**Table 2.** **The Fit Parameters of U L3-edge EXAFS Data of Functionalized MMSNs After Exposure to U in the HSW Simulant**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Samplesa** | **Scattering paths** | **Interatomic distance (Å)b** | **Coordination numberc** | **Debye–Waller factor, σ2 (Å2)b** | **E0** | **R-factor** |
| MMSNs-DIM | U-Oax | 1.80 (1) | 2 | 0.003 (1) | 6.4 ± 2.4 | 0.0024 |
|  | U-Oeq | 2.25 (5) | 3.8 | 0.008 (4) |  |  |
|  | U-Nd | 2.34 (5) | 1.2 | 0.008 (4) |  |  |
|  | U-Si | 3.13 (2) | 0.4 | 0.001 (7) |  |  |
| MMSNs-AD | U-Oax | 1.80 (1) | 2 | 0.002 (1) | 6.6 ± 2.5 | 0.0029 |
|  | U-Oeq | 2.26 (5) | 3.6 | 0.008 (4) |  |  |
|  | U-N | 2.34 (5) | 1.4 | 0.008 (4) |  |  |
|  | U-Si | 3.14 (3) | 0.4 | 0.002 (9) |  |  |
| MMSNs-PP | U-Oax | 1.81 (1) | 2 | 0.003 (1) | 6.8 ± 4.0 | 0.0030 |
|  | U-Oeq | 2.26 (2) | 5.1 | 0.008 (3) |  |  |
|  | U-P | 3.56 (3) | 0.9 | 0.02 (3) |  |  |
|  | U-Si | 3.13 (4) | 0.6 | 0.003 (5) |  |  |
| MMSNs-PPA | U-Oax | 1.80 (1) | 2 | 0.003 (1) | 7.3 ± 2.1 | 0.0028 |
|  | U-Oeq | 2.26 (1) | 4.1 | 0.008 (1) |  |  |
|  | U-N | 2.34 (1) | 0.9 | 0.008 (1) |  |  |
|  | U-Si | 3.13 (2) | 0.7 | 0.003 (5) |  |  |
| MMSNs-PPI | U-Oax | 1.80 (1) | 2 | 0.003 (1) | 7.3 ± 2.3 | 0.0027 |
|  | U-Oeq | 2.25 (4) | 3.4 | 0.007 (3) |  |  |
|  | U-N | 2.34 (4) | 1.6 | 0.007 (3) |  |  |
|  | U-Si | 3.13 (3) | 0.6 | 0.004 (8) |  |  |
| MMSNs-PM | U-Oax | 1.80 (1) | 2 | 0.003 (1) | 6.6 ± 2.1 | 0.0028 |
|  | U-Oeq | 2.25 (4) | 4.3 | 0.008 (4) |  |  |
|  | U-N | 2.34 (4) | 0.7 | 0.008 (4) |  |  |
|  | U-Si | 3.12 (2) | 0.4 | 0.002 (3) |  |  |
| a Amplitude was set at 1 for data fitting of all samples.  b The uncertainty as calculated by Artemis are listed in parentheses, representing the errors in the last digit.  c Coordination number of the axial uranyl oxygen atoms was set at 2. The errors for the other coordination numbers are ±30%.  d Total coordination numbers of the equatorial uranyl oxygen and nitrogen atoms were set at 5, and variations in interatomic distance and Debye–Waller factor of the U-Oeq and U-N paths were set identical. | | | | | | |