PROBING THE FORMATION & EVOLUTION OF COMETS VIA NUCLEAR SPIN TEMPERATURES.

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Introduction: Comets are true remnants of our primordial Solar System, and provide unique clues to its formation and evolution, including the delivery of organics and water to our planet. A key indicator stored in the molecular structure of the nuclear ices is the spin temperature \( T_{\text{spin}} \), derived from spin-isomeric ratios \( R_{\text{spin}} \).

At the time when cometary ices formed, the prevailing temperature defined the relative abundance of the different spin-isomeric species, and herewith \( R_{\text{spin}} \) and \( T_{\text{spin}} \) are normally treated as “remnant thermometers” probing the formation environments of cometary molecules. Radiative and collisional transitions between ortho and para states are strongly forbidden and herewith this indicator is preserved over time.

Most of our knowledge of this indicator comes from measurements of ortho-para ratios in water and \( \text{NH}_2 \) (a proxy for ammonia), suggesting a common \( T_{\text{spin}} \) near 30K [e.g. 1,2 and references therein]. This information is based on a restricted sample of comets, and the measurements are particularly sensitive to the molecular modeling technique and adopted spectral database.

Analysis: Here, we present new methodology for extracting spin temperatures from ethane (\( \text{C}_2\text{H}_6 \)), methane (\( \text{CH}_4 \)), and methanol (\( \text{CH}_3\text{OH} \)), and advanced new models for ortho/para water (\( \text{H}_2\text{O} \)) and ammonia (\( \text{NH}_3 \)). Our \( \text{H}_2\text{O} \) analysis is based on the most complete fluorescence radiative transfer model to date, which incorporates 1,200 million transitions including those originating from high-energy levels that are activated in comets via non-resonance cascade. In a similar fashion, we developed non-resonance fluorescence models for \( \text{NH}_3 \) and \( \text{HCN} \), and quantum band models for the \( \nu_3 \) band of \( \text{C}_2\text{H}_4 \) and \( \nu_3 \) band of \( \text{CH}_3\text{OH} \). All models respect spin symmetry non-conversion radiative rules, and make use of a realistic Solar spectrum for the computation of fluorescence pumps.

Application and discussion: We applied these new methods to derive spin-isomeric ratios for \( \text{H}_2\text{O}, \text{CH}_4, \text{C}_2\text{H}_6, \text{CH}_3\text{OH} \) and \( \text{NH}_3 \) from three high-quality cometary datasets: 1) C/2007 W1 (Boattini), 2) C/2001 A2 (LINEAR), and 3) 8P/Tuttle. We compare our results with the measured organic compositions for these comets, and present possible formation and evolution scenarios.