

A spectroscopist's view of the evolving story of exoplanet K2-18 b

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K2-18 b is the only habitable-zone exoplanet with a detectable atmosphere – initially associated with water vapour, now accepted as being due to methane. Recent observations suggest possible biomarkers. This Comment assesses these shifting conclusions.

K2-18 is an unremarkable, red dwarf star with a temperature of about 3,650 K; there are many such stars in our Galaxy. What makes K2-18 interesting is that it supports a transiting planetary system. Its nearest planet, K2-18 b, orbits in the 'habitable zone' where its temperature is compatible with the state of liquid water. Furthermore, because K2-18 is cooler than our Sun, the habitable zone is much closer to the star and its year is approximately one month, allowing multiple transits to be observed in a single (Earth) year.

The intense interest in exoplanet K2-18 b started in 2019 with observations obtained using the Hubble Space Telescope (HST), which showed the clear signature of an atmosphere. Independent analyses of that spectrum^{1,2} both concluded that the observations indicated a signature due to water, although this signature was compatible with several very different atmospheric compositions. This finding attracted considerable media attention. However, this conclusion was challenged on the basis of an alternative planetary model, which asserted that the observed feature in the spectrum was likely due to methane³. These HST observations were performed in a relatively small window (1.1–1.6 μm) in the near infrared with limited resolution. Figure 1a (from Bézard et al.⁴) illustrates the strong degeneracy of the water and methane spectra represented by only 17 spectral points. This degeneracy indicated the need for better quality data (higher resolution) or at least more observations in a different spectral region.

The launch of the James Webb Space Telescope (JWST) opened the mid-infrared wavelength window – a more promising one for detecting molecular signatures. Observations of K2-18 b using its NIRISS and NIRSpec instruments in the 0.9–5.2 μm range⁵ revealed a carbon-rich atmosphere containing strong detections of methane plus a clear carbon dioxide feature. These observations strongly confirm the conclusions of Bézard et al.⁴ and would therefore appear to settle the issue.

Moreover, the extended spectroscopic coverage and better resolution allowed our focus to expand beyond the main absorbers and to question the planetary formation and constitution of K2-18 b. Based on their observations, Madhusudhan et al.⁵ also detected small features in the 3–3.5 μm range, which were not reproduced by their base planetary model. They associated these features with the complex molecules dimethyl sulphide ((CH_3)₂S or DMS) and methyl chloride (CH_3Cl), while noting that many species have strong spectral features associated with

the widespread C–H stretching excitation. DMS and CH_3Cl had previously been identified as possible signatures of life (biomarkers)⁶. But the weakness of the detection meant that this was generally regarded as extremely speculative.

Earlier this year Madhusudhan et al.⁷ reported further JWST observations using the MIRI LRS instrument to study the spectrum of K2-18 b in the longer, 6–12 μm , wavelength range. These results came from observation of only a single transit and, as the star K2-18 is extremely faint, required considerable binning down (aggregation of data with loss of wavelength resolution) to achieve a spectroscopic signature. Generally, the errors of the MIRI LRS observations are larger than those of NIRISS and NIRSpec instruments on JWST. Madhusudhan et al. interpret their new observations as confirmation of the presence of DMS and the weak detection of the even more complex species dimethyl disulphide ((CH_3)₂S₂ or DMDS). We note that these still rather tentative detections would imply that very considerable quantities of both species are present in the atmosphere of K2-18 b. While the paper itself only makes mild claims about these species indicating signs of life, the associated press releases and resulting press coverage have been much bolder.

The strong focus on a very small subset of the possibly observable molecules whose possible presence does not seem to be based on any objective assessment of the possible chemistry of the exoplanet is very problematic. There are available libraries of observed or calculated infrared spectra of many small molecules that might be important in exoplanetary atmospheres. Thus, for example, Seager et al.⁸ list 59 hydrocarbons that give features similar to the DMS/DMDS combination in models of K2-18 b; indeed four of these hydrocarbons reproduce the observations marginally better than the DMS/DMDS fit. However, these features are extremely unlikely to belong to a single species, be it a hydrocarbon or sulfur-containing molecule, but probably arise from some mixture.

As a response to this point an extensive atmospheric retrieval study of the MIRI spectrum of K2-18 b using a set of 21 species, primarily hydrocarbons, concluded that neither DMS nor DMDS are needed to explain the spectral features in the MIRI spectrum of K2-18 b⁹. But in a more recent study, Pica-Ciamarra, Madhusudhan et al.¹⁰ performed an even more extensive systematic search for trace molecules in K2-18 b; over 650 (mainly complex) species were included in their analysis. Their results reinforced their initial conclusion of DMS and DMDS being among the most promising candidates and suggested methyl acrylonitrile with comparable detection significance. Again, this work seems to focus on the idea that the signal can be associated with a small number (one or two) of species; an assumption for which no justification is offered. A second important issue is that these analyses did not connect the two spectral regions of JWST, MIRI (mid-IR) and NIRISS/NIRSpec (near-IR), into a single retrieval, thus missing out on the obvious potential of resolving degeneracies. When these two observations are combined into a single retrieval¹¹ (Fig. 1b),

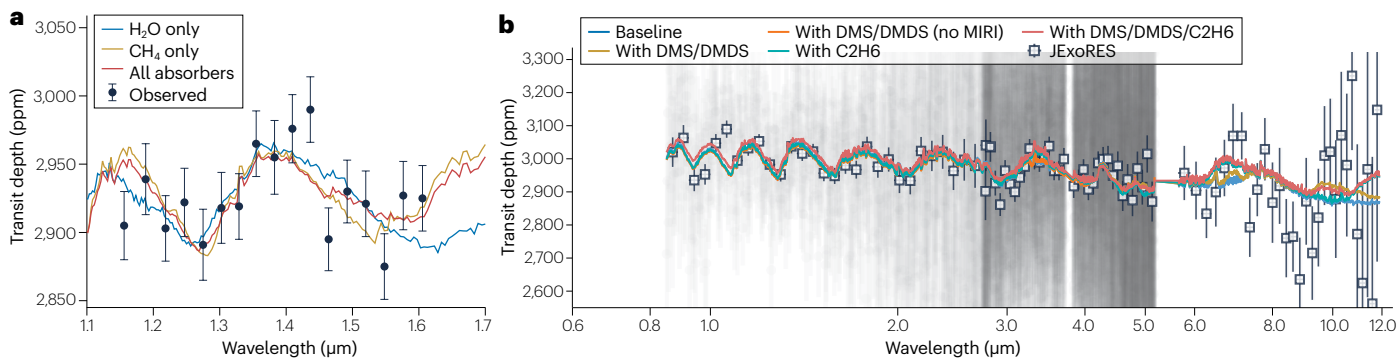


Fig. 1 | Transmission spectra of K2-18 b. **a**, Original K2-18 b HST observations (solid circles²) superimposed on simulations of spectra from water and methane,⁴ illustrating the strong degeneracy of these two alternative compositions of the atmosphere. Adapted from ref. 3, Springer Nature Limited. **b**, Combined analysis of the MIRI and NIRSISS/NIRSpec transmission spectra of

K2-18 b (open squares^{5,7}) with best-fit models of baseline (blue), DMS and DMDS (orange), C₂H₆ (a common hydrocarbon, green), DMS and DMDS without MIRI data (red), and baseline with DMS, DMDS and C₂H₆ (pink). This panchromatic analysis shows no evidence for DMS or DMDS. Adapted from ref. 11, CC BY 4.0.

the more comprehensive analysis strongly contradicts the claimed detections of DMS and DMDS.

All scientists involved in these studies agree on the need for better observational data. A major issue is that observations of transiting exoplanets spectra require special observational capabilities, yet the Spitzer and Hubble Space Telescopes were both launched before the first exoplanet was even discovered! Similarly, the newer JWST, while providing fascinating insights into exoplanetary atmospheres (and much else), was designed prior to the discovery of exoplanets. This means that answers to many of the questions discussed above will simply have to wait for observational facilities to catch up with scientific aspirations.

The scientists also all agree on the need for better laboratory data. Indeed, both the suggested detections of DMS/DMDS or the possible hydrocarbon scenarios were based on the experimental (transmittance) spectra available at three temperatures only (5, 25 and 50° C) as recorded by the Pacific Northwest National Laboratory¹² and currently provided by HITRAN, with no variation in pressure. With such limitations of the laboratory data, proper radiative transfer simulations with altitude variations of temperature and therefore compositions of the species involved are challenging.

Another important question that arises from observational studies in exoplanetary science concerns detection confidence. The original detection of water in K2-18 b, which we now know is not there, was reported with a significance of 3.6 σ (ref. 1) and 3.93 σ (ref. 2). In medical research it is no longer acceptable to ascribe significance to a statistical correlation without some underlying causal relationship. Similarly for exoplanets, chemical models should be linked to assumptions used to interpret observations. Much of the observational work cited above has treated the problem as one of simple spectral fitting. Unless the resolution of the underlying spectroscopic data improves by several orders of magnitude, the degeneracy inherent in these spectra means that this approach will remain fraught with the danger of drawing false conclusions.

The question of when a retrieval becomes a detection is an actively developing subject. It has been proposed that a secure ‘detection’ should correspond to a Bayes factor of 600 or higher,¹³ which corresponds to an odds ratio of 99.8% – close to what a 3 σ result traditionally signifies. Bayes factors $B < 3$ is ‘no evidence’ (as for the 20 molecule analysis⁷), ‘weak evidence’ corresponds to Bayes factor $3 < B < 12$

(as for the two molecule analysis⁷), ‘moderate’ to $12 < B < 150$, and ‘strong’ to $150 < B < 600$.

Regardless of the heated debate, it is very exciting that JWST has started to probe the atmospheres of temperate exoplanets. The spectrum of K2-18 b has shown itself to be open to multiple interpretations, but as a community we are witnessing the formation of a scientific consensus in real time.

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Published online: 16 July 2025

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Competing interests

The authors declare no competing interests.