Astrophysical Masers:
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Quantum-Chemical calculations revealing the effects of magnetic fields on methanol masers

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Abstract. Maser observations of both linearly and circularly polarized emission have provided unique information on the magnetic field in the densest parts of star forming regions, where non-maser magnetic field tracers are scarce. While linear polarization observations provide morphological constraints, magnetic field strengths are determined by measuring the Zeeman splitting in circularly polarized emission. Methanol is of special interest as it is one of the most abundant maser species and its different transitions probe unique areas around the protostar. However, its precise Zeeman-parameters are unknown. Experimental efforts to determine these Zeeman-parameters have failed. Here we present quantum-chemical calculations of the Zeeman-parameters of methanol, along with calculations of the hyperfine structure that are necessary to interpret the Zeeman effect in methanol. We use this model in re-analyzing methanol maser polarization observations. We discuss different mechanisms for hyperfine-state preference in the pumping of torsion-rotation transitions involved in the maser-action.

Keywords. magnetic fields, masers, molecular data, polarization

1. Introduction

The presence of a magnetic field within an astrophysical maser is known to produce partially polarized radiation. Linear polarization provides information on the magnetic field direction, and the magnetic field strength can be determined by comparing the field-induced frequency shifts between left- and right-circularly polarized emission. In OH, H_2O, SiO, and CH_3OH (methanol) masers, polarized radiation has been observed and analyzed for the information it contains on the magnetic field in the regions these masers probe. Extracting quantitative information on the magnetic field in these regions requires knowledge of the Zeeman parameters, describing the response of the maser molecule/atom to a magnetic field. These Zeeman parameters are known for all but methanol masers. Here we describe a quantitative theoretical model of the magnetic properties of methanol, including the complicated hyperfine structure that results from its internal rotation (Lankhaar *et al.* 2016). With this model, we can determine the Zeeman splitting of the hyperfine states within all the known methanol maser transitions. We will use this model in (re-)interpreting methanol maser polarization observations.

Hyperfine interactions and Zeeman effects in methanol

The elucidation of methanol's hyperfine structure has been a challenging problem. The CH_3-group in methanol can easily rotate with respect to the OH-group, which leads to an extension of the usual rigid-rotor hyperfine Hamiltonian with nuclear spin-torsion interactions. In contrast with the nuclear spin-rotation coupling parameters, the torsional hyperfine coupling parameters cannot be obtained from quantum chemical calculations. Experiments probing the hyperfine structure of methanol have proven difficult to interpret, because the hyperfine transitions cannot be individually resolved. Lankhaar *et al.* (2016), revised the derivation of a Hamiltonian which includes the torsional hyperfine interactions and obtained the coupling parameters in this Hamiltonian from *ab initio* calculations and experimental data by Heuvel & Dymanus (1973) and Coudert *et al.* (2015). The hyperfine spectra of methanol calculated from this Hamiltonian agree well with the spectra observed for several torsion-rotation transitions of both A- and E-symmetry.

Zeeman interactions are governed by the same magnetic moments that determine the hyperfine structure, interacting with an external magnetic field. For a diamagnetic molecule as methanol three contributions to the molecules Zeeman effect are important:

- overall rotation. Rotational Zeeman effects are represented by the molecule-specific g-tensor, which for rigid non-paramagnetic molecules has been extensively studied experimentally for its valuable information on the electronic structure. Quantum chemical calculations are able to reproduce these experiments with high accuracy. We carried out quantum chemical calculations to obtain the rotational g-tensor for methanol.
- internal rotation or torsion. Torsional Zeeman interactions are represented by the molecule-specific b-vector. The calculation of the b-vector has not been implemented in the available quantum-chemical program packages. For nitromethane and methyl-boron-difluoride, the torsional Zeeman effect has been investigated experimentally by Engelbrecht *et al.* (1973). In order to estimate the torsional Zeeman effects in methanol, we have extrapolated the torsional b-vectors for these molecules, by comparing their internally rotating CH_3-groups to the CH_3-group of methanol.
- nuclear spins. The nuclear spin of methanol, CH_3OH, comes from the three protons in the CH_3 group and the proton in the OH group. The Zeeman effect of the protons scale with the proton g-factor: $g_p = 5.585$.

We combine these Zeeman interactions with the model of the hyperfine structure to determine the Zeeman splitting of the hyperfine states within all the known methanol maser transitions.

Zeeman interactions are usually described in a first-order approximation by the Landé g-factor. In methanol, each torsion-rotation transition is actually split into a number of transitions between individual hyperfine levels of the upper and lower torsion-rotation states (Figure 1). The Landé g-factors calculated for the different hyperfine transitions differ strongly which is important for the interpretation of the measured maser polarization effects (Lankhaar *et al.* 2017).

Polarization in methanol masers

Methanol maser circular polarization observations have been made for the transitions: 6.7 GHz ($5_{15}\ A_2 \rightarrow 6_{06}\ A_1$) by, *e.g.*, Vlemmings *et al.* (2011), Surcis *et al.* (2012),

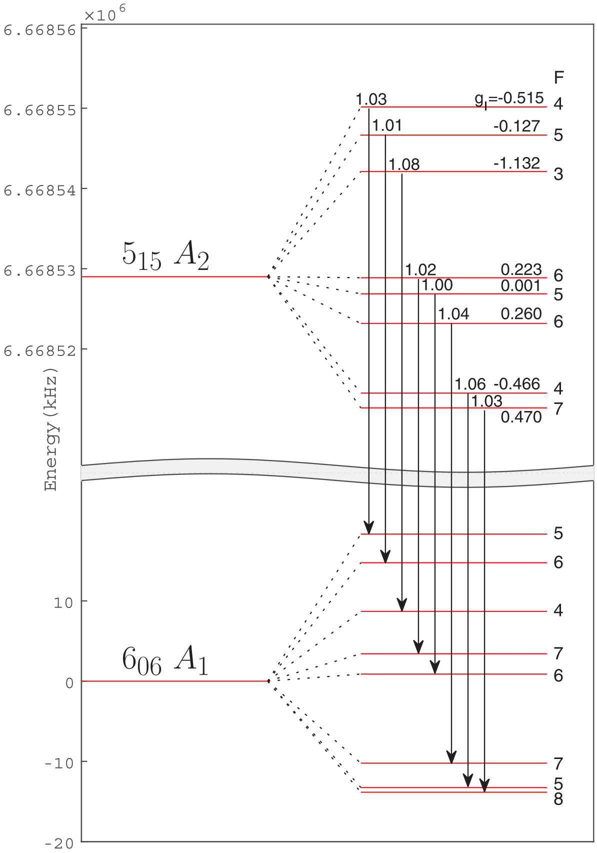

Figure 1. Hyperfine structure of the torsion-rotation levels in the 6.7 GHz ($5_{15}\ A_2 \rightarrow 6_{06}\ A_1$) transition. The energy of the $6_{06}\ A_1$ torsion-rotation level is set to zero. Arrows indicate the strongest hyperfine transitions with $\Delta F = \Delta J = 1$, with the Einstein A-coefficients (in 10^{-9} s^{-1}) indicated above. Landé g-factors of the transitions in a magnetic field of 10 mG are given at the righthand side of the upper energy levels. The rightmost numbers are the F quantum numbers of the hyperfine states.

44 GHz ($7_{07}\ A_2 \rightarrow 6_{16}\ A_1$) by Momjian & Sarma (2016) and 36 GHz ($4_{-1}\ E \rightarrow 3_0$) E by Sarma & Momjian (2009). As the magnetic characteristics of methanol were not known, (hyperfine unspecific) estimates of the Zeeman parameters were used. In the following, we will re-analyze some of the observations using our calculated Zeeman parameters.

Hyperfine-specific effects in the maser action. The individual hyperfine lines are not spectrally resolved, but the maser action can favor specific hyperfine transitions by the following mechanisms:

- different radiative rates for stimulated emission
- kinematic effects, when there are two maser clouds along the line of sight with different velocities, such that a hyperfine transition in the foreground cloud amplifies emission from a different hyperfine transition in the background cloud
- population inversion of the levels involved in maser action is preceded by collisional and radiative de-excitation of higher torsion-rotation levels, with rate coefficients that are hyperfine-state specific.

Polarization observations of class II 6.7 GHz methanol masers. We assume that the transition with the largest Einstein coefficient for stimulated emission, the

$F = 3 \rightarrow 4$ transition, will be favored and that the maser action is limited to this transition. Then, the Zeeman-splitting coefficient is 10 times larger than the value currently used for magnetic field estimates. In the methanol maser regions probed by these class II masers, with an H_2 number density of $n_{\mathrm{H}_2} \approx 10^8$ cm^{-3} , application of our new results to the large sample of maser observations reported in Vlemmings *et al.* (2011) indicates an average field strength of $\langle |B| \rangle \approx 12$ mG. This is in good agreement with OH-maser polarization observations by Wright *et al.* (2004), as well as with the extrapolated magnetic field vs. density relation, see Crutcher (1999).

Polarization observations of class I methanol 36 GHz and 44 GHz masers. We assume that the $F = 3 \rightarrow 2$ (36 GHz) and $F = 5 \rightarrow 4$ (44 GHz) hyperfine lines are favored and that the maser action is limited to these transitions. The observed class I methanol masers are expected to occur in shocked regions of the outflows at densities, an order of magnitude lower in comparison to class II masers. Using our analysis, the Zeeman splitting of the 36 GHz and 44 GHz lines would indicate magnetic field strengths of $20 - 75$ mG. Since, class I masers are shock excited, shock compression is expected to increase the magnetic field strength.

Oppositely polarized masers. Observations have shown reversals in the sign of polarization over areas of small angular extent in the sky. Such reversals have previously been interpreted as a change in field direction. However, reversals on au-scales would be surprising if one considers the agreement between the fields probed by methanol masers and dust emission. A more plausible explanation favored by our results is that in the masers with opposite signs of polarization, the masing process itself is due to the dominance of different hyperfine transitions. Such a mechanism is able to explain opposite circular polarization along the line of sight without assuming a change in magentic field direction, and to obtain magnetic fields comparable with the results from other masers that trace similar areas around the protostar.

Summary

We have presented a model for the Zeeman interactions in methanol, in combination with the hyperfine structure. In contrast to previous models of methanol's Zeeman effect, where a single effective g-factor was assumed, we show that each hyperfine transition in the maser line has its own unique Landé g-factor, and that these g-factors vary over a large range of values. We have applied our results to existing circular polarization measurements, which leads to substantially different conclusions, and confirms the presence of dynamically important magnetic fields around protostars.

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