

Synthesis of 1,3-Benzoxathiol-2-one Derivatives from *N*-(4-Oxocyclohexa-2,5-dien-1-ylidene)ureas

S. A. Konovalova^a, A. P. Avdeenko^{a,*}, V. V. D'yakonenko^b, and S. V. Shishkina^b

^a Donbass State Engineering Academy, Kramatorsk, 84313 Ukraine

^b Institute of Single Crystals, National Academy of Sciences of Ukraine, Kharkiv, 61001 Ukraine

*e-mail: chimist@dgma.donetsk.ua

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Abstract—1,3-Benzoxathiol-2-one derivatives were synthesized by reactions of *N*-(4-oxocyclohexa-2,5-dien-1-ylidene)ureas with potassium thiocyanate or thiourea. In most cases, the highest yields were obtained in the reactions with thiourea in ethanol in the presence of hydrochloric acid, whereas the maximum yield from *N*-(2,6-dimethyl-4-oxocyclohexa-2,5-dien-1-ylidene)urea was achieved using potassium thiocyanate. *N*-(3,5-Dimethyl-4-oxocyclohexa-2,5-dien-1-ylidene)urea reacted with potassium thiocyanate to give 6-(carbamoylamino)-3-hydroxy-2,4-dimethylphenyl thiocyanate, and with thiourea, to produce 5-hydroxy-4,6-dimethyl-2*H*-1,3-benzoxathiol-2-one. The main factor determining the direction of the reaction of *N*-(4-oxocyclohexa-2,5-dien-1-ylidene)ureas with potassium thiocyanate is the energy of primary transition state.

Keywords: 1,3-benzoxathiol-2-one, thiourea, *N*-(4-oxocyclohexa-2,5-dien-1-ylidene)urea, potassium thiocyanate, biological activity

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