

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

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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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