|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Only one So2 is used** |  |  |  |  |  |  |  |
| name | N | S02 | sigma^2 | e0 | delr | Reff | R |
| [YbVO4-zircon.txt] O1\_1 | 4 | **0.869** | 0.00596 | 2.679 | -0.00934 | 2.2789 | 2.26956 |
| [YbVO4-zircon.txt] O1\_2 | 4 | **0.869** | 0.00596 | 2.679 | -0.00982 | 2.3943 | 2.38448 |
| [YbVO4-zircon.txt] V1\_1 | 2 | **0.869** | 0.00297 | 4.179 | 0.03676 | 3.1235 | 3.16026 |
| [YbVO4-zircon.txt] O1\_2 V1\_1 | 8 | **0.869** | 0.00446 | 4.179 | -0.0148 | 3.608 | 3.59321 |
| [YbVO4-zircon.txt] O1\_1 O1\_2 | 8 | **0.869** | 0.00953 | 4.179 | -0.01501 | 3.6605 | 3.64549 |
| [YbVO4-zircon.txt] O1\_1 O1\_2 | 16 | **0.869** | 0.01013 | 4.179 | -0.01576 | 3.8437 | 3.82794 |
| [YbVO4-zircon.txt] V1\_2 | 4 | **0.869** | 0.01344 | 4.179 | 0.00692 | 3.8525 | 3.85941 |
| [YbVO4-zircon.txt] Yb1\_1 | 4 | **0.869** | 0.00681 | 4.179 | 0.00692 | 3.8525 | 3.85941 |
| [YbVO4-zircon.txt] O1\_1 V1\_2 | 8 | **0.869** | 0.0097 | 4.179 | -0.01605 | 3.9148 | 3.89875 |
| [YbVO4-zircon.txt] O1\_1 O1\_1 | 8 | **0.869** | 0.01072 | 4.179 | -0.01608 | 3.9222 | 3.90612 |
| [YbVO4-zircon.txt] O1\_1 V1\_2 O1\_1 | 4 | **0.869** | 0.01385 | 4.179 | -0.01631 | 3.9771 | 3.96079 |
|  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |
| **So2-1 and So2-2 Free parameters – with SS1 fixed at 0.00297** |  |  |  |  |  |  |  |
| name | N | S02 | sigma^2 | e0 | delr | Reff | R |
| [YbVO4-zircon.txt] O1\_1 | 4 | **0.852** | 0.0057 | 2.679 | -0.00987 | 2.2789 | 2.26903 |
| [YbVO4-zircon.txt] O1\_2 | 4 | **0.852** | 0.0057 | 2.679 | -0.01036 | 2.3943 | 2.38393 |
| [YbVO4-zircon.txt] V1\_1 | 2 | **0.897** | 0.00297 | 4.179 | 0.03747 | 3.1235 | 3.16097 |
| [YbVO4-zircon.txt] O1\_2 V1\_1 | 8 | **0.897** | 0.00433 | 4.179 | -0.01562 | 3.608 | 3.59238 |
| [YbVO4-zircon.txt] O1\_1 O1\_2 | 8 | **0.897** | 0.00912 | 4.179 | -0.01585 | 3.6605 | 3.64465 |
| [YbVO4-zircon.txt] O1\_1 O1\_2 | 16 | **0.897** | 0.00969 | 4.179 | -0.01664 | 3.8437 | 3.82706 |
| [YbVO4-zircon.txt] V1\_2 | 4 | **0.897** | 0.01329 | 4.179 | 0.00757 | 3.8525 | 3.86007 |
| [YbVO4-zircon.txt] Yb1\_1 | 4 | **0.897** | 0.00635 | 4.179 | 0.00757 | 3.8525 | 3.86007 |
| [YbVO4-zircon.txt] O1\_1 V1\_2 | 8 | **0.897** | 0.0095 | 4.179 | -0.01695 | 3.9148 | 3.89785 |
| [YbVO4-zircon.txt] O1\_1 O1\_1 | 8 | **0.897** | 0.01026 | 4.179 | -0.01698 | 3.9222 | 3.90522 |
| [YbVO4-zircon.txt] O1\_1 V1\_2 O1\_1 | 4 | **0.897** | 0.01369 | 4.179 | -0.01722 | 3.9771 | 3.95988 |
|  |  |  |  |  |  |  |  |
| **So2-1 and So2-2 Free parameters** |  |  |  |  |  |  |  |
| name | N | S02 | sigma^2 | e0 | delr | Reff | R |
| [YbVO4-zircon.txt] O1\_1 | 4 | **0.756** | 0.00414 | 2.679 | -0.01296 | 2.2789 | 2.26594 |
| [YbVO4-zircon.txt] O1\_2 | 4 | **0.756** | 0.00414 | 2.679 | -0.01361 | 2.3943 | 2.38069 |
| [YbVO4-zircon.txt] V1\_1 | 2 | **1.912** | 0.0108 | 4.179 | 0.05771 | 3.1235 | 3.18121 |
| [YbVO4-zircon.txt] O1\_2 V1\_1 | 8 | **1.912** | 0.00747 | 4.179 | -0.02051 | 3.608 | 3.58749 |
| [YbVO4-zircon.txt] O1\_1 O1\_2 | 8 | **1.912** | 0.00662 | 4.179 | -0.02081 | 3.6605 | 3.63969 |
| [YbVO4-zircon.txt] O1\_1 O1\_2 | 16 | **1.912** | 0.00704 | 4.179 | -0.02185 | 3.8437 | 3.82185 |
| [YbVO4-zircon.txt] V1\_2 | 4 | **1.912** | 0.0124 | 4.179 | 0.0145 | 3.8525 | 3.867 |
| [YbVO4-zircon.txt] Yb1\_1 | 4 | **1.912** | 0.00499 | 4.179 | 0.0145 | 3.8525 | 3.867 |
| [YbVO4-zircon.txt] O1\_1 V1\_2 | 8 | **1.912** | 0.00827 | 4.179 | -0.02226 | 3.9148 | 3.89254 |
| [YbVO4-zircon.txt] O1\_1 O1\_1 | 8 | **1.912** | 0.00745 | 4.179 | -0.0223 | 3.9222 | 3.8999 |
| [YbVO4-zircon.txt] O1\_1 V1\_2 O1\_1 | 4 | **1.912** | 0.01277 | 4.179 | -0.02261 | 3.9771 | 3.95449 |