Probing the formation and evolution of comets via nuclear spin temperatures of C_2H_6, CH_3OH, CH_4, NH_3, and H_2O

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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_{spin}), derived from spin-isomeric ratios (R_{spin}, e.g., ortho/para). At the time when cometary ices formed, the prevailing temperature defined the relative abundance of the different spin-isomeric species, and herewith $\mathrm{R_{spin}}$ and $\mathrm{T_{spin}}$ are normally treated as "remnant thermometers" probing the formation environments of cometary molecules. Radiative and collisional transitions between the ortho and para states are strongly forbidden and herewith this indicator is preserved over time. Most of our knowledge of this indicator comes from the measurements of the ortho-para ratios in water and NH_2 (a proxy for ammonia), suggesting a common T_{spin} near 30 K. 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.

Here, we present new methodologies for extracting spin temperatures from ethane (C_2H_6), methane (CH_4), and methanol (CH_3OH), and advanced new models for ortho/para water (H_2O) and ammonia (NH_3). Our H_2O 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 a non-resonant cascade. In a similar fashion, we developed non-resonant fluorescence models for NH_3 and HCN, and quantum-band models for the ν_7 band of C_2H_6 and ν_3 band of CH_3OH. All models respect spin-symmetry non-conversion radiative rules, and make use of a realistic solar spectrum for the computation of fluorescence pumps.

We applied these new methods to derive spin-isomeric ratios for H_2O, CH_4, C_2H_6, CH_3OH, and 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 to the measured organic compositions for these comets, and present possible formation and evolution scenarios.

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