The ortho-para chemistry of formaldehyde in protoplanetary disks

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The spatial distribution of the chemical reservoirs in protoplanetary disks is key to elucidate the composition of planets, especially habitable ones. However, the partitioning of the main elements among the refractory and volatile phases is still elusive. Key parameters such as the carbon-to-oxygen (C/O) elemental ratio and the ionization fraction remain poorly constrained, with the latter potentially orders of magnitude lower than in the interstellar medium. Moreover, the thermal structure of the gas is also poorly known, despite its deep influence on gas-phase chemistry. In this context, ortho-to-para ratios could provide selective and sensitive probes. Recent ALMA observations have measured the spatially resolved column density of ortho- and para-H_2CO in the transition disk orbiting TW Hya and derived the radial profile of the ortho-to-para ratio. Yet, current disk models do not include the nuclear-spin-resolved chemistry required to interpret these observations. Our work aims to fill this gap, by combining a parametric disk physical model of TW Hya with the UGAN network, updated to include a comprehensive description of the nuclear-spin-resolved chemistry of formaldehyde (H_2CO) [1]. This new model successfully reproduces the observed column density of H_2CO to within a factor of two, as well as the measured ortho-to-para ratio which varies from $\sim$1.5 in the outer disk to $\sim$ 3 inside 90 au. In particular the low value of this ratio beyond $\sim$ 90 au is well explained by our model. However, the statistical value of 3 measured below $\sim$ 70 au in TW Hya and globaly in the disk orbiting HD 163296 cannot be reproduced, suggesting that additional processes involving ices may be involved. Our parameter space exploration shows that the abundance of H_2CO is highly sensitive to the C/O elemental ratio and to the cosmic-ray ionization rate. Future observations of ortho- and para-H_2CO, based on well selected rotational transitions, in a large sample of disks, appear highly desirable.

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References

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