HIGH RESOLUTION FTIR SPECTROSCOPY OF THE ν_4 BANDS OF C_6H_6 AND C_6D_6

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We have re-examined the ν_4 bands (Herzberg numbering) of C_6H_6 and C_6D_6 using high resolution (0.0015 cm^{-1}) Fourier transform infrared spectroscopy. The spectra were taken with the benzene samples in a temperature stabilized cell (4°C), 20 cm in length. The $-h6$ sample spectrum (99.95 atom % $^{12}C_6$) was recorded with an MCT detector and KBr beamsplitter and the $-d6$ sample spectrum was recorded with a silicon bolometer detector and mylar beamsplitter. For the ν_4 band of C_6H_6, we have fit the following preliminary spectroscopic constants: ν_0 = 673.9747(2) cm^{-1}, B' = 0.1896388(13) cm^{-1}, $(C'-B')-(C''-B'')$ = $1.709(2)\times10^{-4}$ cm^{-1}, D'_J = $4.106(60)\times10^{-8}$ cm^{-1}, $D'_K - D''_K$ = $-2.9(9)\times10^{-10}$ cm^{-1}, D'_{JK} = $-6.89(6)\times10^{-8}$ cm^{-1}, B'' = 0.1897739(10) cm^{-1}, D''_J = $4.123(45)\times10^{-8}$ cm^{-1}, D''_{JK} = $-6.94(5)\times10^{-8}$ cm^{-1}. For the ν_4 band of C_6D_6, we have fit the following preliminary spectroscopic constants: ν_0 = 496.2086(1) cm^{-1}, B' = 0.156919(5) cm^{-1}, and B'' = 0.157016(5) cm^{-1}. Band centers of the observed sequences of hot bands for both isotopic modifications will be reported.