Electronic Supplementary Material (ESI) for Analytical Methods.

Investigation on kinetic processes of zeolitic imidazolate framework-8 film growth and adsorption to chlorohydrocarbons by a quartz crystal microbalance

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Supporting Information

Molecular simulation calculation the size of chlorohydrocarbons

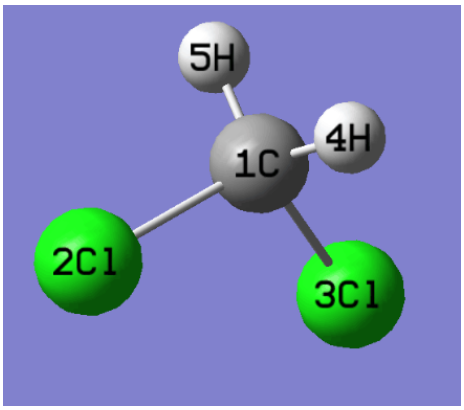
Dichloromethane (DCM)

boiling points : 39.8°C

molecular weight: 84.93

relative density: 1.3266 (20°C)

vapor pressure: 30.55kPa（10°C）



bond length (nm)
1C-4H 0.1069, 1C-5H 0.1069
1C-2Cl 0.183, 1C-3Cl 0.183

bond angle (deg.)
∠4H-1C-5H 113.259，∠4H-1C-2Cl 107.875
∠4H-1C-3Cl 107.875，∠5H-1C-2Cl 107.875
∠5H-1C-3Cl 107.875，∠2Cl-1C-3Cl 112.161

Fig.S1-1 Molecular structure parameters of DCM from molecular simulation calculation

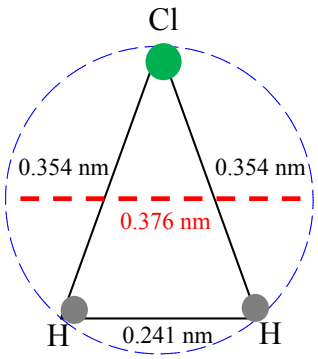


Fig.S1-2 Minimum triangle (ΔHHCl) in the tetrahedral structure of DCM with a kinetic diameter of 0.376 nm.

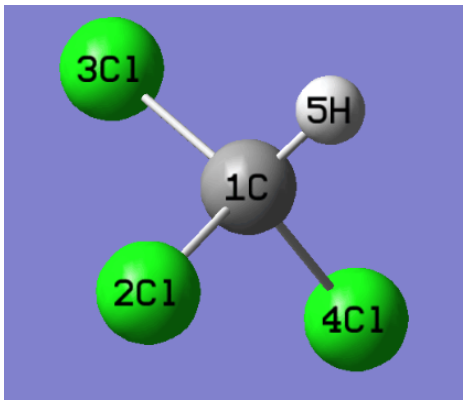
Trichloromethane (TCM)

boiling points : 61.3 °C

molecular weight: 119.39

relative density: 1.50 (20°C)

vapor pressure: 13.33kPa（10°C）



bond length (nm)
1C-5H 0.1067, 1C-2Cl 0.1821
1C-3Cl 0.1821, 1C-4Cl 0.1819

bond angle (deg.)
∠4Cl-1C-5H 107.935，∠4Cl-1C-2Cl 111.152
∠4Cl-1C-3Cl 111.152,∠5H-1C-2Cl 107.704
∠5H-1C-3Cl 107.704，∠2Cl-1C-3Cl 111.017

Fig.S2-1 Molecular structure parameters of TCM from molecular simulation calculation

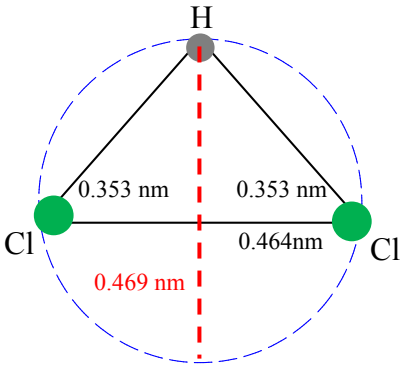


Fig.S2-2 Minimum triangle (ΔHClCl) in the tetrahedral structure of TCM with a kinetic diameter of 0.469 nm.

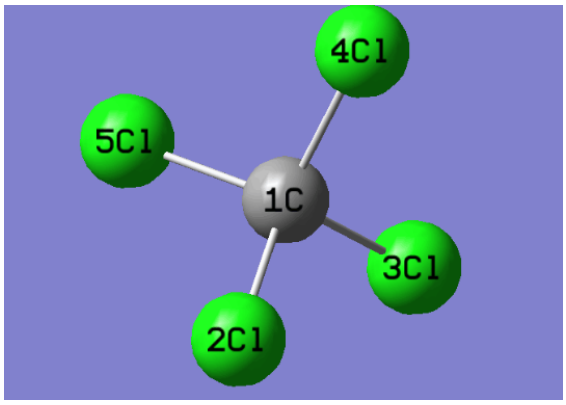
Carbon tetrachloride (CTC)

boiling points : 76.8 °C

molecular weight: 153.84

relative density: 1.595 (20°C)

vapor pressure: 15.26 (25°C)



bond length (nm)
1C-2Cl 0.1822, 1C-3Cl 0.1822
1C-4Cl 0.1822, 1C-5Cl 0.1822

bond angle (deg.)
all the bond angle are 109.524

Fig.S3-1 Molecular structure parameters of CTC from molecular simulation calculation

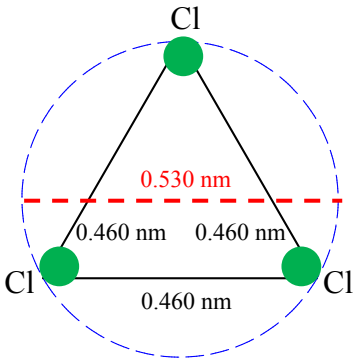


Fig.S3-2 Minimum triangle (ΔClClCl) in the tetrahedral structure of CTC with a kinetic diameter of 0.530 nm.