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**Mechanistic investigation inspired economic synthesis of pyrrole derivatives****Jingping Zhang and Haiyan Yuan**  
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**D**FT investigations are carried out to improve the domino cyclization between gem-dialkylthio vinylallenes and benzylamine ( $BnNH_2$ ). Economic reaction approaches were explored, namely, this reaction can occur under organic solvent-free conditions either catalyzed by trace water or self-catalyzed by  $BnNH_2$ . Three types of reactions (DMSO-assisted, trace water-catalyzed and self-catalyzed by  $BnNH_2$ ) shared the same reaction mechanism with the nucleophilic attack of  $BnNH_2$  on the allenic carbon of thioamide intermediate Re. For trace water-catalyzed reaction another mechanism was also found that the  $BnNH_2$  attacks the carbonyl carbon of the conformational isomer of Re. Among the investigated mechanisms, the trace water catalyzed one is suggested to be the most efficient and convenient synthetic method for pyrroles. Therefore, organic solvent DMSO is not necessary for this reaction, which is further verified by the experimental outcome. Our finding suggests more green chemistry reaction processes by either a trace water catalyst or  $BnNH_2$  self-catalyst and opens a new synthetic strategy for pyrrole derivatives.

**Biography**

Jingping Zhang has completed her PhD from Northeast Normal University and Postdoctoral studies from Kyushu University. She is the Dean of Faculty of Chemistry at Northeast Normal University. She is also the Chief Editor for Journal of Molecular Science. Her research interests are investigation of mechanism for novel organic reactions and design functional materials such as lithium ion battery (cathode and anode) materials. She has published more than 240 papers in Journal of the American Chemical Society, Angewandte Chemie, ACS Catalysis, Green Chemistry, Chemical Communications, Journal of Materials Chemistry A, Advanced Synthesis & Catalysis, The Journal of Organic Chemistry and Journal of Computational Chemistry.

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