|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Sample | path | CN | R (Å) | *σ*2 (Å2) | ΔE (eV) | *χ*2red | *R*-factor |
| BaHAsO4·H2O | As-O | 3 | 1.68±0.005 | 0.0016±0.0003 | 7.6±1.5 | 208 | 0.009 |
|  | As-OH | 1 | 1.76±0.005 |  |  |  |  |
| Ba3(AsO4)2 | As-O | 4 | 1.70±0.006 | 0.0014±0.001 | 6.0±1.9 | 106 | 0.011 |
| Configuration C2 as the initial model |  |  |  |  |  |  |  |
| AT-pH3 | As-O | 3 | 1.66±0.005 | 0.0007±0.0003 | 8.9±1.3 | 6.5 | 0.009 |
|  | As-OH | 1 | 1.77±0.005 |  |  |  |  |
| AT-pH7 | As-O | 3 | 1.67±0.004 | 0.0006±0.0003 | 8.9±1.2 | 26 | 0.007 |
|  | As-OH | 1 | 1.78±0.004 |  |  |  |  |
| AT-pH10 | As-O | 3 | 1.67±0.003 | 0.0007±0.0003 | 8.7±1.3 | 30 | 0.008 |
|  | As-OH | 1 | 1.78±0.003 |  |  |  |  |
| Ba3(AsO4)2 as the initial model |  |  |  |  |  |  |  |
| AT-pH3 | As-O | 4 | 1.69±0.006 | 0.0026±0.0003 | 5.2±1.5 | 8.0 | 0.011 |
| AT-pH7 | As-O | 4 | 1.69±0.006 | 0.0025±0.0003 | 4.9±1.6 | 51 | 0.012 |
| AT-pH10 | As-O | 4 | 1.69±0.006 | 0.0027±0.0004 | 5.1±1.6 | 42 | 0.012 |