Supplementary Information

Isotopic Evidence for a Cold and Distant Origin of 3I/ATLAS

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Supplementary Discussion

Comparison with Other Isotopic Observations of 3I/ATLAS

Our observed isotopic ratios for 3I/ATLAS (D/H = $(0.98 \pm 0.06)\%$ and $^{12}C/^{13}C$ = 123–172) using JWST, are extremely unusual with respect to previous measurements of comets and other Solar System bodies (see Main Text Figure 3). Nevertheless, our results are quantitatively supported by two independent studies of 3I/ATLAS using the Atacama Large Millimeter/submillimeter Array (ALMA) and Very Large Telescope (VLT). Salazar Manzano et al. [1] used ALMA ACA observations of the HDO 241.6 GHz rotational line on 2025-Nov-04 (when 3I/ATLAS was close to perihelion, at $r_H = 1.4$ au), to derive D/H > 0.66% (at 99% statistical confidence), incorporating an upper limit for the water production rate from ACA observations of the 183.3 GHz H_2O line. Although a simultaneous H_2O observation was lacking (leading to only a lower limit for D/H), their result remains consistent with the extremely high D/H found later (at $r_H = 2.4$ au) using JWST. The two sets of HDO observations, obtained using separate telescopes operating in two different wavelength regimes, taken 49 days apart (spanning a factor of up to $\sim 10^2$ in total H_2O production rate of the object — see this study and ref. [2]), demonstrate a consistently high D/H over a large range of r_H. This supports our finding that the 3I/ATLAS nucleus has an intrinsically elevated D/H, which is not strongly affected by activity-dependent isotopic fractionation [*e.g.* 3, 4] or other biases. The conclusions of [1] are also in agreement with our study concerning the requirement of very low temperatures to produce elevated D/H ratios during interstellar (or prestellar/protostellar) ice formation.

Opitom et al. (manuscript submitted) derived a $^{12}C/^{13}C$ ratio of 147^{+87}_{-40} for 3I/ATLAS using VLT UVES spectroscopy of CN fluorescent emission around 387 nm. Due to the weakness of the observed CN isotopic lines, their resulting error bars are somewhat larger than we obtained in the infrared (for CO and CO_2) using JWST. Their range of possible values fully overlaps with our observed $^{12}C/^{13}C$ ranges, thus corroborating our results, and showing that the cause of the ^{13}C enrichment can occur at a similar rate for CO, CO_2 and CN, despite the different chemical formation pathways (and associated isotopic fractionation mechanisms) operating for these three molecules. Higher signal-to-noise observations of all three isotopologue ratios will be worthwhile in the future, to investigate the possibility of differential ^{13}C fractionation among the different gases incorporated into interstellar objects (and Solar System comets). Opitom et al. (manuscript submitted) also observed a lower $^{14}N/^{15}N$ ratio in 3I/ATLAS than previous Solar System comets. This further supports our conclusion that the ISO originated in a relatively low metallicity environment that may have been depleted in ^{15}N in addition to the observed ^{13}C depletion.

Isotopic Insights into the Origin of 3I/ATLAS

The elemental abundances observed in 3I/ATLAS place strict requirements on the chemical profile of its originating star-system, which, combined with dynamical constraints from the object's Galactic orbit (deduced from its inbound velocity vector), result in a set of criteria that help isolate its origin in space and time. Supplementary Table 1 summarises the evidence for a cold and (temporally) distant origin, explained in more detail in this subsection.

Taken at face value, the high CO and CO_2 gas production rates, as well as substantial abundances of organic molecules (including CH_3OH, H_2CO and CH_4 [5, 6] relative to H_2O provide evidence for a carbon- (and oxygen-) rich originating system. Furthermore, since rocky planets and planetesimals can only form in the presence of relatively high metal abundances (characterized by a logarithmic [Fe/H] abundance $\gtrsim -0.6$ relative to the Sun [7, 8]), moderately high overall metallicity is also required. Both these criteria can be fulfilled by an early burst of massive star formation (within a few giga-years of the Galaxy's formation), followed by a slower period of further enrichment of carbon (and other elements) by low-mass AGB stellar outflows. According to the Galactic chemical evolution model of Kobayashi et al. [9], elevated interstellar $^{12}C/^{13}C$ ratios $\gtrsim 130$ can be achieved at relatively high (but still subsolar) metallicity ([Fe/H] ≈ -0.2 to -0.6) under such a scenario. In the Galactic bulge and "thick disk" stellar populations, above-average metallicity and below-average $^{12}C/^{13}C$ ratios occur as a consequence of early, rapid star formation, followed by slower ^{13}C enrichment due to the relative lack of intermediate-mass (IM) AGB stars (with between 4–8 solar masses). Since nitrogen and ^{13}C are both produced more efficiently in IM AGB stars, *via* the CNO cycle [10], deficiencies of both these elements are expected to correlate. The low NH_2 and HCN abundances [5, 11], along with our low HCN/CO ratio (see ALMA Observations section and ref. [12]), could imply a deficiency of elemental nitrogen in 3I/ATLAS relative to C and O. This may therefore also be consistent with the formation of 3I/ATLAS in an environment subject to early, rapid star formation, resulting in enriched interstellar C and O abundances relative to the initial (Big Bang) abundances, but prior to the attainment of the level of ^{13}C and N enrichment typically seen in the present-day Solar System and local Galaxy.

Although the models of Kobayashi et al. [9] indicate that high $^{12}C/^{13}C$ ratios (up to 140) can be most readily achieved at [Fe/H] $\gtrsim -0.6$ in the Galactic bulge, the high velocity dispersion of bulge stars ($\sim 150\,\mathrm{km\,s^{-1}}$) is inconsistent with the present orbit of 3I/ATLAS, which matches better with stars in the Galactic disk [13, 14]. On the other hand, the elemental composition may be consistent with the large population of old stars with elevated C/N and α/Fe ratios, identified by Masseron & Gilmore [15][1]. This chemically-defined stellar population has a higher average vertical motion than non-α-enhanced stars, but remains distinct from the classical "thick disk" stellar component [16]. However, the high vertical motion of 3I/ATLAS's Galactic trajectory is entirely consistent with Masseron & Gilmore [15]'s old, low-metallicity, α-enhanced population ([14, 17] and M. Hopkins 2026, private communication).

In a sample of 63 nearby solar-type stars, [18] obtained $^{12}C/^{13}C$ ratios in the range 71–105. Based on their ages, which range between $\sim$ 0–9 Gyr, [19] inferred a relatively rapid onset of ^{13}C enrichment during the first 4 Gyr of our Galaxy's evolution, as a result of ^{13}C production in novae. The resulting, steep $^{12}C/^{13}C$ curve at early times in their model with 3–8$M_\odot$ white-dwarf nova progenitors (see Supplementary Figure 1), constrains the isotopic age of 3I/ATLAS to the range 11–12 Gyr, assuming an origin in the nearby Galactic disk. For comparison, the secondary $^{12}C/^{13}C$ peak at [Fe/H] = -0.5 in the Kobayashi et al. [9] Fig. 19 (thick-disk model), corresponds to a similar estimated age of $\sim$ 11 Gyr.

Uncertainties in the modeled $^{12}C/^{13}C$ ratios as a function of time are significant due to incomplete knowledge of the stellar initial mass function, star formation rates as a function of time (and Galactocentric radius), gas infall/outflow rates and stellar nucleosynthetic yields. A conclusive age estimate for 3I/ATLAS is further complicated by the interstellar $^{12}C/^{13}C$ gradient as a function of Galactocentric distance (R_{GC}) [20, 21]. Although definitive measurements of interstellar gas $^{12}C/^{13}C$ ratios comparable to the 3I/ATLAS CO_2 lower bound of 141 are lacking, extrapolation of the Luo et al. [21] trend line for HCO^+ to the outer edge of the Galaxy (R_{GC} = 14 kpc) gives $^{12}C/^{13}C = 116 \pm 29$. Therefore, within the uncertainties of the Galactic trend, an origin for 3I/ATLAS in the most distant, metal-depleted outer regions of the Galactic disk is also a possi-

[1] Alpha (α) elements have integer multiples of four nucleons (protons + neutrons), and are synthesized inside stars through alpha capture processes. Examples include C, O, Si and S, but not N.

bility. However, it remains to be demonstrated whether such an origin could be consistent with 3I/ATLAS's present-day trajectory. Furthermore, the observational trend (and models) presented by Yan et al. [20] reach only $^{12}C/^{13}C \approx 80$–120 in the outermost disk (see Supplementary Figure 2). Based on these results, significant temporal evolution would still be required to match the 3I/ATLAS $^{12}CO_2/^{13}CO_2$ ratio, although the age estimate would potentially be shortened to $\sim$ 10–11 Gyr if 3I/ATLAS formed in the outer galaxy, due to slower ^{13}C enrichment of the ISM in those regions. Ultimately, the observed range of $^{12}C/^{13}C$ ratios in 3I/ATLAS can be most readily explained as a result of temporal evolution of the interstellar $^{12}C/^{13}C$ ratio, with a possible additional contribution from the Galactic radial $^{12}C/^{13}C$ gradient.

Insights into the Properties of the 3I/ATLAS Natal Environment from D/H

The D/H ratio for water in 3I/ATLAS demonstrates a surprisingly high deuterium enrichment compared with other (icy and non-icy) Solar System bodies and protostars within the Galaxy (see Main Text Fig. 3). Deuteration of H_2O ice in Solar System comets is theorized to occur primarily in the interstellar and pre-stellar phases, where H_2O (and HDO) are rapidly synthesized on the surfaces of dust grains at very low temperatures ($\lesssim$ 30 K) through atom-atom addition reactions [22, 23]. The D/H ratio is there determined by the balance of gas and grain-surface reactions involving H, D and O atoms, initiated by the conversion of (unreactive) gas-phase HD into (highly reactive) H_2D^+, as a result of the reaction

$$HD + H_3^+ \rightleftharpoons H_2 + H_2D^+. \tag{1}$$

The rate of the reverse reaction (destroying H_2D^+) is highly sensitive to both the gas kinetic temperature (T_{kin}) and the amount of H_2 in its ortho *vs.* para spin states [22, 24], so the resulting H_2O deuterium enrichments become most strongly enhanced for low values of the H_2 ortho/para ratio (OPR) and T_{kin}.

There is significant diversity in water ice D/H ratios in astrochemical models due to varying assumptions regarding the physics and chemistry of star-forming environments [22, 25]. Adopting typical metallicity, temperature and radiation conditions for the nearby Milky Way, Jensen et al. [26] showed that deuteration can remain efficient in star-forming regions as long as the dust temperatures remain below 30 K, while increased ionisation rates actually accelerate the reactions responsible for deuterating H_2O. This occurs as a result of increased H_3^+ abundances, which accelerate the conversion of HD to H_2D^+, leading to more efficient HDO production. Increased ionisation rates also reduce the ortho-to-para conversion timescale for H_2, which further enhances the H_2D^+ deuteration pathway. They also demonstrated that increased D/H ratios $\sim$ 1% could be achieved in the presence of a high cosmic-ray ionisation rate ($\gtrsim$ 10 times the local Galactic value). Such enhanced-ionisation conditions would be expected in the vicinity of the lower-metallicity region of intense, massive star-formation indicated by the high $^{12}C/^{13}C$ ratio and high abundances of α elements in 3I/ATLAS. A reduced CO abundance (relative to hydrogen) in low-metallicity interstellar clouds should further enhance the HDO/H_2O ratio (Furuya et al., in prep.), since CO acts as a chemical inhibitor on the main H_2D^+ deuteration pathway [27]. In the lower metallicity environment implied by our high observed $^{12}C/^{13}C$ ratio, reduced dust grain abundances would result in less-attenuated interstellar radiation fields, and therefore higher gas ionisation rates and associated warmer dust temperatures [28, 29], which can further accelerate the grain-surface chemistry required for efficient HDO formation. Although molecular ice and planetesimal formation is expected to be less efficient in reduced metallicity environments [7, 30], the HDO-rich composition of 3I/ATLAS proves that the cold, ice-rich conditions required for cometary accretion can still be present in the well-shielded midplanes of less metal-rich disks.

Deuterium is slowly destroyed over Galactic timescales as a result of fusion reactions in stellar interiors (astration). Consequently, the elemental D/H ratio has decreased by around 40%, from its initial (Big Bang) value of $\sim 2.5 \times 10^{-5}$, to a present day value of $\sim 1.5 \times 10^{-5}$ in the local ISM [31, 32]. Since the rate of Equation 1 is linearly dependent on the HD abundance, the rate of deuteration via H_2D^+ is also expected to vary linearly with the elemental D/H value [33]. Thus, HDO/H_2O ratios in the early Galaxy can be expected to be up to $\sim$ 40% higher than present day ratios, as a result of astration, further contributing to the elevated value in 3I/ATLAS. We therefore suggest that several physical and chemical factors associated with an old, relatively low-metallicity environment may have worked together to produce 3I/ATLAS's elevated HDO/H_2O ratio.

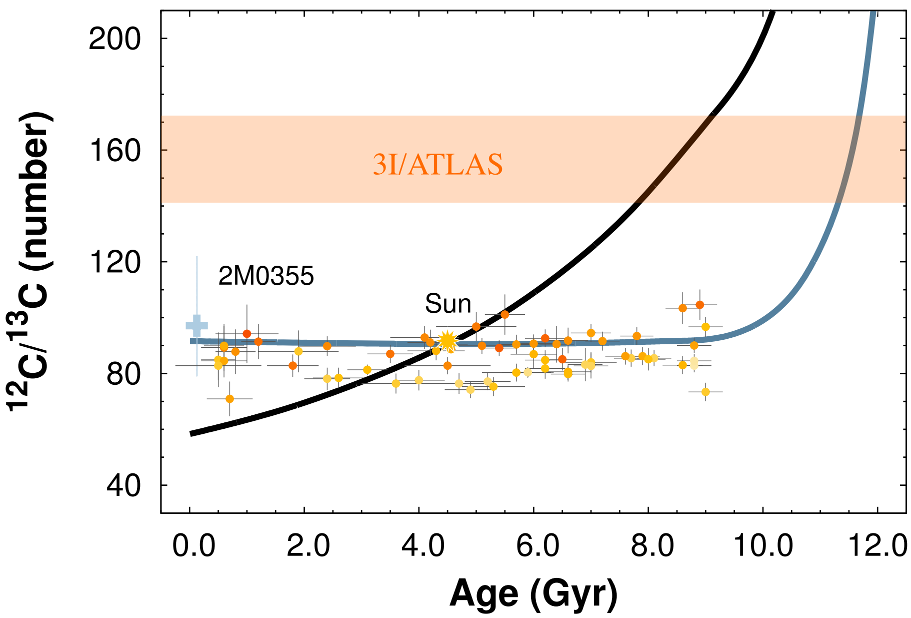
Summarising the Evidence for a Cold and Distant Origin

In summary, our study identifies numerous lines of evidence that help constrain the origin of 3I/ATLAS in space and time, as summarised in Supplementary Table 1. In the table, each line of evidence is assigned a "strength" designation ((S)trong, (M)oderate, and (C)ircumstantial), based on our assessment of its veracity, and the uniqueness of the associated conclusion. The high D/H ratio and presence of abundant hypervolatiles (CO and CH_4) provide strong evidence for the formation and preservation of 3I/ATLAS's ices at temperatures $T < 25$ K. This does not rule out the possibility that some parts of the nucleus have been subjected to higher temperatures, but a dominant component of the observed, outgassed volatiles must have been accreted and maintained at very cold temperatures to preserve frozen CO and CH_4 in the nucleus.

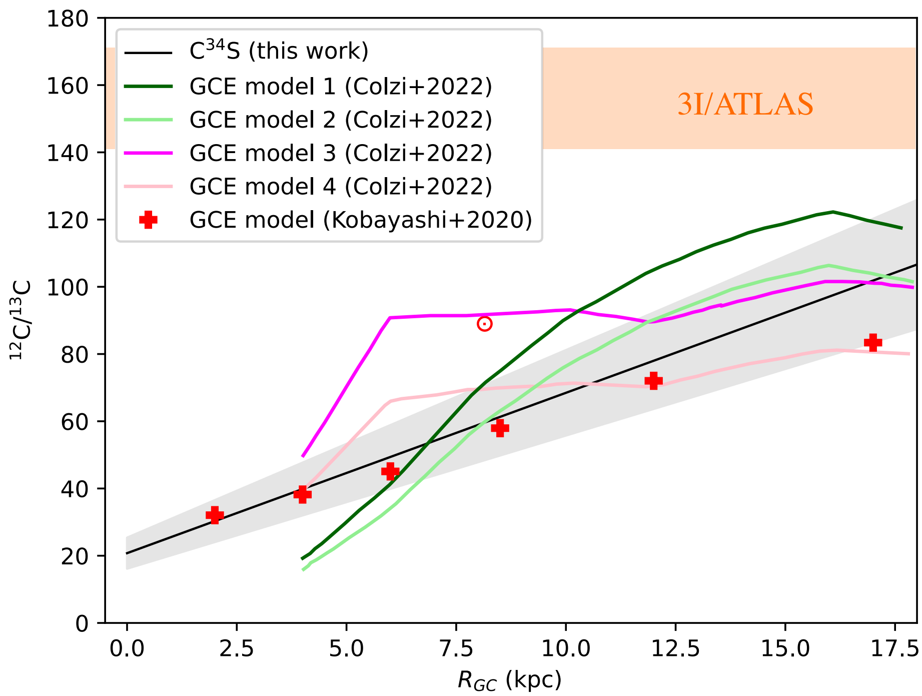
The strongest evidence for formation in a relatively low-metallicity environment (but still high enough to allow planetesimal formation) comes from the $^{12}C/^{13}C$ ratios in CO and CO_2, which are reliable tracers of the elemental carbon isotopic ratio in the ISM. However, formation in a ^{13}C-poor pocket of gas in the nearby (or outer) Milky Way cannot be ruled out from this ratio alone. On the other hand, considering the larger stellar densities at early Galactic times ($\sim$ 10 Gyr ago, during the intense early burst of star formation referred to as "cosmic noon" [34]), an ancient origin for 3I/ATLAS is statistically likely. The high velocity (and associated old dynamical age [17]) for 3I/ATLAS also provides moderately strong evidence for an ancient origin. The presence of abundant α-elements, and theoretical results showing enhanced HDO ice formation under strongly-irradiated interstellar conditions [26] are consistent with this conclusion, but provide only weak (circumstantial) evidence in their own right. Similarly, the low HCN and NH_2 abundances, consistent with an under-abundance of elemental nitrogen, are compatible with the association of 3I/ATLAS with the old, thick-disk stellar population identified by Masseron & Gilmore [15] (again, circumstantially).

Ultimately, our incomplete knowledge of the total elemental inventory of 3I/ATLAS, combined with significant uncertainties in Galactic chemical evolution models, precludes a conclusive statement on the precise origin of 3I/ATLAS in space and time. Nevertheless, we conclude with good confidence that 3I/ATLAS has a cold and temporally/spatially distant origin. Each interstellar object provides a unique snapshot of matter from a particular location and epoch in our Galaxy's chemical history, so further compositional measurements of 3I/ATLAS and future interstellar objects will provide valuable data towards a more complete understanding of the Milky Way's chemical evolution. The abundance of C, H, O, N and S-bearing species in 3I/ATLAS demonstrates the existence of volatile compounds around other stars that could lead to complex, potentially prebiotic chemistry [35], during the early history of our Galaxy.

Supplementary Figures



Supplementary Figure 1: Temporal evolution of the interstellar $^{12}C/^{13}C$ ratio as a function of Galactic age [19]. Observed ratios in 63 solar-type stars are shown (with 1σ error bars), from ref. [18]. Galactic chemical evolution models from Romano et al. [36] are plotted, implementing nova nucleosynthesis with white-dwarf progenitors in the mass range 1–8 $M_\odot$ (black curve), and 3-–8 $M_\odot$ (blue curve). The intersection of the ranges of fit results for $^{12}CO_2/^{13}CO_2$ and $^{12}CO/^{13}CO$ in 3I/ATLAS (141–172) is shown with a shaded orange rectangle. Adapted from Romano [19] under a Creative Commons Attribution 4.0 International License.



Supplementary Figure 2: Interstellar CS gas $^{12}C/^{13}C$ isotopic ratios measured in the present-day Milky Way [20] (black line with gray-shaded 1σ error margins). The red $\odot$ symbol indicates the Solar ratio. Galactic chemical evolution model results [37, 38] are also shown. The intersection of the ranges of fit results for $^{12}CO_2/^{13}CO_2$ and $^{12}CO/^{13}CO$ in 3I/ATLAS (141–172) is shown with a shaded orange rectangle, which is significantly higher than can be explained solely by the Galactic $^{12}C/^{13}C$ gradient, necessitating the formation of 3I/ATLAS at an earlier epoch. Adapted from Yan et al. [20] under a Creative Commons Attribution 4.0 International License.

Supplementary Tables

Supplementary Table 1: Summarising the Evidence for a Cold and Distant Origin for 3I/ATLAS

Evidence for a cold origin
1(S): Large abundances of hypervolatiles (CO and CH_4) $\longrightarrow$ formation and preservation of the nucleus at $T < 25$ K.
2(S): Extremely high HDO/H_2O ratio $\longrightarrow$ water ice formation at $T < 30$ K.
Evidence for a temporally-distant formation epoch
1(M): Very high $^{12}C/^{13}C$ ratios $\longrightarrow$ age > 10 Gyr [19].
2(M): Elevated D/H ratio $\longrightarrow$ consistent with deuterium astration over Galactic time.
3(C): Formation of HDO in a strongly-irradiated ISM $\longrightarrow$ association with a high star-formation rate environment ("cosmic noon").
4(C): Abundant α elements $\longrightarrow$ formation around the epoch of cosmic noon.
5(C): Low NH_2 and HCN abundances $\longrightarrow$ association with old, N-poor, thick-disk stars.
6(M): High velocity trajectory $\longrightarrow$ large dynamical age $\sim$ 3–11 Gyr [17].

Notes — Strength of the evidence is denoted with (S) for strong, (M) for moderate, and (C) for circumstantial.

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