Table S1. Bond valence calculations\* for donnayite-(Y).

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Sr1** | **Sr2** | **Sr3** | **Na4** | **Ca5** | **Y6** | **C1** | **C2** | **C3** | **C4a** | **C4b** | **C5a** | **C5b** | **C6a** | **C6b** | **∑** |
| **O1** | 0.22 | 0.22 |  |  |  | 0.41 | 1.24 |  |  |  |  |  |  |  |  | **2.09** |
| **O2** |  | 0.21 | 0.24 | 0.26 |  |  | 1.46 |  |  |  |  |  |  |  |  | **2.17** |
| **O3** | 0.21 |  | 0.24 |  | 0.32 |  | 1.39 |  |  |  |  |  |  |  |  | **2.16** |
| **O4** |  | 0.23 | 0.22 |  | 0.34 |  |  | 1.36 |  |  |  |  |  |  |  | **2.15** |
| **O5** | 0.22 |  | 0.23 |  |  | 0.42 |  | 1.22 |  |  |  |  |  |  |  | **2.09** |
| **O6** | 0.21 | 0.23 |  | 0.27 |  |  |  | 1.42 |  |  |  |  |  |  |  | **2.13** |
| **O7** | 0.22 |  | 0.23 | 0.28 |  |  |  |  | 1.39 |  |  |  |  |  |  | **2.12** |
| **O8** | 0.23 | 0.21 |  |  | 0.33 |  |  |  | 1.42 |  |  |  |  |  |  | **2.19** |
| **O9** |  | 0.22 | 0.23 |  |  | 0.41 |  |  | 1.24 |  |  |  |  |  |  | **2.10** |
| **O10** |  | 0.31 |  |  |  | 0.21 |  |  |  | 0.66 | 0.69 |  |  |  |  | **1.87** |
| **O11a** |  |  | 0.24 |  |  | 0.34 |  |  |  | 0.46 |  |  |  |  |  | **0.75** |
| **O11b** |  |  | 0.25 |  |  | 0.32 |  |  |  |  | 0.46 |  |  |  |  | **0.75** |
| **O12a** |  | 0.24x0.5↓→ |  | 0.21x0.5↓→ |  |  |  |  |  | 0.75 |  |  |  |  |  | **0.98** |
| **O12b** | 0.27x0.5↓→ |  |  |  | 0.25x0.5↓→ |  |  |  |  |  | 0.75 |  |  |  |  | **1.01** |
| **O13** | 0.29 |  |  |  |  | 0.24 |  |  |  |  |  | 0.75 | 0.67 |  |  | **1.95** |
| **O14a** |  | 0.25x0.5↓→ |  | 0.21x0.5↓→ |  |  |  |  |  |  |  | 0.77 |  |  |  | **1.00** |
| **O14b** | 0.24x0.5↓→ |  |  |  | 0.24x0.5↓→ |  |  |  |  |  |  |  | 0.84 |  |  | **1.08** |
| **O15a** |  |  | 0.26x0.5↓→ |  |  | 0.31x0.5↓→ |  |  |  |  |  | 0.41 |  |  |  | **0.70** |
| **O15b** |  |  | 0.25x0.5↓→ |  |  | 0.34x0.5↓→ |  |  |  |  |  |  | 0.44 |  |  | **0.74** |
| **O16** |  |  | 0.32 |  |  | 0.21 |  |  |  |  |  |  |  | 0.64 | 0.69 | **1.86** |
| **O17a** |  | 0.24x0.5↓→ |  | 0.22x0.5↓→ |  |  |  |  |  |  |  |  |  | 0.79 |  | **1.02** |
| **O17b** | 0.23x0.5↓→ |  |  |  | 0.26x0.5↓→ |  |  |  |  |  |  |  |  |  | 0.84 | **1.09** |
| **O18a** |  |  | 0.25x0.5↓→ |  |  | 0.35x0.5↓→ |  |  |  |  |  |  |  | 0.53 |  | **0.83** |
| **O18b** |  |  | 0.24x0.5↓→ |  |  | 0.35x0.5↓→ |  |  |  |  |  |  |  |  | 0.51 | **0.81** |
| **O19a** | 0.26x0.5↓→ |  |  |  | 0.28x0.5↓→ |  |  |  |  |  |  |  |  |  |  | **0.27** |
| **O19b** |  | 0.26x0.5↓→ |  | 0.23x0.5↓→ |  |  |  |  |  |  |  |  |  |  |  | **0.25** |
| **O20a** | 0.28x0.5↓→ |  |  |  | 0.31x0.5↓→ |  |  |  |  |  |  |  |  |  |  | **0.30** |
| **O20b** |  | 0.26x0.5↓→ |  | 0.25x0.5↓→ |  |  |  |  |  |  |  |  |  |  |  | **0.26** |
| **O21a** | 0.28x0.5↓→ |  |  |  | 0.28x0.5↓→ |  |  |  |  |  |  |  |  |  |  | **0.28** |
| **O21b** |  | 0.29x0.5↓→ |  | 0.27x0.5↓→ |  |  |  |  |  |  |  |  |  |  |  | **0.28** |
| **∑** | **2.38** | **2.40** | **2.46** | **1.51** | **1.80** | **2.91** | **4.09** | **4.00** | **4.05** | **1.87** | **1.90** | **1.93** | **1.95** | **1.96** | **2.04** |  |

\*Bond-valence parameters were taken from Brese and O’Keeffe (1991). Bond-valence sums were calculated taking into account site occupancy factors.