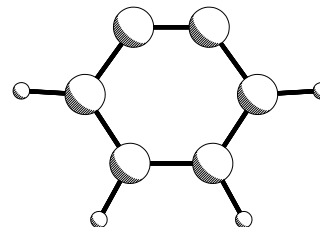


MICROWAVE SPECTRA OF O-BENZYNE PRODUCED IN A DISCHARGE NOZZLE ^a

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Benzynes have been known as reactive intermediates in organic reactions for many years, and have recently been implicated in gasoline combustion reactions and antitumor activity of enediyenes. Rotational transitions were measured for the normal isotopomer, the two unique single-D isotopomers and the ¹³C₆ isotopomer of o-benzyne (o-didehydrobenzene), using a pulsed-beam Fourier transform spectrometer with an electric discharge nozzle source, using a dilute (<1%) mixture of benzene in neon. 27 b-dipole transitions for the normal isotopomer were measured in the 7-40 GHz range to obtain

A = 6989.7303(72), B = 5706.8045(71) and C = 3140.3714(50) MHz, and five centrifugal distortion constants. The inertial defect is $\Delta = 0.06935 \text{ amu \AA}^2$, consistent with a planar structure. Deuterium hyperfine structure for the D₁ (closest to the C-C triple bond) and D₂ (furthest from the triple bond), was analysed to obtain deuterium quadrupole coupling strengths $eQq_{aa} = 231(17) \text{ kHz}$, $eQq_{bb} = -88(13) \text{ kHz}$, for D₁, and $eQq_{aa} = 29(12)$, and $eQq_{bb} = 83(12) \text{ kHz}$, for D₂. The C-D bond axis quadrupole coupling strengths will be compared with values for benzene.



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