A Comment on the Paper "Benzo-1λ⁴, 2-thiazol, a New Bicyclic 10π-System"

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Heterocycle, 2,1-Benzisothiazole

The "novel 10π-system" reported earlier is a 2,1-benzisothiazole, a well-known heterocyclic system.

It was reported [1] that the reaction of lithiated N-(fluorodimethylsilyl)-2,4,6-trimethylaniline with bis(trimethylsilyl)-sulfurdiimide afforded 5,7-dimethylbenzo(c)-1λ⁴,2-thiazole (1), a "new bicyclic 10π system".

1 2

It is the purpose of this Note to point out that (1) is a canonical form of the well-known 2,1-benzisothiazoles, which are usually written as in structure (2). The contribution of structures like (1) to the resonance hybrid has been discussed in several papers, including a review [2] and an X-ray crystallographic structure determination [3]. The S–N bond length in 5-chloro-2,1-benzisothiazole is about 1.636 Å, almost midway between a single bond (1.74 Å) and a double bond (1.56 Å), indicating that (1) is a substantial contributor to the overall structure [3].

The ^1H and ^{13}C NMR data reported in the paper [1] are identical with those reported earlier for 2,1-benzisothiazoles [3, 4], showing clearly that the compound is 5,7-dimethyl-2,1-benzisothiazole.

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