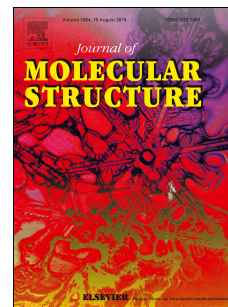


# Accepted Manuscript

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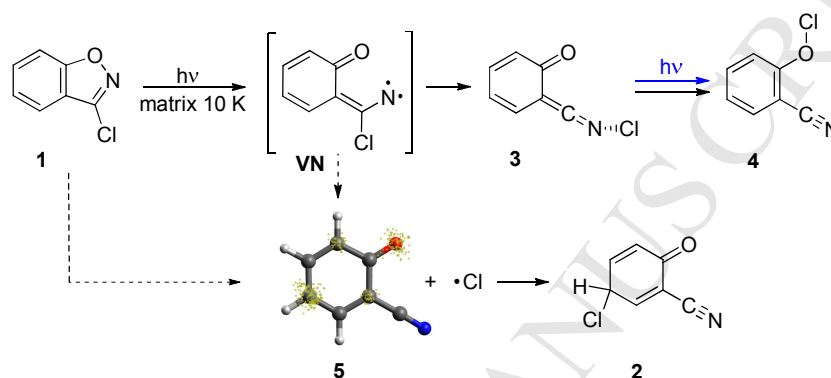
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# Photochemistry of Matrix-Isolated 3-Chloro-1,2-Benzisoxazole: Generation and Characterization of 2-Cyanophenoxy Radical and Other Reactive Intermediates

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**ABSTRACT:** Photochemistry of 3-chloro-1,2-benzisoxazole **1** in  $N_2$  and Ar matrices at 10 K leads to *N*-chloro-ketenimine **3** and 2-cyanophenyl-hypochlorite **4**. The reaction kinetics and the observed photoisomerization of **3** to **4** indicate that ketenimine **3**, possibly formed via an elusive vinylnitrene **VN**, is an intermediate in the formation of hypochlorite **4**. A new pathway involving the formation of 2-cyanophenoxy radical **5**, which was captured only in Ar matrix, was also observed. Radical **5** is possibly formed via photodetachment of Cl atom from **1** (or **VN**) and might explain the formation of 3-chloro-6-oxocyclohexa-1,4-dienecarbonitrile **2** in  $N_2$  and Ar matrices. All the species were characterized by IR spectroscopy and theoretical calculations. The computed geometric and electronic structure of radical **5** is discussed. Overall, the results provided further insight into the mechanism of the photochemistry of 1,2-benzisoxazoles and allowed characterization of new interesting reactive intermediates.

**Keywords:** Reactive intermediates; 1,2-Benzisoxazoles; Photochemistry; Phenoxy radical; IR spectroscopy; Theoretical calculations

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