

the van der Waals dispersion contribution (the universal attractive energy between atoms) arises from electron correlation and decays slowly with molecular separation. The theory of intermolecular forces (8) implies that accurate evaluation of intermolecular interactions requires multibody and many-electron contributions describing the electron correlation. Yang *et al.*'s study is a milestone in the huge effort being made in electronic structure theory for large molecules, clusters, and periodic systems (9, 10).

In condensed phases, small changes in molecular and packing geometry can change the dispersion contribution substantially. The sensitivity to capturing the dispersion contribution is therefore not unique to benzene. Braun *et al.* have shown that the calculated stability order for the polymorphs and energetically competitive CSP-generated structures of molecules from the same drug discovery program change with the dispersion model used to correct periodic electronic structure calculations (11).

Accurate calculation of lattice energies is only the first step to determining the thermodynamics of benzene polymorphs. The methods used by Yang *et al.* are so demanding computationally that the authors must assume a low-temperature crystal structure and cannot relax it to an energy minimum. It remains to be shown how the method fares for the other known polymorphs of benzene, let alone the dozens of other plausible structures generated by CSP methods, although many of these are unlikely to be stable at room temperature (12). Nevertheless, their advances in computational modeling of intermolecular interactions represent an important accuracy benchmark for a molecule that is an important fragment in many protein binding sites and pharmaceuticals. ■

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#### PLANETARY SCIENCE

# Probing the solar system's prenatal history

Radiometric studies can probe the pre-birth conditions of the solar system

By Martin Bizzarro

Stars like our Sun are formed by the gravitational collapse of the densest parts of molecular clouds comprising dust and gas. Collapsing clouds swiftly evolve to form young stars surrounded by disks from which planets originate. The time scales and processes leading to the formation of our own solar system will be important clues to the birth environment of other planetary systems orbiting Sun-like stars, which may exist in greater numbers than previously thought (1). Radiometric age dating of meteoritic inclusions has established that the birth of our solar system occurred  $4567.3 \pm 0.16$  million years ago (2). But there is also life before birth. This distant, recordable past reflects the time when the matter from which the solar system formed became isolated from the chemically evolving interstellar medium. By analogy with a human life, this epoch represents the embryonic and fetal stages of gestation. On page 650 of this issue, Lugaro *et al.* (3) report that the precursor material to the solar system may have been isolated from the galaxy as early as 30 million years before its birth. Considering that it took less than 100 million years for the terrestrial planets to form, this incubation time seems astonishingly long.

The ability to probe the prenatal history of the solar system is counterintuitive. However, this can be achieved by comparing the relative abundances of radioisotopes with short half-lives inferred to have been present at the birth of the solar system with that expected from the chemical evolution of the galaxy. The difference between these two estimates can be translated into a time  $\Delta T$ , which reflects the interval when the matter precursor to the solar system became isolated from the continuous radioactive enrichment of the interstellar medium via stellar nucleosynthesis. In other words,  $\Delta T$  is the period when radioisotopes decay freely to their initial solar system abundances without the addition of freshly synthesized matter. But this approach requires a crisp understanding of the formation pathways of the short-lived radioisotopes

under consideration and robust estimates of their initial abundances in early solar system solids.

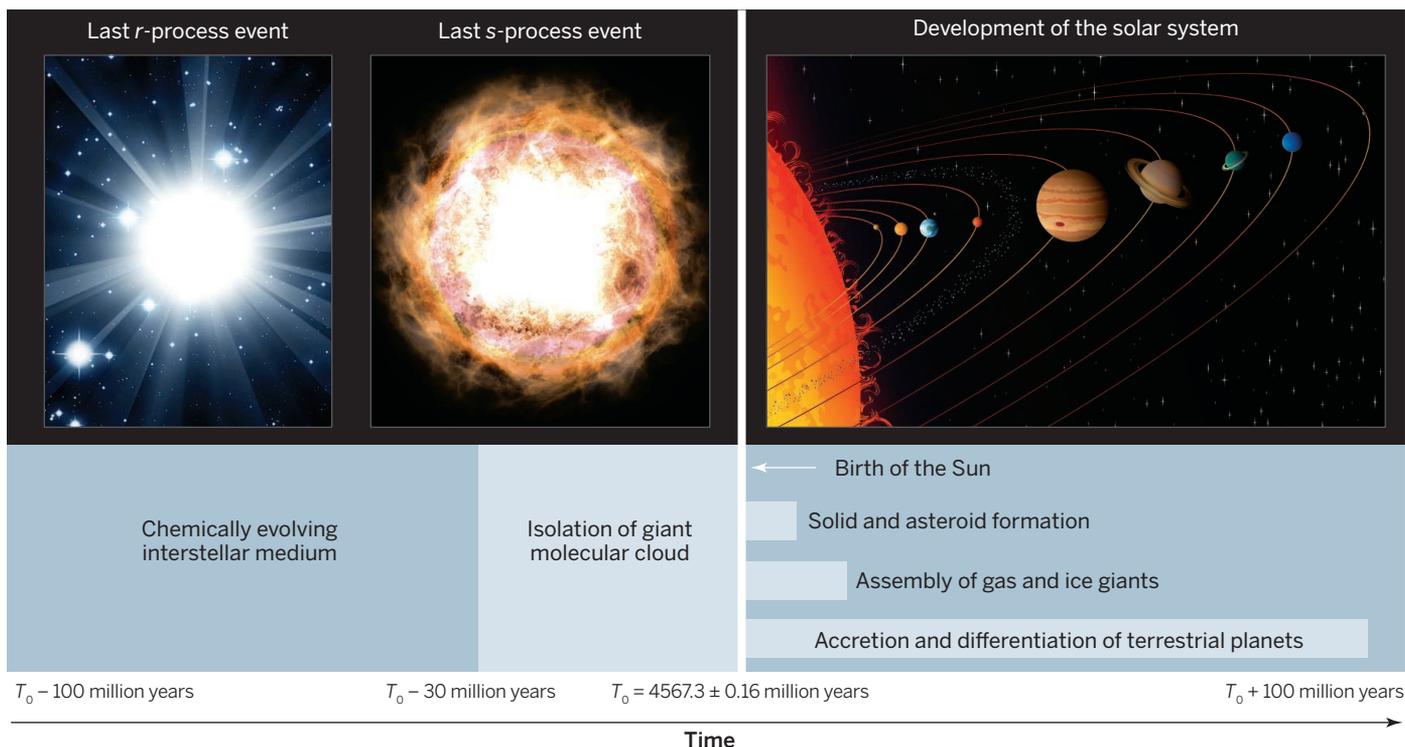
Lugaro *et al.* focus on the  $^{182}\text{Hf}$  and  $^{129}\text{I}$  radioisotopes, with half-lives of ~9 and ~16 million years, respectively, and for which the solar system's initial abundances are well understood. Heavy isotopes such as  $^{182}\text{Hf}$  and  $^{129}\text{I}$  are synthesized by slow and fast neutron capture reactions in stars (4). Sun-like stars live for billions of years, evolving to become asymptotic giant branch (AGB) stars toward

**“The evolutionary cycle of molecular clouds is rather simple—they form, produce stars, and then disperse.”**

the end of their life. These stars are the main sites for the production of isotopes by slow neutron capture reactions (*s* process), which are then ejected into the interstellar medium when the stars die. In contrast, massive stars evolve at much faster rates, ending their lives in titanic supernova explosions after only a few tens of millions of years. This process yields extremely high neutron densities, which promote the synthesis of isotopes by rapid neutron capture reactions (*r* process).

The current paradigm of nucleosynthesis asserts that both the  $^{182}\text{Hf}$  and  $^{129}\text{I}$  radioisotopes are produced by the *r* process. However, under this assumption, conflicting time scales are obtained for the free decay of  $^{182}\text{Hf}$  and  $^{129}\text{I}$  to their solar system abundances, which has led some to hypothesize the existence of two distinct astrophysical sites for *r*-process nucleosynthesis (5). But Lugaro *et al.* point out that the reason for this discrepancy may stem from a gross underestimation of the production rate of  $^{182}\text{Hf}$  by *s*-process nucleosynthesis. Using revised

Centre for Star and Planet Formation, Natural History Museum of Denmark, University of Copenhagen, DK-1350 Copenhagen, Denmark. E-mail: bizzarro@snm.ku.dk



**Solar system formation timeline.** The Sun's age ( $T_0$ ) is inferred from the most accurate estimate for condensation of the solar system's first solids, which occurred  $4567.3 \pm 0.16$  million years ago (Ma) (2). The epoch before the birth of the Sun reflects progressive isolation of the matter precursor to the solar system from the chemically evolving galaxy. This process leads to the formation of the giant molecular cloud from which a dense fragment collapsed to form the Sun and planets. The current architecture of the inner solar system was largely established within 100 million years of solar system formation.

nuclear energy levels for  $^{181}\text{Hf}$  (a branching point leading to  $^{182}\text{Hf}$ ), they show that AGB stars can produce up to 6 times as much  $^{182}\text{Hf}$  as previously recognized, which provides an elegant solution to the conflicting time scale conundrum: Their distinct nucleosynthetic origins must reflect two separate seeding events. In this view, the solar system abundance of  $^{129}\text{I}$  results from an *r*-process last event, whereas that of  $^{182}\text{Hf}$  stems from an *s*-process last event.

Lugaro *et al.* can thus constrain the timing of the *r*- and *s*-process events to have occurred  $\sim 100$  and  $\sim 30$  million years, respectively, prior to the birth of the solar system (see the figure). Reassuringly, these time scales are consistent with those inferred from the  $^{247}\text{Cm}$  and  $^{107}\text{Pd}$  short-lived radioisotopes, which are believed to have been synthesized by similar processes.

Lugaro *et al.* suggest that the isolation time scale of  $\sim 30$  million years inferred from the free decay of  $^{182}\text{Hf}$  provides an upper limit for the lifetime of the giant molecular cloud from which a dense core collapsed to form the solar system. The evolutionary cycle of molecular clouds is rather simple—they form, produce stars, and then disperse. As such, the lifetime of a cloud is to an extent controlled by the star formation rate, as the newly born stars provide some of the energy required to disperse

the cloud. In the solar neighborhood, star-forming clouds appear to be short-lived, with lifetimes of perhaps only a few million years (6). But these are relatively small, and estimates based on more massive clouds ( $>10^4$  solar masses) return much longer lifetimes (7, 8). Therefore, a protracted isolation time scale of  $\sim 30$  million years makes sense if our Sun was born in a giant molecular cloud parental to a high-mass stellar nursery such as the Messier 67 cluster (9).

In addition to  $^{182}\text{Hf}$  and  $^{129}\text{I}$ , meteorites also contain evidence for the former presence of much shorter-lived radioisotopes such as  $^{26}\text{Al}$  (half-life of 730,000 years), which requires late-stage seeding of the protosolar molecular cloud core with freshly synthesized matter just before it collapsed. This observation forms the basis of a popular model (10) in which short-lived radioisotopes were produced in a single supernova explosion and transported by a shock wave that triggered cloud collapse and injected the isotopes. The results of Lugaro *et al.* are a serious blow to this simplistic model and indicate a more complex and dynamic evolution: Some short-lived radionuclides are inherited from the evolving interstellar medium, whereas others (such as  $^{26}\text{Al}$ ) reflect self-pollution of the giant molecular cloud by massive stars formed during its lifetime. This view is supported by the recent discov-

ery of early-formed solar system solids containing the initial solar system inventory of  $^{182}\text{Hf}$  but lacking the expected level of  $^{26}\text{Al}$  (11). Collectively, these observations imply the existence of multiple generations of presolar dust at the start of the solar system, including an older galactic component hosting  $^{182}\text{Hf}$  and young,  $^{26}\text{Al}$ -rich, supernova-derived dust grains.

With the anticipated discovery of Earth-like planets in habitable zones, the development of a unified model for the formation and evolution of our solar system is timely. The study of Lugaro *et al.* nicely illustrates that the integration of astrophysics, astronomy, and cosmochemistry is the quickest route toward this challenging goal. ■

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