Details of relaxed constructed models of dry (no water molecule) biomass

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Biomass source** | **Cell lattice parameters** 1 | | | | | | **seed no.** 2 |
| *No.* | *Source* | *a (A°)* | *b (A°)* | *c (A°)* | *α (°)* | *β (°)* | *γ (°)* |  |
| 1 | Alder | 43.647039 | 44.108986 | 42.991793 | 89.218 | 89.789 | 90.244 | 1284546481 |
| 2 | Aspen | 42.326312 | 43.066786 | 42.710647 | 90.358 | 90.604 | 89.665 | 1425738887 |
| 3 | Bamboo | 42.805401 | 42.029006 | 42.566125 | 90.687 | 90.117 | 89.894 | 342454041 |
| 4 | Beech1 | 40.546749 | 40.480793 | 40.522759 | 89.448 | 89.473 | 89.556 | 363525881 |
| 5 | Beech2 | 37.607596 | 38.750834 | 38.694042 | 90.049 | 91.69 | 89.619 | 364052687 |
| 6 | Cherry wood | 52.313076 | 52.270137 | 51.830211 | 90.195 | 89.92 | 89.044 | 386023521 |
| 7 | Corn cob | 47.542274 | 48.035839 | 47.430179 | 89.591 | 89.512 | 89.186 | 386803553 |
| 8 | Corn leaves | 49.673904 | 49.404933 | 49.24391 | 89.244 | 89.974 | 90.347 | 387994613 |
| 9 | Corn straw | 52.648417 | 53.021025 | 52.934069 | 90.894 | 90.538 | 90.127 | 876877233 |
| 10 | Eastern Red cedar | 64.515841 | 64.931484 | 64.797175 | 90.324 | 90.502 | 89.921 | 66874573 |
| 11 | Fir | 66.318697 | 65.856726 | 65.792252 | 90.866 | 89.893 | 89.757 | 890549973 |
| 12 | Hazelnut shell | 59.947227 | 60.47427 | 59.858123 | 89.434 | 89.822 | 90.075 | 890988781 |
| 13 | Japanese beech | 69.169715 | 68.759867 | 69.087597 | 90.086 | 89.755 | 89.794 | 1069533881 |
| 14 | Japanese cedar | 71.897006 | 71.604279 | 71.751807 | 89.362 | 89.959 | 89.996 | 70381373 |
| 15 | Miscanthus | 67.362632 | 67.796845 | 67.283586 | 90.122 | 89.826 | 89.685 | 876928533 |
| 16 | P.armandii Franch | 61.28267 | 60.847941 | 61.671791 | 90.008 | 89.612 | 90.412 | 1033794961 |
| 17 | Pine | 60.187515 | 60.03546 | 59.637201 | 89.867 | 89.952 | 90.102 | 1165378987 |
| 18 | Poplar | 65.198982 | 64.033846 | 65.217843 | 89.344 | 90.11 | 89.882 | 15498761 |
| 19 | Rice husk | 63.865512 | 65.220071 | 63.381972 | 91.172 | 90.587 | 92.255 | 543897307 |
| 20 | Rice straw1 | 61.455485 | 61.34921 | 61.762343 | 89.2 | 89.676 | 90.54 | 548740547 |
| 21 | Rice straw2 | 62.121657 | 62.521701 | 61.683894 | 90.241 | 89.739 | 90.463 | 549245293 |
| 22 | Spruce1 | 64.611676 | 64.125944 | 64.234211 | 89.861 | 89.555 | 90.426 | 667511327 |
| 23 | Spruce2 | 61.586279 | 62.354946 | 61.715309 | 89.979 | 89.524 | 89.254 | 667395927 |
| 24 | Switch grass | 62.779838 | 62.706649 | 63.527166 | 89.797 | 90.142 | 89.24 | 319554401 |
| 25 | Wheat straw | 71.040291 | 73.105629 | 72.814404 | 92.252 | 89.394 | 87.909 | 318973781 |
| 26 | Willow | 96.494023 | 96.401485 | 96.358021 | 89.997 | 89.978 | 89.928 | 318896907 |
| 1 - *a*, *b*, and *c* are unit cell vectors in *x*, *y* and *z* directions. *α*, *β*, and *γ* are the angle each unit cell vector creates with the unit vectors of Cartesian coordinate.  2 – random seed number used for creating atomistic models. | | | | | | | | |