# <sup>15</sup>NH<sub>3</sub> in the atmosphere of a cool brown dwarf

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David Barrado<sup>1,26⊠</sup>, Paul Mollière<sup>2,26</sup>, Polychronis Patapis<sup>3,26</sup>, Michiel Min<sup>4</sup>, Pascal Tremblin<sup>5</sup>, Francisco Ardevol Martinez<sup>4,6,7,8</sup>, Niall Whiteford<sup>9</sup>, Malavika Vasist<sup>10</sup>, Ioannis Argyriou<sup>11</sup>, Matthias Samland<sup>2</sup>, Pierre-Olivier Lagage<sup>12</sup>, Leen Decin<sup>11</sup>, Rens Waters<sup>4,13</sup>, Thomas Henning<sup>2</sup>, María Morales-Calderón<sup>1</sup>, Manuel Guedel<sup>2,3,14</sup>, Bart Vandenbussche<sup>11</sup>, Olivier Absil<sup>10</sup>, Pierre Baudoz<sup>15</sup>, Anthony Boccaletti<sup>15</sup>, Jeroen Bouwman<sup>2</sup>, Christophe Cossou<sup>16</sup>, Alain Coulais<sup>12,17</sup>, Nicolas Crouzet<sup>18</sup>, René Gastaud<sup>16</sup>, Alistair Glasse<sup>19</sup>, Adrian M. Glauser<sup>3</sup>, Inga Kamp<sup>6</sup>, Sarah Kendrew<sup>20</sup>, Oliver Krause<sup>2</sup>, Fred Lahuis<sup>4</sup>, Michael Mueller<sup>6</sup>, Göran Olofsson<sup>21</sup>, John Pye<sup>22</sup>, Daniel Rouan<sup>15</sup>, Pierre Royer<sup>11</sup>, Silvia Scheithauer<sup>2</sup>, Ingo Waldmann<sup>23</sup>, Luis Colina<sup>1</sup>, Ewine F. van Dishoeck<sup>18</sup>, Tom Ray<sup>24</sup>, Göran Östlin<sup>25</sup> & Gillian Wright<sup>19</sup>

Brown dwarfs serve as ideal laboratories for studying the atmospheres of giant exoplanets on wide orbits, as the governing physical and chemical processes within them are nearly identical<sup>1,2</sup>. Understanding the formation of gas-giant planets is challenging, often involving the endeavour to link atmospheric abundance ratios, such as the carbon-to-oxygen (C/O) ratio, to formation scenarios<sup>3</sup>. However, the complexity of planet formation requires further tracers, as the unambiguous interpretation of the measured C/O ratio is fraught with complexity<sup>4</sup>. Isotope ratios, such as deuterium to hydrogen and <sup>14</sup>N/<sup>15</sup>N, offer a promising avenue to gain further insight into this formation process, mirroring their use within the Solar System<sup>5-7</sup>. For exoplanets, only a handful of constraints on <sup>12</sup>C/<sup>13</sup>C exist, pointing to the accretion of <sup>13</sup>C-rich ice from beyond the CO iceline of the disks<sup>8,9</sup>. Here we report on the mid-infrared detection of the <sup>14</sup>NH<sub>3</sub> and <sup>15</sup>NH<sub>3</sub> isotopologues in the atmosphere of a cool brown dwarf with an effective temperature of 380 K in a spectrum taken with the Mid-Infrared Instrument (MIRI) of JWST. As expected, our results reveal a <sup>14</sup>N/<sup>15</sup>N value consistent with star-like formation by gravitational collapse, demonstrating that this ratio can be accurately constrained. Because young stars and their planets should be more strongly enriched in the <sup>15</sup>N isotope<sup>10</sup>, we expect that <sup>15</sup>NH<sub>3</sub> will be detectable in several cold, wide-separation exoplanets.

The coldest class of brown dwarfs, so-called Y dwarfs, span temperatures from 250 to 500 K (ref. 11). Their atmospheres are dominated by the absorption of water, methane and ammonia, whereas water clouds probably become important for the colder Y dwarfs<sup>12</sup>. Because their emission peaks in the mid-infrared beyond 4 µm, Y-dwarf spectroscopic characterization is challenging and the number of studies has been limited<sup>12-14</sup>. The JWST is transforming the study of Y dwarfs by allowing access to their full luminous range<sup>15</sup>. We analysed JWST/ MIRI Medium Resolution Spectrometer (MRS)<sup>16</sup> observations of the Y-dwarf archetype WISEP J182831.08 + 265037.8 (hereafter WISE J1828), with an effective temperature of about 380 K (ref. 11). We obtain a mid-infrared spectrum at  $R \approx 3,000$  to 1,500, between 4.9 and 27.9 µm. The data reduction is described in Methods. Our observations are presented in Fig. 1, together with an exemplary best-fit model from our analysis, and reveal a spectrum rich in molecular features, namely, a broad water-absorption band at 5–7 μm, methane at 7.6 μm and ammonia at 9–13  $\mu$ m. The ammonia band is also shown in more detail in the lower panels of Fig. 1. We analysed the atmospheric properties of WISE J1828 using several retrieval codes<sup>17-19</sup> and self-consistent atmosphere models in radiative-convective equilibrium (refs. 20,21

1centro de Astrobiología (CAB), CSIC-INTA, Madrid, Spain. 2Max-Planck-Institut für Astronomie (MPIA), Heidelberg, Germany. 3Institute of Particle Physics and Astrophysics, ETH Zurich, Zürich, Switzerland. 4SRON Netherlands Institute for Space Research, Leiden, The Netherlands. 5Université Paris-Saclay, UVSQ, CNRS, CEA, Gif-sur-Yvette, France. 6Kapteyn Institute of Astronomy, University of Groningen, Groningen, The Netherlands. 7School of GeoSciences, University of Edinburgh, Edinburgh, UK. 8Centre for Exoplanet Science, University of Edinburgh, Edinburgh, UK. <sup>9</sup>Department of Astrophysics, American Museum of Natural History, New York, NY, USA. <sup>10</sup>STAR Institute, Université de Liège, Liège, Belgium. <sup>11</sup>Institute of Astronomy, KU Leuven, Leuven, Belgium, 12 Université Paris-Saclay, Université Paris Cité, CEA, CNRS, AIM, Gif-sur-Yvette, France, 13 Department of Astrophysics/IMAPP, Radboud University, Niimegen, The Netherlands, <sup>14</sup>Department of Astrophysics, University of Vienna, Vienna, Austria. <sup>15</sup>LESIA, Observatoire de Paris, Université PSL, CNRS, Sorbonne Université, Université de Paris Cité, Meudon, France. 16Université Paris-Saclay, CEA, IRFU, Gif-sur-Yvette, France, 17LERMA, Observatoire de Paris, Université PSL, CNRS, Sorbonne Université, Paris, France, 18Leiden Observatory, Leiden University, Leiden, The Netherlands. 19 UK Astronomy Technology Centre, Royal Observatory Edinburgh, Edinburgh, UK. 20 European Space Agency, Space Telescope Science Institute, Baltimore, MD, USA. <sup>21</sup>Department of Astronomy, Stockholm University, AlbaNova University Center, Stockholm, Sweden. <sup>22</sup>School of Physics & Astronomy, Space Research Centre, Space Park Leicester, University of Leicester, Leicester, UK. 23Department of Physics and Astronomy, University College London, London, UK. 24School of Cosmic Physics, Dublin Institute for Advanced Studies, Dublin, Ireland. <sup>25</sup>Department of Astronomy, Oskar Klein Centre, Stockholm University, Stockholm, Sweden. <sup>26</sup>These authors contributed equally: David Barrado, Paul Mollière, Polychronis Patapis. 🖾 e-mail: barrado@cab.inta-csic.es

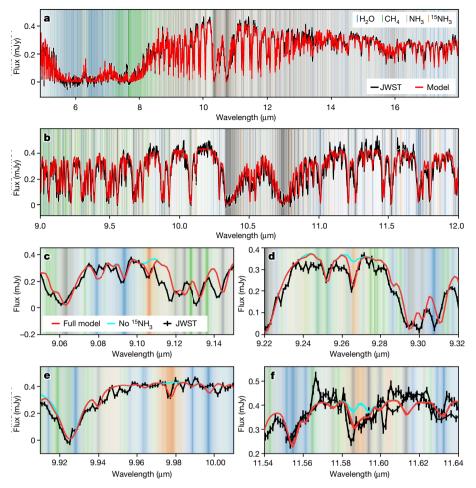


Fig. 1 | MIRI/MRS spectrum and exemplary best-fit model (here, pRT-free) of the Y dwarf WISE J1828. a, Full MIRI wavelength range considered in our models at retrieval resolution ( $\lambda/\Delta\lambda$  = 1,000). All other panels show the data at the original, higher MRS resolution; models have been post-processed to the same resolution. b, As in a but zoomed in to show the NH<sub>3</sub> absorption band at

 $10~\mu m$  in more detail. c-f, Individual  $^{15}NH_3$  lines in the data, including a best-fit retrieval model with and without accounting for the opacity of  $^{15}NH_3$ . The error bars shown for the observations correspond to  $1\sigma$  confidence levels. Panel f contains two overlapping MIRI MRS subchannels. Coloured bands denote the theoretical positions of the absorption lines of  $H_2O$ ,  $CH_4$ ,  $NH_3$  and  $^{15}NH_3$ .

and F.A.M. et al., manuscript in preparation). The best-fit spectra and residuals are shown in Extended Data Fig. 1. As the MIRI observations mostly explore high altitudes in the atmosphere (with the contribution function peaking at approximately 1 bar), we also added archival near-infrared data<sup>14</sup>, which examines deeper layers, at pressures of about 10 bar (Extended Data Fig. 2). Owing to its high luminosity, given its spectral type, WISE J1828 is suggested to be a binary system (However, numerous studies, including recent JWST measurements, all failed at resolving its binarity, putting an upper limit of 0.5 AU on the separation of its components<sup>11,22</sup>). We thus modelled WISE J1828 as an equal-mass binary system, emitting with identical atmospheres.

By combining the results of different retrieval approaches (see Methods), we constrain the  $\log_{10}$  (volume mixing ratios) (VMRs) of the conspicuous absorbers  $H_2O$ ,  $CH_4$  and  $^{14}NH_3$  to be  $-3.03^{+0.18}_{-0.21}$ ,  $-3.65^{+0.21}_{-0.21}$  and  $-4.79^{+0.15}_{-0.25}$ , respectively. The surface gravity of WISE J1828 is constrained to be  $\log(g)=4.34^{+0.42}_{-0.88}$ , the effective temperature is  $378^{+13}_{-18}$  K and the radius is constrained to  $1.37^{+0.26}_{-0.13}$   $R_{\rm Jup}$ . The uncertainties for these values are dominated by the dispersion between the various fitting approaches and are thus larger than the actual uncertainties derived from any single analysis. A posterior plot of the various retrievals is shown in the Extended Data Fig. 3, whereas all retrieval results are summarized in Extended Data Table 1. The self-consistent models constrain the atmospheric properties to be  $\log(g)=4.5\pm1.0$ ,  $R=1.27\pm0.21$   $R_{\rm Jup}$  and  $T_{\rm eff}=450\pm101$  K. Again, the reported uncertainties are dominated by differences between the two models. Our best-fit values

of  $\log(g)$ , R and  $T_{\rm eff}$ , after applying a binary correction to the inferred radii (dividing by  $\sqrt{2}$ ), indicate an age of roughly 5 Gyr for an approximately 15- $M_{\rm Jup}$  equal-mass binary system<sup>23</sup>, which is consistent with our mass constraints (see Extended Data Table 2).

The metallicity we derive for WISE J1828, combining the results of all approaches that included it as a free parameter (retrievals and self-consistent), is consistent with solar:  $[M/H] = 0.02^{+0.12}_{-0.31}$  For C/O, we find  $0.22^{+0.37}_{-0.03}$  (solar is  $0.55\pm0.10$  (ref. 24)), whereas N/O is constrained to  $0.014^{+0.021}_{-0.002}$  (solar is  $0.138\pm0.023$  (ref. 24)). These uncertainties are again dominated by the dispersion between different approaches. The resulting posteriors for the metallicity, C/O and N/O are shown in Extended Data Fig. 3. Our findings thus indicate an atmosphere with a solar bulk metallicity, but depleted in C and N. A probable cause for this is a departure from chemical equilibrium, in which gas poor in both NH<sub>3</sub> and CH<sub>4</sub> is mixed up from the deep interior of the object<sup>25</sup>. The resulting gas would be enriched in N2 and CO, to which our observations are not sensitive. N2 is not spectrally active, and our shortest wavelengths are longer than the location of the fundamental band of CO at roughly 4.5 µm. However, it is questionable whether enough CO can be mixed up from the deep atmosphere to palpably change the inferred C/O ratio<sup>26</sup>.

Also, we detect  $^{15}NH_3$  with a significance ranging from  $4\sigma$  to  $6\sigma$ , with several lines of ammonia clearly visible in the data (see Fig. 1). We derive a VMR of  $-7.68^{+0.24}_{-0.34}$  for  $^{15}NH_3$  and  $^{14}N/^{15}N = 670^{+390}_{-211}$ , averaging over the results of various models. In Fig. 2, we summarize  $^{14}N/^{15}N$  for a range of

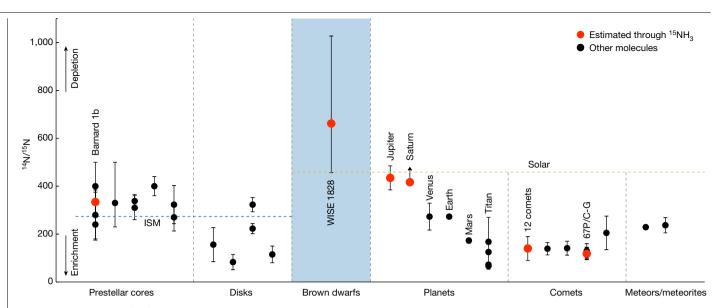
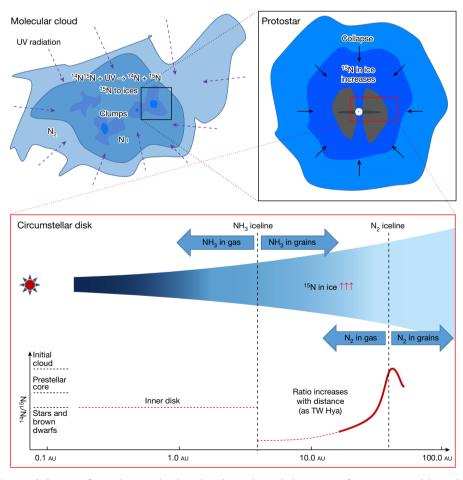


Fig. 2 | Comparison of the <sup>14</sup>N/<sup>15</sup>N ratio in the solar neighbourhood. The values are based on either ammonia isotopologues (red circles) or other molecules (black symbols), in different environments, subdivided by classes<sup>7</sup>. Our estimate for WISE J1828 appears as the brown dwarf class and is consistent with solar

values (dashed yellow line) at the 1–2 $\sigma$  level. Other errors come from the cited compilation. Lower values indicate enrichment in 15N, whereas the dashed blue line represents the current value of the ISM.

astrophysical objects<sup>7</sup>. Our value for WISE J1828 is consistent with solar at the 1–2 $\sigma$  level. Both the Sun and WISE J1828, which we derive to have similar ages, have 14N/15N values above those observed in the interstellar medium (ISM), which has been enriched in <sup>15</sup>N by galactic stellar evolution since their formation<sup>10</sup>. Our measurement thus shows that WISE J1828 most probably formed like a star, as expected<sup>27</sup>. A strong ice enrichment is unlikely and we correspondingly rule out cometary values  $^{14}$ N/ $^{15}$ N < 200 by more than  $3\sigma$ .



 $\textbf{Fig. 3} | \textbf{Different phases of star and planetary formation.} \ \text{We also show the relationship with the ammonia fractionation and the evolution of the $^{14}N/^{15}N$ ratio at $^{14}N/^{15}N$ these stages: inside a molecular cloud with prestellar cores, during the formation of a protostar and in a circumstellar disk around a young star.

Constraints on  $^{14}N/^{15}N$  can serve as a formation tracer. For example, comets in the Solar System, fundamental planetary building blocks, are enriched in  $^{15}N$  by a factor of 2–3 when compared with solar, owing to  $^{15}N$ -rich  $NH_3$  and HCN ice. By contrast,  $N_2$  gas in the solar accretion disk is thought to have been depleted in  $^{15}N$  (ref. 7). In the Solar System, both Jupiter and Saturn are enriched in bulk nitrogen but show  $^{14}N/^{15}N$  values consistent with the Sun. This may mean that they accreted ice cold enough to contain even the volatile  $N_2$  ice, which requires temperatures lower than 30 K, and corresponds to orbital distances greater than 25 AU (refs. 28,29). An enriched nitrogen content through accretion of ice, but at solar  $^{14}N/^{15}N$ , may therefore require accretion close to where even the highly volatile  $N_2$  can condense.

The understanding of how nitrogen fractionation actually occurs is incomplete  $^7$ , but we summarize some processes during different stages of the stellar and planetary evolution in Fig. 3. In the denser parts of the clouds, an increase of  $^{15}$ N in NH $_3$  is inferred, with a candidate for this fractionation being isotope-selective photodissociation  $^{30}$ . Subsequently, NH $_3$  and HCN ices condense in the colder clumps, potentially producing  $^{15}$ N-rich ice. Once a protostar is formed, there is some evidence that  $^{14}$ N/ $^{15}$ N decreases further  $^{31,32}$ . The final consequence is thought to be a  $^{15}$ N increase in the less volatile nitrogen carriers, leading to the observed increase in  $^{15}$ N in HCN for protoplanetary disks and in NH $_3$  and HCN for Solar System comets. We note that models predict  $^{15}$ N-poor NH $_3$  gas in protoplanetary disks  $^{32}$ .

To further assess  $^{14}$ N/ $^{15}$ N as a formation tracer, we used a simplified planet-formation model $^4$ . We tracked  $^{14}$ N/ $^{15}$ N as a function of the mass accreted as icy and rocky material, for a planet located between the N<sub>2</sub> iceline of the disk, at about 20–80 AU, and the NH<sub>3</sub> iceline, ten times closer in  $^{29,33}$ . The ices were therefore probably enriched in  $^{15}$ N. We find that, for Saturn-like metal enrichment (about six times solar  $^{34}$ ), the  $^{14}$ N/ $^{15}$ N decreases by 30–40% when compared with solar (see Extended Data Fig. 4), indicating that  $^{14}$ N/ $^{15}$ N can vary substantially when compared with the stellar value for a planet forming between the N<sub>2</sub> and NH<sub>3</sub> icelines.

With the JWST MIRI, the formation-sensitive isotopologues <sup>14</sup>NH<sub>3</sub> and <sup>15</sup>NH<sub>3</sub> become accessible for objects with low effective temperatures. In the mid-infrared, NH<sub>3</sub> is a dominating absorber from  $T_{\rm eff}$  = 1,000 K (ref. 35) down to at least 380 K, the effective temperature of WISE J1828. As demonstrated above, 14N/15N can constrain formation locations with respect to the NH<sub>3</sub> and N<sub>2</sub> icelines of the disk. This is as well as constraints on N/O, that the detection of H<sub>2</sub>O and NH<sub>3</sub> enables, which has been suggested as another useful formation tracer<sup>36,37</sup>, but which needs careful interpretation owing to chemical disequilibrium processes<sup>25</sup>. Simultaneous constraints on C/O, N/O and  $^{14}$ N/ $^{15}$ N, based on CH<sub>4</sub>, CO, H<sub>2</sub>O and NH<sub>3</sub>, can thus be obtained for cold directly imaged exoplanets, further explaining their formation history. These planets are found in orbits ranging from tens to hundreds of astronomical units, challenging the core-accretion model for planetary formation<sup>38</sup>. They either formed at their detected locations by means of a star-like gravitational instability or originated closer to their star by means of core accretion and subsequent outward migration<sup>39</sup>.

#### **Online content**

Any methods, additional references, Nature Portfolio reporting summaries, source data, extended data, supplementary information, acknowledgements, peer review information; details of author contributions and competing interests; and statements of data and code availability are available at https://doi.org/10.1038/s41586-023-06813-y.

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#### Methods

#### JWST MIRI observations and data processing

The MIRI/MRS targeted WISE J1828 on 28 July 2022 without the use of target acquisition as part of JWST Guaranteed Time Observing programme with PID 1189. All three dichroic/grating settings (SHORT, MEDIUM, LONG) were obtained to cover the full wavelength range, from 4.9 to 27.9  $\mu m$  (ref. 16). The observations were executed with the point-source-optimized two-point dither (negative direction) and the detector set up with 180 frames per integration. No dedicated background observations were obtained.

The JWST pipeline was used (pipeline version: 1.9, CRDS version: 11.16.20, CRDS context: jwst 1045.pmap) to process the data. The raw (level 1B) files were processed with the detector-level pipeline (CALWEBB DETECTOR1) to produce calibrated rate files. This pipeline applies corrections for the nonlinearity of the ramps, dark current, detects jumps in the ramp resulting from cosmic rays and, finally, fits the ramp signal to obtain slope values (rate.fits). The detector images were inspected and no sign of cosmic-ray showers were found<sup>16</sup>. Because the WISE J1828 detector images were clean, we could use the fact that the point source itself is faint to perform a nod subtraction between the two dither points. First, we had to make sure that, for every pair of detector images, the flux levels were on the same level before subtracting them. A small time-dependent difference between the individual integrations has been seen in MRS observations, with the first integration of the visit having a brighter flux level originating from the detector idling before the start of the exposures 16. We used the region between the MRS channels on the detectors that do not contain any astrophysical signal to estimate a single value using the median and subtract it from the whole detector. Next, the two dithers were subtracted from each other to remove the thermal background contribution. For Channel 1 of the MRS, a detector artefact that manifests as vertical stripes was still present after the nod subtraction. These stripes were around 10%of the science signal and, because the dispersion direction also closely follows the detector columns<sup>16</sup>, the stripes affect the continuum of the extracted spectrum. We chose a region of the detector in which the source signal was almost zero and estimated the stripe contribution as the median of ten rows, which was then subtracted from every row of the detector.

With the detector images clean from detector artefacts and the thermal background, the spectroscopy pipeline (CALWEBB SPEC2) was run to obtain calibrated detector images (cal.fits), assigning the astrometric and wavelength information, correcting for the scattered light and detector fringing, and applying the photometric calibration. Finally, with CALWEBB SPEC3, we built the dither combined cubes<sup>40</sup>, with outlier rejection enabled. With background-subtracted cubes, the spectral extraction from the cube is done by performing aperture photometry for each wavelength slice of the cube. We first determined the centre of the point source by fitting a 2D Gaussian in the wavelength-collapsed cube, then placed an aperture of one full width at half maximum centred on the source, applying an aperture correction for each wavelength to account for the missing flux of the point-spread function outside the aperture. Some outliers remain in the extracted spectrum, which were removed for plotting the spectrum in Fig. 1 but not while fitting it. We traced back these outliers to the detector, at which a few cosmic rays overlap with the spectral trace but are not bright enough for the outlier algorithm to detect. We therefore clip these values manually for each spectral band by setting a threshold for the flux. The outliers affected in total 0.4% of the spectrum.

#### Retrieval analysis

We carried out independent analyses of the MIRI/MRS spectra using a diversity of models, namely, with the radiative-convective equilibrium codes ATMO and ARCiS+ML, and with the retrieval codes ARCiS, Brewster and petitRADTRANS (refs. 17–21 and F.A.M. et al., manuscript in

preparation). For computational feasibility, the retrievals with ARCiS, Brewster and petitRADTRANS were run at a resolution of  $\lambda/\Delta\lambda = 1.000$ : the MRS data were binned down correspondingly. For the retrievals, we decided on a setup that assumed vertically constant absorber abundances that were retrieved freely and a flexible parameterization of the pressure-temperature (P-T) structure, which varied slightly between the setups; see below. For the retrievals presented here, we assumed WISE J1828 to be a single object but allowed for a radius prior wide enough to account for an equal-brightness binary scenario. Clouds were neglected, which seems to be justified from a population-wide Y-dwarf retrieval analysis on Hubble Space Telescope (HST) data<sup>41</sup>. We note, however, that the impact of clouds should increase towards longer wavelengths and for colder Y dwarfs<sup>12,42</sup>. As shown in Extended Data Fig. 2, our inferred P-T profiles cross the water saturation vapour pressure curve at the top of the photosphere examined by the HST and the MIRI, so a cloud could have some moderate impact on our results and the effect of its inclusion should be assessed in future studies.

We also observed that the reported uncertainties of the JWST reduction can be much smaller than the differences observed in the overlapping regions of MRS subchannels. Also, all best-fit models had a  $\chi^2$ considerably larger than the number of wavelength channels. We thus opted for retrieving the magnitude of the uncertainties through the  $10^b$  treatment <sup>43</sup>, in which the error bars  $\sigma$  considered during the retrieval are calculated from the uncertainties reported from the reduction  $\sigma_{\rm red}$ as follows:  $\sigma = \sqrt{\sigma_{\rm red}^2 + 10^b}$ . Separate bs were retrieved for MIRI and HST data. The retrieved P-T structures of the retrievals would also exhibit kinks sometimes, which are challenging to reconcile with radiativeconvective equilibrium models. In this case, we implemented a regularization of the P-T structure 43. With this modification, the ARCiS and petitRADTRANS retrievals optionally put a penalty on  $d^2 log T/d log P^2$ , which strives towards a constant power-law dependence between pressure and temperature, as dlog T/dlog P = constant implies  $T \propto P^{\alpha}$ , with  $\alpha$  being the constant power-law coefficient. This setup may therefore also reproduce the relation between pressure and temperature in the deep atmosphere, which is expected to be convective. The individual models we used for the analysis are described below.

The results of all model inferences for WISE J1828 are found in Extended Data Table 1 and the combined result of all retrievals is presented in Extended Data Table 2. Elemental abundance ratios (C/O, N/O,  $^{14}\text{N}/^{15}\text{N}$ ) were computed from the VMR constraints of the retrievals for the atmospheric absorbers. They may thus miss further atoms locked up in clouds (in the case of oxygen) or affected by quenching in species that are spectrally inactive (N $_2$  in the case of N) or have features outside the HST and MIRI wavelength range (CO in the case of C and O). The one-dimensional projection of the posteriors, for key forward model parameters, is shown in Extended Data Fig. 3 for all individual models. In Extended Data Fig. 2, we show the associated P-T uncertainties derived from all model analyses.

**ATMO.** We briefly describe the main properties of the ATMO<sup>20</sup> models and the grids that have been used in our study. These grids are publicly available at https://opendata.erc-atmo.eu. The ATMO models assume that clouds are not needed to reproduce the shape of the spectral energy distribution of brown dwarfs (apart from the 10-µm silicate feature). The authors have proposed that diabatic convective processes<sup>44</sup> induced by out-of-equilibrium chemistry of CO/CH<sub>4</sub> and N<sub>2</sub>/NH<sub>3</sub> can reduce the temperature gradient in the atmosphere and reproduce the reddening previously thought to occur by clouds. The grids assume a modification of the temperature gradient with an effective adiabatic index. The levels modified are between 2 and 200 bar at log(g) = 5.0and are scaled by  $10^{\log(g)-5}$  at other surface gravities. Out-of-equilibrium chemistry is used with  $K_{zz} = 10^5 \text{ cm}^2 \text{ s}^{-1}$  at  $\log(g) = 5.0$  and is scaled by  $10^{2[5-\log(g)]}$  at other surface gravities. The mixing length is assumed to be two scale heights at 20 bar and higher pressures at log(g) = 5.0, and is scaled down by the ratio between the local pressure and the

pressure at 20 bar for lower pressures. The 20-bar limit is scaled by  $10^{\log(g)-5}$  at other surface gravities. The chemistry includes 277 species and out-of-equilibrium chemistry has been performed using a relaxation model<sup>45</sup>. Rainout is assumed to occur for species that are not included in the out-of-equilibrium model. Opacity sources include  $H_2-H_2$ ,  $H_2-He$ ,  $H_2O$ ,  $CO_2$ , CO,  $CH_4$ ,  $NH_3$ , Na, K, Li, Rb, Cs, TiO, VO, FeH,  $PH_3$ ,  $H_2S$ , HCN,  $C_2H_2$ ,  $SO_2$ , Fe, H- and the Rayleigh scattering opacities for  $H_2$ , He, CO,  $N_2$ ,  $CH_4$ ,  $NH_3$ ,  $H_2O$ ,  $CO_2$ ,  $H_2S$  and  $SO_2$ . The grids explore the following parameters: effective temperatures between 250 and 1,200 K; log(g) between 2.5 and 5.5 (step 0.5); effective adiabatic index (reddening) at a value of 1.25. A standard  $\chi^2$ -minimization procedure was used to find the best-fitting model.

petitRADTRANS, petitRADTRANS, or pRT (ref. 18, available from https://petitradtrans.readthedocs.io), is a Python package for the spectral synthesis of exoplanets and allows users to calculate transmission, emission or reflectance spectra. It offers a wide selection of opacities (gas line and continuum, and cloud opacities). Spectra can be calculated at any resolution, up to a wavelength spacing of  $\lambda/\Delta\lambda = 10^6$ .  $Coupled \ to \ a \ Bayesian \ inference \ method \ such \ as \ Py MultiNest^{46,47}, which$ petitRADTRANS provides as a pre-implemented retrieval package, posterior distributions for atmospheric parameters can be derived, given an observation. For WISE J1828, we assumed a forward model setup as described for the retrievals above, with the priors and forward model details set up as described in the following. The prior on log(g)was uniform from 2.5 to 6.0, whereas the radius prior ranged from 0.5 to 3.0 Jupiter radii. Also, the P-T profile was parameterized by retrieving temperature values at ten locations, equidistantly spaced in log-space between 10<sup>-6</sup> and 1,000 bar, and then quadratically interpolating the temperature between these nodes in log(pressure). The priors were set up such that the temperature at 1,000 bar was uniformly sampled between 100 and 9,000 K, and the temperatures at lowerpressure nodes was allowed to be between 0.2 and 1.0 times the temperature of the neighbouring deeper atmospheric node. Because kinks in the P-T profiles could be observed in the standard setup, the P-Tregularization described above was optionally turned on when deriving the atmospheric model posteriors, fitting both MIRI/MRS and the archival HST WFC3 data. Our constraints on <sup>14</sup>N/<sup>15</sup>N are not affected by the regularization. However, we observed a trend that a regularized P-T leads to a higher atmospheric metal enrichment, higher gravity log(g), smaller radii and higher effective temperatures (see Extended Data Fig. 2). For the detection of <sup>15</sup>NH<sub>3</sub>, we only used the MRS data. We also turned the regularization off to allow for maximum model flexibility. This leads to a conservative estimate of the detection significance. The following opacity species were included in the retrievals: H<sub>2</sub>O (ref. 48), CH<sub>4</sub> (ref. 49), CO (ref. 50), CO<sub>2</sub> (ref. 51), <sup>15</sup>NH<sub>3</sub> (ref. 52), H<sub>2</sub>S (ref. 53), NH<sub>3</sub> (ref. 54) and PH<sub>3</sub> (ref. 55). The abundances of said molecules were retrieved using log-uniform priors from 10<sup>-10</sup> to 1 on their mass fractions. For the 15NH3 detection, we used PyMultiNest, with 2,000 live points, constant sampling efficiency set to false and a sampling efficiency of 0.3. The detection significance of <sup>15</sup>NH<sub>3</sub> was determined using a standard method<sup>56</sup>. We report a detection significance of  $4.2\sigma$  for <sup>15</sup>NH<sub>3</sub>. For the retrievals constraining the properties of WISE J1828, which included HST as well as MRS data, we ran in constant sampling efficiency mode, with the efficiency set to 5%. This needed to be done because, otherwise, retrievals ran for 108 models but did not finish. The partially filled weighted posterior files of the 108 model retrievals were consistent with the results using the constant sampling efficiency mode. With petitRADTRANS, we found  $^{14}N/^{15}N = 560_{-115}^{+165}$  for the flexible P-T model and  $^{14}N/^{15}N = 642_{-192}^{+365}$  for the regularized P-Tmodel.

**ARCIS.** The ARtfull Modeling Code for exoplanet Science (ARCIS) is a forward modelling and retrieval code that can be used to analyse and simulate exoplanet atmosphere spectra. It contains many physical and

chemical processes, including cloud formation<sup>57</sup> and disequilibrium chemistry  $^{58}$ . The free P-T structure used in this work is parameterized by the slope at several pressure points in the atmosphere. We parameterize dlog T/dlog P with a prior range between -4/7 and +4/7. The adiabatic gradient expected for a diatomic gas is  $d^2 \log T / d \log P^2 = 2/7$ . so this prior range gives a very generous range. We fix the absolute value of the temperature structure at a pressure of P = 0.1 bar. We retrieve the value of the slope at 12 pressure points distributed equally over the atmosphere in  $\log(-P)$  space. For the detection of <sup>15</sup>NH<sub>3</sub>, we follow this procedure, allowing full flexibility and thereby constructing a conservative detection significance. For the final fits deriving the isotopic ratio and the planet parameters presented, we restrict the gradient of the P-T structure to be positive, as expected for a non-irradiated atmosphere. Following a standard approach<sup>56</sup>, we find evidence that  $^{15}NH_3$  is present in the atmosphere of WISE J1828 at  $6.3\sigma$ . We observe the same trend between metal enrichment, log(g), radii and effective temperature as petitRADTRANS when regularizing the P-T structure (see Fig. 2). However, our derived 14N/15N values are less stable when turning on regularization. Our regularized values are consistent with petitRADTRANS (regularized and flexible P-T), namely,  $^{14}\text{N}/^{15}\text{N}=591^{+432}_{-190}$  . The value derived for the flexible P--T setup is higher  $(^{14}\text{N})/^{15}\text{N}=949^{+322}_{-208})$  . More information on ARCiS can be found at http:// www.exoclouds.com.

ARCiS+ML. For the self-consistent retrieval with ARCiS, we assume a one-dimensional atmosphere in radiative-convective equilibrium. The retrievals were run on the MIRI MRS data only (that is, not including the HST data). The atmospheric composition is parameterized using [M/H], C/O and N/O and we account for disequilibrium chemistry of CH<sub>4</sub>-H<sub>2</sub>O-CO and NH<sub>3</sub>-N<sub>2</sub> owing to vertical mixing<sup>58</sup>, in which the vertical eddy diffusion coefficient  $K_{zz}$  is another free parameter. For WISE J1828, we observed that, although NH<sub>3</sub>-N<sub>2</sub> quenching was active in our models, it quenched from the lowest layer in the atmosphere, in which NH<sub>3</sub> was still the dominating absorber. Probably quenching actually occurs outside our simulated pressure domain, deeper inside the atmosphere. Therefore, the ARCiS+ML constraints may be too low for N/O, similar to the constraints from the retrievals, which are insensitive to the spectrally inactive N<sub>2</sub>. The radiative transfer module was benchmarked<sup>21</sup>. Owing to the high computational load of the self-consistent models, we cannot run nested sampling retrievals, which require millions of model evaluations to converge. Instead, we use a machine-learning method based on sequential neural posterior estimation (SNPE)<sup>59</sup> that allows us to perform the retrieval using on the order of 10<sup>4</sup> models. The details of this retrieval method will be presented in an upcoming publication (F.A.M. et al., manuscript in preparation).

Brewster. Brewster<sup>17,60</sup> is a retrieval code that has mainly been used in the context of exploring clouds in brown dwarfs. However, here, we used a simple, cloud-free retrieval recipe. Brewster uses the two-stream radiative-transfer architecture<sup>61</sup>. We use the default 64-layer atmosphere with intervals of 0.1 dex across the pressures range log P(bar) of -4 to 2.3. The temperature is set using P-T parameterization<sup>62</sup> linked to three atmospheric zones by means of exponential gradients. We included the molecules H<sub>2</sub>O, CH<sub>4</sub>, NH<sub>3</sub>, CO, PH<sub>3</sub> and H<sub>2</sub>S, which originate from a compendium  $^{63,64}$  and updated opacities  $^{17}$ . The abundances of these molecules are modelled assuming vertically constant mixing ratios, which are retrieved as free parameters. The opacities are ingested at a resolution of R = 10,000, putting the native model resolution an order of magnitude above the data being fit. Continuum opacities for H<sub>2</sub>-H<sub>2</sub> and H<sub>2</sub>-He collisionally induced absorption, Rayleigh scattering owing to H<sub>2</sub>, He and CH<sub>4</sub>, and continuum opacities owing to bound-free and free-free absorption by H- and free-free absorption by  $H_2$  are also included. We apply an error inflation 'tolerance' framework<sup>43</sup> and used in all subsequent published works using Brewster. Only the JWST/MIRI

MRS observations were retrieved with Brewster, so the HST data were not included. Here we used the emcee<sup>65</sup> as our sampling algorithm. As we used the standard retrieval recipe for this code, an extensive list of parameter sampling priors has been used<sup>60</sup>.

#### Combining model results

Whenever we report values for the properties of WISE J1828 in the main body of the text, these have been obtained from combining the posteriors of the retrievals at equal weight and calculating the corresponding median and 16th–84th percentile values, corresponding to the  $1\sigma$  credible interval in the case that the resulting distribution is approximately Gaussian. The combined value of the self-consistent codes was obtained by taking the average of their best-fit (ATMO) and median (ARCiS+ML) values, whereas the uncertainty is obtained from calculating the difference d between these two values and then calculating  $\sqrt{d^2+a^2}$ , in which a is the ' $1\sigma$ ' uncertainty obtained from the ARCiS+ML posterior.

#### Exploring 14N/15N as a formation tracer

To approximate the impact of volatile ice accretion between the NH<sub>3</sub> and N<sub>2</sub> icelines in a protoplanetary disk, we generated a simplified planet-formation model for calculating  $^{14}\text{N}/^{15}\text{N}$  as a function of the total solid mass (rock and ices) a planet incorporated during formation. For this, we used a specific framework<sup>4</sup>, which is available at https:// gitlab.com/mauricemolli/formation-inversion. In short, we used a solar disk composition (Table 2 in ref. 4). This means that the mass ratio between NH<sub>3</sub> and N<sub>2</sub> is 1:7 in the disk (combining gas and ice reservoirs). We then assumed, conservatively, that <sup>14</sup>N/<sup>15</sup>N is reduced by a factor of 2 in NH<sub>3</sub> when compared with the total <sup>14</sup>N/<sup>15</sup>N value, whereas the total <sup>14</sup>N/<sup>15</sup>N (summing over all species and phases) is conserved, which we assumed to be 300, and call the ISM value in Extended Data Fig. 4. This figure shows the ratio of the planetary and ISM values of <sup>14</sup>N/<sup>15</sup>N as a function of solids accreted by a planet between the NH<sub>3</sub> and N<sub>2</sub> icelines. Because the solids are rich in NH<sub>3</sub> and N<sub>2</sub> is only in the gas phase, a higher accreted solid mass results in a lower planetary <sup>14</sup>N/<sup>15</sup>N. We note that the picture could be more complicated, as the disk gas could be enriched in <sup>15</sup>N-poor N<sub>2</sub> gas that evaporated off pebbles that drift in from outside the N<sub>2</sub> iceline<sup>66</sup>.

#### Inclusion and ethics

All authors have committed to upholding the principles of research ethics and inclusion as advocated by the Nature Portfolio journals.

#### **Data availability**

The JWST MIRI data presented in this paper are part of the JWST MIRI GTO programme (programme identifier (PID) 1189; PIT. Roellig). The JWST data will be publicly available in the Barbara A. Mikulski Archive for Space Telescopes (MAST; https://archive.stsci.edu/) after 28 July 2023 and can be found either using the programme identifier or using the https://doi.org/10.17909/as3s-x893. The HST WFC3 spectrum is available from https://cdsarc.cds.unistra.fr/viz-bin/cat/J/ApJ/920/20#/ article.

#### **Code availability**

The code used in this publication to extract, reduce and analyse the data is as follows: the data-reduction pipeline of JWST can be found at https://jwst-pipeline.readthedocs.io/en/latest/; the atmospheric model codes used to fit the data can be found at https://www.exoclouds.com/for the ARCiS code<sup>19</sup> and at https://petitradtrans.readthedocs.io/en/latest/for the petitRADTRANS code<sup>18</sup>. The simplified planet-formation model<sup>4</sup> used to study <sup>14</sup>N/<sup>15</sup>N as a function of accreted ice mass can be found at https://gitlab.com/mauricemolli/formation-inversion. The detailed setups of the open-source tools for the analyses presented

here are described in the Methods section of this paper and can be made available to interested parties on request.

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Author contributions All authors played a substantial role in one or more of the following: designing and building the MIRI, development of the original proposal, management of the project, definition of the target list and observation plan, analysis of the data, theoretical modelling and preparation of this paper. Some specific contributions are listed as follows. P.-O.L. is PI of the JWST MIRI GTO European consortium programme dedicated to JWST observations of exoplanet atmospheres. D.B., P.M. and P.P. provided overall programme leadership and management of the WISE J1828 working group. P.-O.L., T.H., R.W., (co-lead of the JWST MIRI GTO European consortium), D.B. and M.Mu. made notable contributions to the design of the observational programme and contributed to the setting of the observing parameters PP\_LA and MS\_reduced the data\_PT\_generated theoretical model grids for comparison with the data, P.M., M.Mi, and N.W. fitted the generated spectrum with retrieval models and M.V. also contributed. F.A.M. applied the radiative-convective equilibrium retrieval to the spectrum. D.B., P.M. and P.P. led the writing of the manuscript. P.-O.L. and L.D. made notable contributions to the writing of this paper. Further contributions were provided by M.M.-C. and L.D. P.B., A.B., J.B., C.C., A.C., N.C., R.G., A.G., A.M.G., S.K., F.L., D.R., P.R., S.S. and I.W. contributed to instrument construction, the programme design and/or the data analysis. P.M., P.P. and D.B. generated the figures for this paper. G.W. is PI of the JWST MIRI instrument, P.-O.L., T.H., M.G., B.V., L.C., E.F.v.D., T.R. and G.Ö. are co-PIs and L.D., R.W., O.A., I.K., O.K., J.P., G.O. and D.B. are co-investigators of the JWST MIRI instrument.

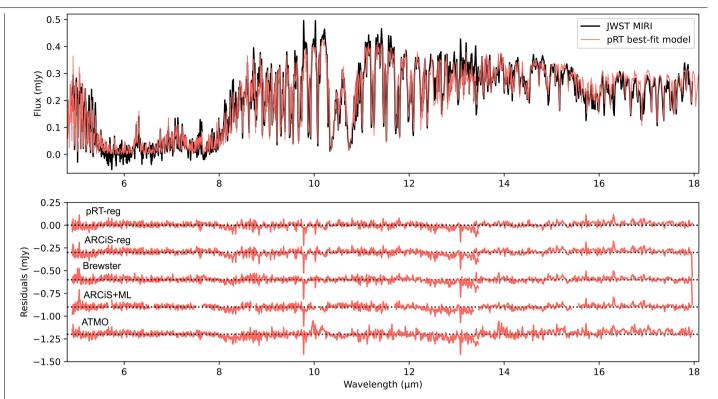
Competing interests The authors declare no competing interests.

#### Additional information

**Supplementary information** The online version contains supplementary material available at https://doi.org/10.1038/s41586-023-06813-y.

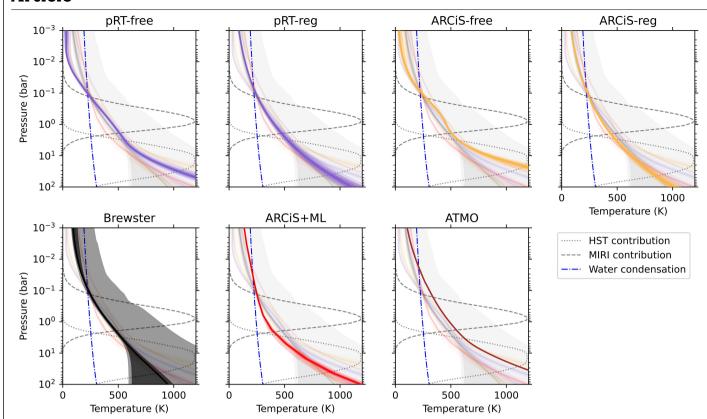
**Correspondence and requests for materials** should be addressed to David Barrado. **Peer review information** *Nature* thanks the anonymous reviewers for their contribution to the peer review of this work. Peer reviewer reports are available.

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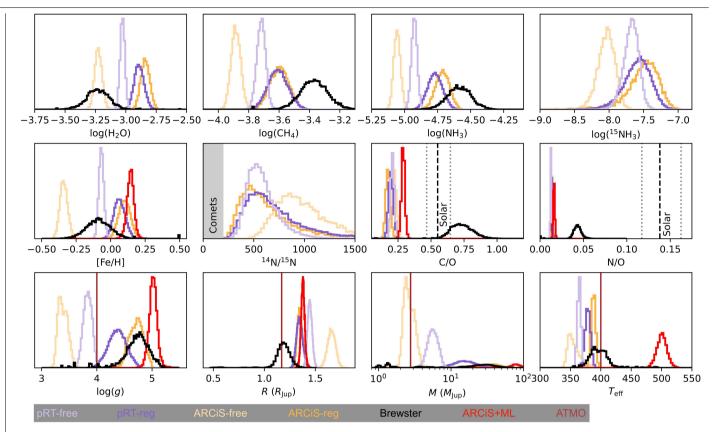
**Extended Data Fig. 1** | **The spectrum of WISE J1828 and the best-fit model.** We show the MIRI/MRS spectrum of WISE J1828 (black solid lines) and the best-fit model of the regularized P-T retrieval of petitRADTRANS (red line).

Residuals (models-observed spectrum) are shown in the bottom panel. pRT-reg and ARCiS-reg stand for the regularized P-T retrieval of petitRADTRANS and ARCiS, respectively.



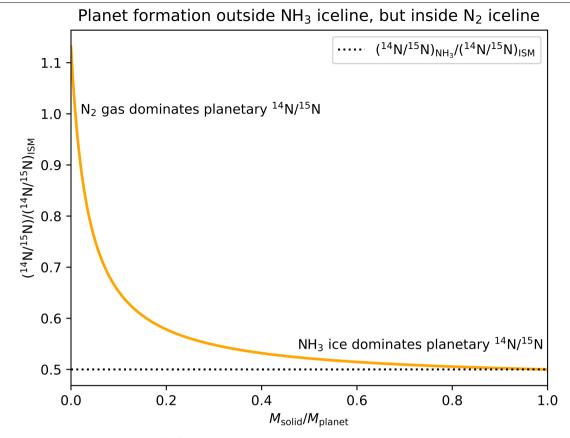
**Extended Data Fig. 2** | **Model inferences on the various** P-T **profiles derived for WISE J1828.** The individual panels always highlight the constraint from one given model, whereas the results of the other models are shown in the background. pRT-reg and ARCiS-reg stand for the regularized P-T retrievals, whereas pRT-free and ARCiS-free stand for the unregularized P-T retrievals of petitRADTRANS and ARCiS, respectively. The contribution functions of the

HST and MIRI observations, constrained from the best-fit pRT-reg model, are shown as dotted and dashed lines, respectively. The condensation curve for water (at solar metallicity) is shown as a blue dash-dotted curve, indicating that, although neglected in our models, water clouds could affect the spectrum in a modest away.



 $\label{lem:projection} \textbf{Extended Data Fig. 3} \ | \ \textbf{One-dimensional projection of the posterior} \\ \textbf{distributions of the WISE J1828 retrievals.} \ \ \text{Values correspond to key} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg} \\ \textbf{atmospheric quantities shown in Extended Data Table 1. pRT-reg and ARCiS-reg and AR$ 

stand for the regularized P-T retrievals, whereas pRT-free and ARCiS-free stand for the unregularized P-T retrievals of petitRADTRANS and ARCiS, respectively.



Extended Data Fig. 4 | Evolution of the planetary  $^{14}N/^{15}N$  as a function of the mass accreted in solids (rock and ice). This computation assumes a planet that forms outside the NH<sub>3</sub> iceline but inside the N<sub>2</sub> iceline. The dotted black line denotes the value expected for pure NH<sub>3</sub> ice.

#### Extended Data Table 1 | Physical constraints on WISE J1828

	Retrieval codes					Self-consistent codes	
Quantity	pRT-free	pRT-reg	ARCiS-free	ARCiS-reg	Brewster	ARCiS+ML	ATMO
$T_{\rm eff}$ (K)	$364^{+3}_{-3}$	$379^{+4}_{-4}$	$354^{+13}_{-7}$	$388^{+3}_{-4}$	$397^{+16}_{-14}$	501_8	400
$\log(g)$	$3.83^{+0.08}_{-0.08}$	$4.37^{+0.16}_{-0.17}$	$3.38^{+0.1}_{-0.08}$	$4.72^{+0.12}_{-0.14}$	$4.74^{+0.19}_{-0.21}$	$5.02^{+0.07}_{-0.07}$	4.0
$R\left(\mathrm{R_{Jup}}\right)$	$1.45^{+0.02}_{-0.02}$	$1.35^{+0.03}_{-0.03}$	$1.65^{+0.04}_{-0.04}$	$1.35^{+0.03}_{-0.03}$	$1.19^{+0.06}_{-0.06}$	$1.38^{+0.02}_{-0.02}$	1.17
$M \left( \mathrm{M_{Jup}} \right)$	$5.76^{+1.04}_{-0.89}$	$17.27^{+6.86}_{-5.01}$	$2.69^{+0.58}_{-0.40}$	$38.57^{+10.92}_{-9.66}$	$31.50^{+14.30}_{-11.60}$	$79.99^{+12.79}_{-10.87}$	2.76
$R_{\rm bin} \left( { m R_{Jup}} \right)$	$1.02^{+0.02}_{-0.02}$	$0.95^{+0.02}_{-0.02}$	$1.17^{+0.03}_{-0.03}$	$0.95^{+0.02}_{-0.02}$	$0.84^{+0.04}_{-0.04}$	$0.98^{+0.01}_{-0.01}$	0.83
$M_{ m bin}$ (M <sub>Jup</sub> )	$2.88^{+0.52}_{-0.45}$	$8.63^{+3.43}_{-2.51}$	$1.34_{-0.2}^{+0.29}$	$19.29^{+5.46}_{-4.83}$	$15.75_{-5.8}^{+7.15}$	$39.99^{+6.4}_{-5.43}$	1.38
${[M/H]}$	$-0.07^{+0.02}_{-0.02}$	$0.06^{+0.04}_{-0.04}$	$-0.34^{+0.03}_{-0.03}$	$0.10^{+0.04}_{-0.04}$	$-0.08^{+0.10}_{-0.09}$	$0.14^{+0.02}_{-0.03}$	solar
C/O	$0.21^{+0.01}_{-0.01}$	$0.20^{+0.02}_{-0.02}$	$0.22^{+0.02}_{-0.02}$	$0.17^{+0.02}_{-0.02}$	$0.73^{+0.08}_{-0.10}$	$0.29^{+0.01}_{-0.01}$	solar
(N/O) /	$0.091^{+0.004}_{-0.004}$	$0.096^{+0.006}_{-0.006}$	$0.107^{+0.006}_{-0.006}$	$0.097^{+0.006}_{-0.006}$	$0.314^{+0.036}_{-0.032}$	$0.117^{+0.006}_{-0.007}$	solar
(N/O) <sub>⊙</sub>							
$^{14}{ m N}/^{15}{ m N}$	$560^{+165}_{-115}$	$642^{+365}_{-192}$	$949^{+322}_{-208}$	$591^{+432}_{-190}$	_	_	_
$\log(H_2O)$	$-3.03^{+0.02}_{-0.02}$	$-2.89^{+0.04}_{-0.04}$	$-3.23^{+0.03}_{-0.03}$	$-2.84^{+0.04}_{-0.04}$	$-3.23^{+0.10}_{-0.10}$	chem	chem
log(CH <sub>4</sub> )	$-3.72^{+0.03}_{-0.03}$	$-3.61^{+0.07}_{-0.06}$	$-3.88^{+0.03}_{-0.03}$	$-3.60^{+0.06}_{-0.06}$	$-3.36^{+0.10}_{-0.09}$	chem	chem
$log(NH_3)$	$-4.93^{+0.02}_{-0.02}$	$-4.77^{+0.06}_{-0.06}$	$-5.06^{+0.03}_{-0.02}$	$-4.71^{+0.05}_{-0.05}$	$-4.58^{+0.10}_{-0.10}$	chem	chem
$\log(^{15}NH_3)$	$-7.67^{+0.10}_{-0.11}$	$-7.58^{+0.17}_{-0.21}$	$-8.03^{+0.11}_{-0.13}$	$-7.49^{+0.18}_{-0.25}$	_	_	_
$\log(K_{\rm zz})$	_	_	_	_	_	$9.01^{+0.19}_{-0.19}$	7

'free' in the code name means that the P-T structure was not regularized, whereas this was done for the 'reg' cases.  $R_{bin}$  model radii have been multiplied by  $1/\sqrt{2}$ , assuming that WISE J1828 is an equal-property binary.  $R_{bin}$  was used for calculating  $M_{bin}$  from the inferred gravity. The units of  $K_{zz}$  are cm² s¹. 'chem' means that absorber abundances have been determined from a chemical model. 'solar' means that the parameter was not varied and that a solar composition was assumed instead.

## Extended Data Table 2 | Physical constraints on WISE J1828, combining different codes

Quantity	Retrievals	Self-consistent codes		
$\overline{T_{\rm eff}}$ (K)	$378_{-18}^{+13} \\ 4.34_{-0.88}^{+0.42}$	$450 \pm 101$		
$\log(g)$	$4.34_{-0.88}^{+0.42}$	$4.5 \pm 1.0$		
$R\left(\mathrm{R_{Jup}}\right)$	$1.37^{+0.26}_{-0.13}$	$1.27 \pm 0.21$		
$M  (\mathrm{M_{Jup}})$	$15.8^{+22.82}_{-12.64}$	41*		
$R_{\rm bin} \left( {\rm R_{Jup}} \right)$	$0.97^{+0.18}_{-0.09}$	$0.90 \pm 0.15$		
$M_{\rm bin}$ (M <sub>Jup</sub> )	$7.91_{-6.34}^{+11.33}$	21*		
$\overline{\mathrm{[M/H]}}$	$-0.05^{+0.15}_{-0.27}$	no comb		
C/O	$0.21^{+0.45}_{-0.03}$	no comb		
(N/O) /	$0.10^{+0.19}_{-0.01}$	no comb		
$(N/O)_{\odot}$				
$^{14}{ m N}/^{15}{ m N}$	$673^{+393}_{-212}$	_		
$log(H_2O)$	$-3.03^{+0.18}_{-0.21}$	chem		
$log(CH_4)$	$-3.65^{+0.21}_{-0.21}$	chem		
$log(NH_3)$	$-4.79_{-0.25}^{+0.15}$	chem		
$\log(^{15}\mathrm{NH_3})$	$-7.68^{+0.24}_{-0.34}$			
$log(K_{zz})$	_	$8 \pm 2$		

 $R_{\rm bin}$  model radii have been multiplied by  $1/\sqrt{2}$ , assuming that WISEJ1828 is an equal-property binary.  $R_{\rm bin}$  was used for calculating  $M_{\rm bin}$  from the inferred gravity. The units of  $K_{zz}$  are cm² s¹. 'chem' means that absorber abundances have been determined from a chemical model. 'no comb' means that the respective parameter was only varied in one of the two codes; see Extended Data Table 1 for the inferred values. \* for the inferred average mass denotes that the distance between the solutions of the two codes was larger than the average value, so no uncertainties, derived as explained in the Methods section, are given here.