

Crystal and molecular structure of two 2-deoxy-2-hydroxyimino derivatives of β -D-*arabino*-hexopyranose.

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The crystal structure of *N*-acetyl-*N*-(3,4,6-tri-*O*-acetyl-2-deoxy-2-hydroxyimino- β -D-*arabino*-hexopyranosyl) amine (**1**) and 3,4,6-tri-*O*-acetyl-2-deoxy-2-hydroxyimino- β -D-*arabino*-hexopyranosyl azide (**2**) were determined by direct methods and refined by fullmatrix least squares to a final value of $R = 0.034$ for 3114 (**1**) and 2924 (**2**) reflections. The pyranoid rings of both compounds have almost identical conformation between the 0S_2 twist-boat and the 3,0B boat. It was found using semi-empirical quantum mechanical calculations that the conformation observed in the solid state for both compounds, similar to that in solution, is more stable than the other possible, 4C_1 conformation. Similarity of geometries of **1** and **2** suggests that the pyranoid ring is less flexible than those with a chair conformation in other 2-hydroxyimino derivatives of pyranosides. On the other hand the observed conformations of **1** and **2** as well as the postulated way for acetyl group migration during hydrogenation of 2-acetoxyimino analog of **2** ($\rightarrow$ **1**) confirm flexibility of the chair conformers. Results of conformation analysis of previous presented crystal structures of 2-oxyimino derivatives with a chair pyranoid ring and both title compounds suggest that the 4C_1 chair $\rightleftharpoons$ 0S_2 twist-boat/ 3,0B boat interconversion via the E_5 half-boat is possible.

Adres publiczny

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