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Combined Experimental and Computational Studies on Molecular Recognition among D-Glucose Molecules

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D-glucose ($C_6H_{12}O_6$) is a strategic chemical for the agri-food and pharmaceutical industries, with a market that is expected to grow in next years. Two anhydrous $P2_12_12_1$ crystal forms, differing in the anomeric (α/β) configuration, plus one hydrated form, are known to date [1]. Due to the presence of a high number of -OH groups with almost null rotational barriers, many low-energy structures are predicted for both anomers in computational studies [2]. Thus, the reasons for the observed conformational monomorphism in glucose are unclear. In this work (Figure 1), an extensive crystallization screening was carried out, which led to the discovery of a new acetonitrile solvate of the β anomer that was crystallized at room temperature. Through high resolution (0.46 Å) single crystal X-ray diffraction experiments at $T = 90(1)$ K, the most common α form was characterized, demonstrating a possible anomeric disorder, never reported before. The experimental charge density study of the crystalline anomer α was obtained from the high-resolution dataset, quantifying the relative strength of hydrogen bonds in the crystal [3]. Finally, Molecular Dynamics simulations of the crystal, liquid and solution states were carried out with the MiCMoS [4] and GROMACS [5] suite of programs at different temperatures. These complemented the static, space-time average picture of standard crystallographic methods with the analysis of the equilibrium dynamics in condensed phase, allowing us to shed new light on the nature of the cohesive forces in D-glucose.

Figure 1. (a) α -D-glucose single crystals obtained from EtOH:pentane. (b) Same, from EtOH:hexane. (c) Crystal structure of the newly discovered β -D-glucose CH_3CN solvate, with the space occupied by the solvent shown as brown cavities. (d) Negative charge density Laplacian ($-\nabla^2\rho$) in the region of one hydrogen bond. Solid lines highlight regions of charge concentration.

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