Molecular modelling insight into the intramolecular methyl transfer of methyl dibenzofuran isomers in oil migration orientation and filling pathways

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Methyl dibenzofuran (MDBF) isomers have been proved to be effective tracers of oil charging orientation, distances and pathways. As reported by Li et al. [1], the relative abundance of 1-MDBF to 4-MDBF in oils decreases with increasing migration distance, due to preferential absorption of 1-MDBF onto the water/silica matrix carrier bed. But beyond that, the impact of intramolecular methyl transfer of MDBF isomers (IMTMI) on the relative abundance of MDBFs in oils cannot be ruled out. Through the density functional theory calculations, detailed methyl transfer mechanisms of MDBFs were systematically considered under different solvents conditions. Two possible transfer routes for IMTMI were explored in our study. The results show that IMTMI is hard to occur owing to its too high activation energies (79.1–84.05 kcal/mol) in gas phase, even the most favourable pathway. In addition, the solvent effect of water could decrease energy barriers (65.96–78.09 kcal/mol) of the proton transfer reaction for IMTMI. It is concluded that IMTMI is difficult to react under geological conditions because of temperature higher than 900 K.

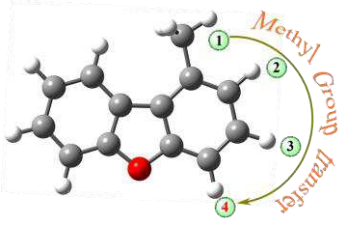

Fig. 1 The intramolecular methyl transfer of MDBF isomers from the 1st site to the 4th position.

[1] Meijun Li et al. (2018), *Org Geochem* **115**, 220-232.