**Annotatsiya.** Asetatsetanilidning konformerlari va tautomerlari DFT (B3LYP/6-311++G\*\*) va IQ spektroskopiya usullari bilan o'rganilgan. Molekulyar O–H···O va N–H···O vodorod bog'lanishi orqali hosil bo'lgan asetoasetanilid dimerlarining geometriyasi va energiya parametrlari olindi. Azot va kislorod atomlarining elektron juftlari va C=O karbonil guruhining antibog'lovchi  $\pi^*$ -orbitallari hamda atsetoasetanilid tautomerlaridagi qo'sh va yakka bog'larning donor-akseptor o'zaro ta'sirining energiyasi NBO usuli yordamida hisoblangan.

**Kalit so'zlar:** asetoasetanilid, tautomerizm, vodorod bog'lanishi, IQ spektroskopiyasi, kvant kimyoviy hisoblashlar.

**Kirish.**  $\beta$ -ketoamidlarning tadqiqotlari ko'p o'rganilgan qiziqarli va muhim birikmalar sinfini tashkil qiladi [1-3].  $\beta$ -ketoamid guruhlari ko'plab tabiiy molekulalarda va terapevtik vositalarda keng tarqalgan (masalan, 4-6). Molekuladagi bir nechta reaktiv joylarga ega  $\beta$ -ketoamidlarning noyob tuzilishi ularning organik sintezda qo'llanilishini ta'minlaydi. Bunday qo'llanilishi asosan  $\beta$ -ketoamidlarning  $\beta$ -dikarbonil birikmalarining tipik vakillari ekanligi va ularning reaktivligi, tuzilishi va tautomer muvozanati bilan bog'liq. Tautomeriya jarayonini tushunish zamonaviy organik va tibbiy kimyo, biokimyo va farmakologiyada reaksiya mexanizmlarini o'rganishda muhim ahamiyatga ega [7]. Shuning uchun  $\beta$ -ketoamidlarda tautomerik muvozanatlarni o'rganish amaliy va nazariy ahamiyatga ega.  $\beta$ -dikarbonil birikmalar orasida  $\beta$ -diketonlar,  $\beta$ -ketoefirlar va  $\beta$ -ketonitrillarning keto-yenol tautomeriyasi turli eksperimental usullar yordamida keng o'rganilgan [8-11]. Biroq,  $\beta$ -ketoamidlarning keto-yenol tautomerizmi (1-sxema) batafsil o'rganilmagan [12-20].  $\alpha$ -amido-  $\beta$ -ketoamidning keto-yenol tautomeriyasi va ikkita  $\alpha$ -alkil-  $\beta$ -ketoamid  $\text{CDCl}_3$  da  $^1\text{H}$  va  $^{13}\text{C}$  NMR spektroskopiyasi yordamida tekshirildi. Natijalar shuni ko'rsatdiki,  $\alpha$ -alkil-  $\beta$ -ketoamidlar keto shaklida mavjud,  $\alpha$ -amido-  $\beta$ -ketoamid esa keto va yenol shakllarini aniqladi [18]. Dipol momentlarini o'lchash va



ISSN (E): 2181-4570 ResearchBib Impact Factor: 6,4 / 2023 SJIF(2023)-3,778 Volume-2, Issue-1

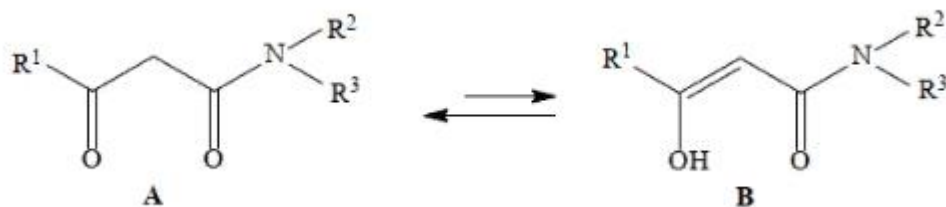
spektroskopiya tahlillari (ayniqsa IQ) eritmada qattiq holatda kuzatilgan metil-6-gidroksi-4-piridon-2 ning keto shakli ham mavjudligini tasdiqladi. Bu shakl ichki va tashqi molekulalararo vodorod bog'lari bilan barqarorlashadi [19]. Gilli va boshqalar  $\beta$ -diketonlarning yenollariga xos bo'lgan  $O=C-C=C-OH$   $\beta$ -enolon fragmenti hosil qilgan g'ayritabiiy kuchli  $O-H\cdots O$  molekula ichidagi vodorod bog'lari bilan barqarorlashgan tautomerlarning konfiguratsiyalangan shakllarini o'rgandilar. Ushbu model  $NH\cdots O$  molekula ichidagi vodorod bog'lariga bir qator geterobog'langan  $O=CC=C-NH$   $\beta$ -yenaminonlar,  $O=CC=N-NH$  ketogidrazonlar va  $O=NC=C-NH$  nitrozoenaminlar uchun qo'llanilishi mumkin. [20]. Bir qator  $\beta$ -ketoamidlarda tautomerizm muvozanatini NMR spektroskopiya yordamida o'rganish shuni ko'rsatdiki, . Ichki molekulyar vodorod bog'lari natijasida keto-yenol muvozanati amido-imidolga nisbatan ustun bo'lib, bu birikmalar asosan ketoamid va yenolamid tautomerlari shaklida mavjud [15]. Asetoasetanilid 1 sintetik organik kimyoda keng qo'llaniladigan  $\beta$ -ketoamidlarning tipik vakili hisoblanadi [21-26]. Rentgen nurlanish tahliliga ko'ra, kristalli atsetoasetanilid  $\beta$ -ketoamid A shaklida mavjud. Kristalda ikkita kristallografik mustaqil molekulalar kuzatilgan, ularning karbamoil guruhlari  $N-H\cdots O=C$  vodorod orqali bog'langan [27]. Asetoasetanilidning vodorod bilan bog'langan birlikni hosil qilish uchun bog'lanishlar monokristalli chiziqli bo'lmagan optik xususiyatlarini namoyon qiladi [28-33]. Ushbu hisobotlarning mualliflari asetasetanilid monokristallarini yetishtirishning yangi usulini ishlab chiqdilar va uning tuzilishini eksperimental (NMR, IR, Raman va UB spektroskopiya, rentgen diffraksiya tahlili) va kvant-kimyoviy (MEP va HOMO-LUMO) usullar bilan o'rgandilar. Biroq, asetasetanilidning keto-yenol tautomerizmi etarlicha o'rganilmagan.  $^1H$  va  $^{13}C$  spektroskopiya ma'lumotlariga ko'ra, 1-birikma asosan eritmada keto shaklida mavjud [34]. Etanol-suv aralashmasida asetasetanilidning yenolizatsiya tezligi (70: 30 v/v) to'xtatilgan oqim spektrofotometriyasi yordamida ham o'rganilgan. Yenolizatsiya tezligi galogenlanish tezligidan o'lchandi va natijalar bu jarayonni  $Ni^{+2}$ ,  $Zn^{+2}$  bilan katalizlashini aniqladi [12]. Benzol,  $CHCl_3$  va dioksanidagi benzoilasetanilid va salitsilanilidning yenol va keto shakllarining muvozanatli molyar fraksiyalari dipol moment o'lchovlari asosida aniqlandi [35]. Ushbu jarayonda asetasetanilid va uning dimerlarining gaz faza, qattiq va eritmada holatlardagi tautomerlarining B3LYP usuli 6-311++G\*\* asosida orqali IQ spektroskopiya va kvant-kimyoviy hisoblar tuzilishini tahlil qildik. Olingan tahlil natijalariga ko'ra, 1-sonli birikmaning beshta tautomer shakli gaz fazasida eng barqaror bo'lgan: ikkita keto-yenol





ISSN (E): 2181-4570 ResearchBib Impact Factor: 6,4 / 2023 SJIF(2023)-3,778 Volume-2, Issue-1

shakli 1a, c va uchta diketon 1b, 1d, 1e (1-jadval va 1-rasm). [36] mualliflari  $\beta$ -ketoefirlarning enol tuzilmalari diketo tautomerlarga qaraganda barqarorroq ekanligini ko'rsatdi. Gaz fazasida eng barqaror bo'lgan keto-yenol tautomerlari 1a, 1c kuchli molekulyar  $\text{OH}\cdots\text{O}=\text{C}$  vodorod bog'i bilan yopilgan 6 a'zoli xelat sikllarini, shuningdek, diketo tautomer 1b ( $\text{NH}\cdots$ ) hosil qilgan.  $\cdot\text{O}=\text{C}$  bog'lanish), kovalent bo'lmagan masofa mos ravishda 1,673, 1,642 va 1,946 Å.



## Ekspirimental va nazariy tadqiqotlar

### 1-rasm

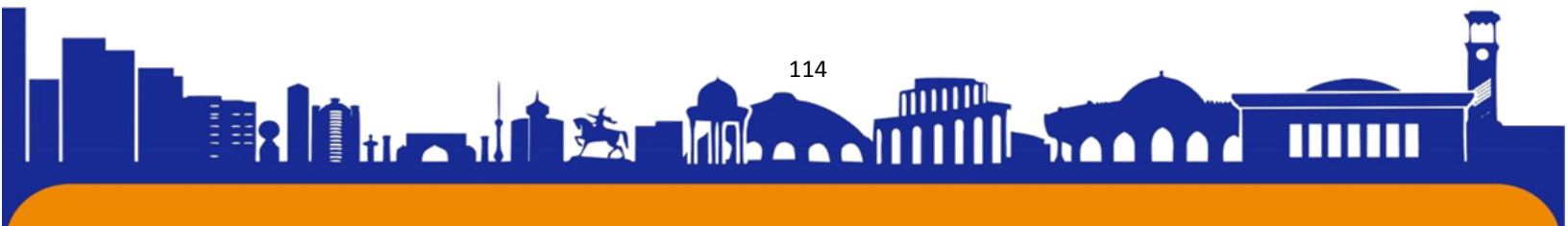
1a-1b, 1a-1d, 1b-1d va 1d-1d chiziqli dimerlar bitta  $\text{N-H}\cdots\text{O}$  bog'i orqali hosil bo'lgan. Hisoblash natijalari 2-jadvalda keltirilgan. Dimerlarning hosil bo'lish energiyasi tenglama (1) yordamida vodorod bog'lanish energiyasi orasidagi farq yordamida aniqlanadi[37].

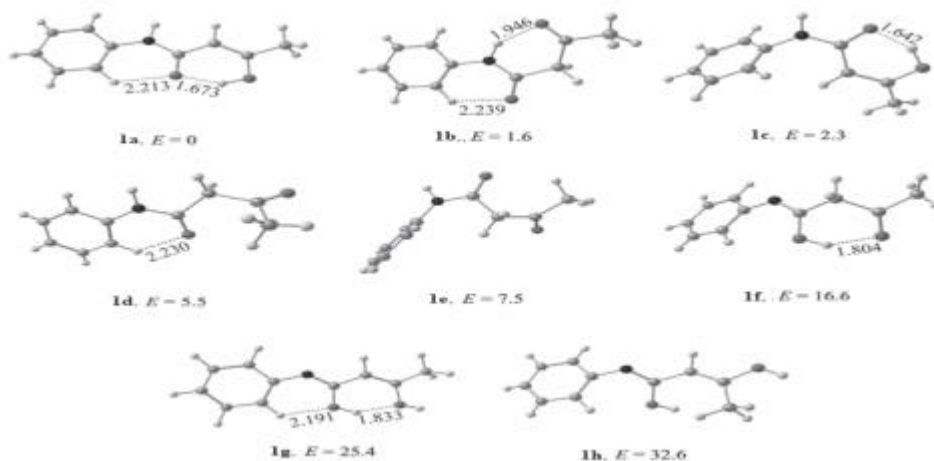
$$DE = E_{\text{dim}} - 2E_{\text{mono}}. (1)$$

1a-1a va 1a-1c dimerlari trisiklik bo'lib, markaziy 4 a'zoli va ikkita yon 6 a'zoli halqalari karbonil kislorod atomlari va vodorod atomlaridagi bilan ikkita tarmoq  $\text{OH}\cdots\text{O}=\text{C}$  vodorod bog'lari orqali o'ralgan. 1a-1a dimeridagi molekula ichidagi vodorod bog'larining uzunligi 1,749 Å ga, molekulararo bog'lanishlar esa 2,482 Å ga teng. 1a-1a va 1a-1c dimerlarida tarmoqlanish vodorod bog'larining hosil bo'lishi molekula ichidagi  $\text{OH}\cdots\text{O}=\text{C}$  vodorod bog'larining uzunligini tautomer 1a bilan solishtirganda mos ravishda 0,076 Å va 0,139 ga oshishiga olib keldi. 1a-1c dimerining 1c komponentidagi bu uzunlik ham monomerga nisbatan 0,044 Å ga oshdi. Yuqori simmetrik dimer 1c-1c markazi 8 a'zoli va ikkita yon 6 a'zoli halqalari bilan trisiklik tuzilishga ega bo'lib, karbonil kislorod atomlarida tarmoqlanish bilan ikkita  $\text{NH}\cdots\text{O}=\text{C}$  vodorod bog'lari orqali bog'langan.

## Ekspirimental va nazariy tadqiqotlar

### Tautomerlarda nisbiy energiya (kkal/mol) va vodorod bog'larining uzunligi





Qisqa molekulararo  $\text{NH}\cdots\text{O}=\text{C}$  vodorod bog'lari (1,867 Å) 12,44 kkal/mol (har bir bog' uchun 6,22 kkal/mol) yuqori dimerlanish energiyasini aks ettirdi, (2-jadval). Monomer 1e ning past barqarorligiga qaramasdan, uning amid guruhining sis-konfiguratsiyasi eng qisqa molekulararo  $\text{NH}\cdots\text{O}=\text{C}$  vodorod bog'lari (1,855 va 1,864 Å) bilan eng barqaror 8 a'zoli siklik dimer 1e-1e hosil bo'lishini ta'minladi. Uning dimerlanish energiyasi har bir bog'lanish uchun 6,92 kkal/molga teng bo'ldi. 1a-1d chiziqli dimerlarining dimerlanish energiyasi 5 va 13 kkal/mol (2-jadval) oralig'ida bo'lgan.

Geteroatomlarning yolg'iz elektron juftlarining donor-akseptor o'zaro ta'siri, shuningdek, bitta va ko'p bog'lanishlar NBO usuli yordamida 1a-1e tautomerlari uchun B3LYP/6-311++G\*\* hisoblashlar olib borildi (3-jadval). Azot atomining yakka elektronning E(2) konfiguratsiya energiyasi karbonil guruhining  $\text{C}=\text{O}$ ,  $n\text{N}\rightarrow p^*\text{C}_1=\text{O}_1$  antibog'lovchi  $p^*$ -orbitali bilan ko'rib chiqilayotgan tautomerlarda ancha yuqori bo'lib, 57–65 ga teng bo'lgan. kkal/mol (2-sxema va 3-jadval). Bundan tashqari, 1a, 1b, 1d tautomerlaridagi azot atomining yolg'iz elektron juftligi benzol halqasining aromatik tizimi ( $n\text{N}\rightarrow p^*$  32–34 kkal/mol) bilan o'zaro ta'sirlashgan.

Bu qiymatlar 1c (E(2) 16,94 kkal/mol) va 1e (E(2) 11,45 kkal/mol) tautomerlari uchun sezilarli darajada past bo'ldi,  $\text{HNCPh}=\text{CPh}$  ikkiburchak burchagi mos ravishda  $-135^\circ$  va  $-125^\circ$  ga teng. 1a va 1c tautomerlardagi konfiguratsion bog'lanish  $\text{C}_2=\text{C}_3$  p-orbitalning karbonil guruhining antibog'lovchi  $p^*$ -orbitali  $p\text{C}_2=\text{C}_3\rightarrow p^*\text{C}_1=\text{O}_1$  bilan 27 kkal/mol ga teng bo'lgan o'zaro ta'sir qilish energiyasi va karbonil guruhining antibog'lovchi  $p^*$ -orbitalining  $\text{C}_2=\text{C}_3$  qo'sh bog'ining antibog'lovchi  $p^*$ -orbitali bilan o'zaro ta'siri bilan tavsiflanadi. 1c tautomeridagi oxirgi o'zaro ta'sirning energiyasi

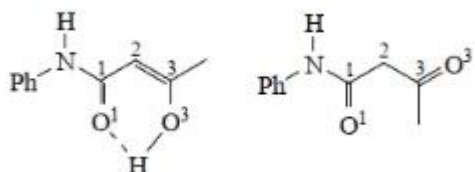






ISSN (E): 2181-4570 ResearchBib Impact Factor: 6,4 / 2023 SJIF(2023)-3,778 Volume-2, Issue-1

$p^*C_1=O_1 \rightarrow p^*C_2=C_3$  tautomer 1a bilan solishtirganda deyarli ikki baravar yuqori (mos ravishda 132,62 va 76 kkal/mol). 1a va 1c keto-enol shakllaridagi  $O_1$  kislorod atomlarining ikkala toq elektron juftlari OH gidroksil guruhining  $s^*$ -orbitali  $nO_1 \rightarrow s^*O_3-H$  antibog'lanish bilan konfiguratsiyada ishtirok etgan.



## 2-sxema

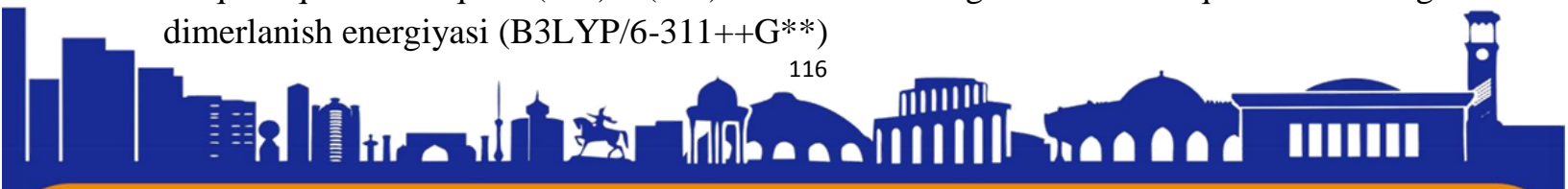
Bu qiymatlar 1c (E(2) 16,94 kkal/mol) va 1e (E(2) 11,45 kkal/mol) tautomerlari uchun sezilarli darajada past bo'ldi, HNCPh=CPh ikkiburchak burchagi mos ravishda  $-135^\circ$  va  $-125^\circ$  ga teng. 1a va 1c tautomerlardagi konfiguratsion bog'lanish  $C_2=C_3$  p-orbitalning karbonil guruhining antibog'lovchi  $p^*$ -orbitali  $pC_2=C_3 \rightarrow p^*C_1=O_1$  bilan 27 kkal/mol ga teng bo'lgan o'zaro ta'sir qilish energiyasi va karbonil guruhining antibog'lovchi  $p^*$ -orbitalining  $C_2=C_3$  qo'sh bog'ining antibog'lovchi  $p^*$ -orbitali bilan o'zaro ta'siri bilan tavsiflanadi. 1c tautomeridagi oxirgi o'zaro ta'sirning energiyasi  $p^*C_1=O_1 \rightarrow p^*C_2=C_3$  tautomer 1a bilan solishtirganda deyarli ikki baravar yuqori (mos ravishda 132,62 va 76 kkal/mol). 1a va 1c keto-enol shakllaridagi  $O_1$  kislorod atomlarining ikkala toq elektron juftlari OH gidroksil guruhining  $s^*$ -orbitali  $nO_1 \rightarrow s^*O_3-H$  antibog'lanish bilan konfiguratsiyada ishtirok etgan.

Dimer	$r, \text{Å}$		$\Delta\nu_{NH}/\nu_{OH}^{calc/exp}, \text{cm}^{-1}$	$\nu_{NH}/\nu_{OH}^{exp}, \text{cm}^{-1}$	$-\Delta E, \text{kkal/mol}$
	intermolecular	intramolecular			
1a-1a, cyclic OH...O	2.482	1.749	309/290	3136	0.82
1a-1c, cyclic OH...O	2.302	1.686	230/230	3196	0.66
	2.544	1.812			
1c-1c, cyclic NH...O	1.866	1.646	305/290	3136	12.44
	1.867	1.647			
1e-1e, cyclic NH...O	1.855	-	326/358	3068	13.84
	1.864				
1a-1b, linear NH...O	1.989	1.664	160/138	3288	7.40
		1.892			
1a-1d, linear NH...O	2.130	1.664	78/53	3375 <sup>b</sup>	5.42
1b-1d, linear NH...O	1.936	1.871	189/173	3253	13.29
1d-1d, linear NH...O	2.078	-	90/129	3297	8.65

Δ

$\nu(NH) = \nu(NH)_{monomer} - \nu(NH)_{dimer}$  104K da IQ ning yutilish diapazoni

2-jadval. Molekulararo va ichki molekular vodorod bog'larining uzunligi, to'lqin raqamlari farqi  $\Delta\nu(NH) \nu(OH)^a$  va 1 birikmaning siklik va chiziqli dimerlarining dimerlanish energiyasi (B3LYP/6-311++G\*\*) Δ





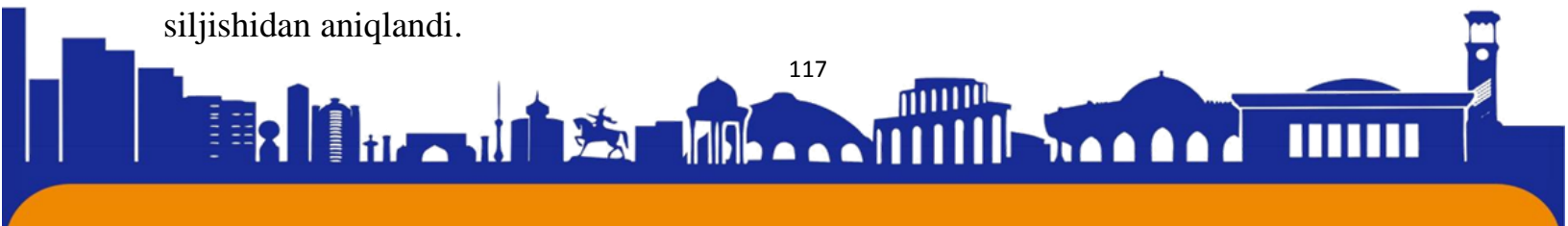
ISSN (E): 2181-4570 ResearchBib Impact Factor: 6,4 / 2023 SJIF(2023)-3,778 Volume-2, Issue-1

IQ spektroskopiya tahliliga ko'ra  $3297\text{ sm}^{-1}$  da kuchli dublet bandining yuqori chastotali maksimali chiziqli dimer 1d-1d uchun tayinlangan.  $3288\text{ sm}^{-1}$  dagi diketo tautomer 1b ning NH guruhlariga to'g'ri keldi, bu (NH) qiymati, 1a yoki 1d tautomerlardagi erkin NH guruhlari va NH guruhlari tebranishlarining hisoblangan chastotasi o'rtasidagi farq bilan tasdiqlanadi. 1b tautomeridagi NH...O=C vodorod bog'lanishida ishtirok etadi,  $136\text{ sm}^{-1}$  ga teng va tajribada kuzatilgan qiymatga to'g'ri keladi (1-2 va 3-jadvallar).

Band	CCl <sub>4</sub>	CH <sub>2</sub> Cl <sub>2</sub>	MeCN	KBr	Film from MeCN
NH	3438 m	3422 m		3426 vw	3426 vw
NH...O=C (intra)	3327 m	3321 m	3348 s	3297 s	3295 m, br
NH...O=C (inter)	3307 m	3301 m	3288 sh	3288 sh	
	3260 vw	3256 vw		3256 vw	3258 s
OH...O=C (inter)			3205 vw	3196 m	3199 m
OH...O=C (intra)	3141 vw	3141 vw	3140 vw	3136 m	3138 m
NH...O=C (inter)				3068 m, br	3082 m, br
C=O (keto)	1716 vs	1714 vs	1725 s		1719 vs
C=O (keto)		1691 sh	1711 sh	1716 vs	
C=O (amide)	1692 vs	1684 vs	1688 vs		1684 sh
C=O (amide)				1684 sh	1662 vs
C=O-C=C-C-OH	1618 w	1619 w	1618 w	1660 vs	
C=O-C=C-C-OH		1600 s	1601 s	1600 vs	1599 vs

3-jadval. Asetoasetilanilid 1 uchun IQ spektroskopiya tahlillari.

CCl<sub>4</sub> va CH<sub>2</sub>Cl<sub>2</sub> dagi asetoasetilanilid 1 spektrlari mos ravishda  $1716$ ,  $1692$  va  $1714$ ,  $1684\text{ sm}^{-1}$  da kuchli  $n(\text{C}=\text{O})$  tasmalarini o'z ichiga olgan. 1b va 1d tautomerlarining hisoblangan tebranish spektrlariga ko'ra, yuqori chastotali diapazon 1d tautomeridagi keto guruhining  $n(\text{C}=\text{O})$  tebranishlari, past chastotali esa C tebranishlari hisobiga yuzaga kelgan. Tautomer 1b dagi karbonil guruhlarining  $n(\text{C}=\text{O})$  tebranishlari molekula ichidagi vodorod bog'larini hosil qilishda ishtirok etib, ikkinchisi bilan bir-biriga yopishgan va yuqori chastotali energiya sifatida namoyon bo'lgan (CCl<sub>4</sub> da  $1699\text{ sm}^{-1}$  va CH<sub>2</sub>Cl<sub>2</sub> da  $1695\text{ sm}^{-1}$ ). [27] dagi ma'lumotlarga ko'ra, qutbli asetonitrildagi keto guruhining  $n(\text{C}=\text{O})$  cho'zilishi inert muhit bilan solishtirganda yuqori chastotaga  $1725\text{ sm}^{-1}$  ga siljidi. 1d tautomerining amid guruhining kuchli  $n(\text{C}=\text{O})$  bandi  $1688\text{ sm}^{-1}$  da kuzatilgan. Tajribada topilgan C=O tebranish chastotalari orasidagi farq ( $37\text{ sm}^{-1}$ ) qiymatga to'g'ri keldi. Xulosa qilib aytganda, IQ spektroskopiya ma'lumotlariga ko'ra, asetoasetilanilid asosan qattiq holatda va eritmalarda diketo tautomerlari va ularning assotsiatsiyalari shaklida mavjud bo'la oladi. Keto-enol tautomer 1a va NH...O bog'li chiziqli dimer gaz fazasida eng barqaror bo'lib, 298-104 K da  $n(\text{NH}) = n(\text{NH}_{\text{erkin}}) - n(\text{NH}_{\text{ass}})$  tebranish chastotalarining qiymatlari vodorod bog'lanishidan kelib chiqqan siljishidan aniqlandi.



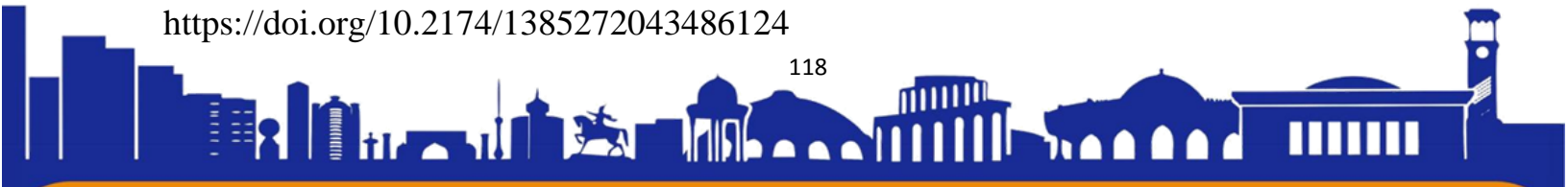


## EXPERIMENTAL

Asetilasetanilidning IQ spektrlari va  $CCl_4$  hamda  $CH_2Cl_2$  dagi eritmalarining natijalari Varian 3100 FT IQ spektrometri yordamida qayd etilgan. Ayniqsa birikmaning IQ spektrlari 298–104 K diapazonida suyuq azot bilan sovutilgan doimiy haroratli kamerada qayd etilgan. Assotsiatsiyalardagi H-bog'larning turlari eksperimental va nazariy hisoblangan  $n(NH)$  qiymatlari yordamida aniqlandi. Kvant-kimyoviy hisob-kitoblar Gaussian'09 dasturiy ta'minoti yordamida to'liq geometriyani optimallashtirish va B3LYP/6-311++G(\*\*) usuli [40] orqali 1 birikma va uning dimerlari uchun tebranish chastotalarini hisoblash bilan amalga oshirildi. Statsionar nuqtalarning minimallarga mos kelishi ijobiy Hessian qiymatlari bilan tasdiqlandi. Nisbiy energiyalar (DE) eng barqaror shaklga nisbatan hisoblangan.

## Foydalanilgan adabiyotlar

1. Hussain, S.M., El-Reedy, A.M., and El-Sherabasy, S.A., J. Heterocycl. Chem., 1988, vol. 25, p. 9. <https://doi.org/10.1002/jhet.5570250102>
2. El-Meligie, S.E.M., Khalil, N.A., El-Nassan, H.B., and Ibraheem, A.A.M., Curr. Org. Chem., 2019, vol. 23, p. 2005. <https://doi.org/10.2174/1385272823666191021120336>
3. Li, W., Zheng, Y., Qu, E., Bai, J., and Deng, Q., Eur. J. Org. Chem., 2021, p. 5151. <https://doi.org/10.1002/ejoc.202100692>
4. Smith, K.M., Bu, Y., and Suga, H., Chem. Biol., 2003, vol. 10, p. 81. [https://doi.org/10.1016/s1074-5521\(03\)00002-4](https://doi.org/10.1016/s1074-5521(03)00002-4)
5. Kim, E.J., Lee, J.H., Choi, H., Pereira, A.R., Ban, Y.H., Yoo, Y.J., Kim, E., Park, J.W., Sherman, D.H., Gerwick, W.H., and Yoon, Y.J., Org. Lett., 2012, vol. 14, p. 5824. <https://doi.org/10.1021/ol302575h>
6. Nogawa, T., Terai, A., Amagai, K., Hashimoto, J., Futamura, Y., Okano, A., Fujie, M., Satoh, N., Ikeda, H., Shin-Ya, K., Osada, H., and Takahashi, S., J. Nat. Prod., 2020, vol. 83, p. 3598. <https://doi.org/10.1021/acs.jnatprod.0c00755>
7. Raczynska, E.D., Kosinska Osmiałowski, W.B., and Gawinecki, R., Chem. Rev., 2005, vol. 105, p. 3561. <https://doi.org/10.1021/cr030087h>
8. Iglesias, E., Curr. Org. Chem., 2004, vol. 8, p. 1. <https://doi.org/10.2174/1385272043486124>

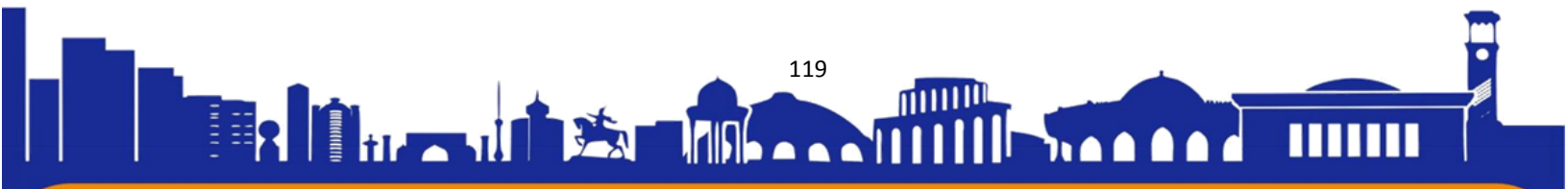






ISSN (E): 2181-4570 ResearchBib Impact Factor: 6,4 / 2023 SJIF(2023)-3,778 Volume-2, Issue-1

9. Smith, K.T., Young, S.C., DeBlasio, J.W., and Hamann, C.S., *J. Chem. Educ.*, 2016, vol. 93, p. 790. <https://doi.org/10.1021/acs.jchemed.5b00170>
10. Sandler, I., Harper, J.B., and Ho, J., *J. Chem. Educ.*, 2021, vol. 98, p. 1043. <https://doi.org/10.1021/acs.jchemed.0c01076>
11. Ruiz, D.L., Albesa, A.G., Ponzinibbio, A., Allegretti, P.E., and Schiavoni, M.M., *J. Phys. Org. Chem.*, 2010, vol. 23, p. 985. <https://doi.org/10.1002/poc.1764>
12. Hynes, M.J. and Clarke, E.M., *J. Chem. Soc. Perkin Trans.*, 1994, vol. 2, p. 901. <https://doi.org/10.1039/P29940000901>
13. Wengenroth, H. and Meier, H., *Chem. Ber.*, 1990, vol. 123, p. 1403. <https://doi.org/10.1002/cber.19901230633>
14. Naoum, M.M. and Saad, G.R., *J. Solut. Chem.*, 1998, vol. 17, p. 67. <https://doi.org/10.1007/BF00651854>
15. Laurella, S.L., Sierra, M.G., Furlong, J.J.P., and Allegretti, P.E., *Open J. Phys. Chem.*, 2013, vol. 3, p. 138. <https://doi.org/10.4236/ojpc.2013.34017>
16. Laurella, S.L., Latorrea, C., Dietricha, R., Furlong, J.J.P., and Allegretti, P.E., *J. Phys. Org. Chem.*, 2012, vol. 25, p. 1365. <https://doi.org/10.1002/poc.305>
17. Newberry, R.W., Orke, S.J., and Raines, R.T., *Org. Lett.*, 2016, vol. 18, p. 3614. <https://doi.org/10.1021/acs.orglett.6b0165>
18. Sung, K., Wu, R.-R., and Sun, S.-U., *J. Phys. Org. Chem.*, 2002, vol. 15, p. 775. <https://doi.org/10.1002/poc.554>
19. Castillo, S., Bouissou, T., Favrot, J., Brazier, J.F., and Fayet, J.P., *Spectrochim. Acta A*, 1993, vol. 49, p. 1591. [https://doi.org/10.1016/0584-8539\(93\)80116-R](https://doi.org/10.1016/0584-8539(93)80116-R)
20. Gilli, P., Bertolasi, V., Ferretti, V., and Gilli, G., *J. Am. Chem. Soc.*, 2000, vol. 122, p. 10405. <https://doi.org/10.1021/ja000921+>
21. Downs, J.R., Grant, S.P., Townsend, J.D., Schady, D.A., Pastine, S.J., Embree, M.C., Metz, C.R., Pennington, W.T., Walsch, R.D.B., and Beam, C.F., *Canad. J. Chem.*, 2004, vol. 82, p. 659. <https://doi.org/10.1139/v04-029>
22. Ke, Z., Lam, Y.-P., Chan, K.-S., and Yeung, Y.-Y., *Org. Lett.*, 2020, vol. 22, p. 7353. <https://doi.org/10.1021/acs.orglett.0c02701>







ISSN (E): 2181-4570 ResearchBib Impact Factor: 6,4 / 2023 SJIF(2023)-3,778 Volume-2, Issue-1

23. Zhang, Z., Gao, X., Yu, H., Bi, J., and Zhang, G., ACS Omega., 2017, vol. 2, p. 7746.

<https://doi.org/10.1021/acsomega.7b01526>

24. Lieby-Muller, F., Constantieux, T., and Rodriguez, J., J. Am. Chem. Soc., 2005, vol. 127, p. 17176. <https://doi.org/10.1021/ja055885z>.

25. Tkachenko, V.V., Muravyova, E.A., Desenko, S.M., Shishkin, O.V., Shishkina, S.V., Sysoiev, D.O., Müller, T.J.J., and Chebanov, V.A., Beilstein J. Org. Chem., 2014, vol. 10, p. 3019. <https://doi.org/10.3762/bjoc.10.320>

26. Azzam, R.A. and Moharebb, R.M., Chem. Pharm. Bull., 2015, vol. 63, p. 1055. <https://doi.org/10.1248/cpb.c15-00685>

27. Kubozono, Y., Kohno, I., Ooishi, K., Namazue, S., Haisa, M., and Kashino, S., Bull. Chem. Soc. Japan, 1992, vol. 65, p. 3234. <https://doi.org/10.1246/bcsj.65.3234>

28. Prabhu, Sh.G. and Rao, P.M., J. Crystal Growth, 2000, vol. 210, p. 824. [https://doi.org/10.1016/0960-8974\(90\)90020-S](https://doi.org/10.1016/0960-8974(90)90020-S)

29. Vijayana, N., Babua, R.R., Gopalakrishnana, R., and Ramasamy, P., J. Crystal Growth, 2004, vol. 267, p. 646. <https://doi.org/10.1016/j.jcrysgr.2004.04.008>

30. Ravikumar, C., Joe, I.H., and Sajjan, D., Chem. Phys., 2010, vol. 369, p. 1.

31. Ravikumar, C. and Joe, I.H., XXII Int. Conf. Raman Spectrosc., 2010, p. 1267. <https://doi.org/10.1063/1.3482727>

32. Senthilkannan, K., Venkatachalam, K., Thamarikannan, P., Kalaipoonguzhali, V., Kannan, S., and Jothibas, M., AIP Conf. Proceed., 2020, vol. 2270, no. 1, p. 040014. <https://doi.org/10.1063/5.0019332>

33. Arjunan, V., Kalaivani, M., Senthilkumari, S., and Mohan, S., Spectrochim. Acta (A), 2013, vol. 115, p. 154. <https://doi.org/10.1016/j.saa.2013.06.003>

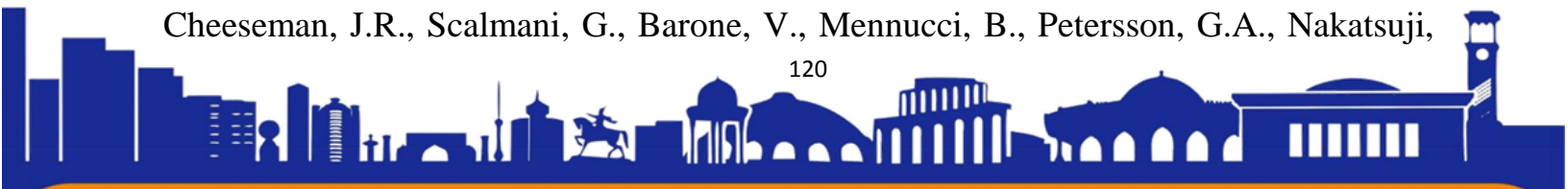
34. Barros, M.T., Geraldies, C.F., Maycock, C.D., and Silva, M.I., J. Mol. Struct., 1986, vol. 142, p. 435. [https://doi.org/10.1016/0022-2860\(86\)85150-X](https://doi.org/10.1016/0022-2860(86)85150-X)

35. Naoum, M.M. and Saad, G.R., Indian J. Chem. (A), 1987, vol. 26, p. 510.

36. Schiavoni, M.M., Di Loreto, H.E., Hermann, A., Mack, H.-G., Ulic, S.E., and Védova, C.O.D., J. Raman Spectrosc., 2001, vol. 32, p. <https://doi.org/10.1002/jrs.701>

37. Karthika, M., Senthilkumar, L., and Kanakaraju, R., Comp. Theor. Chem., 2012, vol. 979, p. 54. <https://doi.org/10.1016/j.comptc.2011.10.015>

40. Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb, M.A., Cheeseman, J.R., Scalmani, G., Barone, V., Mennucci, B., Petersson, G.A., Nakatsuji,





ISSN (E): 2181-4570 ResearchBib Impact Factor: 6,4 / 2023 SJIF(2023)-3,778 Volume-2, Issue-1

H., Caricato, M., Li, X., Hratchian, H.P., Izmaylov, A.F., Bloino, J., Zheng, G., Sonnenberg, J.L., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Montgomery, J.A., Peralta, J.E., Ogliaro, F., Bearpark, M., Heyd, J.J., Brothers, E., Kudin, K.N., Staroverov, V.N., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A., Burant, J.C., Iyengar, S.S., Tomasi, J., Cossi, M., Rega, N., Millam, N.J., Klene, M., Knox, J.E., Cross, J.B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R.E., Yazyev, O., Austin, A.J., Cammi, R., Pomelli, C., Ochterski, J.W., Martin, R.L., Morokuma, K., Zakrzewski, V.G., Voth, G.A., Salvador, P., Dannenberg, J.J., Dapprich, S., Daniels, A.D., Farkas, O., Foresman, J.B., Ortiz, J.V., Cioslowski, J., and Fox, D.J., Gaussian 09, Revision E.01. Gaussian, Inc., Wallingford, CT, 2010.

