**Table. III:** Atomic position, displacement parameters, fractional coordinates and occupation parameters for the series Sr2Mn1-xNixTeO6 with (x = 0.25, 0.5 and 0.75) after Rietveld refinement from XRPD data collected at room temperature.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Atom | **Wyckoff site** | X | y | z | B(Å2) | Occ. |
| x = 0.25 (*P*21/*n*) | | | | | | |
| Sr  Ni1/Mn1/Te1  Ni2/Mn2/Te2  O1  O2  O3 | 4e  2a  2b  4e  4e  4e | 0.4860(14)  0.0000  0.0000  0.958(9)  0.268(8)  0.701(6) | 0.0107(8)  0.0000  0.0000  -0.001(5)  0.247(11)  0.210(6) | 0.2602(9)  0.0000  0.5000  0.744(5)  1.007(7)  0.022(6) | 1.57(5)  0.5(4)  2.1(3)  1.0000  1.0000  1.0000 | 2.0000  0.220(5)/ 0.620(5)/ 0.170(5)  0.030(5)/ 0.13(5)/ 0.840(5)  2.0000  2.0000  2.0000 |
| x = 0.5 (*P*21/*n*) | | | | | | |
| Sr  Ni1/Mn1/Te1  Ni2/Mn2/Te2  O1  O2  O3 | 4e  2a  2b  4e  4e  4e | 0.482(2)  0.0000  0.0000  1.067(8)  0.261(12)  0.802(10) | 0.0117(8)  0.0000  0.0000  0.003(6)  0.270(14)  0.288(12) | 0.253(4)  0.0000  0.5000  0.742(4)  0.999(10)  -0.027(14) | 0.76(11)  0.1(4)  0.9(3)  1.07(2)  1.07(2)  1.07(2) | 2.0000  0.366(4)/ 0.434(4)/ 0.20(4)  0.134(4)/ 0.066(4)/ 0.800(4)  2.0000  2.0000  2.0000 |
| x = 0.75 (*I*2/*m*) | | | | | | |
| Sr  Ni1/Mn1/Te1  Ni2/Mn2/Te2  O1  O2 | 4i  2d  2a  4i  8j | 0.496(3)  0.5000  0.0000  -0.095(5)  0.255(5) | 0.0000  0.5000  0.0000  0.0000 0.259(5) | 0.7631(7)  0.0000  0.0000  0.767(6)  0.984(9) | 1.44(10)  0.17682  2.68(17)  1.00000  1.00000 | 2.0000  0.610(5)/ 0.200(5)/ 0.190(5)  0.140 (5)/ 0.055(5)/ 0.81(5)  2.0000  4.0000 |