**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. |