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Mechanism and implications of methyldibenzothiophene distribution in sedimentary rocks at high maturation

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Dibenzothiophene (DBT) and methyldibenzothiophenes (MDBTs) are important organosulfur compounds in ancient sedimentary organic matter and crude oils. The abundance and distributions of DBTs are influenced by maturity, depositional environment, and lithology. The 4-/1-MDBT (MDR) ratio has been substantially applied as a maturation parameter that shows a different behavior (even a reverse) for a typical MDR-R_o equation at high maturation in some cases. This study conducted gold-tube hydrous pyrolysis experiments to investigate the kinetic characteristics of MDBTs at advanced maturity. Mudstones from Devonian Woodford were selected as reaction samples and heated from 280 to 520 ℃. The relative abundance of MDBTs in the liquid product indicates that the 1-MDBTs are more easily formed before 400 ℃ (corresponding to 1.5% *R*o), and (2+3)-MDBTs are more easily formed after 400℃. It just right suggests that MDBTs are mainly controlled by precursor contribution and is a better indicator parameter of the depositional environment when *R*o<1.5%; in contrast, it is mainly controlled with thermal stability and is a better parameter of thermal evolution when *R*o>1.5%. In addition, we selected (2+3)-MDBT and 4-MDBT for the experiment, respectively, which shows (2+3)-MDBT is more accessible to preserve than 4-MDBT when the geological temperature is greater than 80 ℃. It is concluded that ratio (2+3)-/1-MDBT is a better maturation parameter.