THE r_0 STRUCTURAL PARAMETERS OF EQUATORIAL BROMOCYCLOBUTANE, CONFORMATIONAL STABILITY FROM TEMPERATURE DEPENDENT INFRARED SPECTRA OF XENON SOLUTIONS, AND VIBRATIONAL ASSIGNMENTS

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Variable temperature (-55 to $-100\,^{\circ}$C) studies of the infrared spectra (4000-400 cm^{-1}) of bromocyclobutane, c-C_4H_7Br dissolved in liquid xenon have been carried out. The infrared spectrum (4000-100 cm^{-1}) of the gas has also been recorded. The enthalpy difference between the more stable equatorial conformer and the axial form, has been determined to be 372 $\pm$ 34 cm^{-1} . This experimental value of ΔH is much lower than the average MP2(full) *ab initio* predicted value of 521 $\pm$ 87 cm^{-1}. The percentage of the axial conformer present at ambient temperature is estimated to be 14 $\pm$ 1%. By utilizing previously reported microwave rotational constants for the equatorial conformer combined with *ab initio* MP2(full)/6-311+G(d,p) predicted structural values, adjusted r_0 parameters have been obtained. The determined heavy atom structural parameters for this conformer are with distances($\AA$) C_α-Br = 1.942(3), C_α-C_β = 1.541(5), C_γ-C_β = 1.552(3)$\AA$ and angles in degrees $\angle C_\beta C_\alpha Br$ = 118.4(5), $\angle C_\beta C_\alpha C_\beta$ = 89.7(5), $\angle C_\gamma C_\beta C_\alpha$ = 86.8(5), $\angle C_\beta C_\gamma C_\beta$ = 88.9(5) and $\tau C_\gamma C_\beta C_\beta C_\alpha$ = 29.8(5)$^{\circ}$. The results will be discussed and compared to the corresponding properties of some similar molecules.