Generation and one-pot reactions of ketenes in microwave-assisted flow mode

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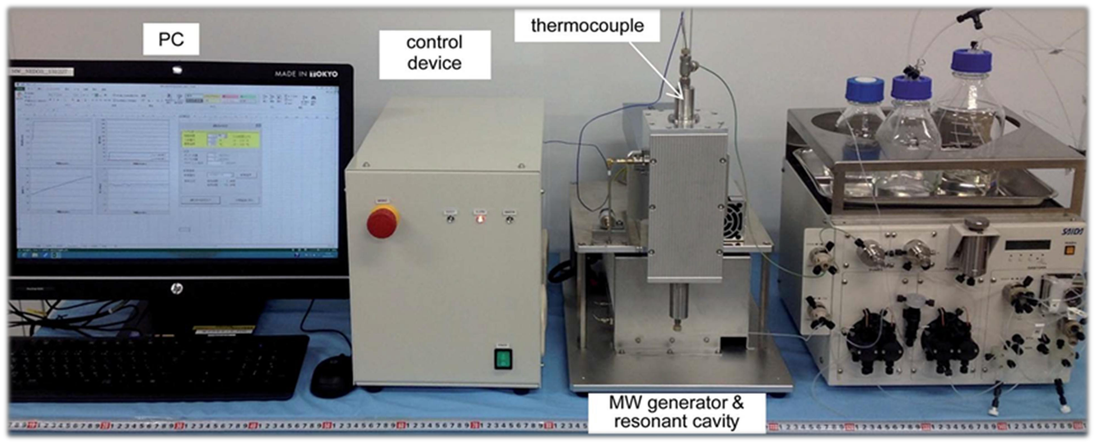
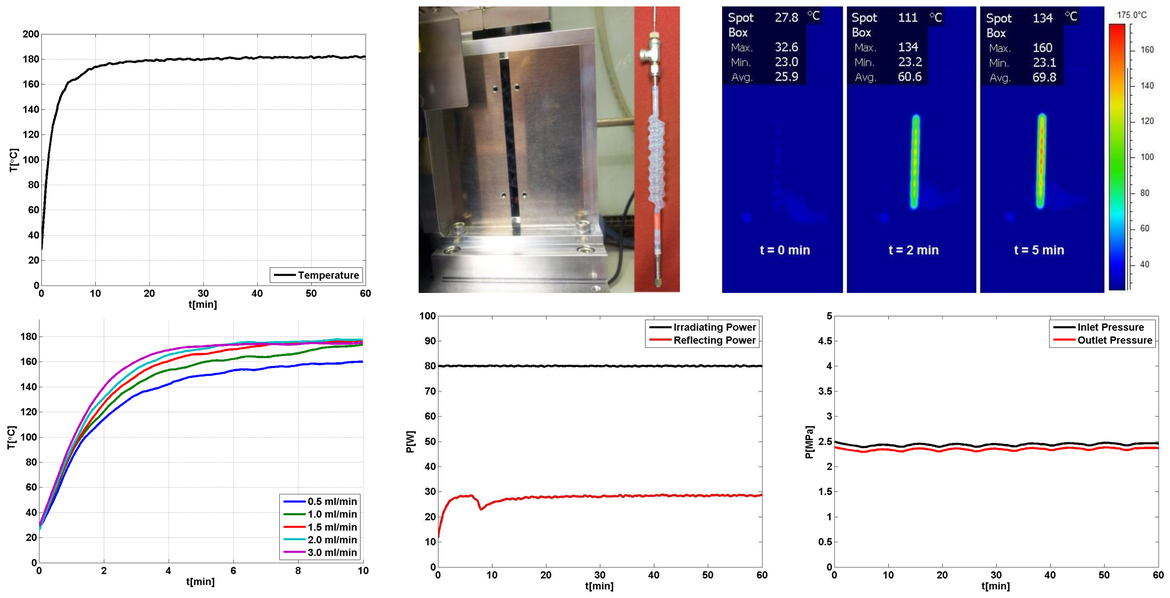
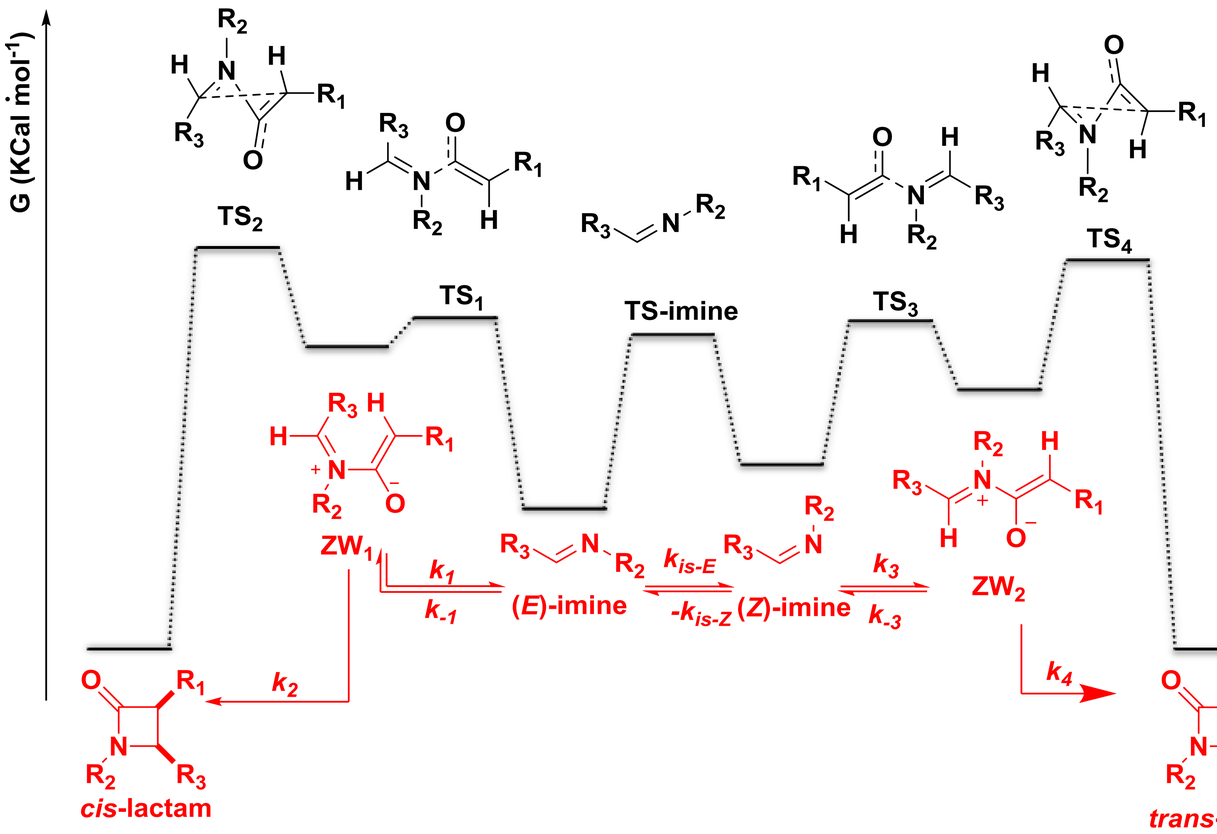
A new single-mode bench-top resonator was evaluated for the microwave-assisted in flow generation of primary ketenes by thermal decomposition of a-diazoketones at high temperature. A number of amides and β-lactams were obtained by in situ ketene generation and reaction with amines and imines in good to excellent yields.

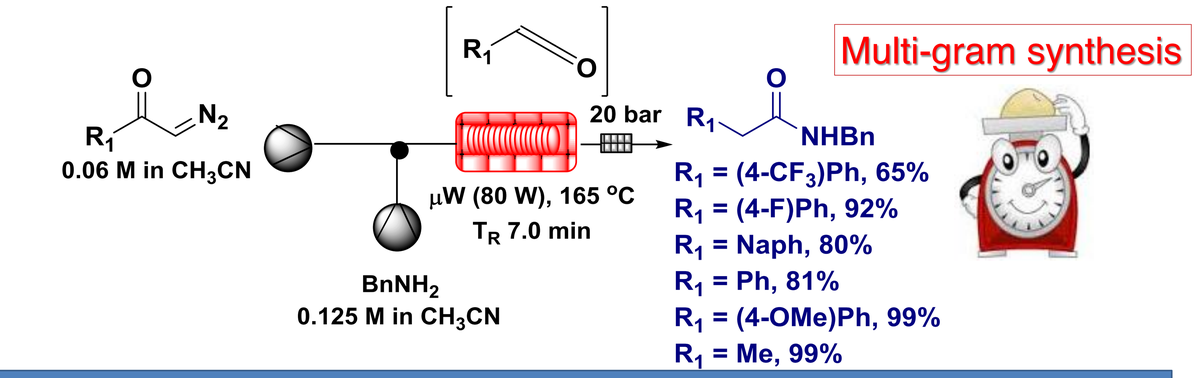


Uniform temperature distribution inside the reactor unit (recorded by a thermocouple and infrared thermal camera) and a good ratio between the irradiating power and the reflecting power over the time is observed.

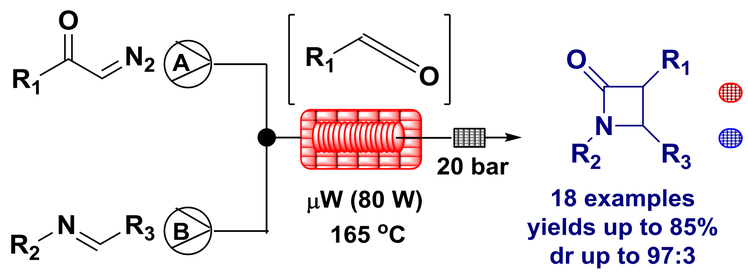


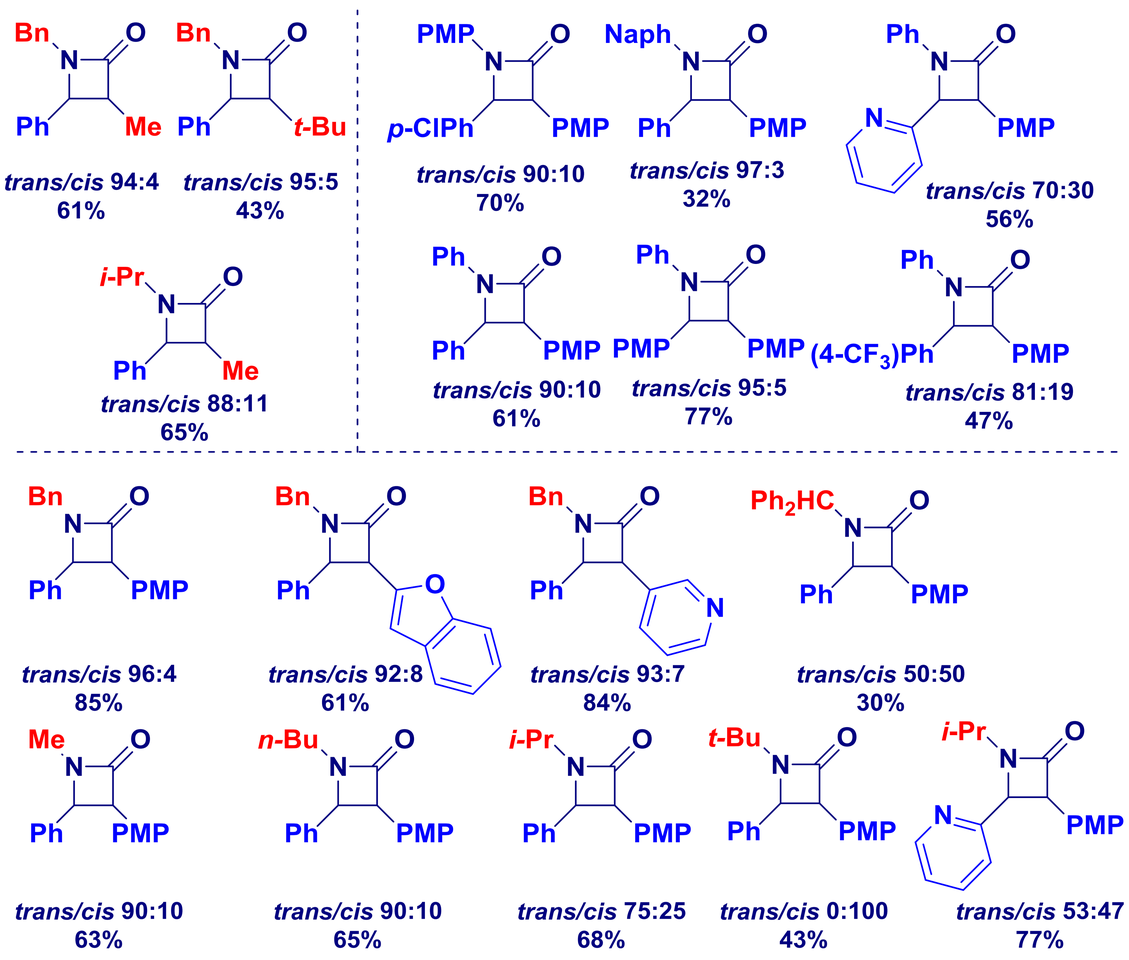
Computational analysis at DFT level (ωB97xD/cc-PVTZ//ωB97xD/cc-PVDZ using the implicit Solvation Model based on Density) of the mechanism of [2+2] Staudinger ketene-imine cycloaddition at high temperature is reported. The relative rates of the key elementary steps were computed and an operational mechanism is suggested for the stereoselective formation of *cis*- and *trans*-lactams.





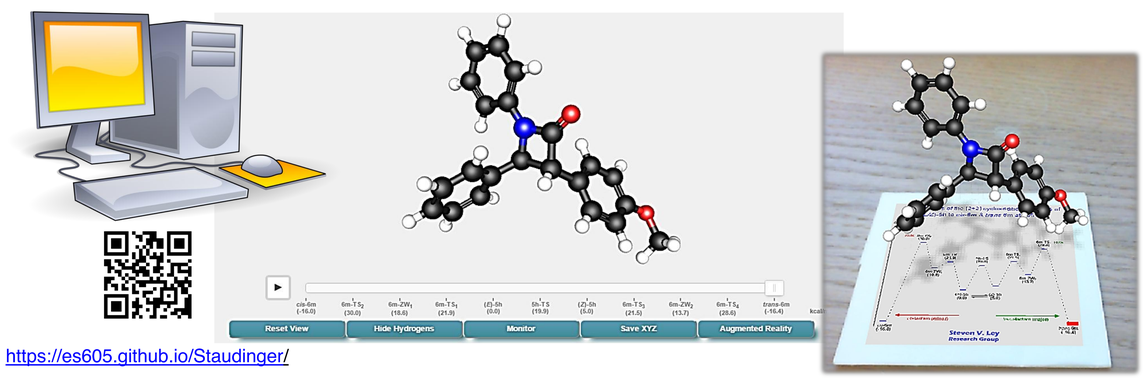
The preferential formation of *trans*-configured β-lactams is observed during the [2+2] Staudinger cycloaddition of a range of ketenes with different imines under controlled reaction conditions (165 °C, 20 bar).





PMP = *p*-(MeO)Ph

A new *web-based molecular viewer*, which takes advantage from augmented reality (AR) technology, is also described for a faster interpretation of computed data.



https://es605.github.io/Staudinger/

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