**The crystal structure of alstonite, BaCa(CO3)2: an extraordinary example of “hidden” complex twinning in large single crystals**

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**Table S1**. Bond-valence sums (in valence units) for alstonite.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Ba1** | **Ba2** | **Ba3** | **Ca1** | **Ca2** | **Ca3** | **C1** | **C2** | **C3** | **C4** | **C5** | **C6** | **C7** | **C8** | **ΣO** |
| **O1** | 0.227\* |  | 0.229 |  |  | 0.245 | 1.205 |  |  |  |  |  |  |  | 1.906 |
| **O2** |  |  | 0.239 | 0.120\* | 0.255\* |  | 1.151 |  |  |  |  |  |  |  | 1.765 |
| **O3** | 0.215\* | 0.346\* |  | 0.165\* |  |  | 1.084 |  |  |  |  |  |  |  | 1.810 |
| **O4** | 0.274\* | 0.205\* |  |  |  | 0.187 |  | 1.452 |  |  |  |  |  |  | 2.118 |
| **O5** |  | 0.278\* |  | 0.181\* | 0.183\* |  |  | 1.314 |  |  |  |  |  |  | 1.956 |
| **O6** |  |  | 0.304 |  | 0.193\* | 0.108 |  | 1.160 |  |  |  |  |  |  | 1.765 |
| **O7** |  | 0.203\* |  | 0.536 |  |  |  |  |  | 1.520$ |  |  |  |  | 2.462 |
| **O8** | 0.221\* |  | 0.202 |  |  | 0.366 |  |  |  |  | 1.231\* |  |  |  | 2.020 |
| **O9** |  |  | 0.227 |  | 0.347 |  |  |  |  |  | 1.379 |  |  |  | 2.180 |
| **O10** |  |  | 0.253 0.231 |  |  | 0.260 |  |  |  |  |  |  | 1.170$ |  | 1.914 |
| **O11** |  |  | 0.236 |  |  | 0.203 0.173 |  |  |  |  |  | 1.361$ |  |  | 1.973 |
| **O12** | 0.239\* |  | 0.205 |  |  | 0.341 |  |  |  |  |  |  |  | 1.286\* | 2.071 |
| **O13** |  |  | 0.227 |  | 0.320 |  |  |  |  |  |  |  |  | 1.492 | 2.266 |
| **O14** |  | 0.214\* |  | 0.556 |  |  |  |  | 1.413$ |  |  |  |  |  | 2.397 |
|  | 2.352 | 2.492 | 2.380 | 2.024 | 1.929 | 1.883 | 3.440 | 3.926 | 4.239 | 4.560 | 3.841 | 4.083 | 3.510 | 4.064 |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

\*Means ×2; $ mean ×