**Table S1.** Infrared band positions and the corresponding hydrogen bond distances[4]

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Tsumeb dioptase** | | **Arizona dioptase** | | **Okatumba dioptase** | |
| Infrared band position (cm-1) | Calculated hydrogen bond distance (Å) | Infrared band position (cm-1) | Calculated hydrogen bond distance (Å) | Infrared band position (cm-1) | Calculated hydrogen bond distance (Å) |
| 3489 | 2.8805 | 3486 | 2.8805 | 3498 | 2.8925 |
| 3363 | 2.7499 | 3363 | 2.7499 | 3363 | 2.7499 |
| 3290 | 2.7384 | 3291 | 2.7384 | 3283 | 2.7353 |
| 3214 | 2.7807 | 3227 | 2.7133 | 3209 | 2.7402 |
| 3108 | 2.6761 | 3140 | 2.6851 | 3168 | 2.6935 |
| 3035 | 2.6575 | 2921 | 2.6329 | 2880 | 2.6251 |