**Table S1.** Relative energies and Boltzmann populations of stable conformers of xylose.

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| --- | --- | --- |
| **Entry No.** | **Δ*E*** **(kcal/mol)** | **Population 1** |
| 1 | 0.00 | 1.000 |
| 2 | 0.22 | 0.690 |
| 3 | 0.45 | 0.468 |
| 4 | 0.99 | 0.188 |
| 5 | 1.23 | 0.123 |
| 6 | 1.41 | 0.093 |
| 7 | 1.51 | 0.078 |
| 8 | 1.78 | 0.051 |
| 9 | 2.38 | 0.018 |
| 10 | 2.62 | 0.012 |
| 11 | 2.72 | 0.010 |
| 12 | 2.75 | 0.010 |
| 13 | 2.93 | 0.007 |
| 14 | 2.94 | 0.007 |

1 Relative population is calculated by the Boltzmann distribution at a temperature of 298 K.