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## **Support Information**

Kinetics and mechanism of decomposition induced by solvent evolution

in ICM-101 solvates: solvent-evolution-induced low-temperature

## decomposition

Yu Chi, Longyu Liao, Qian Yu, Chuande Zhao\*, Guijuan Fan Institute of Chemical Materials, China Academy of Engineering Physics (CAEP), P. O. Box 919-327, Mianyang, Sichuan 621900, People's Republic of China



Fig S1 The DSC curve for ICM-101 and its solvates (5 K min<sup>-1</sup>)

<sup>\*</sup> Corresponding author.

E-mail address:C.D.Zhao@caep.cn (C.D. Zhao)



Fig. S2 The DSC curves of H<sub>2</sub>O evolution induced ICM-101@H<sub>2</sub>O solvate decomposition process at different heating rates



Fig. S3 Infrared spectra of gas products in in the second step of ICM-101@H2O

solvate decomposition at 496 K (a) and in the range of 490-504 K (b)



Fig. S4 The exothermic curve of ICM-101@ $H_2O$  solvate

in adiabatic environment



Fig. S5 The ion flow intensity at different retention times of ICM-101@H<sub>2</sub>O (a) and the first decomposition product of ICM-101@H<sub>2</sub>O (b)

LC-MS analysis condition: All the samples were dissolved in acetonitriles. A reverse phase C18 column (2.1 ×100 mm, 1.8  $\mu$ m particle size) maintained at 35 °C was used for chromatography (UPLC, Thermal). The mobile phases consisted of A (water) and B (acetonitrile). A gradient elution was done at a flow rate of 0.20 mL min<sup>-1</sup> with an injection volume of 1  $\mu$ L. The gradient was as follows: 10 to 90 % B (0-5 min), 90% B (5-7 min), 90% to 10% B (7-8 min), 10% B (8-10min). The in situ mass acquisition was performed on a Exactive Plus EMR Orbitrap (Thermal Corporation) using electrospray ionization (ESI) in negative mode.