## Nano-metal–organic frameworks as corrosion inhibitors for strengthening anti-corrosion behavior of carbon steel in sulfuric acid environment: From synthesis to applications

## **Supplementary Materials**

| N9- Cu8   | 1.866 | Cu8- N7- C8    | 170.24 |
|-----------|-------|----------------|--------|
| N7- Cu8   | 1.879 | N9- C10- Cu11  | 137.36 |
| Cu24- C25 | 1.999 | N2- C1- Cu24   | 177.06 |
| N21- Cu24 | 2.256 | C1- N2- Sn3    | 149.23 |
| Cu11- C29 | 2.008 | Sn3- C4- N5    | 177.40 |
| Cu11- N15 | 2.267 | C10- Cu11- N15 | 107.59 |
| C10- Cu11 | 2.025 | C10- Cu11- N28 | 117.66 |
| C6- Cu24  | 2.032 | C10- Cu11- C29 | 107.00 |
| C1- Cu24  | 2.015 | N15- Cu11- C22 | 104.41 |
| Sn3- Cu7  | 2.270 | N28- Cu11- C29 | 113.93 |
| Sn3- C37  | 2.277 | C1- Cu24- N21  | 103.18 |
| Sn3- C34  | 2.302 | C1- Cu24- C25  | 111.75 |
| Sn3- C4   | 2.313 | C8- Cu24- N21  | 108.69 |
| Sn3- N2   | 2.773 | C1- Cu24- C6   | 112.83 |
| C1- N2    | 1.209 | C6- Cu24- N2   | 108.00 |
| C6- N7    | 1.214 | N2- Sn3- C37   | 89.83  |
| N9- C10   | 1.208 | N2- Sn3- C34   | 80.90  |
| C4- N5    | 1.211 | C4- Sn3- C47   | 93.01  |
| C27- N28  | 1.208 | C4- Sn3- C37   | 89.13  |
| C29- N30  | 1.208 | C34- Sn3- C47  | 124.94 |
| C52-O53   | 1.273 | C37- Sn3- C47  | 103.70 |
| C49- O50  | 1.268 | C34- Sn3- C37  | 128.27 |

Table SF1 Bond lengths (Å) and bond angles (deg.) of NMOF1

| C1—Cu1  | 1.9215(13) | N2—C2—Cu1 | 176.78(11) |  |  |  |
|---|------------|-----------|------------|--|--|--|
| C1—N1   | 1.1566(17) | C2—Cu1—C1 | 125.91(6)  |  |  |  |
| C2—N2   | 1.1569(16) | C2—Cu1—N3 | 110.20(5)  |  |  |  |
| C2—Cu1  | 1.9243(12) | C1—Cu1—N3 | 103.16(5)  |  |  |  |
| C3—Sn1  | 2.1201(13) | C2—Cu1—N4 | 102.48(5)  |  |  |  |
| C4—Sn1  | 2.1210(13) | C1—Cu1—N4 | 113.04(5)  |  |  |  |
| C5—Sn1  | 2.1136(13) | N3—Cu1—N4 | 98.99(5)   |  |  |  |
| Cu1—N3  | 2.1365(11) | C1—N1—Sn1 | 176.61(12) |  |  |  |
| Cu1—N4  | 2.1259(11) | C2—N2—Sn1 | 175.46(11) |  |  |  |
| N1—Sn1  | 2.3229(12) | N1—Sn1—N2 | 178.98(4)  |  |  |  |
| N2—Sn1  | 2.3128(12) | N2—Sn1—C4 | 90.79(5)   |  |  |  |
| Cu1—C1—N1   | 175.89(12) | N1—Sn1—C3 | 89.93(6)   |  |  |  |
| N2—Sn1—C3   | 90.46(6)   | N2—Sn1—C5 | 88.61(5)   |  |  |  |
| C4—Sn1—C3   | 118.64(6)  | C4—Sn1—C5 | 120.32(6)  |  |  |  |
| N1—Sn1—C5   | 90.38(5)   | C3—Sn1—C5 | 121.04(6)  |  |  |  |
| Symmetry codes: (i) $x, -y+3/2, z+1/2$ ; (ii) $-x+2, -y, -z$ ; (iii) $-x+1, -y, -z$ ; |            |           |            |  |  |  |
| (iv) $x, -y+3/2, z-1/2$   |            |           |            |  |  |  |

Table SF2 Selected bond lengths (Å) and bond angles (°) of NMOF2.



Figure SF1 TEM images of NMOF1 (a and b) and of NMOF2 (c and d)