A SEMIEXPERIMENTAL EQUILIBRIUM STRUCTURE OF *cis*-HEXATRIENE FROM MICROWAVE SPECTROSCOPY

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Ground state rotational constants for a full set of carbon and deuterium isotopologues of *cis*-hexatriene, which has a dipole moment of only 0.05 D, have been determined by MW spectroscopy.[a b] Ground state rotational constants were converted into equilibrium rotational constants with spectroscopic alphas computed from force constants found with an MP2/cc-pVTZ model. Corrections for electronic contributions were applied. Despite the availability of a full set of rotational constants for a suite of isotopologues, an accurate structure was not accessible. The mixed estimation method, in which high-quality bond parameters computed by quantum chemistry with appropriate uncertainties were fit simultaneously with the moments of inertia, was applied. A structure good to 0.001 Å was the result. The structural parameters reflect an increase in pi-electron delocalization compared to butadiene.

[a] R. D. Suenram, B. H. Pate, A. Lesarri, J. L. Neill, S. Shipman, R. A. Holmes, M. C. Leyden, N. C. Craig J. Phys. Chem. A 113, 1864-1868 (2009).

[b] N. C. Craig, Y. Chen, H. A. Fuson, H. Tian, H. van Besien, A. R. Conrad, M. J. Tubergen, H. D. Rudolph, J. Demaison, J. Phys. Chem. A 117, in press.