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TABIATSHUNOSLIK VA GEOGRAFIYA FAKULTETI

«UMUMIY KIMYO» KAFEDRASI

URUNOVA MUHAYYO RAJABBOYEVNANING

5440400 KIMYO ta’lim yo’nalishi bo’yicha bakalavr darajasini olish uchun

BITIRUV MALAKAVIY ISHI

Mavzu: 1-METILXINAZOLIN-2,4-DIONNI $FeCl_3 \cdot 6H_2O$ KATALIZATORI ISHTIROKIDA AROMATIK KISLOTA XLORANGIDRIDLARI BILAN ATSILLASH

Ilmiy rahbar: k.f.n. Taxirov Y.R.

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REJA

KIRISH

Mavzuning dolzarbligi. Xinazolin qatoriga kiruvchi birikmalar amaliy nuqtai-nazaridan katta ahamiyatga ega bo'lgan birikmalardir. Xinazolonlarni sintezi va kimyoviy o'zgarishlari ko'proq miqdorda ish talab qiladi. Shunga qaramay ularning soni yil sayin ortib bormoqda. Bu ular orasida ko'pgina biologik faol moddalar (gerbitsidlar, fungitsidlar, bakteritsidlar va boshqa xususiyatlarga ega preparatlar) borligi bilan tushintiriladi. Shu bilan birga xinazalon qatoridagi birikmalar nazariy jihatdan ham muhim ahamiyatga ega. Chunki ular molekulasida bir necha reaktsion markaz mavjud: birinchi va uchinchi holatlardagi azot atomlari, ikkinchi va to'rtinchi holatlardagi karbonil guruhlari hamda aromatik halqa bor. Shuning uchun bu sinf moddalar elektrofil reagentlar bilan har-xil yo'nalishda reaktsiyaga kirishishi mumkin. Xinazolin-2,4-dion qatoridagi elektrofil almashinish reaktsiyalari juda kam o'rganilgan.

Shuning uchun xam xozirgi kunda xinazolin-2,4-dion va uning hosilalarini Lyuis kislotalarining oz miqdori ishtirokida atsillash va olingan moddalar orasidan biologik faol moddalar izlash dolzarb masalalardan biridir.

Ushbu bitiruv malakaviy ishi benzol halqasi bilan kondensirlangan olti a'zoli geterohalqali birikmalar xinazolonlar sinfiga kiruvchi 1-Metilxinazolin-2,4-dionni aromatik kislota xlorangidridlari (benzoilxlorid, p-brombenzoilxlorid, p-nitrobenzoilxlorid) bilan kam miqdor katalizator $FeCl_3 \cdot 6H_2O$ ishtirokida katalitik atsillash reaktsiyalarini o'rganishga bag'ishlangan.

Ishning maqsadi. 1-Metilxinazolin-2,4-dionni aromatik kislota xlorangidridlari bilan o'zaro ta'sirini o'rganish, reaktsiyalarning borish yo'nalishini va sharoitlarini aniqlash.

Ishning vazifalari:

-1-metilxinazolin-2,4-dionni sintezini amalga oshirish;

-1-metilxinazolin-2,4-dionni aromatik kislota xlorangidridlari bilan reaktsiyalarini amalga oshirish, aroillash reaktsiyalarini yo'nalishi va borishini aniqlash;

- 1-metilxinazolin-2,4-dionni aroillash reaktsiyalarida sintez qilingan moddalarning tuzilishini fizik tadqiqot usullari yordamida tasdiqlash va molekula tuzilishini kvant-kimyoviy hisoblashlar qilish.

Ishning yangiligi. 1-metilxinazolin-2,4-dionni aromatik kislota xlorangidridlari bilan reaktsiyalari ilk bor amalga oshirilgan va mahsulot sifatida 1-metil-6-aroilxinazolin-2,4-dionlar hosil bo'lishi ko'rsatilgan.

1-metilxinazolin-2,4-dionni aromatik kislota xlorangidridlari bilan reaktsiyalari 1-metilxinazolin-2,4-dionni molekulasining aromatik yadrosiga borishi va 6-holatga aroil guruhlarining kirishi aniqlangan.

Sintez qilingan mahsulotlarning tuzilishi HyperChem va ChemBio3D Ultra 11.0 programmalari yordamida kvant-kimyoviy hisoblashlar qilingan va ularning fazoviy tuzilishi, elektron zichligi topilgan, molekulalarning IQ-spektrlari olingan.

Tadqiqot natijalarining ilmiy va amaliy ahamiyati. 1-metilxinazolin-2,4-dionni aromatik kislota xlorangidridlari bilan reaktsiyalarida mahsulot sifatida 1-metil-6-aroilxinazolin-2,4-dionlar hosil bo'lishi aniqlangan.

1-Metil-6-aroilxinazolin-2,4-dionlarning aromatik kislota xlorangidridlari bilan reaktsiyalarida aromatik kislota halqasiga elektronoaktseptor guruhlar (Br, NO_2) kiritilganda mahsulotning unumi ortishi ko'rsatilgan.

Sintez qilingan moddalarning fazoviy tuzilishi, elektron zichligi, molekulaning energiyasi hisoblangan va tajriba natijalarining kvant kimyoviy hisoblashlar natijalari bilan mos kelishi aniqlangan.

Himoya ishiga kiritildi:

- antranil kislotani mochevina bilan o'zaro ta'siri natijasida xinazolin-2,4-dionni sintezi;

- N-metilantranil kislotani natriy sianat bilan sikllash natijasida 1-metilxinazolin-2,4-dionni sintezi;

- 1-metilxinazolin-2,4-dionni aromatik kislota xlorangidridlari bilan reaktsiyalari natijasida 1-metil-6-aroilxinazolin-2,4-dionlarning hosil bo'lishi natijalari;

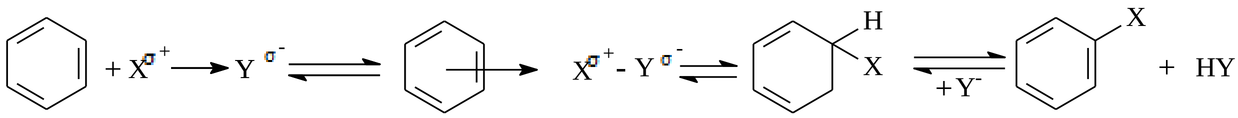
Bitiruv malakaviy ishning tuzilishi va hajmi.

Bitiruv malakaviy ish 57 matn betida bayon qilingan. Kirish, adabiyotlar sharhi, olingan natijalar muhokamasi, tajribalar qismi, xulosalar va ilovalardan iborat bo'lib, 1 ta jadval va 52 ta nomdagi foydalanilgan adabiyotlar ro'yxatini o'z ichiga oladi.

I-BOB. ADABIYOTLAR SHARHI

1-Bob. Organik birikmalarning elektrofil almashinish reaksiyalari

Elektrofil almashinish reaksiyalari aromatik birikmalar uchun keng o’rganilgan. Elektrofil almashinish reaksiyalari deganda musbat zaryadlangan ion yoki dipolning elektron zichligi katta bo’lgan holatga hujumi tushiniladi. Aromatik birikma yadrosidagi elektron zichlikning kattaligi tufayli musbat zaryadlangan ion yoki dipolning musbat qismi tortiladi. Ma’lumki bunga avval π-, keyin esa σ- komplekslar hosil bo’lishi orqali boradigan elektrofil almashinish reaksiyalari sodir bo’ladi [1,2].



π-kompleks σ-kompleks

Aromatik brikmalarni galogenlash, sulfolash, alkillash, atsillash, xlormetillash reaksiyalari elektrofil almashinish mexanizmi bo’yicha boradi, bu reaksiyalar chet el olimlari, shu jumladan O’zbekiston olimlari I.P.Sukervanik, A.R.Abdurasulova, Q.M.Ahmedov, X.Yo’ldoshev va boshqalar tomonidan atroflicha o’rganilgan bo’lib, adabiyotlarda keng yoritilgan [3-7].

Shu sababli aromatik birikmalarning galogenlash, sulfolash, nitrolash, alkillash, xlormetillash reaksiyalariga to’xtalib o’tirmadik.

Biz quyida geterohalqali birikmalarning elektrofil agentlar bilan olib boriladigan reaksiyalari, substratlarning faolligi va elektofil almashinish reaksiyalari ishlatiladigan katalizatorlarning kam miqdori to’g’risidagi ma’lumotlar va boshqa hususiyatlarini keltirib o’tamiz. Shuningdek geterohalqali birikmalarni katalizatorning kam miqdori ishtirokida atsillash reaksiyalariga katta axamiyat berdik, chunki ushbu bitiruv malakaviy ishi katalizatorlarning oz miqdori ishtirokidagi reaksiyalariga bag’ishlangan. Ushbu reaksiyalarning borishi va yo’nalishini aniqlash, hosil bo’ladigan mahsulotlar tuzulishiga geteroatomlarni bevosita ta’sirini o’rganish alohida qiziqish uyg’otadi.

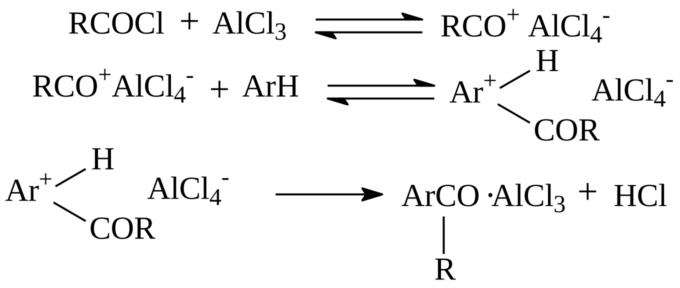
1.1. Aromatik va geterohalqali birikmalarni Fridel-Krafts bo'yicha atsillash reaksiyalari.

Aromatik va geterohalqali birikmalarni Fridel-Krafts bo'yicha atsillash turli organik moddalarni sintez qilishning asosiy usullaridan biri hisoblanadi. Ko'p hollarda ushbu sintezlar aromatik halqa tutuvchi birikmalarni hilma-hil karbon kislatalar xlorangidridlari bilan Luis kislatalari ishtirokida atsillash yordamida amalga oshiriladi [8,9].

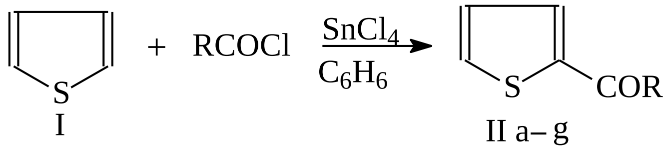
Shuni ta'kidlab o'tish joizki, yuqorida qayd qilingan sintezlarning muvaffaqiyatli amalga oshirilishi substratning, atsillovchi agentlarning hamda katalizatorlarning faolligiga bog'liq.

Karbon kislatalar xlorangidridlarining reaksion qobilyati ularning Luis kislatalari bilan donor-akseptor ta'sirlanish qobilyatiga sezilarli bog'liqligi yaqqol ko'zga tashlanadi.

Ko'pgina adabiyotlardagi ma'lumotlar [8-12] kislorod atomi bo'yicha kompleks hosil bo'lishidan dalolat berganligi tufayli, bu tasirlanish karbonil guruhi kislorodining asosligiga, ya'ni hosil bo'ladigan kompleksning yoki RCO^+ ionning aromatik halqa bilan elektrofil almashinish reaksiyalariga kirishish qobilyati bilan aniqlanadi. Atsillash jarayonini uch bosqichda tasavvur qilish mumkin [10-13].

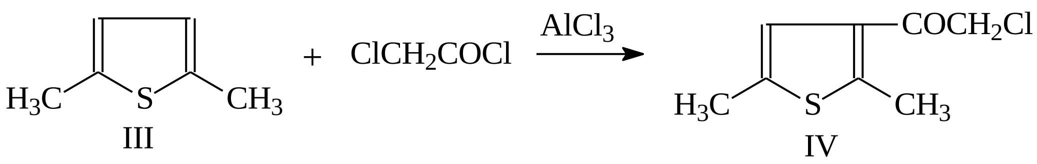


Bunday reaksiyalar Ch.Tomasning monografiyasida [10] va N.N.Lebedevning sharhida [12] atroflicha yoritilgan. Shuning uchun, biz bu bo'limda asosiy e'tiborni adabiyotlarda nisbatan kam yoritilgan geterohalqali birikmalarni Luis kislotalarining ekvimolyar va ortiqcha miqdori ishtirokida atsillash reaksiyalariga qaratdik. Ya.M. Goldfarb tiofenning (I) karbon kislotalar xlorangidridlari bilan reaksiyalarini $SnCl_4$ ning ekvimolyar miqdori ishtirokida o’rganib, qator 1-asetiltiofenlarni (II a-g) yuqori unum bilan olgan [14].

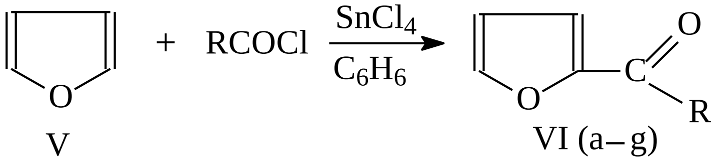


Reaksiya benzol eritmasida, xona haroratida olib borilgan. Ta’kidlab o’tish joizki, ushbu sharoitda erituvchi bilan atsillovchi agentlar reaksiyaga kirishmagan [14].

Agentlar tiofen halqasining 2- va 5-holatlari band bo’lsa, atsillash reaksiyasi uning 3-holatiga ketadi. Masalan, Shirinli V.Z va boshqa mualliflar tomonidan 2,5-dimetil tiofenni (III) xlorasetilxlorid bilan reaksiyasi $AlCl_3$ va piridin ishtirokida o’rganilib, 3-xloratsetil-2,5-dimetiltiofen (IV) yuqori unum bilan olishgan [15].

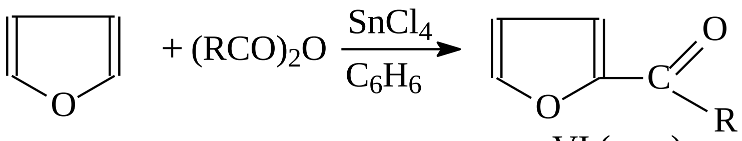


Geterohalqali birikmalarni atsillash bo’yicha izlanishlarni davom ettirib Ya.L.Goldfarb va L.M. Smargonskiy [16] tiofenning kislorodli analogi bo’lgan furanni (V) karbon kislotalar xlorangidridlari bilan $SnCl_4$ ishtirokida benzol eritmasida atsillab, nisbatan past unum bilan (18-31%) tegishli 2-atsilfuranlarni (VI a-g) sintez qilishgan.



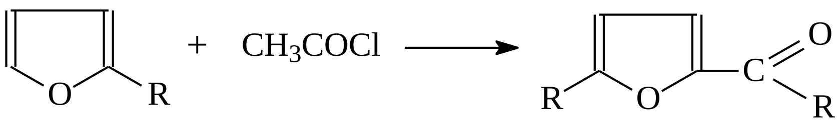
R= CH_3, C_2H_5, C_3H_7, C_6H_5

Ushbu mualliflar tomonidan aniqlanishicha, reaksion aralashmani suv bilan parchalash paytida zich ko’mirsimon massa hosil bo’lib, reaksiya mahsulotlarining unumi keskin kamayib ketishiga olib keladi. Bu massa furanning kislota xlorangidridlari bilan atsillash mahsulotlarini $SnCl_4$ bilan kompleksi hisoblanadi. Komponentlarni qo’shish paytida atsillash mahsulotlari hosil bo’lishi bilan bir qatorda furanning parchalanish va unga $SnCl_4$ ni birikishi oraliq mahsulotlarini hosil qiladi. Bu reaksiyalar erituvchida yaxshiroq boradi. Undan tashqari xlorangidridlar o’rniga tegishli angidridlar qo’llanilsa, 2-atsilfuranlarning VI(a-g) unumi sezilarli ravishda ortadi.[16].



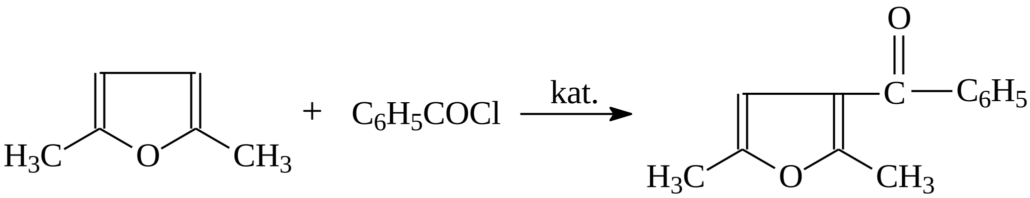
V VI (a– g)

Qayd qilingan natijalar T. Reyxshteynning izlanishlarida o’z ifodasini topdi. U furanni (V) va 2-metilfuranni (VII) $SnCl_4$, $ZnCl_2$ va $AlCl_3$ lar ishtirokida atsetillash reaksiyalari natijasida 2-asetifuran (VI a) va 2-metil-5-atsetilfuranlarni (VIII) tegishli tarzda 10 % va 23% unum bilan olgan[17].



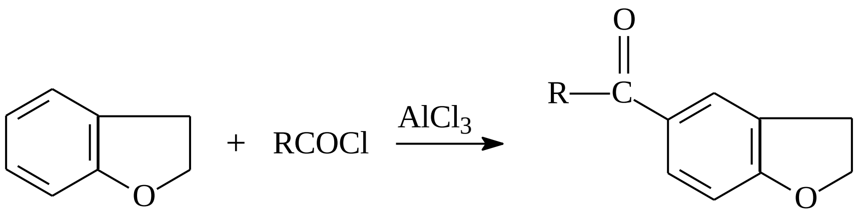
V, VII V, VI a R=H; VII, VIII R=CH_3 VIa, VII

Furan molekulasidagi 2-va 5-holatlar band bo’lsa, atsillovchi agent uning 3-holatiga kiradi. X.Gilman va M.Gallavoy 2,5-dimetilfuranni (IX) turli katalizatorlar ishtirokida benzoillab, 2,5-dimetil-3-benzoilfuranni (X) ajratib olishgan[18].



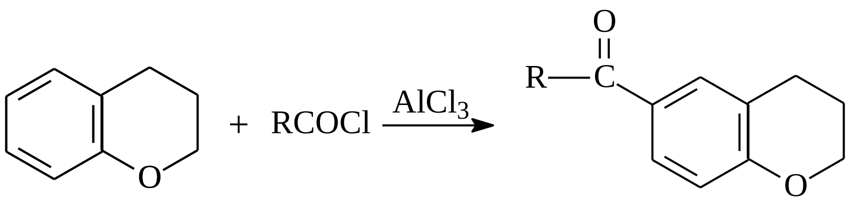
IX kat.=$AlCl_3$, $ZnCl_2$, $SnCl_4$ X

Adabiyotlarda bir yoki ikki aromatik halqa bilan kondensirlangan geterohalqali birikmalarni atsillash bo'yicha ma'lumotlar juda oz keltirilgan. Masalan, kumaranni (XI) karbon kislota xlorangidridlari bilan $AlCl_3$ ishtirokidagi reaksiyalari o'rganilib, 5-atsil hosilalari (XII) yuqori unum bilan olingan[19].



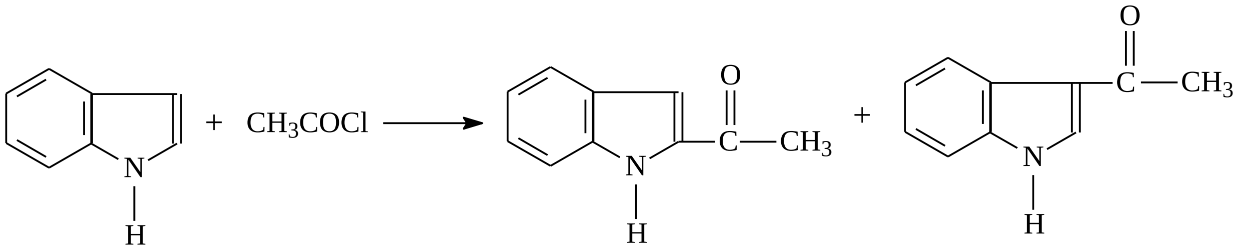
XI R=CH_3, C_2H_5, C_3H_7 XII

Geterohalqaning kamayishi natijasida reaksiya natijasida yo'nalishi o'zgaradi, ya'ni xromanni (XIII) $AlCl_3$ ishtirokida atsillash natijasida 6-atsilhosilalar (XIV) olingan [20].



XIII R= CH_3, C_2H_5 XIV

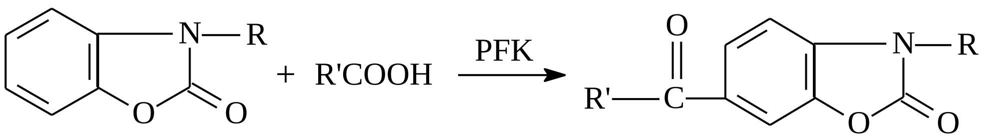
Indollar Fridel-Krafts bo'yicha atsillash reaksiyalariga turlicha kirishadi. Indolni (XV) atsetillash natijasida 2-atsetil (XVI) va 3-atsetilindollar (XVII) aralashmasi hosil bo'ladi [21].



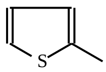
XV XVI XVII

Benzol halqasi bilan kondensirlangan ikki geteroatom tutuvchi besh a’zoli geterohalqali birikmalardan sanalgan benzoksazolin-2-onlarni benzol halqasini atsillash reaksiyalari juda kam o’rganilgan.

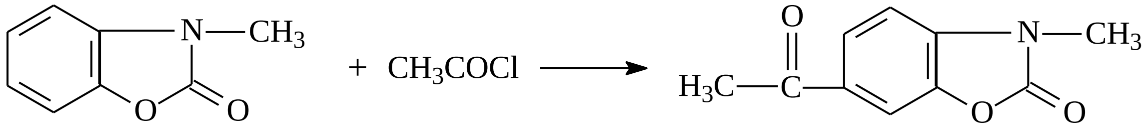
Ch.Lespagnol va hodimlarining [22] ma’lum qilishicha, benzoksazolin-2-onlar (XIX) karbon kislotalar xlorangidridlari bilan $AlCl_3$ ishtirokida reaksiyaga kirishmaydi. Shuning uchun ular 6-atsilbenzoksazolin-2-onlarning (XX) sintezini benzoksazolin-2-onlarni karbon kislotalar bilan polifosfor kislotasi (PFK) ishtirokidagi reaksiyasi natijasida amalga oshirishgan.



XII a –b XX

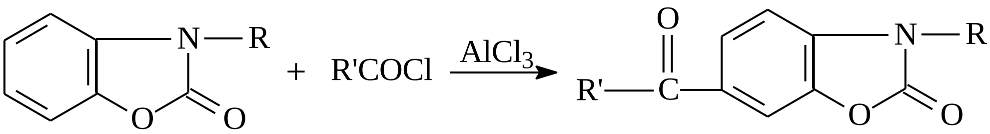
R= H, CH_3; R'= CH_3, CH_2Cl, C_2H_5, C_6H_5, 

Biroq keyinroq N.V.Sabishaya va hammualliflar [23] 3-metil-benzoksazolin-2-onni (XIXB) 4 marta ko’p olingan atsetillorid bilan $AlCl_3$ ishtirokida atsillab, 6-atsetil-3-metilbenzoksazolin-2-on (XX) sintezini amalga oshirgan va Ch.Lespagnolning benzoksazolin-2-onlar Fridel-Krafts bo’yicha atsillanmaydi [22] degan fikrini noto’g’ri ekanini isbotlashgan.



XIX b XX

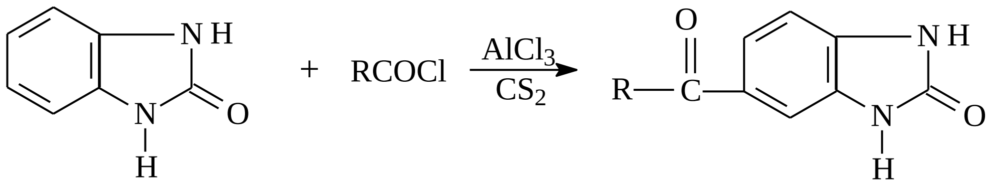
Keyinchalik N.A.Aliyev, N.S.Muhammedovlar boshqa benzoksazolin-2-onlar ham alifatik karbon kislotalari va perftor benzoy kislota xlorangidridlari bilan $AlCl_3$ ishtirokida reaksiyaga kirishib, tegishli 6-atsilbenzoksazolin-2-onlarni (XX) yuqori unum bilan hosil qilish mumkinligini ko'rsatishgan [24].



XIX a,b R=H, CH_3; R'= CH_3, CH_2Cl, C_3H_7, C_4H_9, C_6F_5 XX

Benzoksazolin-2-onlarning navbatdagi vakili bo'lgan benzimidozolin-2-onni (XXI-a) asetilxlorid va n-butiroilxlorid bilan $AlCl_3$ ishtirokidagi ta'siri natijasida 5-asetil va 5-butiroilbenzimidazolin-2-onlar (XXIIa-b) yuqori unum bilan olingan [25].

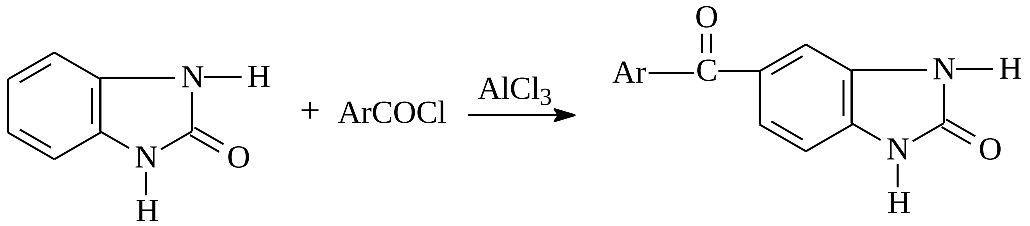
Klark va Pessolono tomonidan yuqorida qayd qilingan usulda benzimidazolin-2-onni (XXIa) boshqa alifatik karbon kislotalarning xlorangidridlari bilan reaksiyalari o'rganilib ,tegishli 6-atsilbenzimidazolin-2-onlar (XXII b-a) olingan [26].



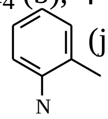
XXI a XXII a - e

R= CH_3 (a), H—C_4H_8 (v), izo - C_4H_9 (g), H—C_7H_{15} (d), H—$C_{13}H_{27}$ (e)

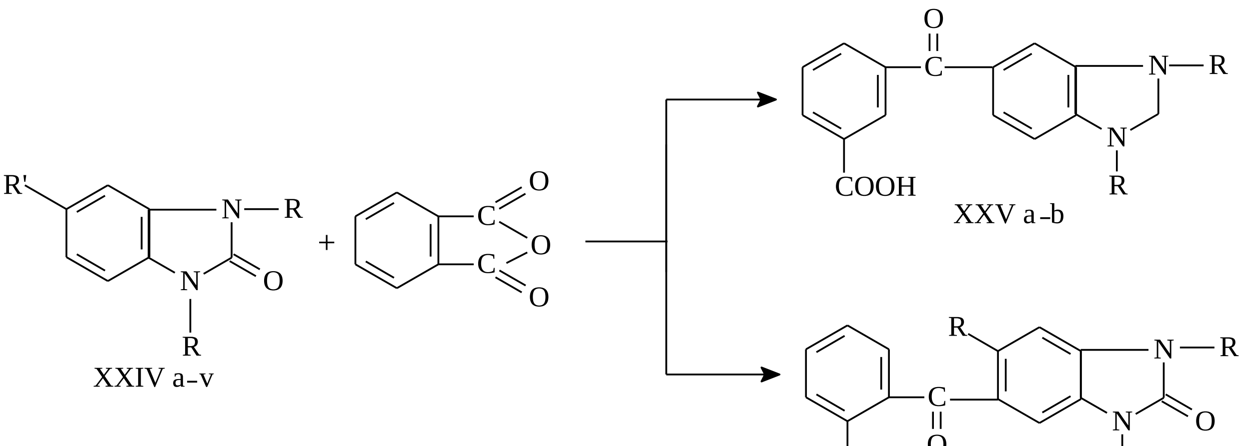
Farmokalogik faol moddalar topish maqsadida Yu.A.Rozin va hamma aliflari [27] tomonidan benzimidazolin-2-onni aromatik va geterohalqali kislotalar xlorangidridlari bilan $AlCl_3$ va ham katalizatorlar ishtirokidagi reaksiyalari o'rganilib, tegishli 5-aroilbenzimidazolin-2-onlar (XXIII a-j) sintez qilingan.



XXI a XXIII a- j

Ar= C_6H_5 (a), 3-$NO_2C_6H_4$ (b), 4-$NO_2C_6H_4$ (v), 3-$H_2NC_6H_4$ (g), 4-$H_2NC_6H_4$ (d), 4-$(CH_3)_2$, N—C_6H_4 (e),  (j).

XXIII a-v moddalar 2 mol $AlCl_3$ ishtirokida nitrobenzolga 70-100^{0}C da tegishli ravishda 47,73 va 80% unum bilan olingan bo'lsa, (XXIII e) modda uchun 7 mol $AlCl_3$ sarflangan.(XXIII j) modda $AlCl_3$, NaCl, KCl, NaF aralashmasi ishtirokida 110-120^{0}C da 49% unum bilan, (XXIII g,d) moddalari esa tegishli nitrohosilalarni (XXIII b,v) qaytarish usuli bilan olingan. L.F.Efrost va hodimlari benzimidazolin -2-onlarni (XXIV a-v) ftal angidridlari bilan $AlCl_3$ ishtirokida atsillashgan [28].Atsillash reaksiyalari dastlabki moddalarni 1:1:3:3 nisbatda 90^{0}C da tetraxlorid etanda 3,5 soat mobaynida qizdirish bilan olib borilib yaxshi unum bilan (57-64%) tegishli 5- va 6- (2-karboksibenzoil) benzimidazolin-2-onlar (XV a-b) olingan [28].

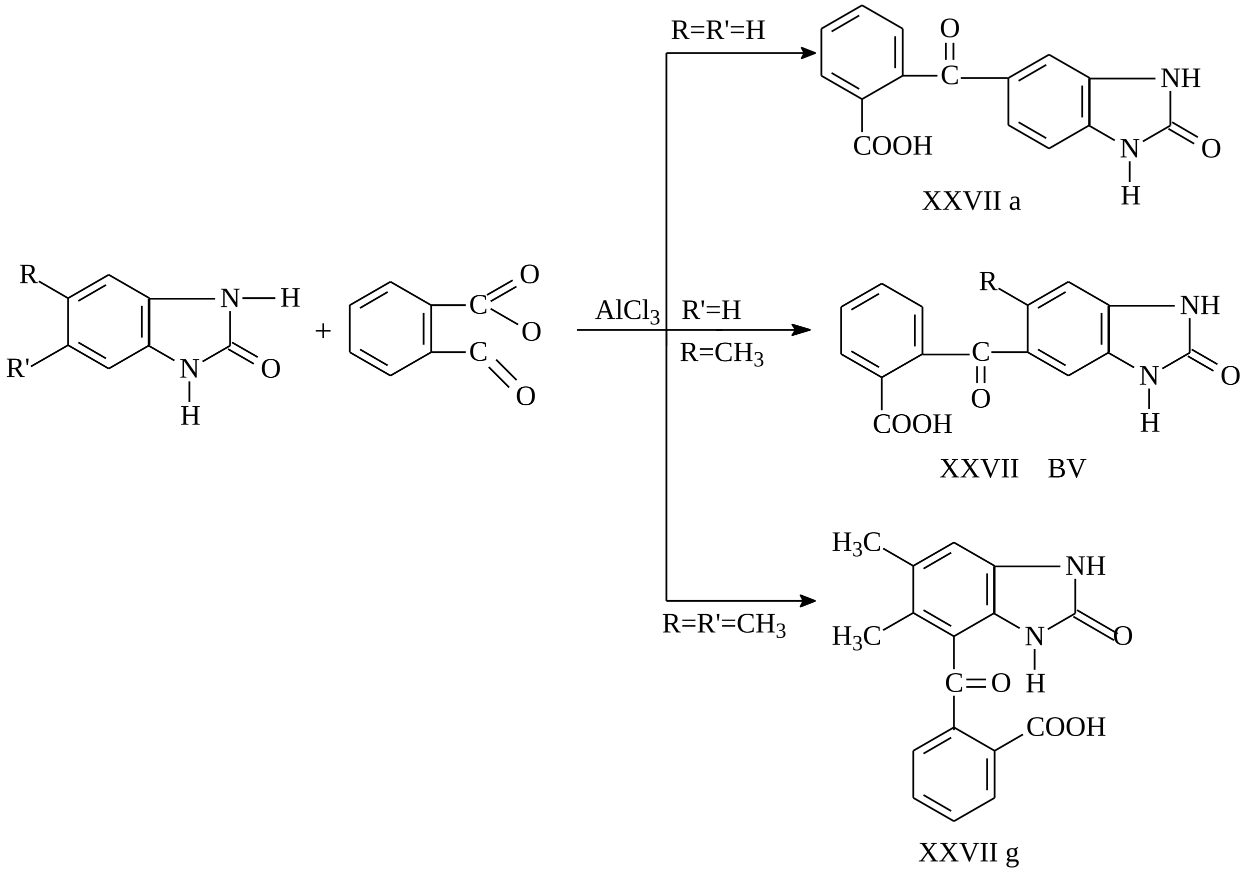


XXIV a–v XXV a–b XXV V

R=R'= H (a); R= CH_3, R'= H(b); R=H, R'=CH_3 (v)

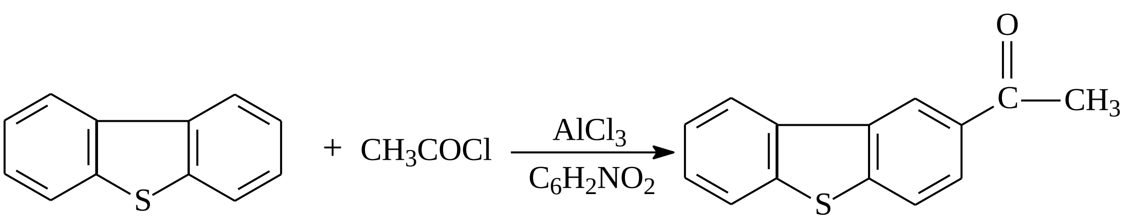
Ch.Sh.Qodirov va hodimlari tomonidan ushbu reaksiya boshqa benzimidazolin-2-onlarga (XXVII a-g) ham tadbiq etilgan va reaksiya natijasida tegishli 5-(2'-karboksibenzoil)-(XXVII a), 5-alkil-6-(2'-karboksibenzoil)-

(XXVII BV) va 4-(2’-karboksibenzoil) benzimidazolin-2-onlar (XXVII g) hosil bo’lishi aniqlangan. Reaksiya mahsulotlarining eng yuqori unumi dastlabki moddalarning 1:1:4 nisbatida va reaksion aralashmani tetraxloretilenda 95-100^0C da 3-soat mobaynida qizdirish yo’li bilan olingan [29].



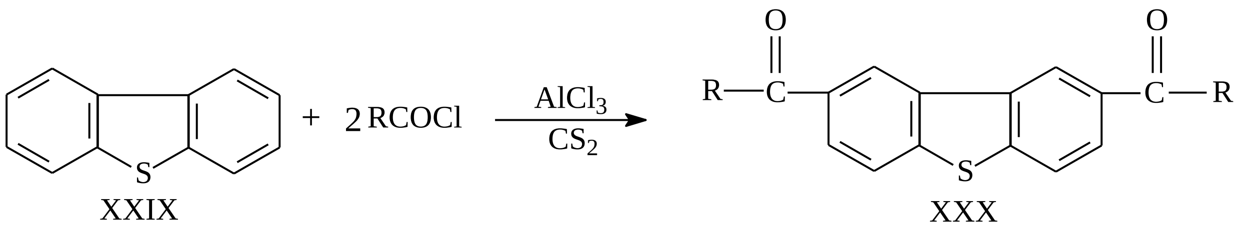
Fridel-Krafts bo’yicha atsillash reaksiyalariga ikki aromatik halqa bilan kondersirlangan 5-azoli geterohalqali birikmalar ham kirishadi.

Masalan, A.Burger va hodimlari tomonidan [30] dibenzotiofenni (XVIII) $AlCl_3$ ishtirokida nitrobenzolga asetillash natijasida 3-asetildibenzotiofen (XIX) olingan.

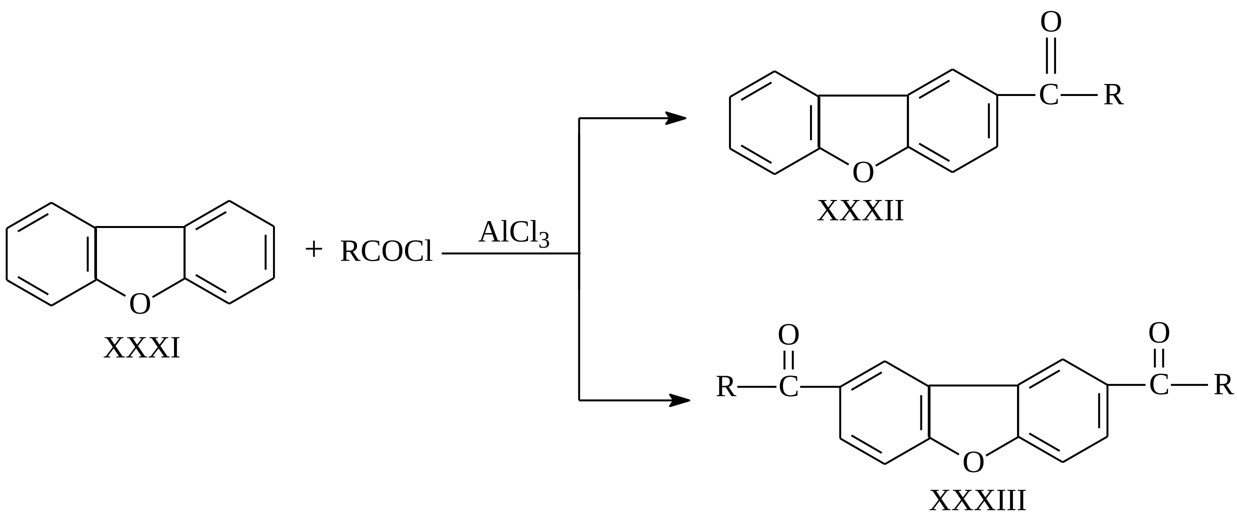


XXVIII XXIX

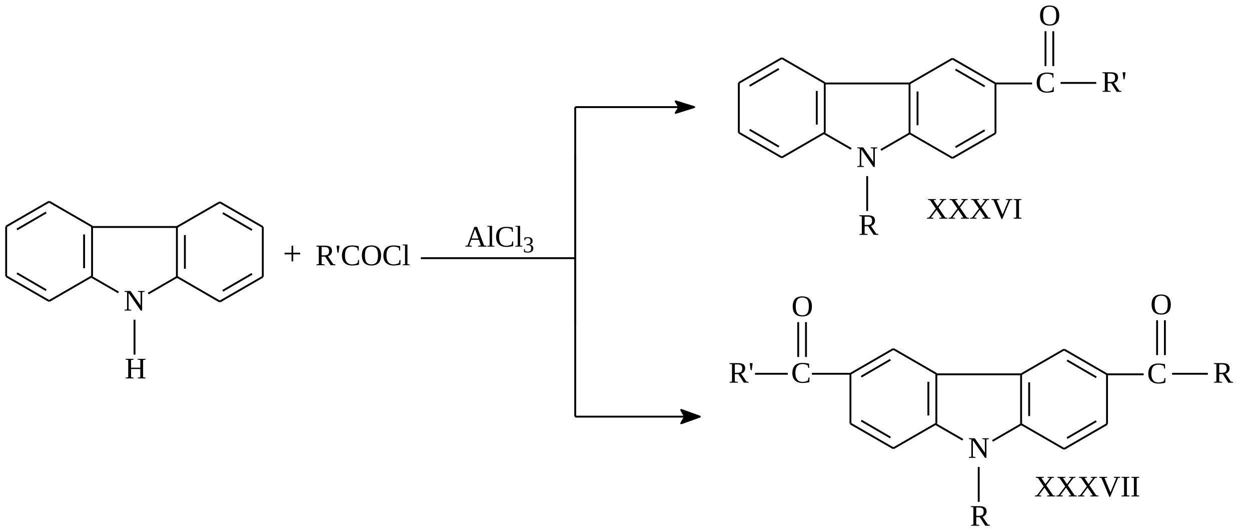
Xuddi shu mualliflar tomonidan dibenzotiofenni CS_2 eritmasida atsillash natijasida diatsilmahsulotlar-3,6-diatsilbenzotiofenlar (XXX) sintez qilingan [30].



Dibenzotiofenning kislorodli analogi dibenzofuranni (XXXI) turli kislotalar xlorangidridlari bilan $AlCl_3$ ishtirokida atsillab, 3-atsildibenzofuranlar (XXXII) olingan. Reagentlar nisbatini va reaksiya sharoitini o’zgartirib,3,6-diatsildibenzofuranlarni (XXXIII) sintezini amalgam oshirgan [31].



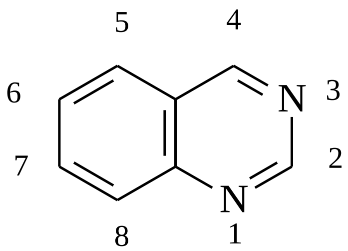
Dibenzotiofen va dibenzofuranning azotli analogi-karbazol Fridel-Krafts bo’yicha atsillash reaksiyalariga o’zining kislorodli va oltingugurtli analoglari singari kirishadi. Masalan,karbazol (XXXIV) va 9-alkilkarbazollar (XXXV) atsillash reaksiyalarining shart-sharoitiga qarab, 3-atsil-(XXXVI) va 3,6-diatsilkarbarbazollarning XXXVII sintezini amalga oshirish mumkin [32].



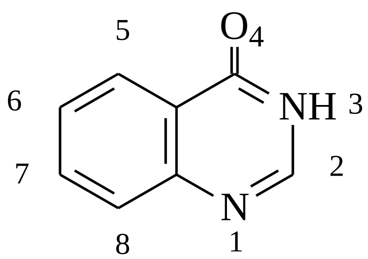
Yuqorida qayd qilinganlar asosida shuni ta’kidlash mumkinki, azot tutuchi geterohalqali birikmalar kislorod va oltingugurt tutuvchi geterohalqali birikmalarga nisbatan Fridel-Krafts bo’yicha atsillash reaksiyalariga nisbatan qiyin kirishadi.

1.2. Xinazolon-4 larning sintez usullari

Xinazolin (XXXVIII) va uning oksidlangan formasi - xinazolon-4 (XXXIX) haqida to’xtalib o’tamiz:



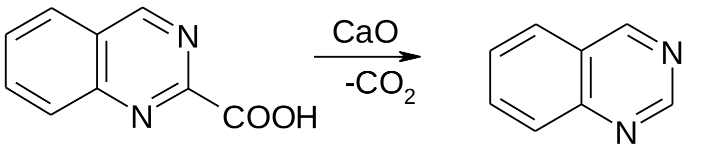
XXXVIII



XXXIX

Bu moddalarning tuzilishidagi farq shundan iboratki, xinazolon-4 molekulasining 4-xolatida karbonil (C=O) guruhining borligidadir.

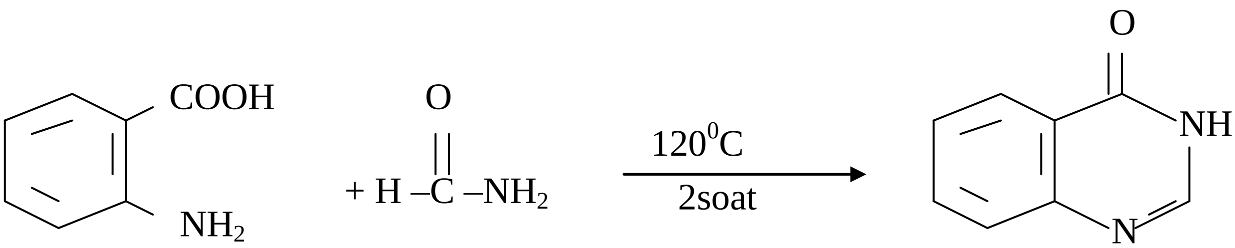
Birinchi bo'lib xinazolin 1895 yilda xinazolin-2-karbon kislotasini dekarboksillash yordamida olingan [33]



I

Xinazolin asos tabiatiga *ega* bo'lgan (pK_a=3,5) modda bo'lib, noorganik kislotalar bilan tuzlar hosil qiladi. Xinazolon-4 esa xinazolinga nisbatan ancha kuchsiz asos hisoblanadi. Bular ham kislotalar xam ishqorlar bilan reaktsiyaga kirishadi va tuzlar hosil qiladi.

Xinazolon-4 (II) sintezining umumiy usuli birinchi marta antranil kislotasi (L) bilan formamid (LI) aralashmasi 120°Cda 2 soat qizdirilganda ikki molekula suv chiqib ketishi xisobiga hosil bo'ladi [34]:

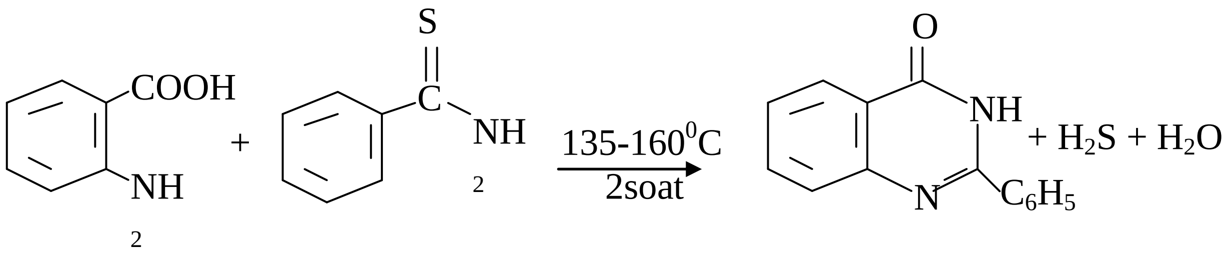


L LI XXXIX

Aromatik xalqada almashingan xinazolon-4 larni sintez qilish uchun antranil kislotasining ham har xil hosilalaridan foydalaniladi. Bunda reaktsiyalarni 180-200°C haroratda va uzoqroq vaqt olib borishga to'g'ri keladi. Tajribalar natijasida aniqlanganki, formamidlarning molekulyar massasi oshishi bilan reaktsiyaning ketishi qiyinlashadi. Hatto reaktsiya maxsulotining unumi deyarli o'zgarmaydi.

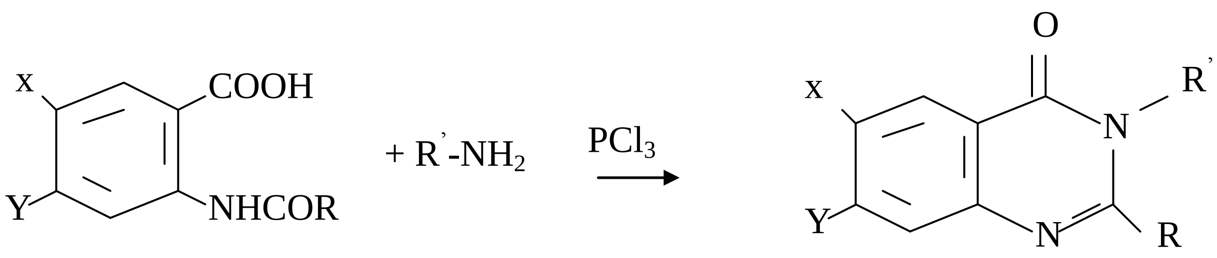
Bunday reaktsiyalarda amidning (LI) o'rniga tioamidlar ishlatilganda xinazolon-4 larning unumi ancha yuqori bo'ladi. Masalan, antranil kislotasining

(L) benzotioamid (LII) bilan reaktsiyasi natijasida 75- 98% unum bilan 2- fenil-xinazolon-4 (LIII) hosil bo’ladi [35]:



L LII LIII

2,3- Di almashgan xinazolon- 4 larni (LV) N-atsetil-antranil kislotasi (LIV) va har xil aminlarning fosfor (III) xlorid yoki polifosfor kislotasi ishtirokida olishning umumiy usuli taklif qilingan [36-38]:



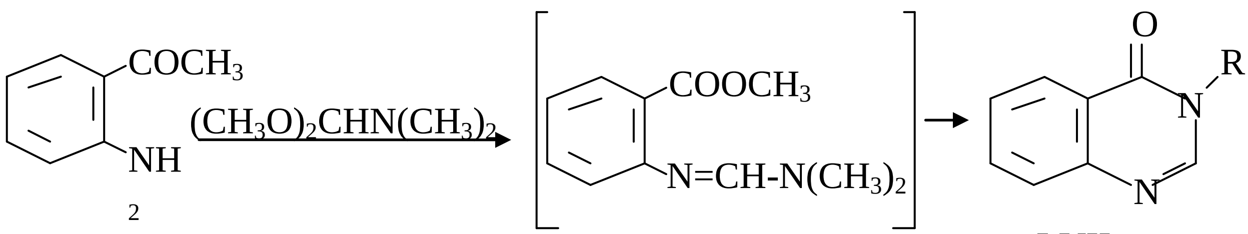
LIV

LV

R=H, CH_3, C_2H_5; R’=aril

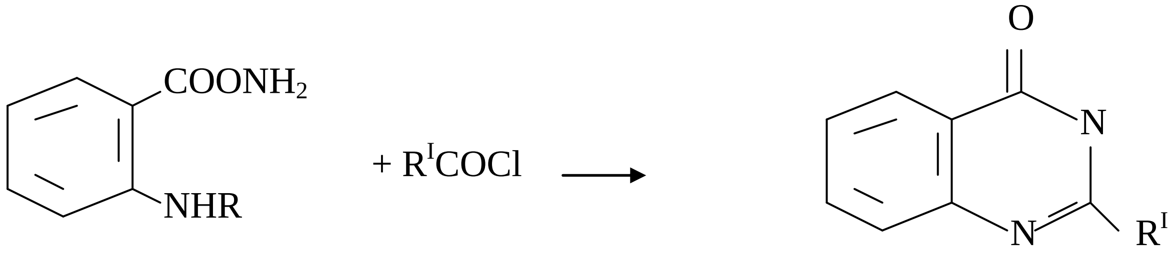
X=Y=H, Cl, NO_2

3-Almashgan xinazolon-4 (LVII) larni sintez qilish uchun antranil kislotasinin metil efir (LVI) bilan dimetilformamidning dimetilatsetali o’zaro ta’sirlashtiriladi. Reaktsiya aminlar ishtirokida ketadi [39]:



LVI LVII

Antranilamid (LVIII) kislotalarning xlorangidridlari bilan kondensatsiyalanishi natijasida tegishli xinazolon- 4lar hosil bo’ladi [40,41]:

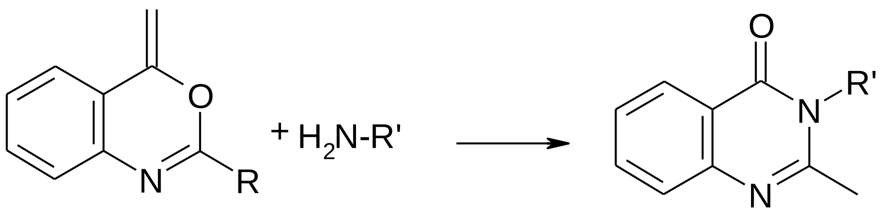


LVIII

LIX

R=H, alkil, aril; R^I=aril

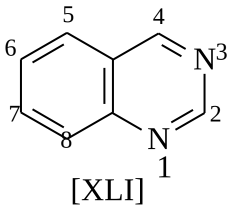
Benzoksazin-3,1-onlarning (XL) birlamchi aminlar bilan reaktsiyalari o’tkazilganda tegishli 2,3-dialmashgan xinazolon- 4 lar (XL) hosil bo’ladi [42]



Bu reaktsiya uchun kerakli benzoksazin-3,1-onlar antranilamid kislotali va kislota xlorangidridlarini sirka angidridda qizdirish bilan olinadi.

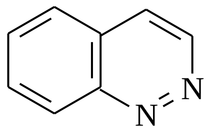
1.3. Xinazolinlarni elektrofil almashinish reaksiyalari.

Xinozolin nomi 1887-yilda halqali sistema [XLI] ni nomlash uchun taklif etildi [43]

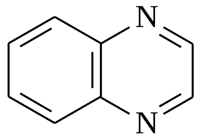


[XLI]

Xinozalin sistemasini nomerlash [XLI] formuladagidek qabul qilingan. O'sha vaqtda xinozalinning xinnolin [XLII] va xinoksolin [XLIII] izomerlari ma'lum edi.



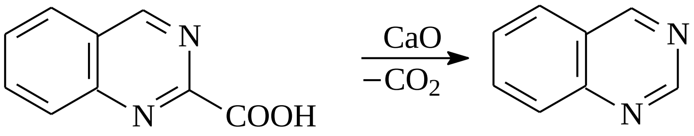
[XLII]



[XLIII]

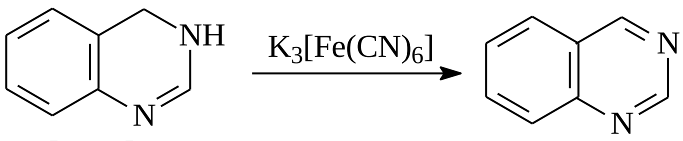
Xinozolin qatorining birinchi vakili 2-siano-3,4-digidroxinozolon-4 1869-yilda sintez qilingan [44].

Xinazolin-2-karbon kislotani [XLIV] dekarboksillab xinozolin olingan[44].



[XLIV] [XLI]

Keyinchalik esa 3,4-digidroxinazolinni [XLV] yumshoq sharoitda ishqoriy muhitda qizil qon tuzi eritmasi bilan oksidlab olingan[44].

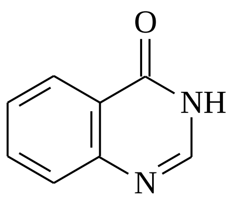


[XLV] [XLI]

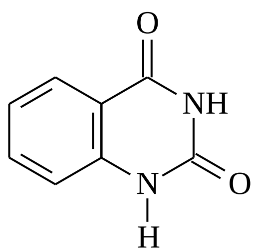
Xinazolin pKa 3,5 pirimidin (pKa 1,31) va 4-metilxinozalin (pKa 2,52) ga nisbatan kuchliroq, 2-metilxinazolin (pKa 4,52) va 2,4-dimetilxinozalinga nisbatan kuchsiz asos xossasiga ega.

Xinazolin mineral kislotalar bilan tuzlar hosil qiladi.

Xinazolin hosilalarini, shu jumladan xinazolon-4 [XLVI] va xinazolin-2,4-dion [XLVII]larni atsillash reaksiyalari juda kam o'rganilgan.



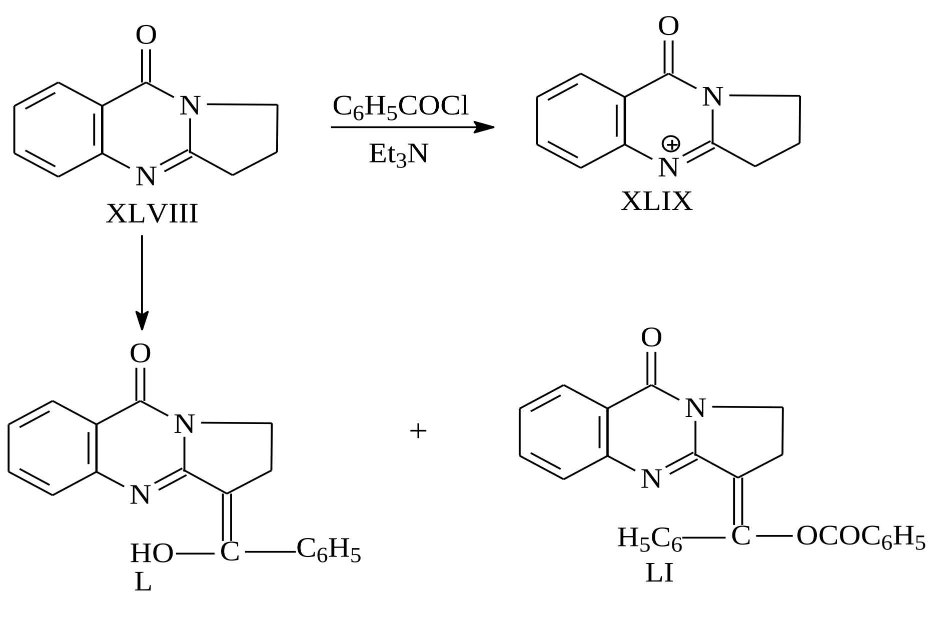
[XLVI]



[XLVII]

Faqatgina xinazolin hosilalaridan uch halqali xinazalonlarni atsillash reaksiyalari o’rganilgan va ularda reaksiya yo’nalishi bir necha omillarga: metilen guruhlar soniga, aromatik halqadagi o’rinbosar tabiatiga , xinazolon va atsillovchi agent mol nisbatlariga bog’liqligi ko’rsatilgan. 1,2,3,9-tetragidropirrolo [2,1-v] xinazolon-9 [XLVIII] ni benzoilxlorid bilan trietilamin ishtirokida reagentlarning mol nisbati 1:1:1,3 bo’lganda faqat N-benzoilxinazolin [XLIX] hosil bo’lgan. Reagentlarning mol miqdori 1:2:1,3 bo’lganda 3-(α-gidroksibenziliden)- 1,2,3,9-tetragidropirrol [2,1-v] xinazolon-9 [LI] (30%) aralashmasi hosil bo’lgan.

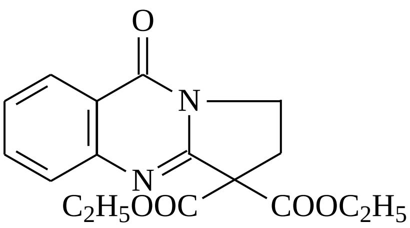
Benzoilxlorid va tetraetilaminni miqdorini oshirish atsillash mahsuloti unumini oshiradi.(masalan: reagentlarning mol nisbati 1:10:10 bo’lganda unum 43% ga oshgan) trietilaminni miqdorini kamayishi mahsuloti unumini pasayishiga olib keladi [44].

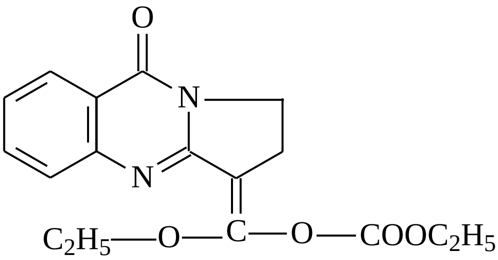


1,2,3,9-tetragidropirrolo [2,1-v] xinozalon-9 o-p-metoksi-, p-nitrobenzoy kislata xlorangidridlari bilan ta’sirlashib (reagentlarning mol nisbati xinazolon-xlorangidrid-TEA 1:4:2) 3-(2-azoiloksiariliden)-1,2,3,9-tetragidro-pirrolo [2,1-v] xinozalon-9 hosilalari olingan [44].

1,2,3,9-tetragidropirrolo [2,1-v] xinozalon-9 ni xlorsirka kislotani etil benzilefiri bilan atsillash natijasida 3,3-dietoksi(butoksi) karbonil-1,2,3,9-

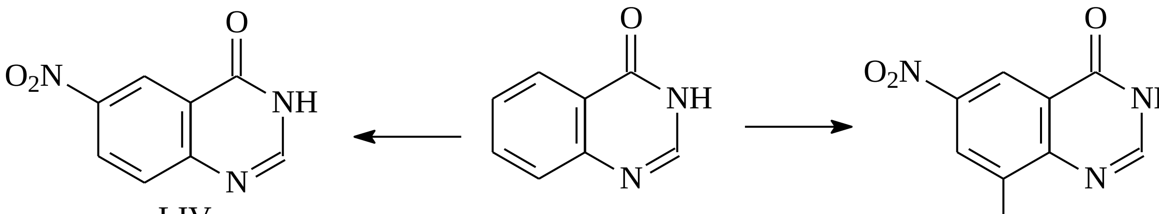
tetragidropirrolo [2,1-v] xinozalon-9 [LII] va 3-(α-etoksi-etoksi karbonil)-1,2,3,9-tetragidropirrolo [2,1-v] xinozalon-9 [LIII] [45].


LII

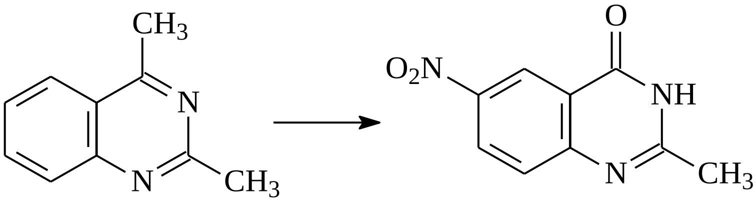

LIII

Qizdirish 150^{O}C da davom ettirilsa birinchi maxsulot, agar reaksiya 8-10 soat davomida olib borilsa ikkinchi mahsulot hosil bo'ladi.

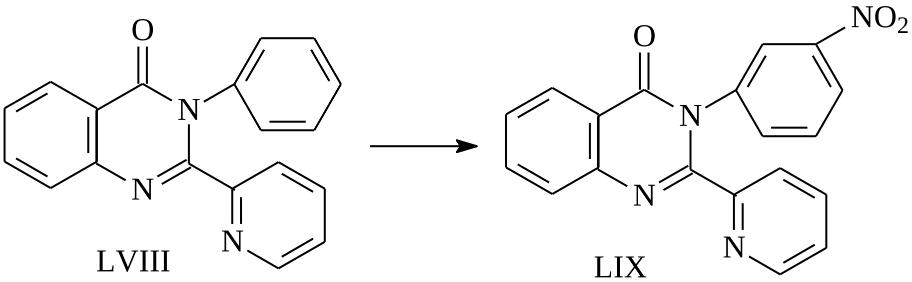
Xinazolon -4 [XLVI]ni nitrolash natijasida faqat 6-nitro-xinazolon-4 [LIV] hosil bo'lgan [37]. Xinazolon-4 ni nisbatan qattiq sharoitda nitrolash natijasida 6,8 –dinitro-3,4-dinitroxinazolin-4 [LV] hosil bo'lgan.


LIV XLVI LV

Xinazolinni nitrolash natijasida ham nitroguruh 6-holatga boradi [47] , 2,4-dimetilxinazolinni [LVI] nitrolashda esa bir vaqtning o'zida 4-holatdagi metil guruh ajralib chiqib, 4-holat oksidlanadi va 2-metil -6-nitroxinazolin-4 [LVII] olingan [48].

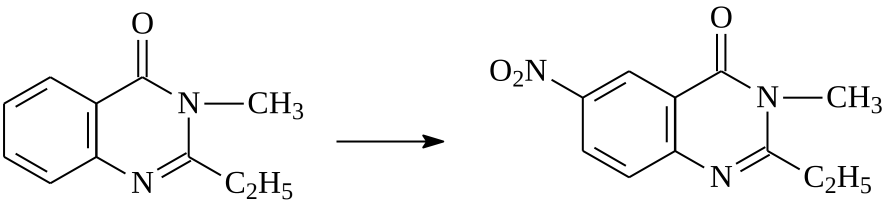

LVI LVII

2-(piridil-2)-3-fenil-3,4-digidroxinazolon-4 [LVIII] ni nisbatan yumshoq sharoitda (0-30^{o}C) nitrolash o'rganilgan. Bunda bir vaqtning o'zida benzol xalqasining 3-holati va xinazolon halqasi nitrolanib 2-(piridil-2)-3-(m-nitrofenil)-6-nitro-3,4-digidro-xinazolon -4 [LIX] hosil bo'lgan. Nisbatan qattiq sharoitda (80^{o}C) bu maxsulotdan tashqari (unimi 12%) 3 ta nitroguruh tutgan mahsulot olingan, lekin olingan moddadagi nitroguruhlarning joylashgan holatini aniqlay olmaganlar [40].



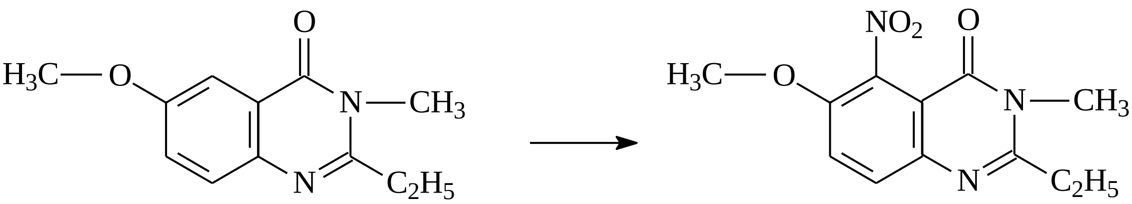
LVIII LIX

2-etil-3-metil-3,4-digidraxinazolin-4[LX] nitrolashda nitroguruh 6-holatga boradi va tegishli 6-nitro-2-etil-3-metil xinazolin-4 [LXI] olingan [44].



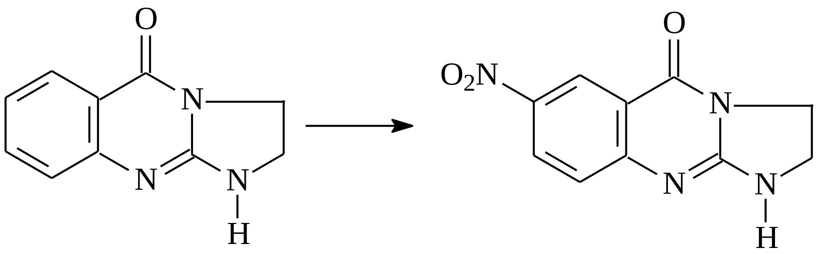
LX LXI

Agar 6- holatda turli o’rinbosar bo’lsa, asosan elektronodonor guruh bo’lganda elektrofil almashinish 5-chi uglerodga boradi. Masalan: 2-etil-3-metil-6-metoksixinazolon-4 [LXII] nitrolanganda 5-nitro-2-etil-3-metil-6-metoksixinazolon-4 [LXIII] hosil bo’lgan.



LXII LXIII

1,2,3,5-tetrogidroimidazo [2,1-v] xinazolon-5 [LXIV] nitrolanganda 7-nitro-1,2,3,5-tetrogidroimidazo [2,1-v] xinazolon-5 [LXV] olingan [50].



Xinazolon-4 [XLVI] ni oleum va xlorsulfon kislata bilan sulfolash va sulfoxlorlash reaksiyasi o’tkazilganda 6-holatdagi vodorod almashinadi va tegishli 6-sulfoksi- va –xlorsulfo almashingan maxsulotlar olingan [46].

2–BOB. 1-Metilxinazolin-2,4–dionni $FeCl_3 \cdot 6H_2O$ katalizatori ishtirokida aromatik kislota xlorangidridlari bilan katalitik atsillash

Fridel-Krafts reaktsiyasi bo'yicha geteroxalqali birikmalarni atsillashda eng yaxshi katalitik samara kuchli ($AlCl_3$) va urtacha kuchli ($FeCl_3$, $ZnCl_2$, $SnCl_4$ va boshqalar) Lyuis kislotalarida namoyon bo'ladi. Ular atsillovchi agentlar bilan mustaxkam donor-aktseptor bog' hosil qilganligi tufayli atsillovchi agent karbonil guruxining qutbliligi ortadi va buning natijasida karbonil uglerodidagi musbat zaryadning ortishiga olib keladi. Bu esa o'z navbatida aromatik va geterotsitslik xalqa tomonidan bo'ladigan nukleofil xujumni osonlashtiradi.

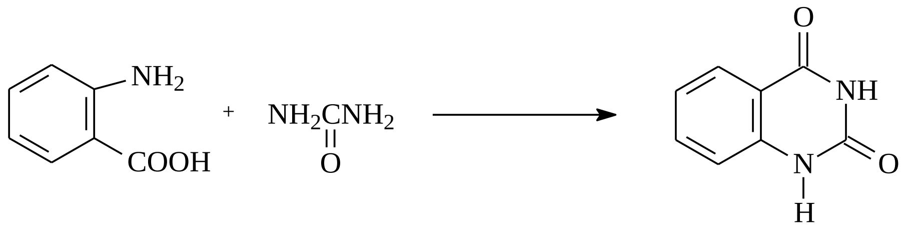
Fridel-Krafts reaktsiyalarida jarayonning borishi Lyuis kislotalarining atsillovchi agentlarni faollashtirish xamda katalizitorning reaksiya maxsuloti bilan mustaxkam kompleks xosil qilishi bilan bog'lik

Adabiyotlardagi ma'lumotlar taxlili shuni ko'rsatadiki benzazolin-2-onlarni Fridel-Krafts buyicha atsillash reaktsiyalari keng o'rganilgan, ammo uni olti a'zoli analogi xinazolin-2,4-dionlar misolida urganilmagan. Shuning uchun biz xinazalonlarni reaksiyalarini o'rganib, ushbu sinf birikmalarining atsil xosilalarini sintezini sodda va qulay usullarini ishlab chiqishni o'z oldimizga maqsad qilib qo'ydik.

Buning uchun zarur bo'ladigan dastlabki moddani quyida keltirilgan tartibda sintezini amalga oshirdik.

2.1. Xinazolin-2,4–dionni olinish usuli

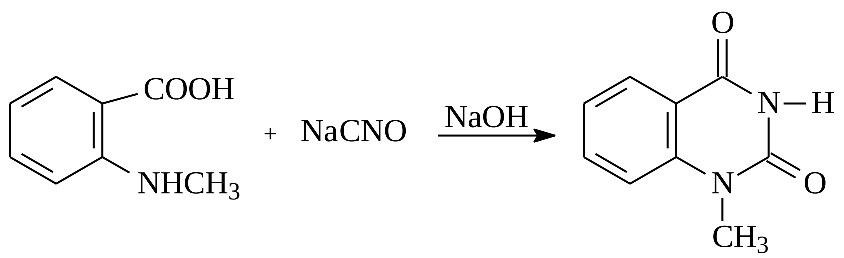
Xinazolin-2,4–dion antranil kislotani mochevina bilan 1:1,5 mol nisbatda 140-150^0 C xaroratda qum xammomida bir og'izli kolbada qizdirish natijasida olindi. Reaksiya 6 soat davom ettirildi. Reaksion aralashma sovutilgach 2% li ishqor eritmasi bilan ishlandi, keyin filtrlandi. Filtrdan o'tgan ishqorli eritma xlorid kislota bilan pH=1 gacha ishlandi. Cho'kmaga tushgan xinazolin-2,4-dion filtrlab olindi va neytralgacha yuvildi, quritildi suyuqlanish harorati 350-352 ^{0}C.



Sintez qilingan xinazolin-2,4-dionning fizik-kimyoviy konstantalari adabiyotlarda keltirilganiga mos keladi.

2.2. 1-Metilxinazolin-2,4-dionni olinish usuli

Fridel-Krafts bo'yicha atsillash reaksiyalarini amalga oshirish uchun tanlangan 1-metilxinazolin-2,4-dion N-metilantranil kislotani natriy sianat bilan 1:1,5 mol nisbatda 70-75 ^{0}C haroratda sikllanishi natijasida olindi. Reaktsion aralashma sovutilgandan keyin tushgan cho'kma filtrlab olindi va neytralgacha yuvildi, quritildi va 75% sirka kislotada qayta kristallandi, suyuqlanish harorati 276-278 ^{0}C.

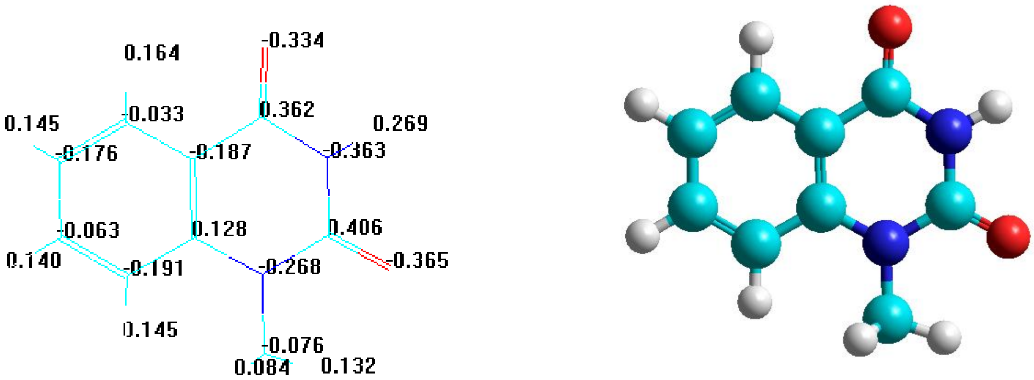


Sintez qilingan 1-metilxinazolin-2,4-dionning fizik-kimyoviy konstantalari adabiyotlarda keltirilganiga mos keladi.

2.3. 1-Metilxinazolin-2,4-dionni aromatik kislota kislota xlorangidridlari bilan katalitik atsillash

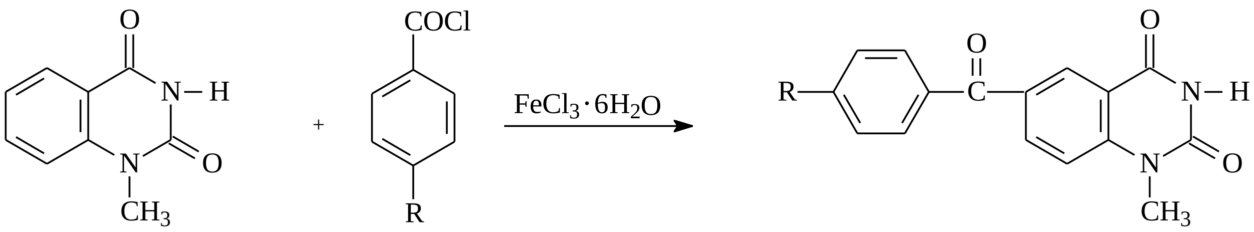
Xinazolin-2,4-dionlarning kimyoviy xossalarini sistematik o'rganish va ular qatorida yangi biologik faol moddalar izlash maqsadida 1-metilxinazolin-2,4-dionni Fridel-Krafts buyicha atsillash reaksiyalarini o'rganish bizda qiziqish uyg’otdi. 1-metilxinazolin-2,4-dionni aromatik xalqasini qaysi xolatiga atsil guruhini borishini o’rganish uchun dastlab uni tuzilishini Hyper Chem programmasi yordamida kvant-kimyoviy xisoblashlar qilindi. Qilingan kvant-kimyoviy hisoblashlar natijasiga ko’ra molekuladagi elektron zaryadlarning taqsimlanishi va molekulaning fazoviy shakli quyidagicha tasvirga ega (1-rasm).

1-metilxinazolin-2,4-dionni molekulasini kvant-kimyoviy hisoblashlar natijasiga ko’ra molekuladagi elektron zaryadlarning taqsimlanishi va molekulaning fazoviy shakli



1-metilxinazolin-2,4-dionni molekulasini kvant-kimyoviy hisoblashlar natijasiga ko’ra molekuladagi elektron zaryadlarning eng ko’p to’plangan joyi bu aromatik xalkadagi 6-xolatdir. Demak atsil guruxi 6-xolatga borishi kerak. Buni amalda tekshirish uchun biz 1-metilxinazolin-2,4-dionni aromatik kislota xlorangidridlari bilan atsillash reaktsiyalarini o’rgandik.

1-metilxinazolin-2,4-dionni **(I)** aromatik kislota xlorangidridlari benzoil xlorid (**II a**), 4-brombenzoilxlorid (**II b**) va 4-nitrobenzoilxlorid (**II v**) bilan $FeCl_3 \cdot 6H_2O$ ishtirokida reagentlarning $I:II:FeCl_3 \cdot 6H_2O = 1:1,5:1 \cdot 10^{-2}$ molyar nisbatlarida erituvchisiz sharoitda 4 soat davomida 150-160^{0}C da qizdirish natijasida tegishli 1-metil-6-aroilxinazolin-2,4-dionlar (**III a-v**) sintezini amalga oshirdik. Tadqiqot natijalari 1-jadvalda keltirilgan.



I **IIa-v** **IIIa-v**

IIa R=H, b R =Br, v R=NO_2;

IIIa R=H, b R =Br, v R=NO_2;

1-jadval

1-Metil-6-aroilxinazolin-2,4-dionlarning (III a-v) ayrim fizik-kimyoviy tavsiflari

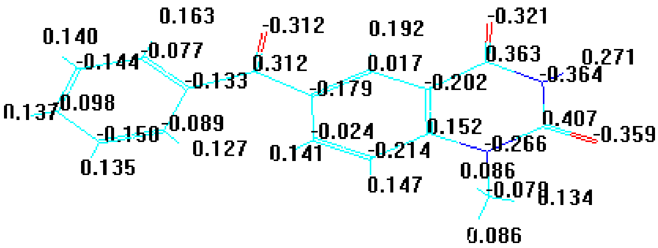
Birikma	Brutto Formula	T.s.,* ^{0}C Qayta kristallash uchun erituvchi	Mass-spektr, $[M^+]$ m/z, %	IQ spektr, ν, sm^{-1} (2-C=O), (4-C=O), (6-C=O)	Unumi, %
IIIa	**$C_{16}H_{12}N_2O_3$**	301-303 (этанол)	280 (32)	1705, 1700, 1665	62
IIIb	**$C_{16}H_{11}BrN_2O_3$**	296-297 (этанол)	361 (38)	1710, 1695, 1670	74
IIIv	**$C_{16}H_{11}N_3O_5$**	309-311 (этанол)	325 (45)	1715, 1695, 1675	82

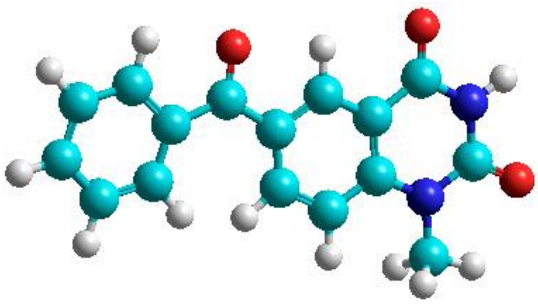
Sintez qilingan 1-metil-6-aroilxinazolin-2,4-dionlarning (**IIIa-v**) tuzilishi IQ-spektroskopiya, mass-spektrometriya usullari va element analiz bilan tasdiqlandi. Ularning IQ-spektrlarida 6-xolat karbonil guruxining valent tebranishlariga (1670-1675 sm^{-1}) va 1,2,4-uch almashgan benzol halqasi CH fragmentining notekis deformatsion tebranishlariga (805-825 va 870-885 sm^{-1}) xos yutilish chiziqlarini kuzatish mumkin.

Moddalarning mass-spektrlarida taklif etilgan tuzilishni tasdiqlovchi molekulyar ionlar va fragmentlarning borligi aniqlandi.

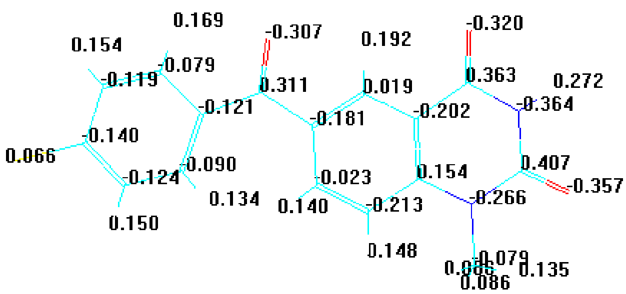
1-metil-6-aroilxinazolin-2,4-dionlarning (**IIIa-v**) tuzilishini HyperChem programmasi yordamida qilingan kvant-kimyoviy hisoblashlar natijasiga ko'ra molekuladagi elektron zaryadlarning taqsimlanishi va molekulaning fazoviy shakli quyidagicha tasvirga ega.

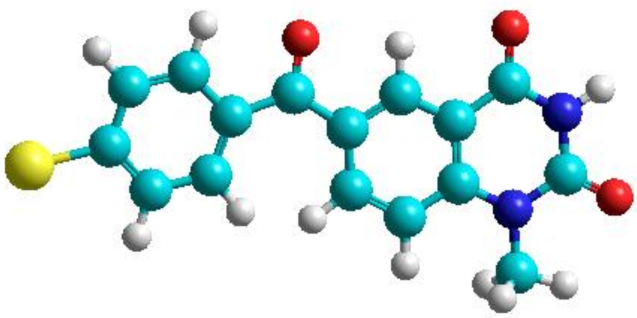
1-metil-6-benzoilxinazolin-2,4-dion



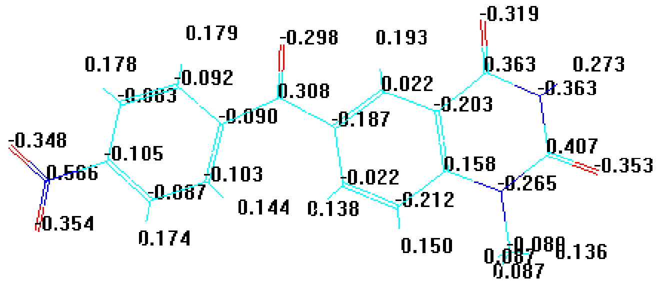


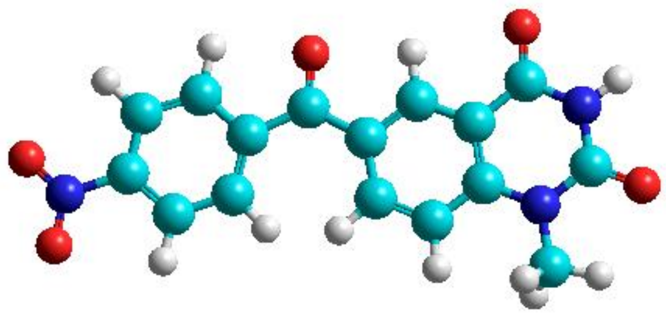
1-metil-6-(4`-brombenzoil)xinazolin-2,4-dion





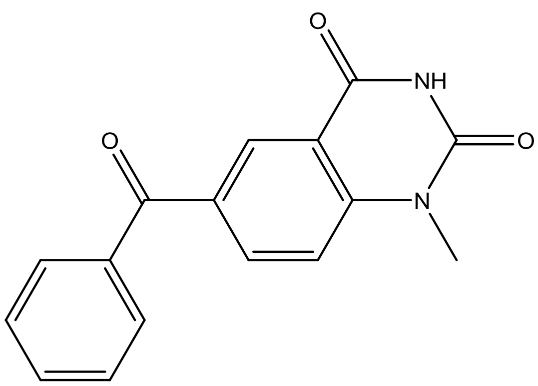
1-metil-6-(4`-nitrobenzoil)xinazolin-2,4-dion

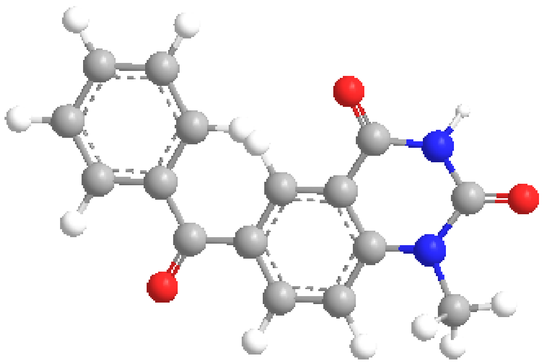


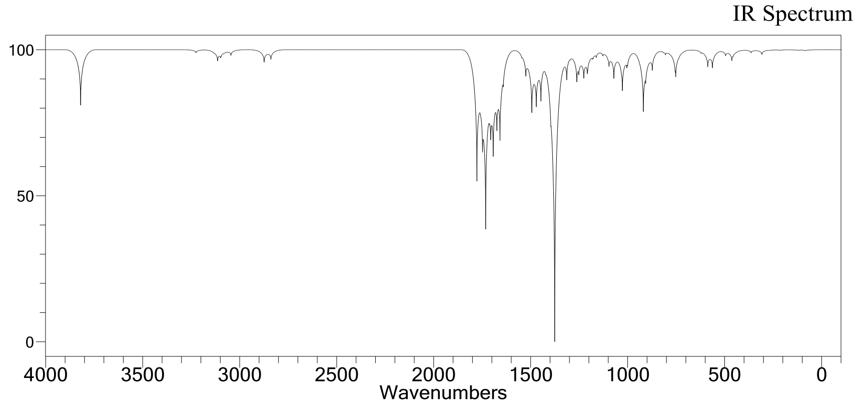


Shunday qilib, 1-metilxinazolin-2,4-dionning aromatik kislota xlorangidridlari bilan reaktsiyalari o’rganilib, yuqori unum bilan 1-metil-6-aroil-xinazolin-2,4-dionlar sintezi amalga oshirildi. Mahsulotlarning (**IIIa-v**) shar-sterjenli fazoviy ko’rinishi va atomlardagi elektronlar zichligi hisoblandi, IQ-spektrlari olindi.

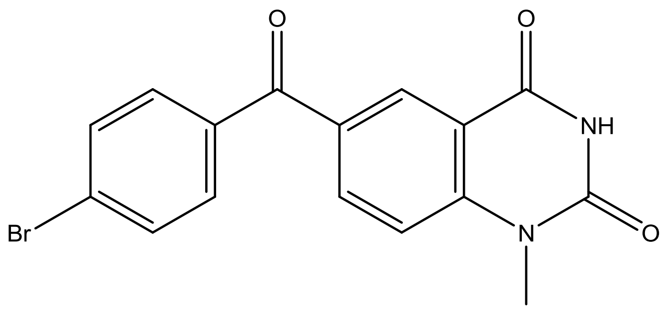
1-metil-6-benzoilxinazolin-2,4-dion

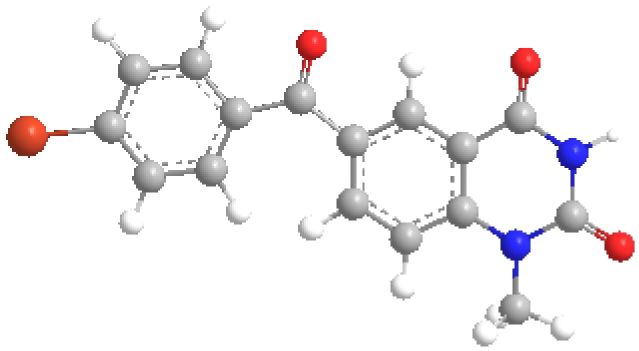


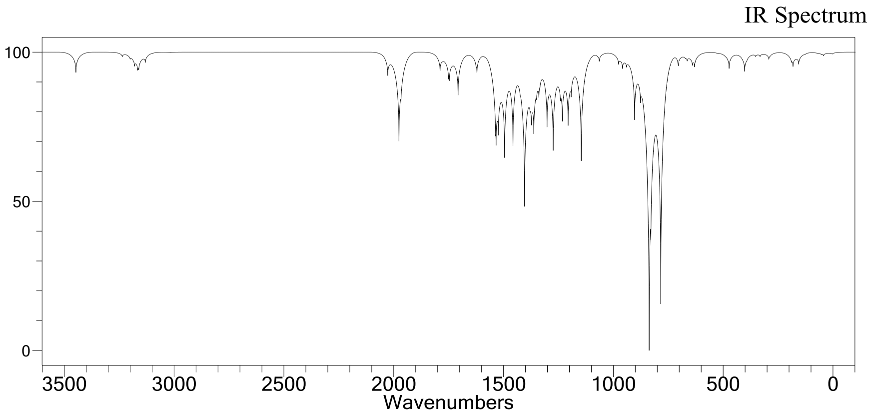




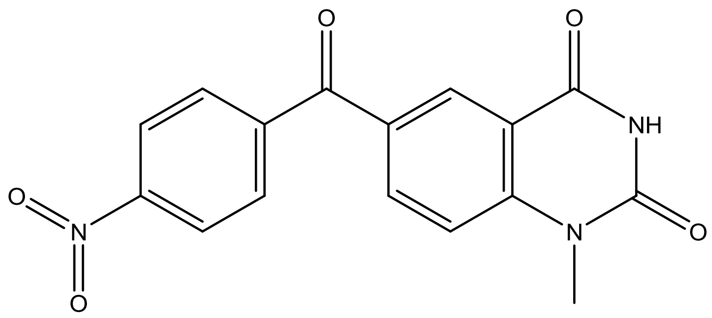
1-metil-6-(4`-brombenzoil)xinazolin-2,4-dion

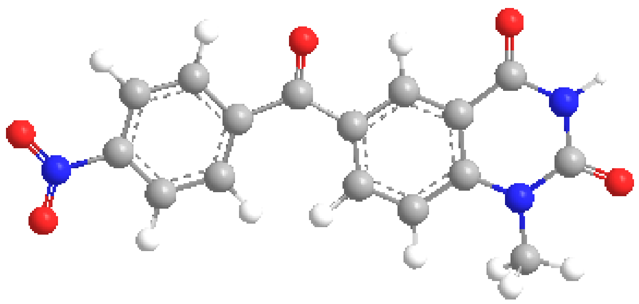


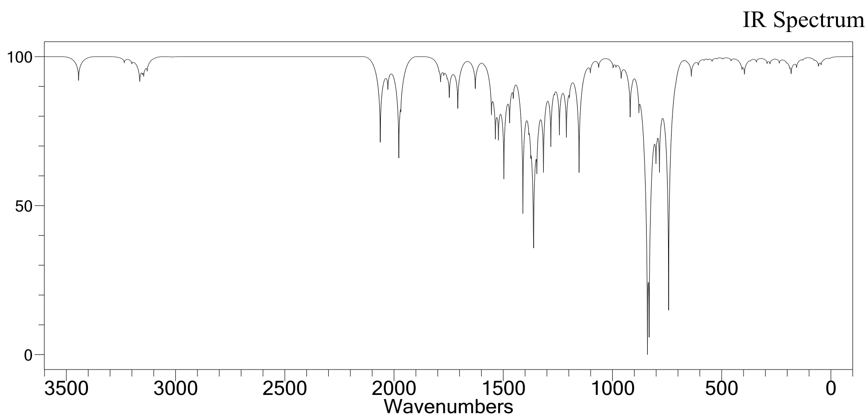




1-metil-6-(4`-nitrobenzoil)xinazolin-2,4-dion







3 – BOB. TAJRIBA QISMI

Reaktsiyalar borishini va moddalarning tozaligini yupqa qatlamli xromotografiya (YUQX) usuli bilan nazorat qilindi (Silufol UV-254, ochuvchi (proyavitel)–1 g $KMnO_4$ + 4 ml konts.H_2SO_4 + 96 ml H_2O).

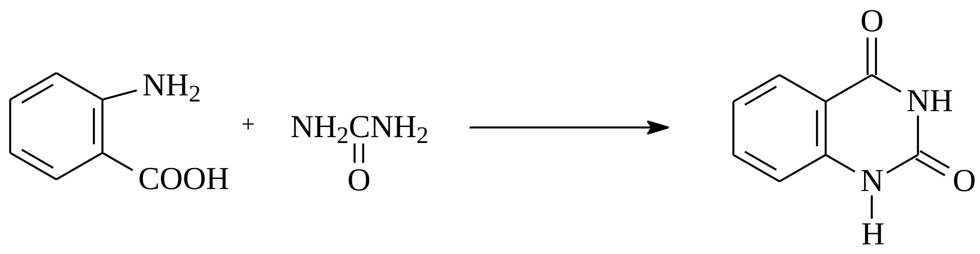
Moddalarning IQ-spektrlari UR-20 spektrometrda KBr tabletkasida olindi.

Mass-spektrlar MS 25-RF (Kratos) spektrometri ion manbasiga namunani bevosita kiritish yo'li bilan olindi (ionlantiruvchi elektronlarning energiyasi 70 eV, ion manbasining harorati 250^0C, namunani kiritish tizimining harorati 200^0C).

Barcha foydalanilgan moddalarning tavsiflari adabiyotlarda keltirilganlariga mos keladi.

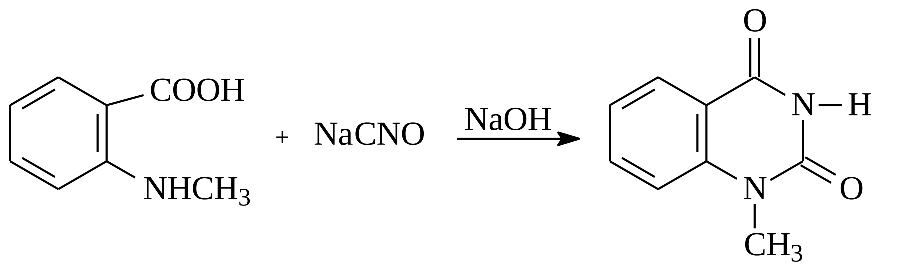
3.1. Xinazolin-2,4-dionni sintezi

Xinazolin-2,4-dion (I). Yumaloq tubli kolbaga 20,55 g (0,15 mol) antranil kislota va 11,2 g (0,2 mol) mochevina xovvonchada ezilgan aralashmasi solinib 200-210 ^{0}C da moy hammomida 4 soat mobaynida qizdirildi. So'ngra aralashma sovitilib unga 10 % li $NaHCO_3$ eritmasi solindi. Tushgan cho'kma filtrlanib 5% li NaOH da eritildi 30 g aktivlangan ko'mir solib qaynatildi va filtrlandi. Sovutilgan filtratga pH 3-4 oraligiga kelguncha 10% li HCl kislota eritmasi quyildi, tushgan cho'kma filtrlandi va neytral muhitgacha suv bilan yuvildi. Cho'kma kuritildi va 18,2 g (75 %) xinazolin-2,4-dion olindi, suyuqlanish harorati 350-352 ^{0}C.



3.2. 1-Metilxinazolin-2,4-dionni sintezi

Yumaloq tubli kolbaga 15,1 gr (0,1 mol) N-metilantranil kislota va 40 ml 50% li sirka kislota eritmasidan quyildi va aralashtiririlib turgan holda 9,1 gr (0,14 mol) natriy sianat kristallari solindi. Reaksion aralashmaning harorati 40 ^{0}C ushlab turilgan holda 60 gr (1,5 mol) NaOH kristallari solinib, 75 ^{0}C da 4 soat mobaynida qizdirildi. Hosil bo'lgan cho'kma filtirlab olindi va 200 ml suvda quyildi. Sovitilgan filtratga pH 1-2 oraligiga kelguncha sulfat kislota quyildi, tushgan cho'kma filtrlandi va neytral muhitgacha suv bilan yuvildi, quritildi, 50% li sirka kislota bilan qayta kristallandi va 14,7 gr (84 %) 1-metilxinazolin-2,4-dion olindi , suyuqlanish harorati 276-278 ^{0}C. **R_f**= 0.42. $C_8H_6N_2O_2$. Adabiyotda keltirilgan suyuqlanish harorati 277-279 ^{0}C.



3.3. 1-Metilxinazolin-2,4-dionni aromatik kislota xlorangidridlari bilan reaksiyalari

1-Metil-6-Benzoilxinazolin-2,4-dion (IIIa) sintezi. Tubi dumaloq uch og'izli kolbaga 3,52 g (0,02 mol) 1-metilxinazolin-2,4-dion (**I**) solib ustiga 4,2 g (0,03 mol) benzoilxlorid va 0,054 g (0,0002 mol) $FeCl_3 \cdot 6H_2O$ katalizatori kushildi. So'ngra reaktsion aralashma 140-150^{0}C da HCl ajralishi susayguncha 4 soat davomida aralishtirgichda aralashitirildi. Reaktsiya tugagach, reaktsion aralashma xona xaroratigacha sovitildi va suv bilan, so'ngra $NaHCO_3$ bilan ishlandi. Cho'kma filtrlab olindi, quritildi va benzolda qayta kristallantirildi.

3,47 g (62%) **IIIa** mahsulot olindi, suyuqlanish harorati 301-303^{0}C
$C_{16}H_{12}N_2O_3$

Mass-spektr, m/z: 280 (M^+ ,

IQ-spektr, sm^{-1}: 1705 (ν_{CO}– 2 holat), 1700 (ν_{CO}–4 holat), 1665 (ν_{CO}–6 holat).

Jadvalda keltirilgan boshqa 1-metil-6-aroilxinazolin-2,4-dionlar (**III b,v**) yuqorida keltirilgan usul bo’yicha sintez qilindi.

XULOSALAR

1. 1-Metilxinazolin-2,4-dionni aromatik kislota xlorangidridlari bilan atsillash reaktsiyalari kam miqdor katalizator $FeCl_3 \cdot 6H_2O$ ishtirokida ilk bor o'rganilib, 1-metil- 6-aroilxinazolin-2,4-dionlarning sintezi amalga oshirildi.

2. 1-Metilxinazolin-2,4-dionni atsillashda aromatik xalqaga elektronoaktseptor guruhlar (Br, NO_2) kiritilganda maxsulotning unumi ortishi kuzatildi.

3. Sintez qilingan moddalarning tuzilishi zamonaviy fizik tadqiqot usullari yordamida tasdiqlandi.

4. 1-Metilxinazolin-2,4-dion va sintez qilingan mahsulotlarning tuzilishi Hyper Chem va Chem Bio 3D Ultra 11.0 programmalari yordamida kvant-kimyoviy hisoblashlar qilindi va ularning fazoviy tuzilishi, elektron zichliklari aniqlandi.

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ILOVALAR

Ilova 1

1-Metilxinazolin-2,4-dionning HyperChem programmasi bo'yicha kvant-kimyoviy hisoblash natijalari

HyperChem log start -- Mon Jun 03 16:29:28 2013.

Geometry optimization, SemiEmpirical, molecule = (untitled).

AM1

PolakRibiere optimizer

Convergence limit = 0.0100000 Iteration limit = 50

Accelerate convergence = YES

Optimization algorithm = Polak-Ribiere

Criterion of RMS gradient = 0.0100 kcal/(A mol) Maximum cycles = 315

RHF Calculation:

Singlet state calculation

Number of electrons = 66

Number of Double Occupied Levels = 33

Charge on the System = 0

Total Orbitals = 60

Starting AM1 calculation with 60 orbitals

E=0.0000 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=7 Diff=0.00688]

E=-2292.1512 kcal/mol Grad=47.259 Conv=NO(0 cycles 1 points) [Iter=1 Diff=59.47530]

E=-2292.1512 kcal/mol Grad=47.259 Conv=NO(0 cycles 1 points) [Iter=2 Diff=11.92049]

E=-2292.1512 kcal/mol Grad=47.259 Conv=NO(0 cycles 1 points) [Iter=3 Diff=4.27918]

E=-2292.1512 kcal/mol Grad=47.259 Conv=NO(0 cycles 1 points) [Iter=4 Diff=3.15577]

E=-2292.1512 kcal/mol Grad=47.259 Conv=NO(0 cycles 1 points) [Iter=5 Diff=0.51784]

E=-2292.1512 kcal/mol Grad=47.259 Conv=NO(0 cycles 1 points) [Iter=6 Diff=0.07683]

E=-2334.1879 kcal/mol Grad=0.031 Conv=NO(40 cycles 91 points) [Iter=1 Diff=0.00000]

E=-2334.1880 kcal/mol Grad=0.014 Conv=NO(41 cycles 92 points) [Iter=1 Diff=0.00003]

E=-2334.1880 kcal/mol Grad=0.009 Conv=YES(43 cycles 96 points) [Iter=1 Diff=0.00000]

ENERGIES AND GRADIENT

Total Energy = -53426.4791668 (kcal/mol)

Total Energy = -85.140503491 (a.u.)

Binding Energy = -2334.1879588 (kcal/mol)

Isolated Atomic Energy = -51092.2912080 (kcal/mol)

Electronic Energy = -272672.0949695 (kcal/mol)

Core-Core Interaction = 219245.6158028 (kcal/mol)

Heat of Formation = -34.2439588 (kcal/mol)

Gradient = 0.0087776 (kcal/mol/Ang)

MOLECULAR POINT GROUP

CS

EIGENVALUES(eV)

Symmetry:	1 A'	2 A'	3 A'	4 A'	5 A'
Eigenvalue:	-41.893326	-39.356244	-39.057846	-36.624462	-35.047315
Symmetry:	6 A'	7 A'	8 A'	9 A'	10 A'
Eigenvalue:	-32.330216	-31.114875	-28.037822	-25.689573	-24.558590
Symmetry:	11 A'	12 A'	13 A'	14 A'	1 A"
Eigenvalue:	-22.694378	-20.555344	-20.202809	-18.609415	-17.246018
Symmetry:	15 A'	16 A'	17 A'	18 A'	2 A"
Eigenvalue:	-17.199406	-16.915965	-16.463006	-15.793586	-15.419664
Symmetry:	19 A'	20 A'	3 A"	4 A"	21 A'
Eigenvalue:	-15.368346	-15.095130	-14.545055	-13.701291	-13.535016

ATOMIC ORBITAL ELECTRON POPULATIONS

AO:	1 S C	1 Px C	1 Py C	1 Pz C	2 S C
	1.218245	0.991108	0.911598	0.912055	1.217253
AO:	2 Px C	2 Py C	2 Pz C	3 S C	3 Px C
	0.914553	0.998095	1.046060	1.193905	0.895081
AO:	3 Py C	3 Pz C	4 S C	4 Px C	4 Py C
	0.941448	1.156905	1.218515	0.980802	0.929472
AO:	4 Pz C	5 S C	5 Px C	5 Py C	5 Pz C
	0.934369	1.216148	0.953512	0.937229	1.084464

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.033005	-0.98921	-2.14294	-0.00000	12.01100
2	6	-0.175961	0.20914	-2.84504	-0.00000	12.01100
3	6	-0.187339	-0.98842	-0.74357	-0.00000	12.01100
4	6	-0.063157	1.41915	-2.14607	0.00000	12.01100
5	6	-0.191353	1.44611	-0.75803	0.00000	12.01100
6	6	0.127654	0.23497	-0.02376	0.00000	12.01100

7	6	0.362380	-2.27476	-0.02126	-0.00000	12.01100
8	8	-0.334035	-3.39029	-0.56942	-0.00000	15.99900
9	7	-0.363473	-2.20664	1.37633	-0.00000	14.00700
10	7	-0.268333	0.22357	1.37604	-0.00000	14.00700
11	6	-0.076476	1.46018	2.11353	0.00000	12.01100
12	6	0.405910	-0.99823	2.08962	-0.00000	12.01100
13	8	-0.365247	-1.01616	3.33996	-0.00000	15.99900
14	1	0.163619	-1.95866	-2.67023	-0.00000	1.00800
15	1	0.144818	0.20632	-3.94453	-0.00000	1.00800

ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom) x	y	z
1	6	0.00680	0.01702	0.00000
2	6	0.00392	0.00685	0.00000
3	6	-0.00992	-0.02274	-0.00000
4	6	-0.01090	0.00569	-0.00000
5	6	-0.01989	0.00927	-0.00000
6	6	0.02025	-0.00845	-0.00000
7	6	0.00169	0.00737	0.00000
8	8	-0.00156	0.01524	0.00000
9	7	-0.02086	-0.01527	0.00000
10	7	-0.00569	0.00663	-0.00000
11	6	0.00692	0.00675	-0.00000
12	6	0.00981	-0.00801	-0.00000
13	8	-0.00269	0.00460	-0.00000
14	1	-0.00673	-0.01175	0.00000
15	1	0.00385	-0.00139	0.00000

Dipole (Debyes)	x	y	z	Total
Point-Chg.	3.978	-1.919	0.000	4.417
sp Hybrid	-0.017	0.180	0.000	0.181
pd Hybrid	0.000	0.000	0.000	0.000
Sum	3.961	-1.739	0.000	4.326

HyperChem log stop -- Mon Jun 03 16:33:11 2013.

Ilova 2

1-Metil-6-benzoilxinazolin-2,4-dionning HyperChem programmasi bo'yicha kvant-kimyoviy hisoblash natijalari

HyperChem log start -- Fri Jun 14 14:15:27 2013.

Geometry optimization, SemiEmpirical, molecule = (untitled).

AM1

PolakRibiere optimizer

Convergence limit = 0.0100000 Iteration limit = 50

Accelerate convergence = YES

Optimization algorithm = Polak-Ribiere

Criterion of RMS gradient = 0.0100 kcal/(A mol) Maximum cycles = 495

RHF Calculation:

Singlet state calculation

Number of electrons = 104

Number of Double Occupied Levels = 52

Charge on the System = 0

Total Orbitals = 96

Starting AM1 calculation with 96 orbitals

E=-3662.1175 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=1 Diff=19858.83083]

E=-3662.1175 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=2 Diff=206.80205]

E=-3662.1175 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=3 Diff=26.07845]

E=-3662.1175 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=4 Diff=2.55008]

E=-3662.1175 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=5 Diff=0.52953]

E=-3662.1175 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=6 Diff=0.19020]

ENERGIES AND GRADIENT

Total Energy = -82726.9766665 (kcal/mol)

Total Energy = -131.833812662 (a.u.)

Binding Energy = -3790.9263025 (kcal/mol)

Isolated Atomic Energy = -78936.0503640 (kcal/mol)

Electronic Energy = -517955.1096837 (kcal/mol)

Core-Core Interaction = 435228.1330172 (kcal/mol)

Heat of Formation = -26.7853025 (kcal/mol)

Gradient = 0.0095868 (kcal/mol/Ang)

MOLECULAR POINT GROUP

CS

EIGENVALUES(eV)

Symmetry:	1 A'	2 A'	3 A'	4 A'	5 A'
Eigenvalue:	-42.123010	-40.679307	-39.468830	-39.211313	-38.433015
Symmetry:	6 A'	7 A'	8 A'	9 A'	10 A'
Eigenvalue:	-36.654381	-35.174901	-32.898666	-32.090072	-31.799719
Symmetry:	11 A'	12 A'	13 A'	14 A'	15 A'
Eigenvalue:	-31.346259	-28.294768	-26.275865	-25.816110	-24.411916
Symmetry:	16 A'	17 A'	18 A'	19 A'	20 A'
Eigenvalue:	-23.468339	-22.758820	-22.001954	-20.644874	-20.008210
Symmetry:	21 A'	22 A'	23 A'	1 A''	24 A'
Eigenvalue:	-18.745768	-18.184646	-17.511590	-17.405260	-17.197183
Symmetry:	25 A'	26 A'	27 A'	28 A'	2 A''
Eigenvalue:	-16.764592	-16.523765	-16.028768	-15.878163	-15.559129

ATOMIC ORBITAL ELECTRON POPULATIONS

AO:	1 S C	1 Px C	1 Py C	1 Pz C	2 S C
	1.226337	0.988512	0.922547	0.845549	1.201994
AO:	2 Px C	2 Py C	2 Pz C	3 S C	3 Px C
	0.927266	0.938038	1.111624	1.193430	0.900048
AO:	3 Py C	3 Pz C	4 S C	4 Px C	4 Py C
	0.938075	1.170475	1.216237	0.983991	0.918552
AO:	4 Pz C	5 S C	5 Px C	5 Py C	5 Pz C
	0.904757	1.216025	0.944049	0.946873	1.106606
AO:	6 S C	6 Px C	6 Py C	6 Pz C	7 S C
	1.190260	0.937757	0.815222	0.904992	1.201639

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	0.017055	-1.47515	0.13749	-0.00000	12.01100
2	6	-0.178921	-0.19424	-0.44888	0.00000	12.01100
3	6	-0.202028	-1.65036	1.51955	-0.00000	12.01100
4	6	-0.023537	0.90363	0.41691	0.00000	12.01100
5	6	-0.213553	0.75651	1.79885	0.00000	12.01100

6	6	0.151769	-0.52704	2.38974	0.00000	12.01100
7	6	0.363101	-3.01705	2.07750	-0.00000	12.01100
8	8	-0.321275	-4.05678	1.39901	-0.00000	15.99900
9	7	-0.364257	-3.12057	3.47443	-0.00000	14.00700
10	7	-0.266436	-0.70815	3.77332	0.00000	14.00700
11	6	0.406784	-2.01175	4.33198	-0.00000	12.01100
12	6	-0.078562	0.42851	4.65794	0.00000	12.01100
13	8	-0.358901	-2.17930	5.57030	0.00000	15.99900
14	6	0.312029	-0.18337	-1.93694	-0.00000	12.01100
15	8	-0.311773	-1.30011	-2.49433	-0.00000	15.99900
16	6	-0.133443	1.00597	-2.83208	-0.00000	12.01100
17	6	-0.077228	0.70698	-4.21339	0.00000	12.01100
18	6	-0.144305	1.71216	-5.17375	0.00000	12.01100
19	6	-0.097746	3.05140	-4.78336	0.00000	12.01100
20	6	-0.149947	3.36381	-3.42717	-0.00000	12.01100
21	6	-0.088781	2.35266	-2.46338	-0.00000	12.01100
22	1	0.192236	-2.37789	-0.50711	-0.00000	1.00800
23	1	0.140921	1.93727	0.04963	0.00001	1.00800
24	1	0.147032	1.66008	2.42750	0.00000	1.00800
25	1	0.271369	-4.02264	3.90258	-0.00000	1.00800
26	1	0.085622	1.05206	4.47405	-0.91600	1.00800
27	1	0.134354	0.08175	5.72685	0.00000	1.00800
28	1	0.085622	1.05206	4.47405	0.91601	1.00800
29	1	0.163368	-0.34992	-4.53401	0.00000	1.00800
30	1	0.140016	1.44816	-6.24192	0.00000	1.00800
31	1	0.136883	3.85089	-5.53882	0.00000	1.00800
32	1	0.135233	4.41603	-3.10532	-0.00000	1.00800
33	1	0.127300	2.68100	-1.41918	-0.00001	1.00800

ATOMIC GRADIENTS

Atom Z Gradients(kcal/mol/Angstrom)

		x	y	z
1	6	-0.01667	0.03254	0.00000
2	6	-0.00511	-0.00955	-0.00000
3	6	-0.02196	-0.00940	0.00000
4	6	0.00158	0.00342	-0.00001

5	6	-0.01356	-0.00925	-0.00001
6	6	0.00961	0.00852	-0.00000
7	6	0.00761	-0.00563	0.00001
8	8	-0.01432	-0.00435	0.00001
9	7	-0.01030	0.00748	0.00000
10	7	0.04200	0.00178	-0.00000
11	6	-0.00449	0.01245	0.00000
12	6	-0.03060	-0.01179	0.00000
13	8	0.00844	0.00338	0.00000
14	6	0.01508	0.00588	0.00000
15	8	-0.00801	-0.01197	0.00001
16	6	0.01551	0.00831	0.00000
17	6	0.00049	-0.00719	-0.00001
18	6	0.02327	-0.00167	-0.00001
19	6	-0.02344	0.00936	0.00000
20	6	-0.00942	0.00739	0.00001
21	6	-0.00458	-0.00479	0.00002
22	1	-0.01175	-0.00632	0.00001
23	1	0.00720	-0.00544	-0.00003
24	1	0.00470	0.00076	-0.00002
25	1	0.00778	0.00312	0.00000
26	1	0.00606	-0.00353	0.00418
27	1	0.00283	-0.00490	0.00000
28	1	0.00606	-0.00353	-0.00419
29	1	0.00165	0.00024	-0.00002
30	1	0.00911	0.00475	-0.00002
31	1	0.00920	-0.00261	-0.00000
32	1	0.00035	0.00285	0.00002
33	1	-0.00431	-0.01029	0.00004

Dipole (Debyes)	x	y	z	Total
Point-Chg.	5.835	-0.546	0.000	5.861
sp Hybrid	0.370	0.441	0.000	0.576
pd Hybrid	0.000	0.000	0.000	0.000
Sum	6.205	-0.105	0.000	6.206

HyperChem log stop -- Fri Jun 14 14:16:10 2013.

Ilova 3

1-Metil-6-(4`-brombenzoil)xinazolin-2,4-dionning HyperChem programmasi bo’yicha kvant-kimyoviy hisoblash natijalari

HyperChem log start -- Fri Jun 14 15:14:27 2013.

Geometry optimization, SemiEmpirical, molecule = (untitled).

AM1

PolakRibiere optimizer

Convergence limit = 0.0100000 Iteration limit = 50

Accelerate convergence = YES

Optimization algorithm = Polak-Ribiere

Criterion of RMS gradient = 0.0100 kcal/(A mol) Maximum cycles = 495

RHF Calculation:

Singlet state calculation

Number of electrons = 110

Number of Double Occupied Levels = 55

Charge on the System = 0

Total Orbitals = 99

Starting AM1 calculation with 99 orbitals

E=-3633.1286 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=1 Diff=19873.20159]

E=-3633.1286 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=2 Diff=258.42675]

E=-3633.1286 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=3 Diff=37.48148]

E=-3633.1286 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=4 Diff=4.69396]

E=-3633.1286 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=5 Diff=0.66060]

E=-3633.1286 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=6 Diff=0.25331]

ENERGIES AND GRADIENT

Total Energy = -90558.1097588 (kcal/mol)

Total Energy = -144.313516075 (a.u.)

Binding Energy = -3760.1493968 (kcal/mol)

Isolated Atomic Energy = -86797.9603620 (kcal/mol)

Electronic Energy = -557037.6788822 (kcal/mol)

Core-Core Interaction = 466479.5691234 (kcal/mol)

Heat of Formation = -21.3703968 (kcal/mol)

Gradient = 0.0081594 (kcal/mol/Ang)

MOLECULAR POINT GROUP

CS

EIGENVALUES(eV)

Symmetry:	1 A'	2 A'	3 A'	4 A'	5 A'
Eigenvalue:	-42.205703	-40.877681	-39.629975	-39.308767	-38.634572
Symmetry:	6 A'	7 A'	8 A'	9 A'	10 A'
Eigenvalue:	-36.746475	-35.244257	-33.822892	-32.668597	-32.165131
Symmetry:	11 A'	12 A'	13 A'	14 A'	15 A'
Eigenvalue:	-31.638258	-30.622425	-28.348485	-26.290164	-25.844128
Symmetry:	16 A'	17 A'	18 A'	19 A'	20 A'
Eigenvalue:	-24.442848	-23.811072	-22.851834	-22.105819	-20.746428

ATOMIC ORBITAL ELECTRON POPULATIONS

AO:	1 S C	1 Px C	1 Py C	1 Pz C	2 S C
	1.226227	0.987772	0.922939	0.844450	1.200943
AO:	2 Px C	2 Py C	2 Pz C	3 S C	3 Px C
	0.928531	0.935174	1.116749	1.193531	0.900770
AO:	3 Py C	3 Pz C	4 S C	4 Px C	4 Py C
	0.937783	1.170119	1.215902	0.982467	0.919318
AO:	4 Pz C	5 S C	5 Px C	5 Py C	5 Pz C
	0.905205	1.216065	0.944851	0.946155	1.106018
AO:	6 S C	6 Px C	6 Py C	6 Pz C	7 S C
	1.190346	0.937557	0.815898	0.902260	1.201435

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	0.018612	-3.06387	1.16251	-0.00000	12.01100
2	6	-0.181398	-1.78412	0.57350	0.00000	12.01100
3	6	-0.202203	-3.23582	2.54487	-0.00000	12.01100
4	6	-0.022892	-0.68402	1.43687	0.00001	12.01100
5	6	-0.213090	-0.82808	2.81880	0.00001	12.01100
6	6	0.153940	-2.11068	3.41279	0.00000	12.01100
7	6	0.363004	-4.60159	3.10561	-0.00000	12.01100
8	8	-0.320372	-5.64209	2.42845	-0.00000	15.99900
9	7	-0.363922	-4.70218	4.50257	-0.00000	14.00700
10	7	-0.266061	-2.28875	4.79621	0.00000	14.00700

11	6	0.406779	-3.59160	5.35780	-0.00000	12.01100
12	6	-0.079081	-1.15029	5.67881	0.00000	12.01100
13	8	-0.356972	-3.75610	6.59630	-0.00000	15.99900
14	6	0.311198	-1.77691	-0.91317	-0.00000	12.01100
15	8	-0.307122	-2.89260	-1.47178	-0.00000	15.99900
16	6	-0.120807	-0.58784	-1.81140	-0.00000	12.01100
17	6	-0.079042	-0.88790	-3.19161	0.00000	12.01100
18	6	-0.118610	0.11226	-4.15659	0.00000	12.01100
19	6	-0.139999	1.45559	-3.76873	-0.00000	12.01100
20	6	-0.124037	1.77062	-2.41005	-0.00000	12.01100
21	6	-0.090180	0.75919	-1.44697	-0.00001	12.01100
22	35	0.065767	2.81321	-5.05558	0.00000	79.90900
23	1	0.192402	-3.96820	0.52011	-0.00000	1.00800
24	1	0.139873	0.34879	1.06744	0.00001	1.00800
25	1	0.147971	0.07679	3.44573	0.00001	1.00800
26	1	0.271990	-5.60347	4.93258	-0.00000	1.00800
27	1	0.086070	-0.52726	5.49387	-0.91613	1.00800
28	1	0.135007	-1.49524	6.74834	0.00000	1.00800
29	1	0.086070	-0.52726	5.49388	0.91614	1.00800
30	1	0.169356	-1.94533	-3.51269	0.00001	1.00800
31	1	0.154456	-0.16303	-5.22337	0.00001	1.00800
32	1	0.149645	2.82221	-2.08142	-0.00001	1.00800
33	1	0.133644	1.09224	-0.40375	-0.00001	1.00800

ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	0.00289	0.00217	0.00001
2	6	-0.00208	-0.00167	-0.00001
3	6	0.00585	-0.00337	0.00000
4	6	-0.00409	-0.02003	-0.00003
5	6	-0.00994	-0.00927	-0.00002
6	6	0.00515	0.01449	-0.00000
7	6	-0.02027	-0.00230	0.00001
8	8	0.00782	0.00715	0.00001

9	7	0.01206	0.01442	0.00001
10	7	-0.00138	0.01626	-0.00000
11	6	0.00955	-0.04933	0.00000
12	6	0.00010	-0.00605	-0.00000
13	8	0.00004	0.02424	0.00000
14	6	-0.01124	-0.00493	0.00001
15	8	0.00365	0.00096	0.00001
16	6	0.01093	0.01547	0.00001
17	6	-0.00221	-0.00089	-0.00001
18	6	-0.00168	-0.00037	-0.00002
19	6	0.00842	-0.00015	-0.00000
20	6	0.00051	-0.00532	0.00002
21	6	-0.00852	0.00670	0.00003
22	35	0.00790	0.00866	-0.00001
23	1	-0.00423	-0.00755	0.00002
24	1	-0.00506	-0.00001	-0.00006
25	1	0.00803	0.00528	-0.00003
26	1	0.00089	-0.00132	0.00001
27	1	0.00145	0.00082	-0.00566
28	1	-0.00360	-0.01127	0.00000
29	1	0.00146	0.00081	0.00565
30	1	-0.00650	-0.00327	-0.00003
31	1	-0.00132	0.00295	-0.00003
32	1	-0.00173	0.00290	0.00004
33	1	-0.00287	0.00380	0.00007

Dipole (Debyes)	x	y	z	Total
Point-Chg.	5.121	0.251	0.000	5.127
sp Hybrid	-0.011	0.787	0.000	0.787
pd Hybrid	0.000	0.000	0.000	0.000
Sum	5.110	1.038	0.000	5.215

HyperChem log stop -- Fri Jun 14 15:18:03 2013.

Ilova 4

1-Metil-6-(4`-nitrobenzoil)xinazolin-2,4-dionning HyperChem programmasi bo'yicha kvant-kimyoviy hisoblash natijalari

HyperChem log start -- Fri Jun 14 15:32:49 2013.

Geometry optimization, SemiEmpirical, molecule = (untitled).

AM1

PolakRibiere optimizer

Convergence limit = 0.0100000 Iteration limit = 50

Accelerate convergence = YES

Optimization algorithm = Polak-Ribiere

Criterion of RMS gradient = 0.0100 kcal/(A mol) Maximum cycles = 525

RHF Calculation:

Singlet state calculation

Number of electrons = 120

Number of Double Occupied Levels = 60

Charge on the System = 0

Total Orbitals = 107

Starting AM1 calculation with 107 orbitals

E=-3711.7457 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=1 Diff=20858.43327]

E=-3711.7457 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=2 Diff=12713.16061]

E=-3711.7457 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=3 Diff=51529.77713]

E=-3711.7457 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=4 Diff=7388.88905]

E=-3711.7457 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=5 Diff=7312.72351]

E=-3711.7457 kcal/mol Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=6 Diff=6571.81999]

ENERGIES AND GRADIENT

Total Energy = -101885.6191178 (kcal/mol)

Total Energy = -162.365049045 (a.u.)

Binding Energy = -3965.4768218 (kcal/mol)

Isolated Atomic Energy = -97920.1422960 (kcal/mol)

Electronic Energy = -639089.5549953 (kcal/mol)

Core-Core Interaction = 537203.9358776 (kcal/mol)

Heat of Formation = -21.3198218 (kcal/mol)

Gradient = 0.0097902 (kcal/mol/Ang)

MOLECULAR POINT GROUP

CS

EIGENVALUES(eV)

Symmetry:	1 A'	2 A'	3 A'	4 A'	5 A'
Eigenvalue:	-43.591359	-42.388283	-41.185499	-39.833479	-39.475346
Symmetry:	6 A'	7 A'	8 A'	9 A'	10 A'
Eigenvalue:	-38.896339	-38.024161	-36.944401	-35.399010	-33.569897
Symmetry:	11 A'	12 A'	13 A'	14 A'	15 A'
Eigenvalue:	-32.715890	-32.568949	-31.816116	-28.673998	-28.080948
Symmetry:	16 A'	17 A'	18 A'	19 A'	20 A'
Eigenvalue:	-26.330633	-25.773042	-24.532991	-24.096782	-23.054242

ATOMIC ORBITAL ELECTRON POPULATIONS

AO:	1 S C	1 Px C	1 Py C	1 Pz C	2 S C
	1.226102	0.983206	0.926900	0.842104	1.199005
AO:	2 Px C	2 Py C	2 Pz C	3 S C	3 Px C
	0.931335	0.928898	1.127461	1.193743	0.902972
AO:	3 Py C	3 Pz C	4 S C	4 Px C	4 Py C
	0.936451	1.169520	1.215321	0.981157	0.919258
AO:	4 Pz C	5 S C	5 Px C	5 Py C	5 Pz C
	0.905973	1.216180	0.943891	0.947384	1.104916

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	0.021688	-2.53018	0.98365	-0.00000	12.01100
2	6	-0.186699	-1.23882	0.41966	0.00000	12.01100
3	6	-0.202686	-2.72891	2.36213	-0.00000	12.01100
4	6	-0.021708	-0.15541	1.30486	0.00001	12.01100
5	6	-0.212371	-0.32660	2.68295	0.00001	12.01100
6	6	0.158435	-1.62124	3.25239	0.00000	12.01100
7	6	0.362831	-4.10598	2.89574	-0.00000	12.01100
8	8	-0.318526	-5.13160	2.19652	-0.00000	15.99900
9	7	-0.363267	-4.23411	4.29012	-0.00000	14.00700
10	7	-0.265243	-1.82612	4.63086	0.00000	14.00700
11	6	0.406769	-3.14071	5.16725	-0.00000	12.01100

12	6	-0.080157	-0.70530	5.53632	0.00000	12.01100
13	8	-0.352736	-3.32845	6.40190	-0.00000	15.99900
14	6	0.308069	-1.20483	-1.06415	-0.00000	12.01100
15	8	-0.297610	-2.30617	-1.64894	-0.00000	15.99900
16	6	-0.089671	0.00331	-1.94466	-0.00000	12.01100
17	6	-0.092255	-0.27591	-3.32900	0.00000	12.01100
18	6	-0.082649	0.73519	-4.28200	0.00000	12.01100
19	6	-0.104707	2.07210	-3.85556	-0.00000	12.01100
20	6	-0.086738	2.37644	-2.48913	-0.00001	12.01100
21	6	-0.103448	1.34237	-1.55140	-0.00001	12.01100
22	7	0.565786	3.17129	-4.85913	0.00000	14.00700
23	8	-0.348155	2.89088	-6.02694	0.00000	15.99900
24	8	-0.353920	4.30888	-4.47184	0.00000	15.99900
25	1	0.192754	-3.42246	0.32445	-0.00001	1.00800
26	1	0.138159	0.88481	0.95711	0.00002	1.00800
27	1	0.149894	0.56564	3.32797	0.00001	1.00800
28	1	0.273308	-5.14396	4.70226	-0.00000	1.00800
29	1	0.086979	-0.07893	5.36395	-0.91628	1.00800
30	1	0.136424	-1.07168	6.59879	0.00000	1.00800
31	1	0.086979	-0.07893	5.36395	0.91629	1.00800
32	1	0.179098	-1.32888	-3.66732	0.00001	1.00800
33	1	0.177767	0.49047	-5.35853	0.00001	1.00800
34	1	0.173609	3.42791	-2.15246	-0.00001	1.00800
35	1	0.143998	1.65336	-0.50089	-0.00002	1.00800

ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	-0.01489	-0.01197	0.00001
2	6	0.01111	0.01462	-0.00001
3	6	0.03260	0.00502	0.00001
4	6	-0.00130	0.00508	-0.00004
5	6	-0.00562	-0.02075	-0.00003
6	6	-0.01650	0.01860	-0.00001
7	6	-0.03275	0.00640	0.00001

8	8	0.00983	0.01502	0.00002
9	7	-0.00559	-0.01280	0.00001
10	7	-0.00070	-0.02676	-0.00000
11	6	-0.00074	0.02197	0.00000
12	6	0.01182	0.00557	-0.00000
13	8	0.00908	-0.00889	0.00000
14	6	-0.00060	-0.00788	0.00001
15	8	-0.00475	-0.00685	0.00002
16	6	0.00187	0.00189	0.00001
17	6	-0.00163	0.01166	-0.00002
18	6	0.00620	0.00982	-0.00002
19	6	-0.00392	-0.00564	0.00000
20	6	0.00347	0.00882	0.00003
21	6	0.00477	-0.01217	0.00004
22	7	-0.02919	-0.02132	-0.00001
23	8	0.00640	0.00705	-0.00001
24	8	0.03011	0.01335	0.00000
25	1	-0.00963	0.00042	0.00002
26	1	-0.00771	0.00636	-0.00008
27	1	-0.00989	-0.00051	-0.00004
28	1	-0.00640	0.00792	0.00001
29	1	-0.00097	-0.00783	0.00208
30	1	0.01101	-0.00113	0.00000
31	1	-0.00096	-0.00784	-0.00209
32	1	0.00903	-0.00140	-0.00004
33	1	0.00065	-0.00296	-0.00004
34	1	-0.00046	-0.00404	0.00005
35	1	0.00626	0.00118	0.00010

Dipole (Debyes)	x	y	z	Total
Point-Chg.	1.489	3.903	0.000	4.177
sp Hybrid	0.471	0.300	0.000	0.559
pd Hybrid	0.000	0.000	0.000	0.000
Sum	1.960	4.203	0.000	4.638

HyperChem log stop -- Fri Jun 14 15:34:46 2013.