

~OH Projection: the Latest Frontier to Define Geometry of Carbohydrates

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The high relative abundance of different conformations of carbohydrates in aqueous solution at room conditions is due to their energy values, which differ from each other within a range of 0.5 kcal/mol. It happens because these compounds have several hydroxyl groups that interact in different orientations, generating several conformations. Since only *ab initio* descriptions may get close to this precision for energy difference values, we present a simple computational code (CONFPO) able to univocally classify and generate input files for *ab initio* calculations of all conformational possibilities for pentoses. D-Ribose was used as a test case, and within the set of stable conformers found some were not identified by common samplings. To do so, we developed a 1-3-6 numerical identification code that works as a univocal representation of the hydroxyl groups for each orientation possible, in a way that these degrees of freedom may properly receive attention (Figure 1).¹

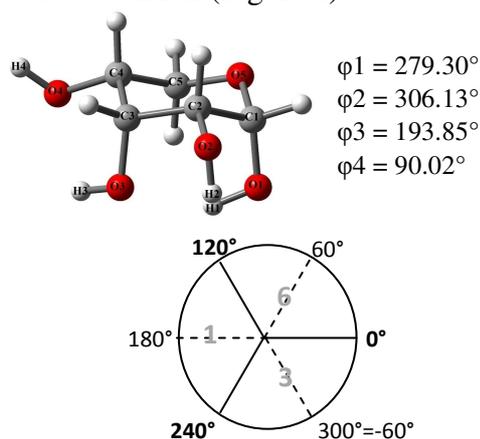


Figure 1. Dihedral angle values that establish each hydroxyl group orientation ($\phi_1 = \text{H1-O1-C1-O5}$, $\phi_2 = \text{H2-O2-C2-C1}$, $\phi_3 = \text{H3-O3-C3-C2}$ and $\phi_4 = \text{H4-O4-C4-C3}$), define the name of ribose conformation: 3316. The circle is a transversal section across the axis

of the $\text{O}_x\text{-C}_x$ bond, $x=1, 2, 3$ or 4 . The arrows in indicate the hydroxyl groups orientation, in this proposed OH projection.

The absence of an experimental property able to distinguish these conformations has left this issue untouched in the literature, but recently a theoretical *ab initio* description may support such a discussion. It starts with the investigation of all conformation possibilities for pentoses in aqueous solution, and is followed by the calculation of the specific rotation values of the conformers found as the most abundant in aqueous solution.

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¹. (a) R. R. Andrade, C. O. Silva, *Carbohydr. Res.*, 2012, 350, 62; (b) B. A. França, C. O. Silva, *Phys. Chem. Chem. Phys.*, 2014, 16, 13096; (c) A. V. Orlova, A. I. Zinin, R. R. Andrade, C. O. Silva, L. O. Kononov, *ChemPhysChem*, 2014, 15, 195.