QUANTUM-CHEMICAL CALCULATIONS REVEALING THE EFFECTS OF MAGNETIC FIELDS ON METHANOL

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Maser observations of both linear and circular emission have provided unique information on the magnetic field in the densest regions of star forming regions. While linear polarization observations provide morphological constraints, the magnetic field strength determination is done by comparing the Zeeman-induced velocity shifts between left- and right-circularly polarized emission of molecular maser species. Soon, full-polarization observations with be possible with ALMA, making magnetic field measurements with unprecedented spatial resolution possible. In particular, methanol is of special interest as it is the most abundant maser species and its different transitions probe unique areas of high-mass protostellar disks and outflows. However, its exact Zeeman-parameters are unknown. Experimental efforts to determine the Zeeman-parameters have failed. Here we present quantum chemical calculations to the Zeeman-parameters of methanol, along with calculations to the hyperfine structure, which are also necessary to interpret the Zeeman effect in methanol. We present the proper treatment of the torsional motion in computing hyperfine and Zeeman effects. Our results on the hyperfine structure show good agreement with recent experimental data. We find that the Zeeman-effect in methanol is non-linear and comment on its applicability in astronomical magnetic field studies. We give an outlook on rigorously treating non-linear Zeeman effects in radiative transfer modeling of maser-species interacting with a magnetic field.