ANALYSIS OF THE ROTATIONAL STRUCTURE IN THE HIGH-RESOLUTION IR SPECTRUM OF trans-
HEXATRIENE-3-\textsuperscript{d1}

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For use in determining the semiexperimental structure of trans-hexatriene, its 3-\textsuperscript{d1} isotopologue has been synthesized and the high-resolution (0.0015 cm\textsuperscript{-1}) IR spectrum has been recorded. The rotational structure in four C-type bands has been analyzed. These bands are for $\nu_{26}$ at 997.4, $\nu_{28}$ at 908.8, $\nu_{29}$ at 902.2, and $\nu_{32}$ at 678.6 cm\textsuperscript{-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\textsuperscript{-1}. The inertial defect is –0.2009 amu Å\textsuperscript{2}, which confirms planarity for this molecular species. The ultimate intent of this investigation is to evaluate the degree to which the “=C” bonds are lengthened and the sp\textsuperscript{2}–sp\textsuperscript{2} “C–C” bonds are shortened in comparison with localized bonds and with butadiene.