Supporting Information

Collision-Induced Dissociation of Cellobiose and Maltose

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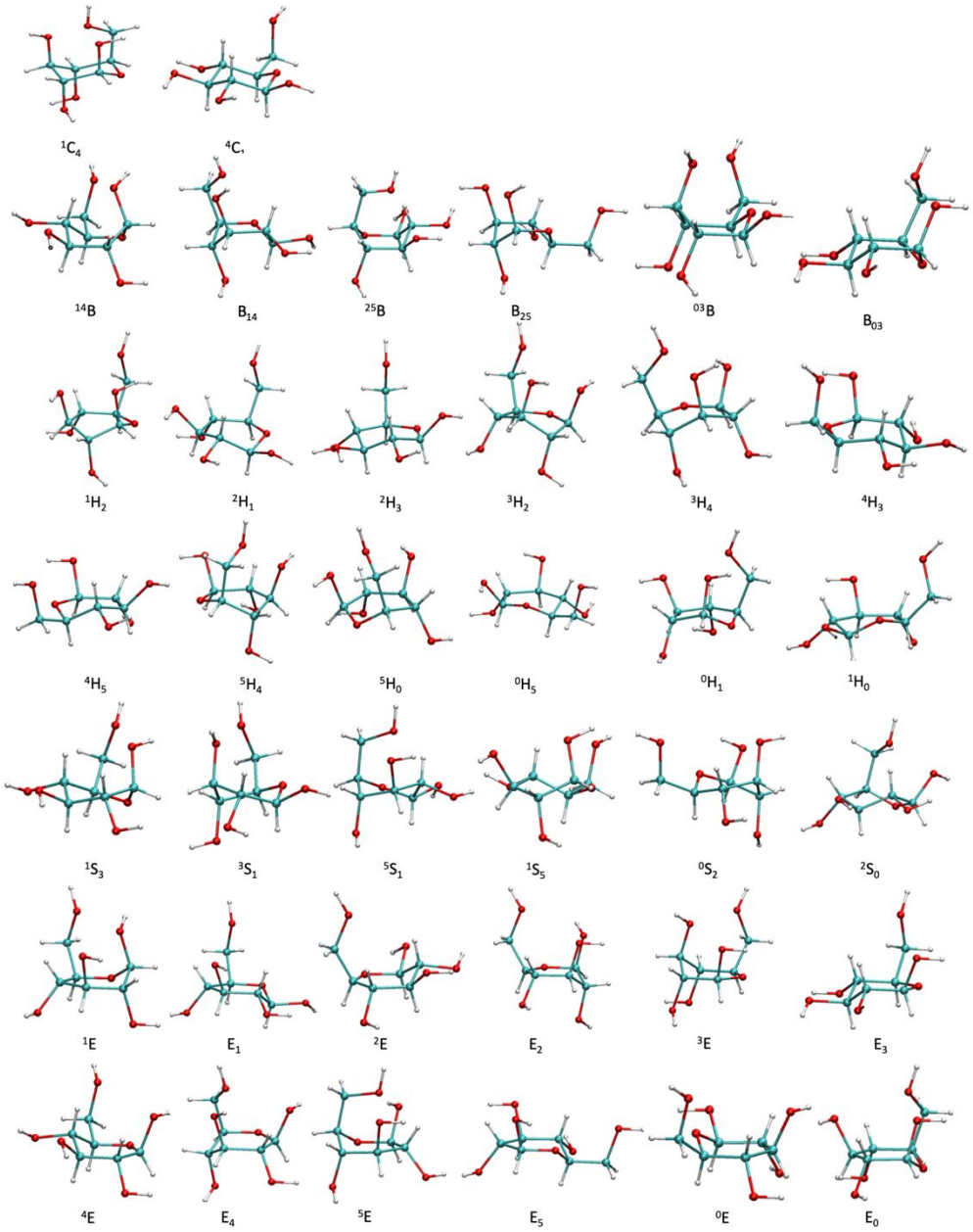

Figure S1. The schematic drawing of β-glucose molecules with 38 different Cremer-Pople[1] puckering forms.

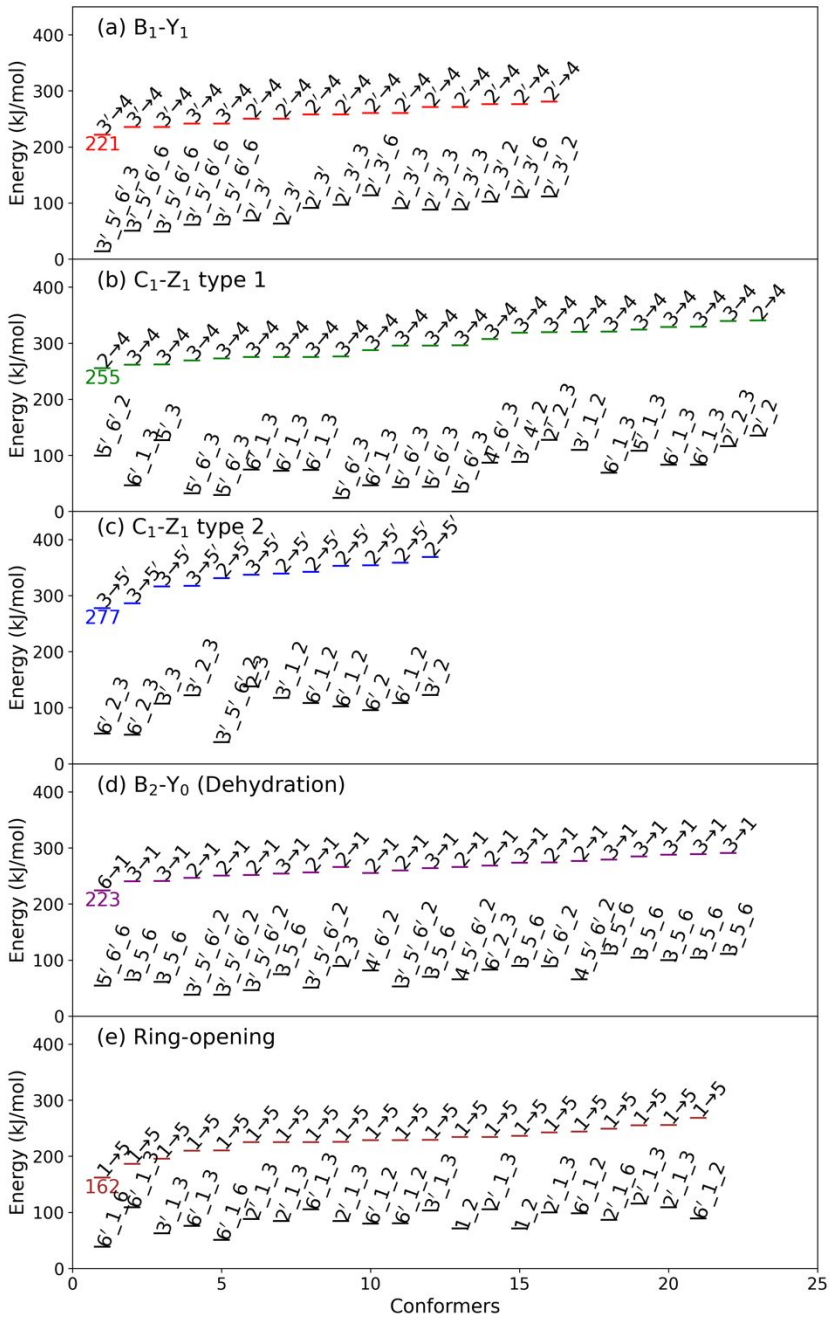

Figure S2. The energies of the transition states (TS) and the reactants of β-cellobiose obtained by DFT/B3LYP calculations for different reactions. (a) B_1-Y_1 fragmentation, (b) C_1-Z_1 type 1 fragmentation, (c) C_1-Z_1 type 2 fragmentation, (d) B_2-Y_0 fragmentation (dehydration) and (e) ring-opening. The energy is relative the energy of global minimum structure. The red, green, blue, purple, and brown lines mark the TS energies. Right about the TS dash lines, the H-atom transfer that responsible for the TS is written, where A→B means H-atom transfer from atom A to atom B. The black dash lines right below each TS dash line marks the energies of the reactant states corresponds to each TS, where the series of numbers represent the O-atoms that bind to a sodium ion.

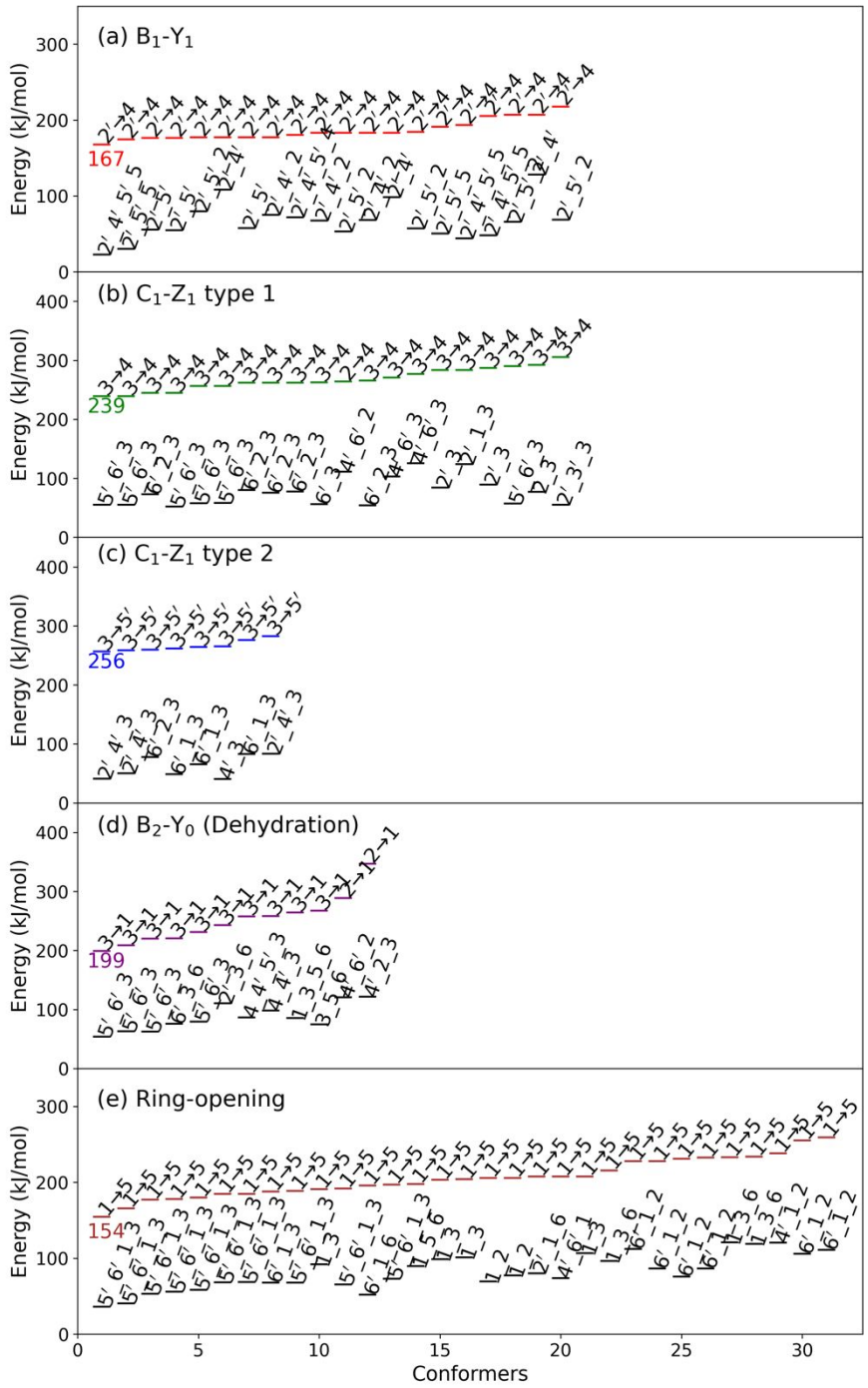

Figure S3. The energies of the transition states (TS) and the reactants of β-maltose obtained by DFT/B3LYP calculations for different reaction. (a) B_1-Y_1 fragmentation, (b) C_1-Z_1 type 1 fragmentation, (c) C_1-Z_1 type 2 fragmentation, (d) B_2-Y_0 fragmentation (dehydration) and (e) ring-opening. The energy is relative the energy of global minimum structure. The red, green, blue, purple, and brown lines mark the TS energies. Right about the TS dash lines, the H-atom transfer that responsible for the TS is written, where A→B means H-atom transfer from atom A to atom B. The black dash lines right below each TS dash line marks the energies of the reactant states corresponds to each TS, where the series of numbers represent the O-atoms that bind to a sodium ion.

Reference

1. Cremer, D. t.; Pople, J., General definition of ring puckering coordinates. *J. Am. Chem. Soc.* **1975,** *97* (6), 1354-1358.