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Letter to the Editor

Ammonia-methane ratios from *H*-band near-infrared spectra of late-T and Y dwarfs

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ABSTRACT

Aims. Our goals are to investigate the relative absorption strengths of ammonia and methane using low-resolution *H*-band (1.5−1.7 microns) spectra obtained in the laboratory and compared with observational spectra of late-T and Y dwarfs, and to estimate what can be expected from the wide-angle low-resolution near-infrared spectroscopic survey that will be provided by the upcoming *Euclid* space mission.

Methods. Gas cells containing ammonia and methane at atmospheric pressure were custom-made in our chemical laboratory. Low-resolution near-infrared spectroscopy of these gas cells was collected in our optical laboratory. It is compared with simulated spectra using the high-resolution transmission molecular absorption database (HITRAN) for temperatures of 300 K and 500 K, and with near-infrared spectra of late-T dwarfs, Y dwarfs, Jupiter, and Saturn. We selected for this investigation the spectral region between 1.5 and 1.7 microns (*H* band) because it is covered by the *Euclid* red grism, it is particularly sensitive to the relative proportions of ammonia and methane opacity, and it is free from strong contributions of other abundant molecules, such as water vapor.

Results. The laboratory spectra showed that the ammonia and methane features present in the simulations that used the HITRAN database are incomplete. Using our laboratory spectra, we propose a modified version of the NH3-H spectral ratio with expanded integration limits that increases the amplitude of variation in the index with respect to spectral type. Combinations of our laboratory spectra were used to find the best fits to the observed spectra with the relative absorption ratio of ammonia to methane as a free parameter. A relationship was found between the $T_{\rm eff}$ and the ratio of ammonia to methane from spectral classes T5 to Y2 (1100 K–350 K), in fairly good qualitative agreement with theoretical predictions for high-gravity objects and temperatures from 1100 K to 500 K. The ammonia-to-methane ratios in late-T and Y dwarfs are similar to that of Jupiter, suggesting a similar chemical composition. Simulations of the spectroscopic performance of *Euclid* suggest that it will yield $T_{\rm eff}$ values and ratios of ammonia to methane for over 10^3 late-T dwarfs in the entire wide survey.

Key words. molecular processes – methods: laboratory: molecular – techniques: spectroscopic – brown dwarfs – stars: abundances

1. Introduction

Brown dwarfs (BDs) do not stabilize on the hydrogen (H) burning main sequence, and hence they keep cooling down to very low temperatures. The coolest BDs have been spectroscopically classified as T dwarfs and Y dwarfs, based on the presence of methane and ammonia in near-infrared spectra, respectively (Burgasser et al. 2002; Delorme et al. 2008; Cushing et al. 2011), although the presence of ammonia has been established not only in Y dwarfs but also in late-T dwarfs (Bochanski et al. 2011; Canty et al. 2015).

The Wide Field Infrared Survey Explorer (WISE; Wright et al. 2010) has been very effective in discovering Y dwarfs and low-resolution spectroscopic follow-up has been carried out from the ground and from space. In particular, homogeneous sets of low-resolution near-infrared spectra have been collected with the Keck Near Infrared Spectrometer (NIRSPEC) and with the *Hubble* Space Telescope (HST) for late-T and Y dwarfs down to spectral class Y2 (McLean et al. 2003; Schneider et al. 2015; Cushing et al. 2021).

Estimates of the effective temperature ($T_{\rm eff}$) of Y dwarfs are difficult because theoretical fits to their spectral energy distribution are of modest quality, which indicates that the chemistry calculations and/or the sources of opacity may be incomplete. Furthermore, values estimated from their luminosity and assumed radii using the Stefan-Boltzmann law are hampered by uncertainties due to possible effects of unresolved binarity (Leggett et al. 2013; Luhman & Esplin 2016).

The appearance of ammonia in the near-infrared spectra of ultra-cool dwarfs has been discussed by several authors (Saumon et al. 2000; Leggett et al. 2007; Warren et al. 2007; Bochanski et al. 2011; Burgasser et al. 2012; Canty et al. 2015). A spectral index named NH3-H was defined by Delorme et al. (2008) to quantify the effects of ammonia absorption from 1.53 to

1.56 microns. Their NH3-H index has been adopted for spectral type quantification for dwarfs of classes T5 to Y2 (Cushing et al. 2021).

The upcoming *Euclid*[1] space mission is expected to provide the next order of magnitude leap in the numbers of detected ultra-cool dwarfs. By the end of its six-year nominal mission, the *Euclid* wide survey is expected to reach 15 000 square degrees of the extragalactic sky observed at a single epoch, and the *Euclid* deep surveys are expected to cover between 40 and 50 square degrees at multiple epochs. The Near Infrared Spectrometer and Photometer (NISP) is a two-channel instrument for the *Euclid* space mission. The photometric channel is equipped with three broadband filters, and the spectroscopic channel is equipped with three identical low-resolution grisms that cover the spectral range from 1250 nm to 1850 nm with a spectral resolving power of $R = 380$ as well as one grism that covers the spectral range from 920 nm to 1250 nm. This last grism is expected to be used only for the *Euclid* deep fields and not for the wide survey. The spectroscopic observations will be made in survey mode without any slit. The NISP field of view is 0.53 square degrees covered with a matrix of 4×4 Teledyne detectors, each of them with 2040×2040 18-micron pixels with a scale of 0.3 arcsec per pixel.

Updated simulations of the number counts of ultra-cool dwarfs in the *Euclid* wide survey using the most recent information on the photometric passbands were provided in Solano et al. (2021). In this Letter we provide updated simulations for the number of T and Y dwarfs expected to be detected with the NISP spectroscopic mode in the *Euclid* wide survey. We show that *Euclid* will provide useful low-resolution *H*-band spectra for an unprecedentedly large number of T dwarfs ($\geq 10^3$ for T5–T8 subclasses). Consequently, it is important to investigate efficient methods for deriving $T_{\rm eff}$ values for T dwarfs using NISP spectra. Our first goal is to confirm that the NH3-H spectral index is really an indicator of the absorption of ammonia in late-T and Y dwarfs, and to adjust its integration limits using our laboratory spectra. Our second goal is the determination of the ammonia-to-methane ratio as a probe of the atmospheres of ultra-cool dwarfs using low-resolution *H*-band spectra.

This Letter presents laboratory spectra of gas cells filled with ammonia and methane, which were made with the aim of helping with the identification of these molecules in the atmospheres of ultra-cool dwarfs. The rest of the paper is organized as follows: Sect. 2 describes the experimental setup for the laboratory measurements. Section 3 compares the laboratory spectra with simulated spectra using the high-resolution transmission molecular absorption database HITRAN and redefines the NH3-H index. Section 4 compares the laboratory spectra with observed near-infrared spectra from the Infrared Telescope Facility (IRTF), *Hubble*, and Keck for dwarfs with spectral types from T5 to Y2 as well as for Jupiter and Saturn. Ammonia-to-methane ratios are derived using a best matching algorithm on the laboratory and the observed spectra. Section 5 summarizes our results and their implications.

2. Low-resolution laboratory spectra

Custom-made gas cells were created to fit into the spectrophotometer Cary 5000 located at the optical laboratory of the Instituto de Astrofísica de Canarias (IAC). They are G2 Infrasil cells from International Crystal Lab, 13 cm long and with a window size 38 mm in diameter and 6 mm thick.

The cells were filled with different molecular gases using a vacuum pump system in our laboratory located in the chemistry department of the Universidad de La Laguna. The procedure for filling the cells with gas is described in more detail in Valdivielso et al. (2010). The gas cells with ammonia (NH3), argon (Ar), and methane (CH4) were completely filled with each of those gases at the atmospheric pressure.

The gas cells were taken to the IAC and were left to settle to the ambient conditions inside the Cary 5000 for at least five hours before the measurements were taken. The Cary 5000 has two channels, which allows for two gas cells to be measured simultaneously. In one channel we placed a gas cell filled with ammonia or methane, and in the other channel we placed an identical gas cell filled with Ar so that the instrumental response would be corrected by the instrument's software.

The laboratory spectra of all the gas cells were taken on July 8 and 9, 2021, with an integration time of 0.2 s for each step of 0.5 nm. The total time to measure a spectrum from 800 nm to 3000 nm was 6.3 h. The ambient conditions in the laboratory were a temperature of 298 K and a humidity level of 57%.

3. Comparison between laboratory and simulated spectra

Our laboratory spectra for ammonia and methane were compared with simulated spectra for the same molecules using the HITRAN database (Gordon et al. 2017) for temperatures of 300 K and 500 K. The comparisons in the full spectral range from 1.0 to 2.5 microns are shown in Fig. 1. The agreement between 2.0 and 2.5 microns is quite good, but the differences increase toward shorter wavelengths. This is not a surprise because it had previously been reported that HITRAN is very incomplete for hot bands and high-J molecular transitions (Bailey & Kedziora-Chudczer 2012; Wong et al. 2019).

We used our laboratory spectrum of ammonia to propose a redefinition of the integration limits for the spectral index NH3-H, which was originally defined using HITRAN opacity data (Delorme et al. 2008). These authors used as numerator the spectral region from 1.53 to 1.56 microns, and as denominator the region from 1.57 to 1.60 microns. Based on the appearance of the ammonia band in our laboratory spectra, we propose redefining the NH3-H index using as numerator the region from 1.50 to 1.57 microns, and as denominator the region from 1.57 to 1.61 microns. These integration limits are shown in the bottom part of Fig. 1. They sample a region dominated by the ammonia absorption and not by methane.

The increased wavelength range chosen for our proposed modification of the NH3-H spectral index was motivated by a desire to better understand the ammonia absorption in this region, and it has the advantage of increasing the flux collected in each passband for the classification of ultra-faint objects of T and Y type detectable with NISP. The comparison between the previous NH3-H index and ours of dwarfs from spectral type T5 to Y2 is shown in Fig. 2.

4. Comparison between laboratory and HST spectra

Different combinations of the relative strengths of ammonia and methane were computed using our laboratory spectra. An example of the typical combination that provides the best fit is shown in Fig. 3 together with HST spectra of a T8 dwarf and two Y dwarfs (Schneider et al. 2016; Cushing et al. 2014). This combination, denoted with a blue line, corresponds to the case where

[1] http://sci.esa.int/euclid/

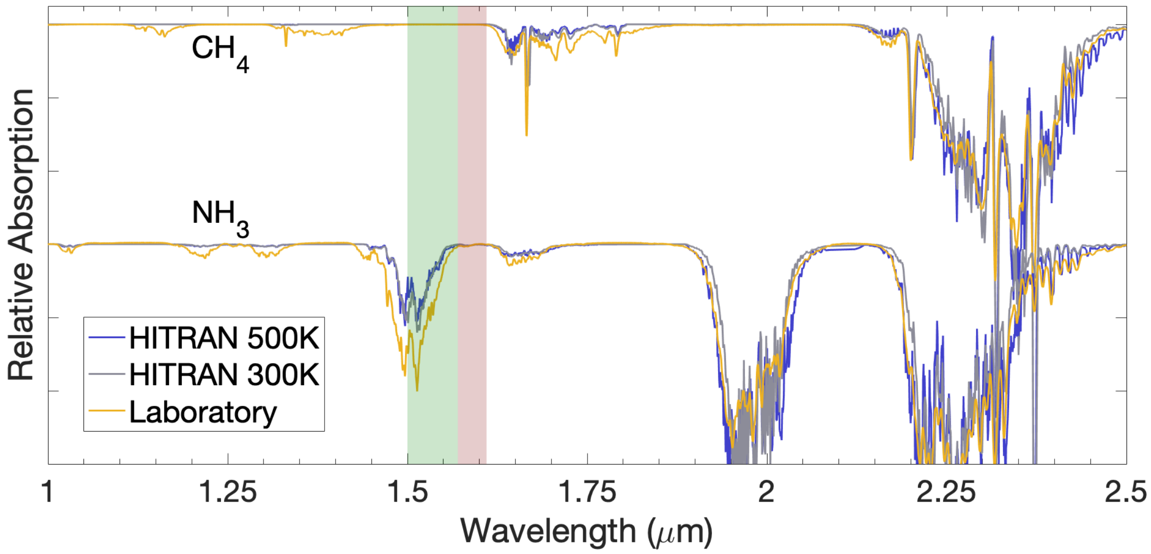

Fig. 1. Our laboratory spectrum for ammonia and methane compared to simulated spectra of the same molecules using HITRAN for temperatures of 500 K and 300 K. The wavelength regions proposed for the new NH3-H index are marked with color bands: green for the numerator, red for the denominator.

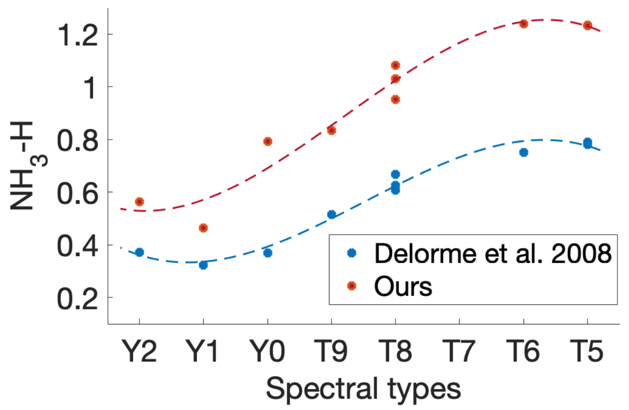

Fig. 2. Redefined NH3-H index using our laboratory spectra. It has a higher sensitivity to spectral class (larger amplitude of variation) than the original definition by Delorme et al. (2008) based on HITRAN data. Third-order polynomial fits to the relationship between the indices and the spectral types are denoted with dashed lines of different colors, as labeled.

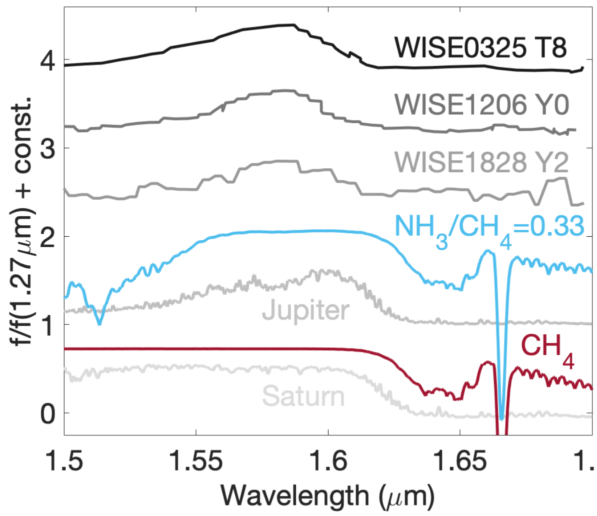

Fig. 3. Our laboratory spectra for a combination of ammonia and methane (blue) and for pure methane (red), compared to HST spectra of a T8 dwarf and two Y dwarfs, and IRTF spectra of two giant gas planets.

we scaled our laboratory spectrum of ammonia by a factor of 0.33 and added it to our laboratory spectrum of methane.

The spectral region from 1.5 to 1.7 microns is particularly sensitive to the effects of changing the relative contribution of ammonia with respect to methane. Furthermore, this spectral region is thought to be free from a significant contribution of other molecules, such as water vapor (Delorme et al. 2008; Canty et al. 2015).

A least square fit and a confidence interval estimate were computed using the `lsqcurvefit` and `nlparci` routines available in the Optimization Toolbox and the Statistics and Machine Learning Toolbox in the MATrix LABoratory (MATLAB). We found that the best fit to the HST and NIRSPEC spectra of late-T and Y dwarfs in the spectral window from 1.5 to 1.7 microns was achieved with the ratios of ammonia to methane shown in Fig. 4.

Using the same method as described above, we also derived the ammonia-to-methane ratio in the spectra of Jupiter and Saturn that we downloaded from the NASA IRTF archive (Vacca et al. 2003). Our ratio for Jupiter is plotted in Fig. 4, and it is consistent (within the 1 sigma uncertainty) with that found in the literature using models and observations of the Galileo spacecraft (0.26; Taylor et al. 2007). Our ratio for Saturn agrees with that of Owen et al. (1977), who reported on the non-detection of ammonia in high-resolution spectra of Saturn obtained at Palomar Observatory in the wavelength region relevant for this work.

In Fig. 4 (lower panel) we show the comparison of our ammonia-to-methane ratios with the theoretical predictions for high-gravity objects ($g = 10^5\,\mathrm{cm\,s^{-2}}$) from Zahnle & Marley (2014). To compare the behavior of the models with other data, we used the ratios of theoretical column densities scaled by a constant factor to produce two values that reach an agreement at 600 K. There is a good qualitative agreement in the sense that

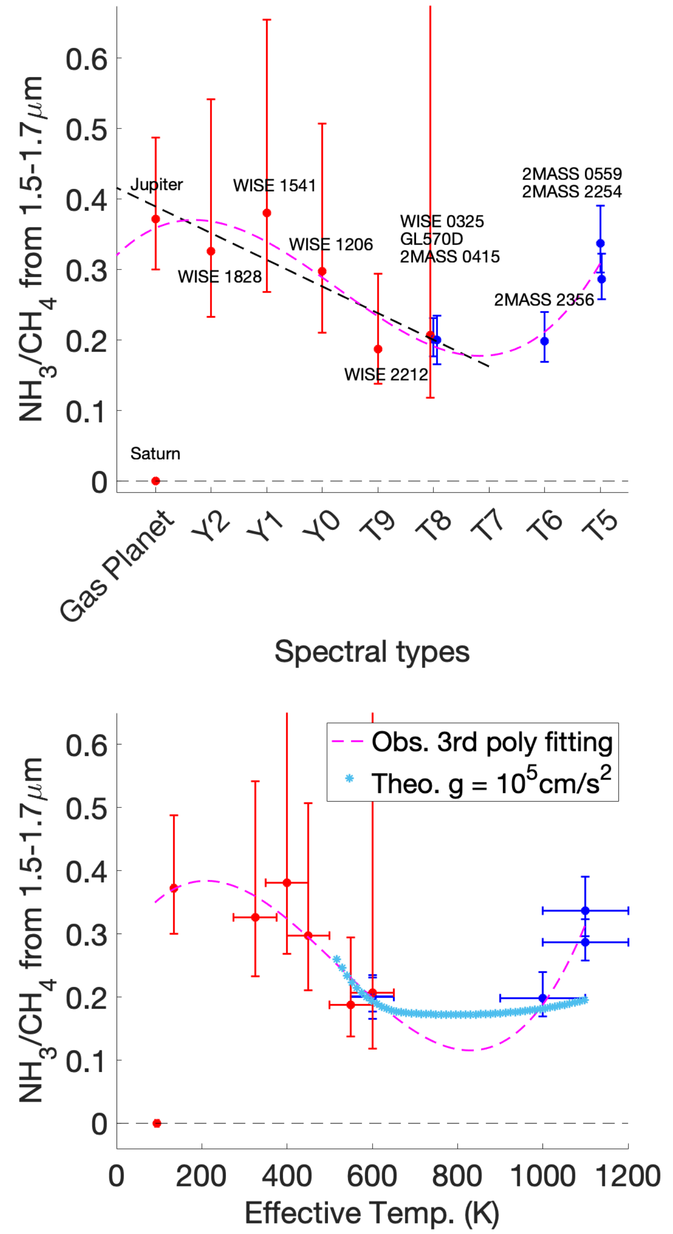

Fig. 4. Ammonia-to-methane ratios derived for late-T dwarfs and Y dwarfs with a 95% confidence level from NIRSPEC data (blue) and HST data (red) compared with those of Jupiter and Saturn from IRTF data (red) as functions of spectral type (*upper panel*) and $T_{\rm eff}$ (*lower panel*). The $T_{\rm eff}$ of T dwarfs, Y dwarfs, Jupiter, and Saturn adopted in this work are listed in Table 1. The dashed pink curves are the third-degree polynomial fittings for all objects (except Saturn) against spectral type and $T_{\rm eff}$, and the dashed black line is a linear fitting just for objects from T8 to Y2. In the *lower panel*, the results are compared with the scaled theoretical ratios of molecular column densities estimated from Zahnle & Marley (2014), which are shown in light blue.

the models predict a ratio that has a minimum around 800 K and increases toward cooler and hotter temperatures.

5. Discussion and final remarks

Our laboratory spectra of ammonia and methane contain absorption features that are too weak or not present in the HITRAN database. We used our laboratory spectrum of ammonia to redefine the spectral index NH3-H in late-T and Y dwarfs. This index

Table 1. Adopted $T_{\rm eff}$ values and uncertainties for the different spectral types and giant gas planets considered in this work.

Type	$T_{\rm eff}$ (K)	References
T5	1100 ± 100	Dupuy & Liu (2017)
T6	1000 ± 100	Dupuy & Liu (2017)
T8	600 ± 50	Schneider et al. (2015)
T9	550 ± 50	Schneider et al. (2015)
Y0	450 ± 50	Schneider et al. (2015)
Y1	400 ± 50	Schneider et al. (2015)
Y2	300 ± 50	Cushing et al. (2021)
Jupiter	134 ± 4	Aumann et al. (1969)
Saturn	97 ± 4	Aumann et al. (1969)

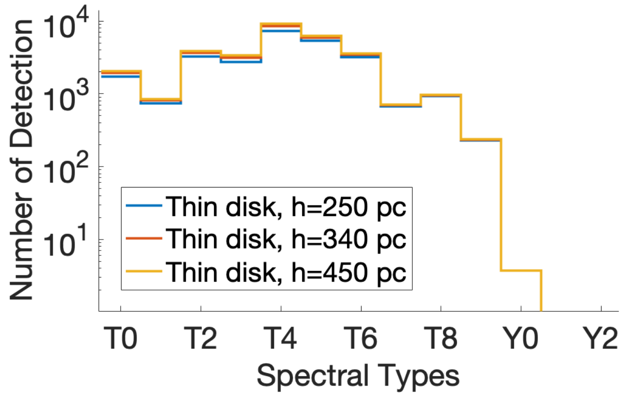

Fig. 5. Simulated number counts of T and Y dwarfs detectable ($S/N \geq 10$) in the full *Euclid* wide survey with the spectroscopic mode of NISP for different values of the Galactic scale height of the BD population in the thin disk.

is a sensitive indicator of the spectral type of ultra-cool BDs, and it can be used to calibrate the data provided by the slitless spectroscopic mode of the NISP instrument on *Euclid*. Our new defined NH3-H index has broader integration limits and an amplitude of variation with spectral type that is almost twice as large as the one based on HITRAN and originally proposed by Delorme et al. (2008).

There is a smooth relation between the ammonia-to-methane ratio derived from our best fits to the observed spectral region from 1.5 to 1.7 microns and the $T_{\rm eff}$ of the objects considered, which is qualitatively in agreement with theoretical predictions taken from the ratio of the theoretical column densities of ammonia and methane under a high surface gravity environment ($g = 10^5$ cm s^{-2}) (Zahnle & Marley 2014). All the late-T and Y dwarfs considered in this work have ammonia-to-methane ratios consistent with that of Jupiter within the uncertainties, suggesting that they have similar chemical abundances.

Using the same assumptions as in Solano et al. (2021) and the densities of objects of different spectral types in the solar neighborhood (Kirkpatrick et al. 2021), we provide here estimates of the numbers of dwarfs with spectral types from T0 to Y2 that could be detected by NISP spectroscopy with $S/N > 10$ in the *Euclid* wide survey (Fig. 5). We note that the number of T5 to T8 dwarfs spectroscopically characterized by NISP is expected to be $\geq 10^3$, and this number rapidly decreases in the Y dwarf domain due to the intrinsic faintness at near-infrared wavelengths of those sources. The results of this work indicate that ammonia-to-methane ratios can be measured in late-T and Y dwarfs using low-resolution near-infrared spectra such as those that will be provided by *Euclid*/NISP. These ratios measured in a large sample with NISP will be useful for exploring the diversity of chemical and physical properties that are likely to exist among the coolest objects in the solar vicinity.

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References

Aumann, H., Gillespie, C., Jr., & Low, F. 1969, ApJ, 157, L69
Bailey, J., & Kedziora-Chudczer, L. 2012, MNRAS, 419, 1913
Bochanski, J. J., Burgasser, A. J., Simcoe, R. A., & West, A. A. 2011, AJ, 142, 169
Burgasser, A. J., Kirkpatrick, J. D., Brown, M. E., et al. 2002, ApJ, 564, 421
Burgasser, A. J., Gelino, C. R., Cushing, M. C., & Kirkpatrick, J. D. 2012, ApJ, 745, 26
Canty, J. I., Lucas, P. W., Yurchenko, S. N., et al. 2015, MNRAS, 450, 454
Cushing, M. C., Kirkpatrick, J. D., Gelino, C. R., et al. 2011, ApJ, 743, 50
Cushing, M. C., Kirkpatrick, J. D., Gelino, C. R., et al. 2014, AJ, 147, 113
Cushing, M. C., Schneider, A. C., Kirkpatrick, J. D., et al. 2021, ApJ, 920, 20
Delorme, P., Delfosse, X., Albert, L., et al. 2008, A&A, 482, 961
Dupuy, T. J., & Liu, M. C. 2017, ApJS, 231, 15
Gordon, I. E., Rothman, L. S., Hill, C., et al. 2017, J. Quant. Spectr. Rad. Transf., 203, 3
Kirkpatrick, J. D., Marocco, F., Caselden, D., et al. 2021, ApJ, 915, L6
Leggett, S. K., Saumon, D., Marley, M. S., et al. 2007, ApJ, 655, 1079
Leggett, S. K., Morley, C. V., Marley, M. S., et al. 2013, ApJ, 763, 130
Luhman, K. L., & Esplin, T. L. 2016, AJ, 152, 78
McLean, I. S., McGovern, M. R., Burgasser, A. J., et al. 2003, ApJ, 596, 561
Owen, T., McKellar, A., Encrenaz, T., et al. 1977, A&A, 54, 291
Saumon, D., Geballe, T. R., Leggett, S. K., et al. 2000, ApJ, 541, 374
Schneider, A. C., Cushing, M. C., Kirkpatrick, J. D., et al. 2015, ApJ, 804, 92
Schneider, A. C., Greco, J., Cushing, M. C., et al. 2016, ApJ, 817, 112
Solano, E., Gálvez-Ortiz, M. C., Martín, E. L., et al. 2021, MNRAS, 501, 281
Taylor, F. W., Atreya, S. K., Encrenaz, T., et al. 2007, The Composition of the Atmosphere of Jupiter, 59
Vacca, W. D., Cushing, M. C., & Rayner, J. T. 2003, PASP, 115, 389
Valdivielso, L., Esparza, P., Martín, E. L., Maukonen, D., & Peale, R. E. 2010, ApJ, 715, 1366
Warren, S. J., Mortlock, D. J., Leggett, S. K., et al. 2007, MNRAS, 375, 213
Wong, A., Bernath, P. F., Rey, M., Nikitin, A. V., & Tyuterev, V. G. 2019, ApJS, 240, 4
Wright, E. L., Eisenhardt, P. R. M., Mainzer, A. K., et al. 2010, AJ, 140, 1868
Zahnle, K. J., & Marley, M. S. 2014, ApJ, 797, 41