# THERMAL SYNTHESIS OF CARBOCYCLIC EIGHT-MEMBERED RINGS SUPPORTED BY DFT CALCULTIONS

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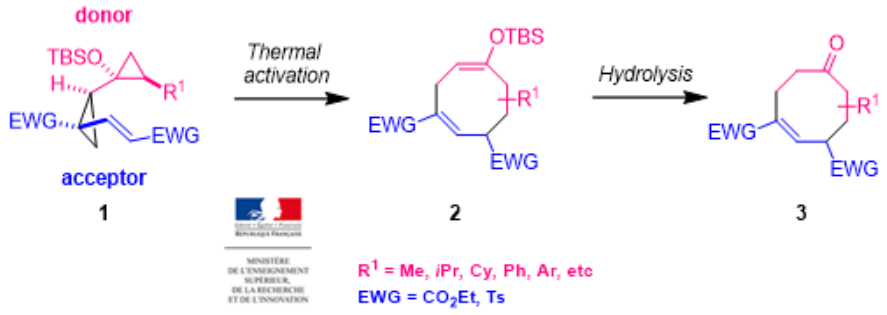
The development of efficient synthesis of eight-membered carbocyclic ring systems represents a particularly important area of research, given the number of biologically potent targets that incorporate such ring[1]. However, owing to ring strain and transannular interactions, the formation of eight-membered carbocyclic rings has sometime proven difficult[2].

In this regard, the donor-acceptor cyclopropanes (DACs) represent a valuable class of intermediates for organic synthesis due to their high reactivity based on the inherent strain of the cyclopropane ring[3]. These molecules can easily undergo a ring opening reaction induced and oriented by the presence of the two antagonist groups. A valuable 1,3-dipole synthetic building block is thus delivered and has been used in plethora of reactions. Some of the resulting molecules have been used as advanced materials in the construction of biologically relevant materials[4].

Quite recently, a new class of DACs **1** has been developed in our laboratory combining a silyl protected cyclopropanol with an α,β-unsaturated ester. Gratifyingly, we found out that DAC **1**, under purely thermal conditions, reacts intramolecularly to afford regio-and diastereoselectively, a functionalized all carbon 8-membered ring **2** (Scheme 1). Furthermore, a mild acidic hydrolysis allows the preparation of cyclooctenones **3** with good overall yields.




*Scheme 1: Thermal synthesis of carbocyclic eight membered rings*

The full details of our investigation, including a mechanistic investigation supported by DFT calculations, will be presented.

[1] G. Mehta, V. Singh, *Chem. Rev*., **1999**, 881–930.

[2] J. R. Donald, W. P. Unsworth, *Chem. Eur. J.*, **2017**, 8780–8799.

[3] O. A. Ivanova, I. V. Trushkov, *Chem. Rec.*, **2019**, 19., 2189–2208.

[4] I. Marek, A. Masarwa, P.-O. Delaye, M. Leibeling, *Angew. Chem. Int. Ed.*, **2015**, 54, 414–429.