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Chemical composition of planets for different scenarios of formation of volatile species in the disc

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Abstract

We investigate the effects of three different scenarios for the formation of volatile species in protoplanetary discs on the chemical composition of planets formed in the solar system. The main objective of this work is to provide valuable theoretical data on chemical composition for models of planet formation and evolution, and future interpretation of chemical composition of solar and extra-solar planets. To do this, we combine the results of models of planet formation and ice formation in protoplanetary discs to obtain the chemical composition for planets in stellar systems of solar chemical composition.

1. Introduction

Solar and extrasolar planets are the subject of numerous studies in order to determine their chemical composition and internal structure. The determination of the chemical composition of planets is important as it governs partly their potential habitability. Moreover, observational determination of chemical composition of planetary atmospheres is becoming available, especially for transiting planets. Different models are developed to understand the processes at play, especially for volatile species (whose condensation temperature is lower or equal to that of the water). The present works aims at determining the chemical composition of volatile species in planetesimals and planets formed in stellar systems with the composition of the solar nebula, using these different models. The main objective of this work is to provide valuable theoretical data of chemical composition for models of planetesimals, comets, planet formation and evolution, and future interpretation of chemical composition of solar and extra-solar planets. It is also an opportunity to compare the different models using the same set of initial physical conditions. To do this, we use different models of formation of volatile species [1-3], starting from different initial chemical assumptions (atoms, or gas species, or ice species) and which allow us to calculate the chemical composition of planetesimals and planets for different surface densities of discs, the insolation (irradiated and non irradiated discs), and the initial abundance of elements (atoms or volatile species).

2. Method

We compute the chemical evolution of solids and volatiles in a viscously evolving protoplanetary disc using a large chemical network [2,3]. We probe the effects of the assumed initial reservoirs (atomic or molecular) and the effect of including irradiation by the central star, on the final molecular abundances. We consider three different disc masses across the mass regime. The results of our simulations are used as an input into a planet population synthesis code [5] and the resulting compositions of planets are compared with those determined using model in which chemistry during evolution is not considered [4].

2.1. Computation of ices in planetesimals

Starting from volatiles in the gas phase, in the solid phase, or as gas-phase atoms in the disc, models of chemical composition of grains in discs [2, 3] provide the chemical composition of planetesimals everywhere in the disc for several volatile species such as H_2O, CO_2, CO, CH_3OH, CH_4 , NH_3, N_2, and H_2S, and for different initial surface densities. The abundances of solids is determined by the relative rates of "freeze out" or condensation of volatiles onto dust grain mantles to thermal "desorption" or sublimation. In this way, the locations of ice lines of important volatile species are determined as a function of time. We include dissociation of ice species by UV photons generated internally by cosmic rays and grain-surface reactions between reactive radicals within and on the ice mantle. Thus, we also consider the chemical processing of ices as the protoplanetary disc evolves which depends on the ionization rate in the disc midplane.

2.2. Computation of volatiles species in planets

In order to determine the chemical composition of planets, we consider several planetary systems assumed to emerge from a protoplanetary disc, whose initial density profile, mass and lifetime, is different, and follows, as much as possible, observational characteristics (see [5,6]). The model of planet formation [4, 5] allows us to determine the formation pathway of the ten initial embryos in the disc and their growth during their migration for the three different surface densities of discs, and for different initial distances to the star. We combine the results of the planet formation model, which provides the amount of planetesimals accreted by every planet as a function of the distance to the central star, with the chemical composition of planetesimals and gas everywhere in the disc to derive the composition of planets.

The abundances of gas species are computed using a large gas-phase chemical network based on the UMIST Database for Astrochemistry (McElroy et al. 2013). Both neutral-neutral and ion-neutral reactions are considered, the latter of which is also dependent on the assumed ionisation rate in the disc midplane. Volatiles can also be ionised and dissociation via cosmic-ray-induced UV photons. The depletion of volatiles from the gas phase onto icy grain mantles depends also on the relative rates of freeze out and desorption. Thus we can probe whether the evolving conditions in the disc affect the relative abundances of volatiles in the gas phase which are then incorporated into planetary atmospheres.

3. Results

Preliminary results without grain-surface chemistry suggest that the final abundances at a time of 2 Myr are sensitive both to the assumed initial abundances (whether atomic or molecular) and the evolving conditions. The partitioning of C/N/O into different volatiles by 2 Myr varies as a function of radius and time. For example, we find that H_2O ice reaches a lower abundance at 10 AU when starting with atomic abundances (roughly 10% that when starting with molecular abundances) because the gas-phase formation routes to water are less efficient than grain-surface (or in-situ) formation. The results of all simulations will be used in a planet population synthesis model to test if chemical evolution during the disc lifetime has an effect on the resulting composition of planetesimals which in turn are the primary reservoirs of C/N/O incorporated into planetary atmospheres.

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