1. **The data of the pore and framework structures of three MOFs:**

Crystal data are as: **IRMOF-3**, cubic, Fm-3m, a= 25.747(1) Å, V=17067(2) Å3, Z=8, R1=0.1160; and they show well-shaped and smooth faces (Fig. 4a). The BET surface area of IRMOF-3 was 2450 m2g−1 (pore volume = 1.01 cm3/g).

The BET surface area of **IRMOF-3-PI** smaller than IRMOF-3 and indicating that the Schiff base formed upon treatment with pyridine-2-aldehyde occupied space in IRMOF-3 pores.

**IRMOF-3-PI-Ru** shows the BET surface area of a value of 1374 m2g−1 with pore volume of 0.77 cm3/g. Change in surface area as well as pore volume IRMOF-3-PI-Ru was smaller than IRMOF-3. It seems space occupied by the Schiff-base moiety has not changed substantially after complex formation with ruthenium. After ruthenium loading, which is connected with heating and stirring of the sample followed by evaporation of the solvent, the particles show some damage. The former particles are broken into compartments of irregular shapes (Fig. 4b).

1. **Products**:

**Pyrene-4,5-dione (1a)** m.p. 299–302 ºC, FTIR (KBr): ν (cm−1): 703, 837, 1267, 1350, 1429, 1517, 1610, 1663, 2850, 2923, 3068. 1H NMR (500 MHz, CDCl3, 25 ºC): δ = 7.52 (t, *J*= 7.6 Hz, 2H), 7.61 (s, 2H), 7.95 (d, *J*= 7.4 Hz, 2H), 8.18 (d, *J*= 6.8 Hz, 2H) ppm. 13C NMR (125 MHz, CDCl3, 25 ºC): δ = 127.52, 128.21, 128.44, 130.11, 130.21, 132.22, 136.04, 180.50 ppm.

**Pyrene-4,5,9,10-tetraone (1b)** m.p. >350 ºC, FTIR (KBr): ν (cm−1): 711, 808, 908, 1054, 1276, 1336, 1421, 1446, 1562, 1676, 2923. 1H NMR (500 MHz, DMSO-d6, 25 ºC): δ = 7.62 (t, *J*= 7.7 Hz, 2H), 8.38 (d, *J*= 7.7 Hz, 4H) ppm. 13C NMR (125 MHz, DMSO-d6, 25 ºC): δ = 131.29, 131.44, 134.80, 136.82, 178.13 ppm.

**Chrysene-5,6-dione (2a)** m.p. 189–191 ºC, FTIR (KBr): ν (cm−1): 660, 713, 756, 835, 957, 1040, 1086, 1250, 1298, 1364, 1447, 1483, 1595, 1662, 1693, 1767, 2927, 3066. 1H NMR (500 MHz, CDCl3, 25 ºC): δ = 7.52 (t, *J*= 7.5 Hz, 1H), 7.60 (t, *J*= 7.7 Hz, 1H), 7.74 (t, *J*= 8.5 Hz, 1H), 7.77 (t, *J*= 8.1 Hz, 1H), 7.87 (d, *J*= 7.9 Hz, 1H), 8.12 (d, *J*= 8.6 Hz, 2H), 8.18 (d, *J*= 7.4 Hz, 1H), 8.20 (d, *J*= 8.6 Hz, 1H), 9.43 (d, *J*= 8.8 Hz, 1H) ppm. 13C NMR (125 MHz, CDCl3, 25 ºC): δ = 121.54, 125.64, 126.34, 127.62, 128.09, 129.09, 130.32, 130.45, 131.09, 131.28, 132.67, 134.23, 136.49, 137.06, 137.78, 138.29, 182.45, 184.63 ppm.

**Anthracene-9,10-dione(anthraquinone) (3a)** m.p. 286 ºC, FTIR (KBr): ν (cm−1); 695, 721, 810, 820, 912, 937, 1084, 1171, 1287, 1306, 1333, 1455, 1581, 1593, 1660, 3074, 3323, 3426. 1H NMR (500 MHz, CDCl3, 25 ºC): δ = 7.82 (t, 2H), 8.33 (d, 2H), ppm. 13C NMR (125 MHz, CDCl3, 25 ºC): δ = 127.14, 133.11, 134.48, 183.50 ppm.

**9,10-Phenanthrenequinone (4a)** m.p. 209-210 ºC, FTIR (KBr): ν (cm−1); 638, 766, 770, 925, 1231, 1283, 1294, 1306, 1333, 1452, 1581, 1593, 1660, 1875, 3067, 3088, 3108. 1H NMR (500 MHz, CDCl3, 25 ºC): δ = 7.72 (m, *J*=7.9 2H), 7.83 (m, *J*=8,7 2H) 7.92 (d, *J*=7.9 2H), 8.79 (d, *J*=8.7 2H), ppm. 13C NMR (125 MHz, CDCl3, 25 ºC): δ = 123.90, 129.52, 130.51, 135.88, 136.13, 180.50 ppm.

**Phthalaldehyde (5a)** m.p. 56 ºC, FTIR (KBr): ν (cm−1): 627, 765, 860, 998, 1190, 1201, 1273, 1310, 1481, 1578, 1593, 1688, 1722, 2850, 2902, 3360. 1H NMR (500 MHz, CDCl3, 25 ºC): δ = 7.80 (m, 2H), 7.96 (m, 2H), 10.53 (s, 2H), ppm. 13C NMR (125 MHz, CDCl3, 25 ºC): δ = 131.11, 133.87, 136.48, 192.50 ppm.

**Benzoic acid (6a,7a)** m.p. 122 ºC, FTIR (KBr): ν (cm−1); 666, 709, 812, 1003, 1075, 1296, 1327, 1428, 1466, 1690, 2564, 2607, 2886, 3012, 3073. 1H NMR (500 MHz, CDCl3, 25 ºC): δ = 7.44 (m, 2H), 7.62 (m, 1H), 8.12 (d, 2H), 1210 (s, 1H), ppm. 13C NMR (125 MHz, CDCl3, 25 ºC): δ = 128.59, 129.64, 130.48, 133.84, 172.50 ppm.

**Benzophenone (8a)** m.p. 48 ºC, FTIR (KBr): ν (cm−1): 639, 698 706, 768, 919, 946, 998, 1162, 1177, 1281, 1324, 1450, 1578, 1593, 1628, 1666, 2919, 3067, 3291. 1H NMR (500 MHz, CDCl3, 25 ºC): δ = 7.47 (m, 2H), 7.56 (m, 1H), 7.79 (m, 2H), ppm. 13C NMR (125 MHz, CDCl3, 25 ºC): δ = 128.11, 129.87, 132.48, 137.52, 196.50 ppm.

**1-Benzothiophene 1,1-dioxide (9a)** m.p. 138-139 ºC, FTIR (KBr): ν (cm−1): 520, 621, 683, 759, 865, 1149, 1285, 1452, 1548, 3062, 3105. 1H NMR (500 MHz, CDCl3, 25 ºC): δ = 6.76 (d, *J*= 6.8 Hz, 2H), 7.26 (d, *J*= 7.2 Hz, 2H), 7.41 (d, *J*= 7.4 Hz, 4H), 7.59 (m, *J*= 7.6 Hz, 4H), 7.71 (d, *J*= 7.7 Hz, 4H) ppm. 13C NMR (125 MHz, CDCl3, 25 ºC): δ = 121.29, 121.89, 122.81, 123.77, 124.44, 132.80, 139.82, 140.85 ppm.

**Dibenzothiophene S,Ś-dioxide (10a)** m.p. 233 ºC, FTIR (KBr): ν (cm−1); 540, 569, 600, 697, 712, 759, 865, 944, 1048, 1121 1166, 1285, 1452, 1548, 3065, 3086. 1H NMR (500 MHz, CDCl3, 25 ºC): δ = 7.51 (d, 2H), 7.60 (m, 2H), 7.66 (d, 2H), 7.80 (m, 4H), ppm. 13C NMR (125 MHz, CDCl3, 25 ºC): δ = 121.52, 122.89, 124.31,126.67, 135.54, 139.82, ppm.

**4,6-Dimethyldibenzothiophene S,Ś-dioxide (11a)** m.p. 243–244ºC ºC, FTIR (KBr): ν (cm−1): 569, 596, 697, 712, 759, 866, 944, 1048, 1121 1158, 1255, 1313 1478, 1573, 3066. 1H NMR (500 MHz, CDCl3, 25 ºC): δ = 2.70 (s, 6H), 7.25 (d, 2H), 7.47 (t, 2H), 7.55 (d, 2H) ppm.

**4-Methyldibenzothiophene S,Ś-dioxide (12a)** m.p. 168-169 ºC, FTIR (KBr): ν (cm−1): 569, 600, 712, 759, 865, 944, 1048, 1121 1166, 1285, 1452, 1548, 3065, 3086. 1H NMR (500 MHz, CDCl3, 25 ºC): δ = 2.624 (s, 3H), 7.259 (s, 1H), 7.33 (s, 1H), 7.45 (s, 1H), 7.48 (s, 1H), 7.60 (s, 1H), 7.80 (s, 1H), 7.98 (s, 1H), ppm.