ANALYSIS OF THE ANOMERIC EFFECT USING ROTATIONALLY RESOLVED ELECTRONIC SPECTRA OF 1,3-BENZODIOXOLE IN THE GAS PHASE.[a]

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The anomeric effect, observed in molecules containing -O-CH_2-O- groups, occurs when there is an overlap of an oxygen atom lone pair orbital with an antibonding molecular orbital from the adjacent C-O bond, and leads to a distortion of the molecule along some out-of-plane coordinate. An example of a molecule containing this sequence is 1,3-benzodioxole. In this molecule, the anomeric effect leads to a puckering of the five-membered ring, breaking conjugative links between the two rings. Rotationally resolved spectra of the origins and several vibronic bands of 1,3-benzodioxole will be compared to an analog, 2,3-dihydrobenzofuran (coumaran), which contains only one oxygen atom. Each of these molecules has two rings that are able to bend with respect to one another along the shared bond. In addition, each contains a nonconjugated ring that has the ability to pucker. The rotationally resolved spectra will be used to determine whether the bending or puckering modes predominate in each molecule.

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