The Molecular Zeeman Effect of Norbornadiene, its *g*-Values, Magnetizability Anisotropies, and Molecular Electric Quadrupole Moment; A High-Resolution Microwave Fourier-Transform Study Combined With Quantum Chemical Calculations

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The molecular Zeeman effect is reported for norbornadiene at fields near 18 kG. The experimental results are for the molecular g-values: g_{aa} = 0.02860(16), g_{bb} = 0.05271(11), g_{cc} = 0.00142(26), for the magnetizability anisotropies: $2\xi_{aa} - \xi_{bb} - \xi_{cc} = -0.41(26) \cdot 10^{-6}$ erg G^{-2} mol^{-1}, $2\xi_{bb} - \xi_{cc} - \xi_{aa}$ = +40.72(27) $\cdot 10^{-6}$ erg G^{-2} mol^{-1} and for the molecular electric quadrupole moments: $Q_{aa} = -1.78(20) \cdot 10^{-26}$ esu cm^2, Q_{bb} = 3.73(20) $\cdot 10^{-26}$ esu cm^2, $Q_{cc} = -1.94(30) \cdot 10^{-26}$ esu cm^2, with the c-axis of the molecular inertia tensor aligned to the C_{2v}-axis of the equilibrium configuration. The results of *ab-initio* calculations, using London type atomic orbitals as basis functions, are reported for the g-tensor, the magnetizability tensor and the molecular electric quadrupole moment tensor and are compared to the experimental findings. The possibilities of strain induced magnetizability exaltations and of systematic differences between gas phase and bulk phase magnetizabilities are discussed.

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