

ANALYSIS OF THE ROTATIONAL STRUCTURE IN THE HIGH-RESOLUTION IR SPECTRUM OF *trans*-HEXATRIENE-3- d_1

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For use in determining the semiexperimental structure of *trans*-hexatriene, its 3- d_1 isotopologue has been synthesized and the high-resolution (0.0015 cm^{-1}) IR spectrum has been recorded. The rotational structure in four C-type bands has been analyzed. These bands are for ν_{26} at 997.4, ν_{28} at 908.8, ν_{29} at 902.2, and ν_{32} at 678.6 cm^{-1} , which are all out-of-plane modes. Ground state rotational constants are $A_0 = 0.7952226(8)$, $B_0 = 0.0446149(7)$, and $C_0 = 0.0422661(4)$ cm^{-1} . The inertial defect is -0.2009 amu \AA^2 , which confirms planarity for this molecular species. The ultimate intent of this investigation is to evaluate the degree to which the “C=C” bonds are lengthened and the $\text{sp}^2\text{-sp}^2$ “C-C” bonds are shortened in comparison with localized bonds and with butadiene.