Supplementary data 1.

The atomic coordinates of the optimized computational model of TPDA-TDTACOF-1 pore.

Supplementary data 2.

atomic coordinates of the optimized computational model of TPDA-BTCOF-1 pore.

Supplementary data 3.

The atomic coordinates of the optimized computational model of TPDA-ViBTCOF-1 pore.