Table 5. Thermal parameters for non-hydrogen atoms in pascoite. (FOR DEPOSIT)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **ATOM** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** | **Ueq** |
| V(1) | 0.02065 | 0.01748 | 0.02341 | 0.00000 | 0.01503 | 0.00000 | 0.01878 |
| *esd* | 0.00019 | 0.00018 | 0.00019 | 0 | 0.00016 | 0 | 0.00009 |
|  |  |  |  |  |  |  |  |
| V(2) | 0.01583 | 0.02424 | 0.01682 | 0.00000 | 0.01032 | 0.00000 | 0.01806 |
| *esd* | 0.00018 | 0.00020 | 0.00018 | 0 | 0.00015 | 0 | 0.00009 |
|  |  |  |  |  |  |  |  |
| V(3) | 0.01395 | 0.02971 | 0.01724 | 0.00000 | 0.00903 | 0.00000 | 0.01982 |
| *esd* | 0.00018 | 0.00022 | 0.00018 | 0 | 0.00015 | 0 | 0.00010 |
|  |  |  |  |  |  |  |  |
| V(4) | 0.02453 | 0.04379 | 0.02252 | -0.01440 | 0.01444 | -0.01248 | 0.02917 |
| *esd* | 0.00016 | 0.00021 | 0.00015 | 0.00014 | 0.00013 | 0.00014 | 0.00009 |
|  |  |  |  |  |  |  |  |
| Ca(1) | 0.04838 | 0.04160 | 0.02908 | 0.00000 | 0.01989 | 0.00000 | 0.03967 |
| *esd* | 0.00054 | 0.00050 | 0.00042 | 0 | 0.00040 | 0 | 0.00021 |
|  |  |  |  |  |  |  |  |
| Ca(2) | 0.02163 | 0.02780 | 0.02750 | 0.00000 | 0.01552 | 0.00000 | 0.02429 |
| *esd* | 0.00023 | 0.00026 | 0.00025 | 0 | 0.00021 | 0 | 0.00011 |
|  |  |  |  |  |  |  |  |
| O(1) | 0.01842 | 0.04222 | 0.02593 | 0.00000 | 0.01403 | 0.00000 | 0.02762 |
| *esd* | 0.00083 | 0.00115 | 0.00091 | 0 | 0.00075 | 0 | 0.00041 |
|  |  |  |  |  |  |  |  |
| O(2) | 0.01551 | 0.02170 | 0.01643 | 0.00000 | 0.00896 | 0.00000 | 0.01752 |
| *esd* | 0.00073 | 0.00080 | 0.00073 | 0 | 0.00062 | 0 | 0.00032 |
|  |  |  |  |  |  |  |  |
| O(3) | 0.01781 | 0.02070 | 0.02021 | -0.00062 | 0.01198 | -0.00218 | 0.01853 |
| *esd* | 0.00052 | 0.00055 | 0.00054 | 0.00044 | 0.00045 | 0.00044 | 0.00023 |
|  |  |  |  |  |  |  |  |
| O(4) | 0.03116 | 0.02278 | 0.03097 | -0.00637 | 0.02078 | -0.00608 | 0.02605 |
| *esd* | 0.00068 | 0.00062 | 0.00066 | 0.00052 | 0.00058 | 0.00052 | 0.00027 |
|  |  |  |  |  |  |  |  |
| O(5) | 0.02087 | 0.03409 | 0.02695 | 0.00000 | 0.01630 | 0.00000 | 0.02543 |
| *esd* | 0.00084 | 0.00101 | 0.00090 | 0 | 0.00075 | 0 | 0.00038 |
|  |  |  |  |  |  |  |  |
| O(6) | 0.02350 | 0.02995 | 0.02187 | -0.00682 | 0.01483 | -0.00430 | 0.02362 |
| *esd* | 0.00059 | 0.00066 | 0.00058 | 0.00050 | 0.00050 | 0.00051 | 0.00026 |
|  |  |  |  |  |  |  |  |
| O(7) | 0.02006 | 0.04070 | 0.02298 | -0.00924 | 0.01269 | -0.00970 | 0.02714 |
| *esd* | 0.00058 | 0.00077 | 0.00060 | 0.00056 | 0.00050 | 0.00055 | 0.00029 |
|  |  |  |  |  |  |  |  |
| O(8) | 0.02058 | 0.05854 | 0.01722 | 0.00000 | 0.00902 | 0.00000 | 0.03242 |
| *esd* | 0.00088 | 0.00142 | 0.00083 | 0 | 0.00072 | 0 | 0.00047 |
|  |  |  |  |  |  |  |  |
| O(9) | 0.03933 | 0.06232 | 0.03821 | -0.02982 | 0.02295 | -0.02309 | 0.04519 |
| *esd* | 0.00085 | 0.00116 | 0.00084 | 0.00084 | 0.00072 | 0.00083 | 0.00045 |
|  |  |  |  |  |  |  |  |
| O(10) | 0.05048 | 0.08458 | 0.06707 | 0.00000 | 0.02143 | 0.00000 | 0.07139 |
| *esd* | 0.00186 | 0.00282 | 0.00232 | 0 | 0.00166 | 0 | 0.00097 |
|  |  |  |  |  |  |  |  |
| O(11) | 0.06283 | 0.11815 | 0.03343 | 0.00000 | 0.01764 | 0.00000 | 0.07471 |
| *esd* | 0.00224 | 0.00357 | 0.00153 | 0 | 0.00149 | 0 | 0.00112 |
|  |  |  |  |  |  |  |  |
| O(12)A | 0.03247 | 0.03871 | 0.02732 | 0.00480 | 0.00937 | -0.01242 | 0.03559 |
| *esd* | 0.00163 | 0.00187 | 0.00155 | 0.00139 | 0.00129 | 0.00144 | 0.00072 |
|  |  |  |  |  |  |  |  |
| O(12)B | 0.04401 | 0.04780 | 0.03963 | 0.00926 | 0.01580 | -0.01510 | 0.04642 |
| *esd* | 0.00207 | 0.00234 | 0.00204 | 0.00174 | 0.00169 | 0.00182 | 0.00092 |
|  |  |  |  |  |  |  |  |
| O(131) | 0.17834 | 0.02009 | 0.08633 | 0.00000 | 0.11207 | 0.00000 | 0.07442 |
| *esd* | 0.00939 | 0.00223 | 0.00489 | 0 | 0.00587 | 0 | 0.00271 |
|  |  |  |  |  |  |  |  |
| O(132) | 0.07060 | 0.05154 | 0.08259 | 0.01896 | 0.04684 | 0.00727 | 0.06472 |
| *esd* | 0.00296 | 0.00253 | 0.00343 | 0.00241 | 0.00273 | 0.00226 | 0.00119 |
|  |  |  |  |  |  |  |  |
| O(14) | 0.06703 | 0.03801 | 0.05255 | -0.01115 | 0.04300 | -0.02391 | 0.04680 |
| *esd* | 0.00124 | 0.00094 | 0.00108 | 0.00082 | 0.00102 | 0.00089 | 0.00046 |
|  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |
| O(15) | 0.08156 | 0.03811 | 0.16234 | 0.00000 | 0.10306 | 0.00000 | 0.07521 |
| *esd* | 0.00237 | 0.00152 | 0.00389 | 0 | 0.00281 | 0 | 0.00122 |
|  |  |  |  |  |  |  |  |