NEW ELECTRONIC STATES OF MgCl: THE PURE ROTATIONAL SPECTRUM IN THE $(3)^2\Sigma^+$ AND $(4)^2\Sigma^+$ STATES

TYLER J HERMAN, <u>RAJAT RAVI</u>, Department of Chemistry and Biochemistry, University of Arizona, Tucson, AZ, USA; LUCY M. ZIURYS, Dept. of Astronomy, Dept. of Chemistry, Arizona Radio Observatory, The University of Arizona, Tucson, AZ, USA; ROBERT W FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, USA.

The millimeter/submillimeter spectrum of magnesium chloride (MgCl) has been recorded in electronic excited sates not previously measured, using direct absorption spectroscopy in the range of 210-450 GHz. The molecule was synthesized by reacting chlorine gas (Cl₂) with magnesium vapor, produced using a Broida-type oven, in the presence of argon carrier gas. Two distinct rotational patterns were observed, with significantly different rotational constants (B=5504 and 6349 MHz). The first vanishes at N=30 \leftarrow 29, while the latter only appears at and above N=26 \leftarrow 25, with this effect being observed across all vibrational states. There is no evidence of perturbations in either pattern prior to their disappearance. In the first pattern, at least seven rotational transitions in each of six isotopologues (²⁴Mg³⁵Cl, ²⁴Mg³⁷Cl, ²⁵Mg³⁵Cl, ²⁵Mg³⁷Cl, ²⁶Mg³⁵Cl, ²⁶Mg³⁷Cl) were measured in the ground vibrational state, with numerous vibrationally excited satellite lines (v=1-13) also being observed for each species. For the second pattern, measurements were taken for v=0-2. From both sets of data, rotational and fine structure parameters were determined for ²⁴Mg³⁵Cl, as well as equilibrium constants and the equilibrium bond lengths, $\mathbf{r}_e = 2.54$ Å and 2.36 Å. From the first pattern, constants for the other five isotopologues were also established, including ²⁵Mg hyperfine parameters. Based on comparison with theoretical calculations, one excited state has been identified as the (3)² Σ ⁺ state, and the other may arise from the (4)² Σ ⁺ state. The excited state manifold of MgCl has already been the subject of several computational studies, and the unexpected formation of these states emphasizes the need to further investigate both this molecule, as well as other alkaline earth metal halides.