**Experimental and theoretical investigation of carbene catalyzed isomerisation of dimethyl maleate to dimethyl fumarate**

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Abstract: Isomeraization of dimethyl maleate to dimethyl fumarate catalyzed by an N-heterocyclic carbene (NHC) namely 3-benzylbenzothiazolylidene is reported for the first time.

 

On the basis of theoretical investigation of a model reaction scheme, a plausible mechanism has been proposed.

 

The reaction of 3-benzylbenzothiazolylidene with maleic anhydride affords 2-(3-benzylbenzothiazolylidene)succinic anhydride through Michael type attack followed by a 1,2-proton shift.

Thrust area: Organic Synthesis Category: Research