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Synthesis of Salicylic Acid Compounds Retaining the Thiomachevin Fragment

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ABSTRACT: The synthesis of compounds that retain the thiourea moiety of salicylic acid and their new derivatives consists in identifying the active sites of N -carbomathiol-2 and benzoylthiocyanate compounds and synthesizing new compounds.

KEYWORD: Salicylic acid, thiourea, synthesis, benzoylthiocyanate, N -carbomathiol-2, electron density, mesomeric effect, atom, GaussView, synthesis.

Current day come salicylic acid acids new to properties have substances synthesis do attention _ _ more increases. Literature analysis from do salicylic acid is known acid derivatives wide biological to activity be _ _ fever laxative, rheumatic, antipyretic, anti-inflammatory _ _ as well as pain _ _ Leader, blood Thinning, antiseptic, silga against drugs cooking derivative considered _thiourea fragment kept compounds one series properties, including herbicidal, fungicidal, antioxidant, antimicrobial, etc. e. _ s together with HIV infection, bacteria, cancer as well as malaria With dependent _ _ disease per potential therapeutic tools as too much application _ _ cited [1-1].

This in field scientific research development one How many? theories there is of which _ _ _ one pharmacophore fragment countable thiourea fragment input as a result harvest was substances assets centers find them new compounds, biogen metals With harvest did complexes synthesis do as well as medical importance o ' study Current from problems considered _

One How many? an experience based this acceptable syntheses Performed increased _ This per originally N - carbamothioyl-2 - hydroxybenzamide synthesis Performed increase need _ N - carbamothioyl-2 - hydroxybenzamide synthesis Performed increase per salicylic acid acids chlorine to anhydride equivalent amount thiourea in acetone solution 1 hour during drop by drop was poured as well as slowness With confused rises _ A yellowish oily liquid was obtained. Several factors have been shown to influence the response.

Synthesis in the process temperature at the level of 40-50 C * take when will you go free sulfur as well as hydrogen sulfide harvest to be increased reaction yield up to 30 % fell _ Temachevina With together take walked in reactions temperature growth _ _ with substances stability decline has been determined. Next reactions relatively short by temperature Performed warmed up. reaction room by temperature take when will you go sulfur compounds harvest be _ _ relatively decline has been determined. That's all due to key reactions Cold in the bathroom Performed increase through planning reactions at a temperature of 5-10 C * Achieved increased in that reaction product relatively high it happened _ _ and 60-65 % organize did _

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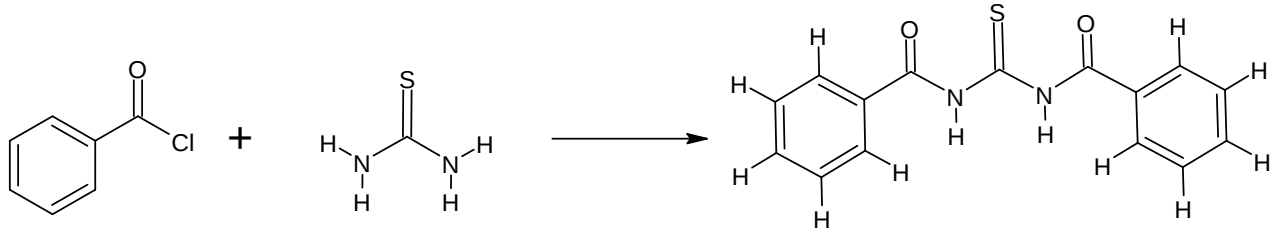
Mixing mechanic Effect as a result too much harvest was initially N - carbamothioyl-2 - hydroxybenzamide in the mixer to sulfur turn stuck stay observed. From this key reactions go per to reaction introductory components concentration reduced your reaction duration extended. fashion one to one influenced slow down as well as reaction general volume according to _ _ go per thiourea solution drop by drop poured _ reaction last in minutes flask from Ohist With shocked got up _

In synthesis productive increase per one How much solvents With take went _ Thiourea per main solvent calculated water using Reaction Performed failed to increase. Salicylic acid acids chlorine anhydride very assets when The fact is that per water small With to reaction input care can _ reaction according to Kui Performed increases.

Benzoyl chloride water With influenced due to reagents per general calculated solvents using solutions prepared. Solvents between acetone relatively melting good the fact that it's fruitful high The fact is that per with acetone under the circumstances synesis Performed increased _

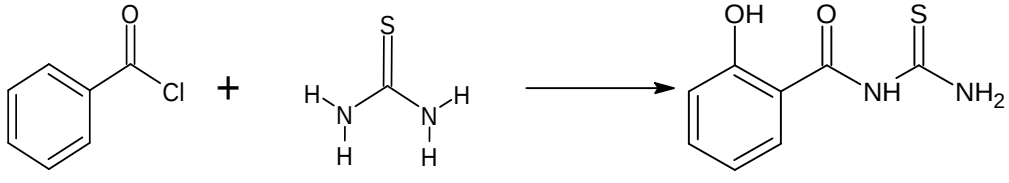
In Thiourea equals strong one as NH _ $_2$ Group what was it reaction in the process count was _ _ N - carbamothioyl-2 - hydroxybenzamide in the composition - NH $_2$ groups Events a lot of decreases. That's all in spite of benzoyl chloride With merger at the expense productive more increase possible no _ _ _



N,*N*'-carbonothioyldibenzamide

Harvest was _ _ N, N - carbonothioldibenzamide from harvest to be of a possible 15-20% was determined not to exceed as well as key corresponding catalysts in experiments using productive more increase possible has been determined.

The preparation of N -carbamothioyl-2-hydroxybenzamide was carried out according to the following reaction equations substance separate get to solvent vacuum under driving received _ As a result hungry yellow work _ colorful powdery substance received



Received product N - carbamothioyl-2 - hydroxybenzamide The fact is that chemical analyzes through completely _ _ own _ _ confirmation _ _ found _ Chemical structure when studying _ one How much active to the centers have i.e. malekulani _ organize doer atoms each other make an impact at the expense such reaction centers number increase has been determined. [2-4].

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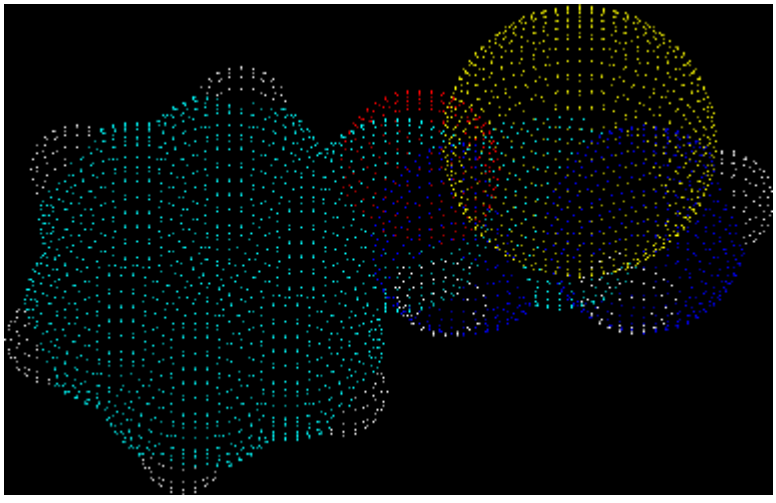
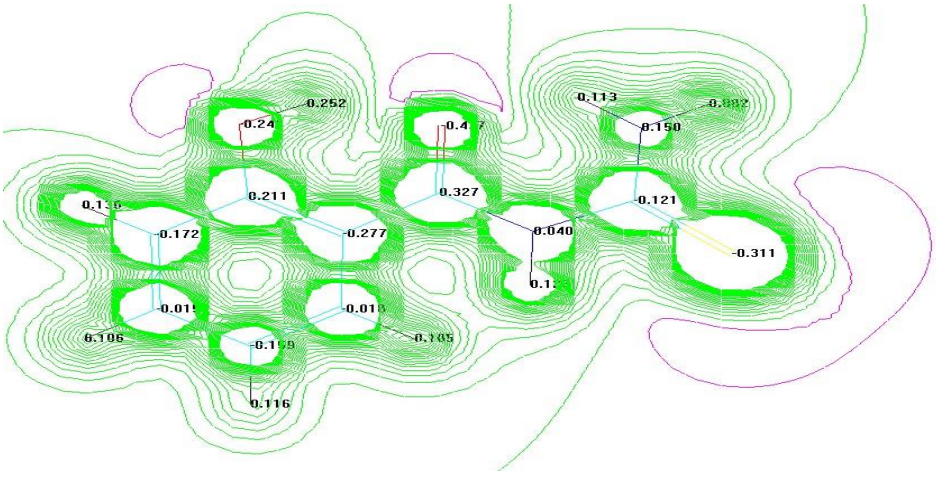


Molecule structure when saw _ too much to benzene bound (-OH _) negative _ _ inductive Effect at the expense in benzene ortho as well as paragraph situation assets to be With together excitable _ _ _ _ due to vadarodly (-OH). too much one How much reactions Performed increase possible all see _ _ you can _ that's all With together benzene ring attached carbonyl Group Effect too much taking into account get important have be _ _ this is Group too much benzene ring Effect achieve With together relative electro negativity high was _ _ oxygen atom as well as hydroxide Group in the middle _ vadarod garden harvest _ be _ _ probability very high_N _ _ - carbamothioyl-2 - hydroxybenzamide in a molecule relatively to reactions Get in probability high was _ _ thiourea (-NH _ 2) group in fragment rest to the centers relatively a lot of active nucleophile to the center turn rest as well as electrophile particles With pair electrons on his account to reactions input assume done _ molecules Events Gauss View program using analysis when done too much this is thoughts own _ _ confirmation _ _ found _ Kidagi on the picture electron clouds density as well as Minus accusations basically nitrogen atom near relatively high what has been determined. These taking into account received without N - carbamothioyl-2 - hydroxybenzamide nucleophile to the center have molecules Effect reaching new products get possibility there is The fact is that has been determined. [3-3].



Charges and electron density of atoms of the N -carbamothioyl-2-hydroxybenzamide molecule

N -carbamothioyl-2-hydroxybenzamide molecule containing a thiourea fragment by this method does not exceed 70-75% productivity, since the product is very active, it is necessary to provide an optimal environment, which creates difficulties for subsequent reactions.. [4-2].

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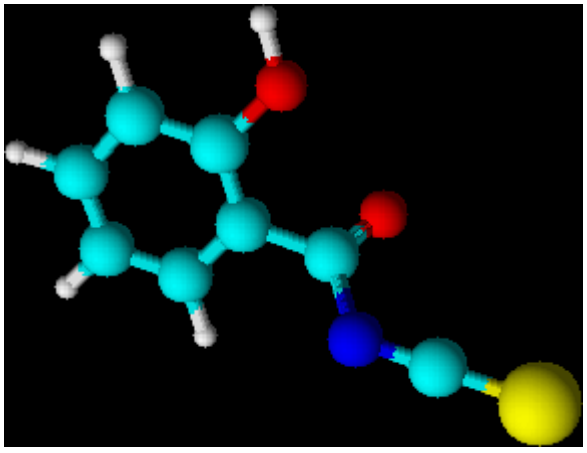
Thus, the analysis of the literature confirmed that the addition of the thiourea fragment to the acid chloride of salicylic acid can be carried out not due to the thiourea effect, but due to monovalent radanite salts containing the same bonds and atoms. [5-3].

To do this, an acetone solution containing 11.6 g of salicylic acid containing an acid chloride is slowly stirred and a solution of KCNS in 9.7 g of acetone is added dropwise over 1-1.5 hours. After the reaction is completed, acetone is removed from the mixture under a vacuum pump. A yellowish-red substance is obtained,

The reaction yield of benzoyl thiocyanate was above 75-80% and the product was stable.

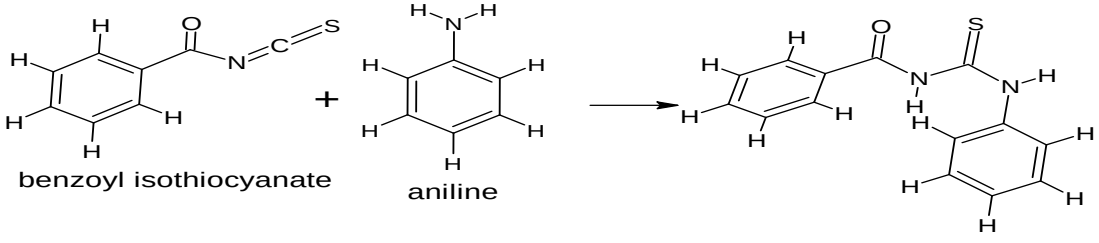


It was found that the resulting substance has the above structure. When determining the active centers, it turned out that the carbon atom that attached the atoms (= S) and (N -) to itself was able to attach electron donor atoms due to the observation of the +M effect. It allows many molecules to enter into nucleophilic coupling reactions, keeping the thiourea fragment in the molecule [6-2].

Based on the foregoing, initial syntheses of benzoyl thiocyanate with amino group-retaining molecules were carried out for use in medicine.

Initial syntheses were carried out with relatively highly active aniline.

In these reactions, the choice of alternative solvents is important. When the reaction is carried out in an acetone medium, the acetone molecule is a relatively polar solvent molecule, therefore, Schiff bases, hydrazones and oximes are formed. Therefore, the reactions were continued using inert non-polar solvents. Among solvents, solubility in DMSO is much better, and the yield of the product was relatively high. Therefore, an alternative solvent was chosen. [1-2].benzoyl thiocyanate in DMSO was slowly heated and stirred in a three-necked flask until the activation energy was reached, isolated and a dark red powder was obtained. The reaction was carried out according to the following scheme



For the following reactions, biologically active substances with undistributed electron-pair-retaining nitrogen were selected and the reactions were carried out in the above order. The products obtained as a result of the

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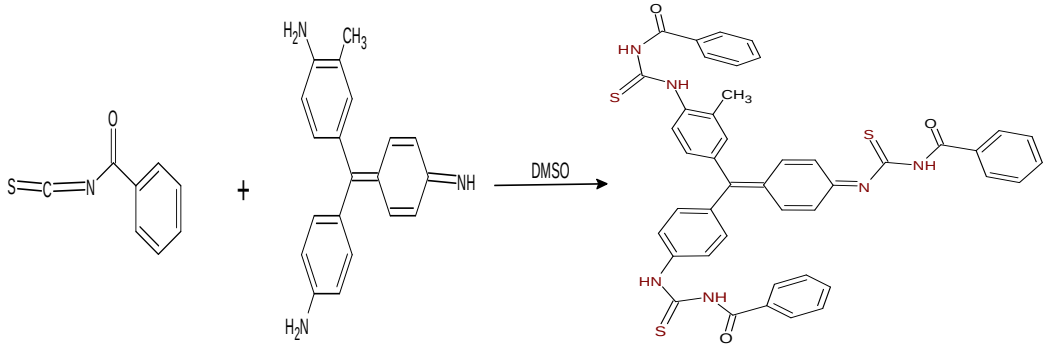
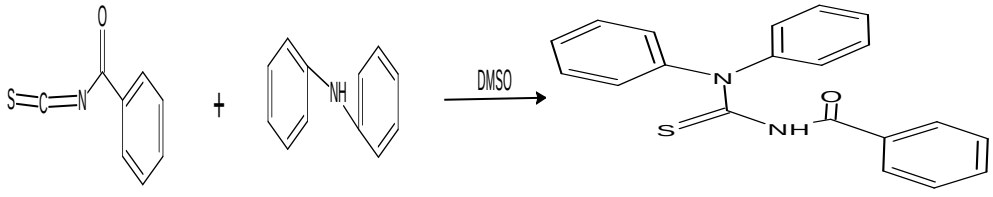
reactions are crystals of different colors and are salicylic acid bases containing an increased thiourea fragment. [7-2].

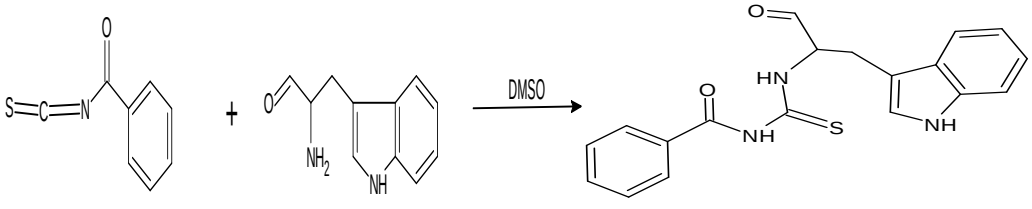
benzoyl thiocyanate in DMSO was slowly heated and stirred in a three-necked flask until the activation energy was reached, isolated and a dark red powder was obtained. The reaction was carried out according to the following scheme



benzoyl thiocyanate in DMSO was slowly heated and stirred in a three-necked flask until the activation energy was reached, isolated and a green powder was obtained. The reaction was carried out according to the following scheme



benzoyl thiocyanate in DMSO was slowly heated and stirred in a three-necked flask until the activation energy was reached, isolated and a woody powder was obtained. The reaction was carried out according to the following scheme



In short, since the synthesis of salicylic acid bases containing a thiourea moiety, their biological activity, their use as industrial raw materials, or the preparation of their compounds with other molecules is considered very important, the synthesis of salicylic acid derivatives containing a thiourea moiety has been carried out and several acceptable methods have been identified. Factors influencing the synthesis, side reactions inhibiting the course of the reaction were identified, high productivity was ensured. It was planned to conduct medical and biological laboratory studies on the use of the synthesized molecules as industrial dyes, their activity against bacteria and parasites.

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