A Uniform Retrieval Analysis of Ultra-cool Dwarfs. III. Properties of Y Dwarfs

Joseph A. Zalesky, Michael R. Line, Adam C. Schneider, and Jennifer Patience
School of Earth and Space Exploration, Arizona State University, Tempe, AZ 85287, USA; joezalesky@asu.edu

Received 2019 January 11; revised 2019 March 27; accepted 2019 April 5; published 2019 May 20

Abstract

Ultra-cool brown dwarfs offer a unique window into understanding substellar atmospheric physics and chemistry. Their strong molecular absorption bands at infrared wavelengths, Jupiter-like radii, cool temperatures, and lack of complicating stellar irradiation make them ideal test beds for understanding Jovian-like atmospheres. Here, we report the findings of a uniform atmospheric retrieval analysis on a set of 14 Y- and T-type dwarfs observed with the Hubble Space Telescope Wide Field Camera 3 instrument. From our retrieval analysis, we find the temperature structures to be largely consistent with radiative-convective equilibrium in most objects. We also determine the abundances of water, methane, and ammonia, as well as upper limits on the alkali metals sodium and potassium. The constraints on water and methane are consistent with predictions from chemical equilibrium models, while those of ammonia may be affected by vertical disequilibrium mixing, consistent with previous works. Our key result stems from the constraints on the alkali metal abundances where we find their continued depletion with decreasing effective temperature, consistent with the trend identified in a previous retrieval analysis on a sample of slightly warmer late T-dwarfs in Line et al. (2017). These constraints show that the previously observed Y−J color trend across the T/Y transition is most likely due to the depletion of these metals, in accordance with predictions from equilibrium condensate rainout chemistry. Finally, we simulate future James Webb Space Telescope observations of ultra-cool dwarfs and find that the Near Infrared Spectrometer (NIRSpec) PRISM offers the best chance at developing high-precision constraints on fundamental atmospheric characteristics.

Key words: brown dwarfs – infrared: stars – methods: statistical – radiative transfer – stars: abundances – stars: atmospheres

1. Introduction

Brown dwarfs have raised intriguing questions since their discovery several decades ago (Becklin & Zuckerman 1988; Oppenheimer et al. 1995; Rebolo et al. 1995). While not massive enough to to fuse hydrogen into helium (Hayashi & Nakano 1963; Kumar 1963), they are still too massive to be considered “traditional” planets according to the ~13 \( M_{\text{Jup}} \) definition based on the fusion of deuterium (Shu 1977; Saumon et al. 1996). More recently, there have been arguments that formation pathways, rather than mass limits, are more useful when defining the difference between brown dwarfs and planets (Boss 2001; Bate et al. 2003). This has placed the study of brown dwarfs at an interesting crossroads between planetary science and stellar astrophysics. Efforts to understand the physics of brown dwarfs have thus pulled methodologies from both fields, in order to measure these objects’ physical characteristics and understand their evolution (for a review, see Marley & Robinson (2015)).

There are two primary motives for studying the atmospheres of brown dwarfs. First, brown dwarfs do not have a stable internal energy source, and thus their evolution is highly dependent upon their initial formation mass (e.g., Baraffe et al. 2003) and the specific physical/chemical structure of their atmosphere (e.g., Saumon & Marley 2008). Second, brown dwarfs offer a chance to study planetary-like atmospheric conditions without having to include the complication of an irradiating host star. Understanding the physical and chemical mechanisms at work in cooler brown dwarf atmospheres thus provides constraints on both their evolution and the characteristics of planetary-like atmospheres.

The bulk properties of field brown dwarfs (mass, radius, \( T_{\text{eff}} \), etc.) have been well-studied over the past several decades (for a review, see Burrows et al. (2001)). With cool effective temperatures (200 K \( \leq T_{\text{eff}} \leq 3000 \) K) over photospheric pressures (300 \( \leq P \leq 10^{-4} \) bar), their thermal emission predominantly radiates in the near- to mid-infrared, with their spectra being sculpted by strong molecular and atomic opacities of species such as hydrogen and helium (\( \text{H}_2/\text{He} \)), water (\( \text{H}_2\text{O} \)), methane (\( \text{CH}_4 \)), and ammonia (\( \text{NH}_3 \)), as well as alkali metals such as potassium (K) and sodium (Na), for the coolest objects. For the hottest objects, carbon monoxide and dioxide (CO, \( \text{CO}_2 \)), \( \text{H}_2\text{O} \), \( \text{H}_2/\text{He} \), and metal hydrides and oxides are more dominant (Fegley & Lodders 1996; Lodders & Fegley 2002; Lodders 2003). The precise molecular and cloud compositions, as well as their evolution with temperature, give rise to spectral signatures that define the L-T-Y spectroscopic classes (Oppenheimer et al. 1995; Kirkpatrick et al. 1999; Cushing et al. 2005, 2011; Kirkpatrick 2005).

While empirical approaches exist (e.g., Cruz et al. 2009; Filippazzo et al. 2015), the primary method of choice for inferring atmospheric properties relies upon detailed comparisons between theoretical models and the observed spectra. This often takes the form of precomputing a large grid of theoretical spectra across a range of key physical parameters (Allard et al. 1996, 2012; Marley et al. 1996; Tsuji et al. 1996). Most commonly, these grids have included effective temperature and gravity, but more recently they have been modified to include variable cloud models (Ackerman & Marley 2001; Marley et al. 2002), eddy diffusion within the atmosphere (Saumon et al. 2006), rainout of specific condensates, and varying metallicity and carbon-to-oxygen (C/O) ratios (Marley et al. 2017; Mollière et al. 2017; Samland et al. 2017). These large grid models are then interpolated between grid points and fit via standard maximum likelihood comparisons (e.g., Cushing et al. 2008) or modern MCMC methods (e.g.,
Though this grid modeling approach provides a useful baseline for beginning the analysis of infrared spectra, it has been shown to fail to accurately reproduce key spectral features, and it often provides poor fits to the data (e.g., Leggett et al. 2017). For example, Patience et al. (2012) have demonstrated that grid models from different groups cannot reproduce statistically similar results for the same data set of young brown dwarf companions. These inconsistencies between grid model fitting and the observational data suggest that the established grid model are not properly accounting for all of the possible atmospheric physics and chemistry. Despite this, a more recent effort in Baudino et al. (2017) found greater consistency between several widely used grid models, though outstanding issues in abundance determinations still remain. These inconsistencies motivate the need for a new methodology to complement the grid-modeling approach, in order to reach a more complete understanding of brown dwarf spectra.

Realizing the limitations of the grid modeling approach, Line et al. (2015, 2017) (hereafter Parts I & II) applied well-established atmospheric retrieval (Tinney et al. 1997; Fletcher et al. 2007; Benneke & Seager 2012; Lee et al. 2012; Line et al. 2012) tools to the problem by performing a uniform retrieval analysis on a sample of late-T dwarfs. In Part I, the authors were able to validate their model on two benchmark T-dwarfs by showing that the overall retrieved abundances and C/O ratios were consistent with the objects’ stellar companion. With the larger sample (11 T7-T8 targets) in Part II, they found a strong depletion of the combined Na+K abundances with decreasing $T_{\text{eff}}$. This had long been a theoretical expectation from rainout chemistry (Fegley & Lodders 1994) and hypothesized from trends of near-infrared colors (Marley et al. 2002; Leggett et al. 2010; Liu et al. 2012; Lodieu et al. 2013), but the measured abundance depletion had never been directly detected. These investigations demonstrate that the retrieval method as applied to brown dwarf atmospheres is able to constrain key atmospheric properties often overlooked in traditional methods.

Our primary goals in this work, Part III, are to both expand the previously analyzed data set into the cooler, early-Y–dwarf (Y0-Y1) regime to see if the trends identified in Part II continue to cooler temperatures, and to test the various model assumptions made in Parts I & II. This is accomplished by performing a retrieval analysis on a set of objects from Schneider et al. (2015), which contains near-IR (0.9–1.7 μm, Y, J, H band) spectra of 6 late-T and 16 early-Y–dwarfs using the Hubble Space Telescope’s Wide Field Camera 3 (HST,WFC3).

In Section 2, we briefly outline the methods of our atmospheric retrieval model. Section 3 discusses the data set from WFC3 and the history of our targets. Constraints on the temperature structure (Section 4.1), evolutionary parameters (Section 4.2), and chemical abundances (Section 4.3) are then discussed. We also perform a comparison of our retrieval method with a recently published grid model in Section 4.4. In Section 5, we predict how well the future James Webb Space Telescope (JWST) will be able to improve our constraints. Finally, we list our primary conclusions in Section 6.

## 2. Methods

We utilize the same basic retrieval framework and forward model as described in Parts I and II, briefly summarized here.

| Table 1 |
| --- |
| The 31 Free Parameters in Our Retrieval Model |
| Parameter | Description |
| $\log(f)$ | Seven log(constant-with-altitude volume mixing ratios) |
| $\log(g)$ | log(GM/R$^3$) [cm s$^{-2}$] |
| $(R/D)^2$ | radius-to-distance scale [R$_{\text{app}}$/pc] |
| $T$ | temperature at 15 pressure levels [K] |
| $\Delta$ | wavelength calibration uncertainty [nm] |
| $b$ | error bar inflation exponent |
| $\gamma$, $\beta$ | TP-profile smoothing hyperparameters |
| $\nu_0$, $\rho_0$, $\alpha$ | Cloud profile parameters |

The model includes 31 free parameters, including: constant-with-altitude volume mixing ratios for H$_2$O, CH$_4$, NH$_3$, CO, CO$_2$, and H$_2$S; a combined alkali [Na+K] fixed at a solar ratio (seven in total), gravity, radius-to-distance scale factor $(R/D)^2$, 15 independent temperature–pressure $(TP)$ profile points implemented within a Gaussian-process–like smoothing framework; and a simple cloud parameterization (Burrows et al. 2006). These parameters are summarized in Table 1. All of our molecular and alkali cross sections are those of Freedman et al. (2008, 2014). We have also implemented new Na and K cross sections from Allard et al. (2016), but found no substantial change to our retrieved abundances.

One aspect we wish to reiterate is that we neglect scattering, which may break down in the presence of strongly forward-scattering clouds. Part II did not find any strong evidence for the presence of optically thick clouds in the late-T dwarf sample, as expected for cooler brown dwarfs (e.g., Kirkpatrick 2005), though the alkali depletion trend was consistent with the expected trend in the Na$_2$S and KCl condensation-temperature–pressure profile intersections. Y dwarfs are cooler than late-T dwarfs, permitting the possible formation of water-ice clouds at low pressures (Morley et al. 2014), though we note that the presence of water clouds would have minimal impact over the 1.0–1.7 μm wavelength range covered by WFC3 (see Figure 16 (b) of Morley et al. (2018)).

At the WFC3 spectral resolution $(R \sim 140)$ and signal-to-noise ratio (J-band $S/N \sim 20$), the alkalis’ overall spectral signal, if present, is blended together to create a continuum-like absorption feature along the red portion of the Y-band, due to the broad wings of the 0.59 and 0.77 μm resonance lines, as well as weak features at 1.24 μm in the J-band. For this reason, as was done in Parts I & II, we have combined their signatures and kept the [Na/K] fixed to the solar ratio. We have experimented with relaxing this assumption and allowing both Na and K to be retrieved independently, but find no substantial difference in our results.

To solve the parameter estimation problem, we use the affine-invariant MCMC sampler emcee (Foreman-Mackey et al. 2013), initialized using a grid-model profile $(TP)$ profile from Marley et al. (1996) interpolated to our 15 level parameterization. We choose an approximate $T_{\text{eff}}$ and gravity for each object, based on the spectral type from Schneider et al. (2015) and approximate thermochemical equilibrium abundances for a representative pressure. As in Parts I & II, we have checked that our MCMC chains have converged (typically
WISEA J032504.52-504403.0 T8 19.980
WISEA J040443.50-642030.0 T9 20.328
WISEA J173835.52-693121.6 T9 20.166
WISEA J041022.75 T9 20.166
WISEA J140518.32
WISEA J221216.27-693121.6 T9 20.282
WISEA J040443.50-642030.0 T9 20.328
WISEA J041022.75-150247.9 Y0 20.328
WISEA J094306.00+360723.3 T9.5 19.766
WISEA J154212.00+223005.2 T9.5 19.467
WISEA J140518.32+553421.3 Y0.5 21.351
WISEA J154151.65-225024.9 Y1 20.461

Table 2
Basic Photometric Properties of Our Sample

| WISE/AIWSE Name | Spec. Type | $J_{MKO}$ (mag) | $H_{MKO}$ (mag) | $K_{MKO}$ (mag) | Dist. (pc) |
|----------------|-----------|----------------|----------------|----------------|-----------|
| WISEA J032504.52-504403.0 | T8 | 19.980 ± 0.027 | 19.935 ± 0.024 | 19.423 ± 0.027 | 27.2 ± 2.2\textsuperscript{a} |
| WISEA J040443.50-642030.0 | T9 | 20.328 ± 0.032 | 19.647 ± 0.025 | 19.970 ± 0.033 | 21.9 ± 1.4\textsuperscript{b} |
| WISEA J173835.52-693121.6 | T9 | 20.282 ± 0.023 | 19.737 ± 0.024 | 20.225 ± 0.036 | 12.2 ± 0.4\textsuperscript{c} |
| WISEA J041022.75-150247.9 | Y0 | 20.328 ± 0.022 | 19.937 ± 0.026 | 20.520 ± 0.045 | 11.6 ± 0.6\textsuperscript{d} |
| WISEA J094306.00+360723.3 | T9.5 | 19.766 ± 0.025 | 20.315 ± 0.038 | 10.7 ± 0.3\textsuperscript{e} |
| WISEA J154212.00+223005.2 | T9.5 | 20.461 ± 0.028 | 19.937 ± 0.026 | 20.520 ± 0.045 | 11.6 ± 0.6\textsuperscript{d} |
| WISEA J041022.75-150247.9 | Y0 | 19.325 ± 0.024 | 19.897 ± 0.038 | 6.52 ± 0.17\textsuperscript{e} |
| WISEA J173835.52-693121.6 | Y0 | 20.870 ± 0.041 | 20.354 ± 0.029 | 21.069 ± 0.071 | 15.1 ± 1.2\textsuperscript{f} |
| WISEA J140518.32+553421.3 | Y0.5 | 21.33 ± 0.057 | 21.061 ± 0.035 | 21.501 ± 0.073 | 6.76 ± 0.49\textsuperscript{f} |
| WISEA J154151.65-225024.9 | Y1 | 20.461 ± 0.028 | 19.934 ± 0.026 | 20.520 ± 0.045 | 5.98 ± 0.14\textsuperscript{f} |

Notes.
\textsuperscript{a} Synthetic Photometry from Schneider et al. (2015).
\textsuperscript{b} Distances from Kirkpatrick et al. (2019).
\textsuperscript{c} Distances from Martin et al. (2018).

3. Data Set

In both Part I & II, ground-based near-IR spectra from the SpeX Prism Library (Burgasser 2014) were used. As our aim is to extend into the cooler Y-dwarf regime, we turn to space-based spectroscopy in order to have comparable S/N on cooler targets. Our chosen data set includes the 6 late-T and 16 early-Y objects observed with the HST’s WFC3 in Schneider et al. (2015), which details the WFC3 data reduction process. This sample was chosen because it provides the most complete, uniformly reduced spectra of the known Y dwarfs.

For all of our targets, we have used the most recent distance estimates available in the literature (Martin et al. 2018; Kirkpatrick et al. 2019). We have also done an analysis assuming parallax estimates from several other authors, the results of which are presented in Section 4.2 (Dupuy & Liu 2012; Luhman & Esplin 2016; Smart et al. 2017).

We first performed an initial retrieval on all 22 of our targets. While the retrieval technique obtains constraints on various atmospheric parameters, it is ultimately a data-driven technique that requires precise spectroscopy to properly converge. We found that 8 of our 22 targets had low enough S/N to prevent our retrieval model from converging upon physically realistic TP profiles, and thus have not included them in our analysis.

A brief review of the remaining 14 objects, specified by their Wide-field Infrared Survey Explorer (WISE) identification, is provided below. Key observational quantities (YJHK magnitudes and distance estimates) are summarized in Table 2.

WISEA J02504.52-504403.0 (W0325, T8). This is one of several new brown dwarf discoveries from Schneider et al. (2015). The object spectroscopically matches the T8 spectral standard well (Burgasser et al. 2006). Follow-up work was done by Leggett et al. (2017), who published an archival J-band magnitude.

WISEA J040443.50-642030.0 (W0404, T9). This is another new discovery from Schneider et al. (2015), who found the spectrum to closely match the T9 spectral standard (Cushing et al. 2011).

WISEA J221216.27-693121.6 (W2212, T9). Another new discovery of Schneider et al. (2015) that is also in good agreement with the T9 spectral standard.

WISEA J033515.07+431044.7 (W0335, T9). This object was discovered in the Mace et al. (2013) study, along with 86 other T dwarfs, and given the classification of T9. Both Beichman et al. (2014) and Schneider et al. (2015) found good agreement with this classification. Leggett et al. (2015) published new ground-based YJHK photometry from Gemini Observatory for this target, and they noted an unusually faint K-band measurement with respect to their other T dwarfs. They found that current equilibrium models could not well-explain their photometric measurements unless the assumed NH$_3$ abundance was halved and/or there were systematic issues with the CH$_4$ line list. Leggett et al. (2017) used archival photometry combined with nonequilibrium models from Tremblin et al. (2015) to conclude that this target may have subsolar metallicity.

WISEA J094306.00+360723.3 (W0943, T9.5). W0943 was initially discovered by Cushing et al. (2014), who published WISE and Hubble photometry along with WFC3 G141 spectroscopy. It was given a classification of T9.5, which agrees well with the results from Schneider et al. (2015).

WISEA J154214.00+223005.2 (W1542, T9.5). W1542 was also discovered in the Mace et al. (2013) study. It was given the classification of T9.5, which is in agreement with other similar studies (Beichman et al. 2014; Schneider et al. 2015).

WISEA J041022.75+150247.9 (W0410, Y0). This is a well-studied object that was part of the initial classification of Y dwarfs as distinct from their T dwarf counterparts (Cushing et al. 2011). These measurements helped establish the extreme blueshift of Y-J colors across the T/Y transition (e.g., Kirkpatrick et al. 2012; Liu et al. 2012). Cushing et al. (2014) obtained the first space-based spectrum of this object and confirmed Y0 classification. Leggett et al. (2013) found that fitting YJHK photometry from the Near-Infrared Imager on Gemini North with cloudy models from Morley et al. (2012) results in effective temperatures, gravities, and low-level cloud sedimentation efficiencies consistent with previous analyses of early-Y dwarfs. Spectra from Schneider et al. (2015) agree well...
with the photometry of Leggett et al. (2013). Leggett et al. (2015) highlighted that current equilibrium models were unable to reproduce their updated photometry for early-Y dwarfs and that retrieval techniques are needed to understand these objects. Leggett et al. (2017) visually fit the spectra of Schneider et al. (2015) with cloud-free, vertical disequilibrium models from Tremblin et al. (2015). They found that, while the Y and H bands are visually well-fit, the J-band model spectrum was ~20% brighter.

WISEA J073444.03-715743.8 (W0734, Y0). This is another object initially discovered by an early WISE Survey (Kirkpatrick et al. 2012). Follow-up photometric work by both Tinney et al. (2014) and Leggett et al. (2015) noted the rather red Y–J color for this object, more consistent with a late-T than an early-Y dwarf.

WISEA J173835.52+273258.8 (W1738, Y0). This object is probably one of the most well-studied cool brown dwarfs, as it represents the Y0 spectral standard (Cushing et al. 2011). Saumon et al. (2012) updated the collisionally induced H2 and NH3 opacities and found improved fits to observed infrared colors. Lodieu et al. (2013) provided Z-band imaging of this and several other cool brown dwarfs. Leggett et al. (2013) noted the rather blue Y–J colors now seen in many Y dwarfs. Rajan et al. (2015) performed the first photometric monitoring of such a cool target, but this object proved too faint to provide the precision needed to confirm variability in the J band. Recent ground-based spectra have revealed that nonequilibrium models from Tremblin et al. (2015) better-fit the entire near-infrared spectrum of this object, but a majority of the Y band is not well fit (Leggett et al. 2016a). Leggett et al. (2016b) found a peak-to-peak 3% Spitzer [4,5] variability consistent with W1738’s rotation period of roughly 6 hr.

WISEA J205628.88+145953.6 (W2056, Y0). W2056 represents another archetype WISE early-Y dwarf also analyzed in the Cushing et al. (2011) and Kirkpatrick et al. (2012) studies. Leggett et al. (2013) obtained ground-based YJHK photometry and far-red spectra for this object. They noted that cloudy models from Morley et al. (2012) fit both the red spectra and K band well overall, but were too faint near 1.0, 1.5, and 1.65 μm. This was attributed both to overly strong NH3 absorption due to vertical mixing of NH3 not being included in the models, and to incomplete CH4 molecular line lists. Leggett et al. (2017) provided new ground-based M’ observations for this object, and visually fit cloud-free models from Tremblin et al. (2015) to archival WFC3 spectra. Due to poor S/N and sparse sampling in their grid model, the archival WFC3 spectra were fit only by eye.

WISEA J22055.34-362817.5 (W2220, Y0). W2220 was initially discovered as a new Y dwarf in the Kirkpatrick et al. (2012) study. Chosen as part of an astrometric survey, Beichman et al. (2014) noted that W2220 provided tentative evidence for variability, due to the archival J- and H-band measurements differing by over an order of magnitude. Leggett et al. (2017) concluded that this object is consistent with a solar-metallicity and solar-age field dwarf.

WISEA J163940.84-684739.4 (W1639, Y0 Pec.). W1639 was first discovered by Tinney et al. (2012) after carefully resolving the near-infrared counterpart to the WISE point source with ground-based imaging. Though J-band spectroscopy matches well to the Y0 standard, both Y-band spectra and Y-J colors deviate from the standard, leading to the Y0-Peculiar classification (Schneider et al. 2015). Opitz et al. (2016) searched for—but found no evidence of—another companion to the known Y dwarf to within 2 au. Leggett et al. (2017) found that, while their nonequilibrium models matched $T_{\text{eff}}$ estimates from Schneider et al. (2015), the nonequilibrium models resulted in a significantly lower gravity for this object.

WISEA J140518.32+553421.3 (W1405, Y0.5). W1405 is an early-Y dwarf that was identified by a methane-induced H-band feature (Cushing et al. 2011; Kirkpatrick et al. 2011). Morley et al. (2012) obtained ground-based YJH photometry in order to draw comparisons with a suite of models that incorporated various condensates, including several sulfides, KCl, and Cr. They found that these models fit near-infrared data better than completely cloud-free models. Using updated YJHK photometry, Leggett et al. (2013) found that this object should be cool enough to display effects from the presence of water clouds, but their model grid did not extend down to cool enough temperatures for a reliable water-cloud model fit. Lodieu et al. (2013) obtained lower-limit Z-band measurements for this dim object. Schneider et al. (2015) reclassified this object as Y0.5, due to its J-band spectroscopy being narrower than the Y0 spectral standard. Cushing et al. (2016) obtained Spitzer 3.6 and 4.5 μm light curves and found the first evidence for variability in a Y dwarf, with 3.6% variability detected with an 8.2 hr period. Leggett et al. (2017) found this object to also be consistent with solar metallicity and age.

WISEA J154151.65+225024.9 (W1541, Y1). W1541 is the latest-type Y dwarf we have analyzed; it was reclassified as Y1, based upon the width of J-band spectroscopic measurements (Schneider et al. 2015). This object is another of the Y dwarfs included in the initial WISE discovery papers (Cushing et al. 2011; Kirkpatrick et al. 2011, 2012). Morley et al. (2012) obtained ground-based Y- and J-band photometry of this object, and they note that their cloudy (rather than cloud-free) models better reproduce the observed colors of their Y-dwarf photometry. However, Saumon et al. (2012) noted that, with improved NH3 opacities, their cloud-free models matched the observed colors. Ground-based YJHK photometry was obtained by Leggett et al. (2013), whose cloud-free models estimate $T_{\text{eff}}$ ~ 325 K. Leggett et al. (2015) obtained improved H-band measurements, and compared measured colors with a suite of both water-cloud and cloud-free models. Though they find that several colors are better-fit with the inclusion of water clouds, there are still magnitude-scale systematic offsets between the models and data. Leggett et al. (2017) was able to successfully reproduce either Y- or J-band spectroscopy, but a simultaneous fit to the entire YJHK spectrum could not be obtained.

4. Results

Here, we present our results from the analysis of our 14 late-T/early-Y dwarfs. Full posteriors of all model parameters are available online.1 Figure 1 summarizes the fits with the WFC3 data in black, best-fit spectra in blue, and residuals in red. Several objects only have 1.1–1.7 μm coverage, as full YJK coverage requires both G105 and G141 spectra from HST (Schneider et al. 2015). A visual inspection shows that there is no systematic structure in the residuals and most of our objects have a $\chi^2_v$ between 1 and 3. W2056 has a higher $\chi^2_v = 5.05$, but this is due to an over-subtraction artifact, with fluxes between

---

1 Zenodo link: http://doi.org/10.5281/zenodo.2611930.
Figure 1. WFC3 observations (black points), best-fit retrieval model (blue), and residuals (lower, red) for the WFC3 sample sorted by the Schneider et al. (2015) spectral classification (upper left). The retrieved log($g$) [cgs] and derived effective temperature [K] are given in the upper right-hand corner of each panel.
### Table 3
Retrieved and Derived Evolutionary Parameters

| WISEA ALLWISE Name | Spec. Type | $T_{\text{eff}}$ (K) | log$(g)$ (cgs) | $R$ ($R_{\text{Jup}}$) | Mass ($M_{\text{Jup}}$) | Prior |
|-------------------|------------|----------------------|----------------|---------------------|---------------------|-------|
| WISEA J032504.52-504403.0 | T8 | 664 ± 26 | 4.97 ± 0.19 | 1.08 ± 0.11 | 44 ± 23 | Free |
| WISEA J040443.50-642030.0 | T9 | 646 ± 24 | 5.06 ± 0.36 | 1.10 ± 0.11 | 56 ± 32 | Constrained |
| WISEA J221216.27 -693121.6 | T9 | 659 ± 35 | 5.20 ± 0.23 | 0.81 ± 0.06 | 42 ± 25 | Constrained |
| WISEA J035151.07+431051.8 | T9 | 540 ± 37 | 5.25 ± 0.29 | 0.71 ± 0.02 | 36 ± 17 | Constrained |
| WISEA J094306.00+360723.3 | T9.5 | 484 ± 26 | 4.87 ± 0.22 | 0.87 ± 0.06 | 23 ± 10 | Free |
| WISEA J154214.00-223005.2 | T9.5 | 488 ± 20 | 5.16 ± 0.15 | 0.61 ± 0.05 | 21 ± 8 | Free |
| WISEA J041022.75+150247.9 | Y0 | 530 ± 24 | 5.30 ± 0.23 | 0.73 ± 0.08 | 43 ± 21 | Free |
| WISEA J073444.03-715743.8 | Y0 | 467 ± 21 | 5.39 ± 0.17 | 0.71 ± 0.07 | 50 ± 21 | Free |
| WISEA J173855.22+273225.8 | Y0 | 371 ± 30 | 5.43 ± 0.13 | 0.71 ± 0.05 | 59 ± 15 | Free |
| WISEA J205628.88+145935.6 | Y0 | 493 ± 30 | 4.95 ± 0.11 | 0.67 ± 0.05 | 16 ± 6 | Free |
| WISEA J220553.34-362817.5 | Y0 | 443 ± 24 | 4.93 ± 0.25 | 0.72 ± 0.02 | 18 ± 14 | Constrained |
| WISEA J163940.84+684739.9 | Y0 | 654 ± 18 | 4.37 ± 0.08 | 0.40 ± 0.02 | 1.5 ± 0.3 | Free |
| WISEA J140518.32+553421.3 | Y0.5 | 327 ± 31 | 4.39 ± 0.28 | 0.66 ± 0.12 | 4.4 ± 3.9 | Free |
| WISEA J154151.65+225024.9 | Y1 | 323 ± 31 | 5.00 ± 0.48 | 0.33 ± 0.05 | 5.4 ± 3.4 | Free |

Note.

* Retrieval model could not converge upon a physically realistic TP profile.

### Table 4
Retrieved Atmospheric Abundances

| WISEA ALLWISE Name | Spec. Type | H$_2$O$^a$ | CH$_4$$^a$ | CO$^b$ | CO$_2$ | C/O$^b$ | H$_2$S | NH$_3$$^a$ | Na+K | Na+K$^a$ |
|-------------------|------------|-----------|-----------|-------|-------|--------|-------|--------|-------|--------|
| WISEA J032504.52-504403.0 | T8 | -3.3 ±0.12 | -3.05 ± 0.11 | -0.13 | -3.16 | 0.99 ± 0.18 | -5.0 | -4.49 ± 0.12 | -5.52 ± 0.07 |
| WISEA J040443.50-642030.0 | T9 | -3.0 ±0.11 | -2.74 ± 0.10 | -0.13 | -3.16 | 1.02 ± 0.16 | -5.0 | -4.63 ± 0.20 | -6.0b |
| WISEA J221216.27-693121.6 | T9 | -2.50 ± 0.18 | -2.56 ± 0.16 | -0.16 | -3.16 | 3.3 ± 0.09 | -6.8 | -4.40 ± 0.13 | -5.0b |
| WISEA J035151.07+431051.8 | T9 | -3.3 ±0.09 | -3.48 ± 0.11 | -0.11 | -3.8 | 0.57 ± 0.07 | -5.3 | -4.78 ± 0.12 | -5.97 ± 0.07 |
| WISEA J094306.00+360723.3 | T9.5 | -3.35 ± 0.15 | -3.13 ± 0.17 | -0.15 | -3.3 | 1.22 ± 0.25 | -5.0 | -4.46 ± 0.16 | -5.2b |
| WISEA J154214.00+223005.2 | T9.5 | -3.04 ± 0.09 | -2.92 ± 0.08 | -0.10 | -4.2 | 0.95 ± 0.15 | -6.0 | -4.32 ± 0.12 | -6.7b |
| WISEA J041022.75+150247.9 | Y0 | -2.90 ± 0.15 | -2.63 ± 0.17 | -0.19 | -3.3 | 4.1 | -0.33 | -4.3 | -4.11 ± 0.19 | -5.0b |
| WISEA J073444.03-715743.8 | Y0 | -2.91 ± 0.13 | -2.77 ± 0.14 | -0.19 | -3.4 | 0.78 ± 0.16 | -6.0 | -4.29 ± 0.14 | -6.0b |
| WISEA J173855.22-273228.8 | Y0 | -2.87 ± 0.13 | -2.75 ± 0.12 | -0.10 | -3.3 | 4.1 | -0.19 | -4.3 | -4.11 ± 0.19 | -5.0b |
| WISEA J205628.88+145935.6 | Y0 | -3.18 ± 0.15 | -2.89 ± 0.15 | -0.21 | -4.2 | 1.33 ± 0.17 | -5.5 | -4.46 ± 0.14 | -5.5b |
| WISEA J220553.34-362817.5 | Y0 | -3.04 ± 0.10 | -3.00 ± 0.12 | -0.12 | -4.2 | 0.63 ± 0.10 | -5.8 | -4.40 ± 0.19 | -6.8b |
| WISEA J163940.84-684739.4 | Y0 | -3.3 ± 0.04 | -3.42 ± 0.05 | -0.04 | -4.3 | 0.46 ± 0.06 | -6.3 | -4.72 ± 0.04 | -7.0b |
| WISEA J140518.32+553421.3 | Y0.5 | -3.24 ± 0.13 | -3.33 ± 0.16 | -0.16 | -3.6 | 0.46 ± 0.10 | -5.0 | -4.84 ± 0.16 | -6.0b |
| WISEA J154151.65+225024.9 | Y1 | -2.68 ± 0.18 | -2.80 ± 0.16 | -0.26 | -3.5 | 0.45 ± 0.17 | -5.0 | -4.43 ± 0.21 | -6.4b |

Notes.

* All abundances are reported as the log of the volume mixing ratio log (VMR), where the remainder of the gas is taken to be H$_2$He at a fixed solar ratio.

* All of these measurements represent 3σ upper limits (see text).

* These are not relative to solar. Solar [C/O] is 0.55 in this table.
the $J$ and $H$ bands being $\sim 2\sigma$ below zero. We have experimented with removing such data from our fit, but found no impact on our results (see Section 4.2).

We first discuss the implications of our constraints on the temperature structure and evolutionary properties of these objects. Our retrieved evolutionary parameters are enumerated in Table 3. We then highlight our retrieved abundances, which are listed in Table 4. Finally, we discuss how observations of these objects with JWST will impact our ability to characterize them.

4.1. Vertical Temperature Structure

For any nonirradiated substellar object, the energy balance—and hence, the thermal structure of the atmosphere—is governed by the flow of internal heat flux through the atmosphere, controlled by the gravity and atmospheric opacity. These properties are directly set by both the mass and age of the system (e.g., Allard et al. 1996). In ultra-cool dwarfs, energy is primarily transported through radiation and convection (Marley & Robinson 2015).

Late-T/early-Y type objects are ideal for the characterization of the $TP$ profile structure, due to the high degree of spectral modulation (which maps to a wide range of probed pressures) and the presumed lack of optically thick clouds (Morley et al. 2012). As before, we make few a priori assumptions regarding the thermal structure of the atmosphere, and instead allow the observations to drive the solutions. By subsequently making comparisons between our results and those of self-consistent models, we can then investigate where “atypical” atmospheric processes, such as deviations from radiative-convective equilibrium, may be occurring. Should any significant deviations be found, such information can be utilized in order to improve grid-based models’ treatment of atmospheric structure by inclusion of other possible sources of heating. (e.g., Sorahana et al. 2014; Tremblin et al. 2015).

Figure 2 summarizes the resulting $TP$ profiles. The median $TP$ profile is shown in black, with $1\sigma$ and $2\sigma$ confidence intervals outlined in red. Overlaid atop the retrieval results are radiative-convective equilibrium profiles (blue) derived using the ScCHIMERA modeling tool described in Piskorz et al. (2018) and Bonnefoy et al. (2018), generated using the $T_{eff}$ and log($g$) range derived from the retrieval results. We compute the effective temperature as in Parts I and II by numerically integrating for the bolometric flux of the retrieved spectral spread for each object from 1 to 20 $\mu$m. Contribution functions (gray) from the WFC3 observations are also overlaid; these can be treated as the effective photosphere probed by WFC3. As was noted in Part II, we reiterate that the atmospheric structure above and below these regions is largely driven by our $TP$ profile smoothing parameter (described in Part I), and that interpretation of such structure should be done with caution.

The WFC3 observations probe pressures from roughly 1–100 bars with typical $1\sigma$ temperature uncertainties of $\sim 50$–100 $K$, consistent with the SpeX T-dwarfs from Part II. For a large majority of objects, the retrieved structures appear consistent with the assumption of radiative-convective equilibrium. Though this is true for most objects, W1639 stands out in stark contrast. The retrieved $TP$ profile shows almost no consistency with that of radiative-convective equilibrium, as well as an interesting “kink” structure at roughly 10 bars. The unique atmospheric structure also suggests that our WFC3 wavelents are sensitive to much lower pressures of roughly 0.1–0.01 bars.

4.1.1. WISEA J1639-6847

W1639 is the only object in our sample with a classification of “Y0: Peculiar” (Schneider et al. 2015). Though the object’s $J$-band spectra well-match the Y0 spectral standard, the overall $Y$-$J$ color is significantly bluer due to a bright $Y$-band. Additionally, the overall position of the $Y$-band is significantly blueshifted when compared to the $T9$ spectral standard. These features, remarked upon by Schneider et al. (2015), are not just an artifact of the WFC3 data, as the bright $Y$-band has also been observed with the ground-based FIRE instrument (Tinney et al. 2012). These unique properties motivated Schneider et al. (2015) to invest more of their limited WFC3 time to this object, resulting in much better $Y$-band constraints than the other objects in our sample (see Figure 1). This is the main contributor to the improved $TP$ profile constraints relative to our other objects. Though the W1639 spectrum seems well-fit by our model (reduced $\chi^2$ of $\sim 2$), there are several lingering issues with the resulting best-fit parameters.

The first issue is that, despite the object being in the Y0 Pec. classification, we derive an effective temperature of 654$^{+35}_{-38}$ $K$. It has been suggested that double-diffusive convection can result in much shallower thermal structures than predicted by equilibrium grid models (Tremblin et al. 2015). This would be consistent with the profile we retrieve for W1639. However, using basic energy balance arguments and thermodynamics, Leconte (2018) demonstrated that this mechanism would result in steeper, not shallower, temperature gradients, in contrast to Tremblin et al. (2015) and the profile of W1639. Release of latent heat due to condensation of various cloud species may also result in shallower adiabats. However, Figure 2 shows that the main contributor to such heat—namely, water—would negligibly impact our objects, based on the intersection of the retrieved $TP$ profile with water’s equilibrium condensation curve.

Additionally, our estimate for log($g$) is the lowest out of our 11 objects at log($g$) = 4.35$^{+0.1}_{-0.1}$, requiring a radius of $R = 0.4^{+0.03}_{-0.02} R_{\text{Jup}}$ and $M = 1.5^{+0.3}_{-0.3} M_{\text{Jup}}$ (see Section 4.2, Table 3). These constraints are significantly smaller than allowed by typical field dwarfs; combined with the peculiar $TP$ profile, this leads us to conclude that our data-driven retrieval model may not be well-suited to explaining the physical characteristics of this single unique object. However, we reiterate that the remaining object’s $TP$ profiles seem to agree well with assumptions of radiative-convective equilibrium.

4.2. Effective Temperature, Gravity, Radius, and Mass

The effective temperature, gravity, radius, and mass are diagnostic of brown dwarf evolutionary history (e.g., Burrows et al. 2001; Baraffe et al. 2003; Saumon & Marley 2008). Evolution models suggest that our late-T ($\geq T8$) and early-Y ($\leq Y1$) sample should have values of $T_{eff}$ ranging from 800 to 350 $K$ (Pecaut & Mamajek 2013). Field-age late-T and early-Y dwarfs are expected to have log($g$) $\approx 5$ with a relatively strong upper bound at log($g$) $\approx 5.3$ for even the oldest and coldest brown dwarfs possible (e.g Saumon & Marley 2008). Field-aged objects over the 10–80 $M_{\text{Jup}}$ range are expected to have radii within $\sim 20\%$ of Jupiter’s.
Figure 2. Retrieved TP profiles for all targets. Black lines are median values with red 1σ and 2σ confidence intervals. In gray are the contribution functions of the atmosphere from the WFC3 observations; these can be thought of as the effective photosphere. Overlaid (blue) are solar-composition radiative-convective equilibrium profile spreads derived from the retrieved spread in effective temperature and gravity. Finally, we also include solar-composition equilibrium condensation curves (dashed lines) for several important species (Morley et al. 2012, 2014). Most systems’ retrieved TP profiles are in good agreement with radiative-convective equilibrium, save for W1639 (see text).
In this work, the total \((R/D)^2\) scaling factor is a free parameter. By using constraints on the distance \(D\) from the literature and our retrieved constraints on \((R/D)^2\), we are then able to derive constraints on the photometric radius \(R\). Using this derived constraint, along with our retrieved \(\log(g)\), we can then derive the total mass of the object \(M\), with a prior upper limit of \(80\, M_{\text{Jup}}\). Table 3 and Figure 3 summarize the retrieved and derived estimates for these evolutionary parameters under two sets of model assumptions.

4.2.1. Free Retrieval

We first focus on a less constrained, “free” retrieval, which only incorporates the \(80\, M_{\text{Jup}}\) mass prior upper limit, as has been done in Parts I and II. Our retrieved \(\log(g)\) and derived \(T_{\text{eff}}\) for this case are shown as red symbols in Figure 3. In general, we find that the uncertainties in both \(\log(g)\) and \(T_{\text{eff}}\) are consistent with the results from Part II, with respective \(1\sigma\) errors between 0.1–0.5 dex and 30–90 K. This is encouraging because both our data set in this work and the data set in Part II had comparable S/N on the observed spectra. For a majority of objects, our derived effective temperatures agree with the spectral types given in Schneider et al. (2015) when compared to the table provided in Pecaut & Mamajek (2013). The notable exception to this trend is W1639, whose unique \(\text{TP}\) profile is discussed in Section 4.1.

Overplotted on Figure 3 are (blue, dashed) curves of constant age from the upcoming Sonora grid of evolutionary models (M. S. Marley et al. 2019, in preparation). Several objects appear to have gravities that extend well beyond those anticipated by the 10 Gyr curve, though our retrieved uncertainties are large enough to be consistent with the oldest models at \(\sim 2\sigma\). This result is not unique to our retrieval approach—Schneider et al. (2015) also noted that grid-model comparisons resulted in a similar result, with several objects’ \(\log(g)\) estimates requiring gravity values higher than computed in their grid model. In addition to high gravity estimates, we also found several objects to have smaller radii than expected for our late-T, early-Y sample, with several objects below a lower limit value of \(\sim 0.7\, R_{\text{Jup}}\) (Saumon & Marley 2008). Both the uncomfortably high gravities and small radii prompted us to explore the robustness of our results through a battery of tests.

We first investigated the possibility of an unknown systematic error in the observed spectra biasing the fits. We considered this because it was noticed that the observed fluxes fell below zero, well outside of the reported \(1\sigma\) uncertainties in some cases, in the deep absorption bands for several objects (namely W2056, W2220, and W1541; see Figure 1). This is due to oversubtraction when attempting to remove background fluctuations. To test this, we introduced a free parameter to uniformly shift the model spectra fluxes to within the \(1\sigma\) error estimates of the data, but found that it did not produce any considerable change in parameter estimates.

Next, we explored some of the key assumptions made within our model. In this initial set of “free” retrievals, we had assumed a hard prior upper limit of \(80\, M_{\text{Jup}}\) on the mass. This prior rejects combinations of radii and gravities that would exceed this mass limit. We tested the sensitivity of our results to this mass upper limit by effectively removing the prior. These resulted in significantly higher retrieved gravities, with some objects such as W1738 reaching as high as \(\log(g) = 5.7_{-0.32}^{+0.18}\). This indicated to us that the data was indeed favoring higher masses and gravities along with lower radii.

We then explored how radius assumptions (through \((R/D)^2\))—assuming a distance—could influence the retrievals by fixing the radii to a realistic \(0.9\, R_{\text{Jup}}\) (and turning the mass upper limit prior back on). For the case of W0734 (originally retrieved \(R \sim 0.71\, R_{\text{Jup}}\), \(\log(g) = 5.39_{-0.28}^{+0.17}\)), we found that the fixed radius resulted in a decreased gravity (\(\log(g) = 5.12_{-0.33}^{+0.28}\)). However, the resulting marginalized posterior is highly non-Gaussian due to the enforcement of the \(80\, M_{\text{Jup}}\) cutoff. This suggests that, despite enforcing these priors, the high-gravity solution is still favored.

4.2.2. Constrained Retrieval

We finally decided to run a completely separate set of retrievals on all of our objects, with more stringent priors based on results from evolutionary models that we have labeled as “constrained” retrievals. This included restricting \(0.7\, R_{\text{Jup}} < R < 2.0\, R_{\text{Jup}}\), \(3.5 < \log(g) < 5.5\) and effectively removing the mass upper limit. The results of this analysis are shown as black symbols in Figure 3 and are enumerated in Table 3. Objects whose “constrained” retrieval results are within \(1\sigma\) of the “free” retrieval are translucent, while those whose \(\log(g)\) change by \(> 1\sigma\) are opaque.

We obtained two key results from this constrained retrieval test. The first is that, regardless of our priors on evolutionary parameters, the data suggest that these objects have anomalously high gravity estimates. This can be seen in Figure 3, where most objects still lie above the 10 Gyr trend for both the “constrained” (black) and “free” (red) retrieval. For the Y0 objects, we find a consistent decrease in their \(\log(g)\) estimates by upward of 0.3 dex, and a slight increase in the radii estimates to roughly \(0.75\, R_{\text{Jup}}\). Though this places our retrieval results in better agreement with evolutionary models, our posterior distributions for \(\log(g)\) are consistently non-Gaussian and push against the \(\log(g) = 5.5\) upper limit, suggesting that the high-gravity solution is still favored.

Our second result is that, regardless of our priors on evolutionary parameters, we still obtain the same constraints on our chemical abundances to within \(1\sigma\). This was a bit

![Figure 3. \(T_{\text{eff}}\) and \(\log(g)\) 1\sigma constraints for our free retrieval results (red) and constrained retrieval (black). Each object has its own unique symbol. Most objects, save the coldest two (W1405, W1541) and W1639 (see text) show consistent results between the free and constrained retrievals at \(1\sigma\).](image-url)
surprising as there is a well-known correlation between the gravity and overall metallicity for these objects. We ensured this by picking three of our objects with anomalously high gravities (W2212, W0734, and W1738) and enforcing that log (g) = 5.0. We found that our retrieved metallicity did indeed decrease as expected, but our overall fit to the data was much worse under this assumption, with an average delta $\chi^2$ of 6.5, indicating that our original retrieved metallicities and high gravities are the statistically favored solution.

4.2.3. Caveats & Exceptions

There were four objects in total that did not follow these trends; these are the opaque points in Figure 3. Though W2212 obtains plausible constraints on the mass and $T_{\text{eff}}$, it requires a radius of $R = 0.47^{+0.05}_{-0.03}$ under the “free” retrieval assumption. Our “constrained” retrieval does result in a more physically realistic $R = 0.71^{+0.02}_{-0.02}$, and we find that our constraints on the chemical abundances change by $\sim 2\sigma$. We ran a separate retrieval on this target, using a different distance estimate from Kirkpatrick et al. (2012). In that case, we obtained a physically realistic $R = 0.68^{+0.06}_{-0.05}$ and our chemical abundances did not change beyond $1\sigma$, though the retrieved gravity is still the largest of our sample at log$g = 5.5^{+0.11}_{-0.17}$. Full model posteriors for this additional retrieval on this target, using a different distance estimate from Kirkpatrick et al. (2012). In that case, we obtained a physically realistic $R = 0.68^{+0.06}_{-0.05}$ and our chemical abundances did not change beyond $1\sigma$, though the retrieved gravity is still the largest of our sample at log$g = 5.5^{+0.11}_{-0.17}$.

For W1639, our retrieval model could not converge upon a physically realistic TP profile given the assumptions in the constrained retrieval, and thus there is no corresponding black star in Figure 3. For both W1405 and W1541 (represented by a diamond and a cross, respectively), we find that though our retrieval model converges upon solutions for both objects, they are largely nonphysical. By enforcing stronger constraints on the radius, we find that a Jupiter-like mass and significantly lower gravities (by $\sim 2\sigma$) are needed in order to well-match the spectra under these assumptions. Additionally, our constraints on the chemical abundances change by upward of $3\sigma$. Though we include these four objects in the results of subsequent sections, we strongly caution against overinterpretation of their chemical abundance constraints, given that they significantly change under different model assumptions.

The one technique that proved successful in reducing the retrieved gravity of an object without encountering non-Gaussian posteriors or changes in chemical abundances was changing the assumed parallax. Our distance estimates had been taken from two specific sources in the literature (Martin et al. 2018; Kirkpatrick et al. 2019). These were chosen in order to use the most updated parallax estimates from the Spitzer instrument. However, several other campaigns have previously measured parallaxes for several of our targets (e.g., Luhman & Esplin 2016; Smart et al. 2017). In most cases, the distances proved consistent with our previous assumptions and our retrieved parameters remained the same, as expected. However, using the parallax measurement for W2056 from Smart et al. (2017) resulted in a more physically realistic log (g) = 4.58$^{+0.33}_{-0.37}$. Though we did not find similar results for the other distance estimates from Smart et al. (2017), we note that this result shows how sensitive our evolutionary parameters are to measured parallaxes. If the distance estimates are systematically biased in a similar fashion, this may also account for the fact that our radii estimates are slightly lower than expected from evolutionary models.

4.3. Composition

One of the key advantages of retrievals is their ability to directly determine the molecular abundances in an atmosphere, rather than assuming them from elemental abundances and equilibrium chemistry. From the molecular abundances, we can derive the atomic abundance ratios (e.g., metallicity, C/O, N/O etc.), and more importantly, explore trends in these abundances that are diagnostic of atmospheric chemical mechanisms. The primary motivations for looking at molecular abundances in the Y-dwarf regime are: (1) to determine at what temperature the alkali metals completely disappear, and whether it is consistent with grid-model chemical predictions; and (2) to determine the role of ammonia, as it is anticipated to be strongly influenced by disequilibrium vertical mixing. Again, our retrieval forward model assumes constant-with-altitude (pressure) molecular mixing ratios. The retrieved abundances are therefore representative of column-integrated abundances over the photosphere probed by WFC3.

Table 4 summarizes the molecular abundance constraints (median and 68% confidence interval). We find well-defined, bounded constraints for H$_2$O, CH$_4$, NH$_3$, and in two cases, Na + K, but obtain only upper limits for CO, CO$_2$, H$_2$S, and the alkalies. Upper limits are consistent with a nondetection as shown in Part II. These results are also broadly consistent with expectations from chemical equilibrium predictions: H$_2$O, CH$_4$, and NH$_3$ are expected to be more dominant species than CO, CO$_2$, H$_2$S, and the alkali metals (Burrows & Sharp 1999).

Section 4.3.2 highlights trends identified in both NH$_3$ and alkali metals. First, we discuss the derived bulk atmospheric metallicity and C/O ratios.

4.3.1. Metallicity and C/O

The elemental abundance inventory of a substellar object is important to its evolutionary history, as it governs the total atmospheric opacity and therefore the cooling rate as well (Burrows et al. 2001). It is important to understand the elemental abundances in brown dwarfs in order to place them into compositional context with both higher-mass stars and lower-mass planets.

One would expect the population of field brown dwarfs to have an elemental abundance pattern similar to that of stars, given that both objects are thought to form via fragmentation within a molecular cloud. To contrast this, planets that are formed in protoplanetary disks can undergo migration within that disk. The existence of ice lines and dynamical models of migration have led to a range of predictions regarding planet mass atmospheric elemental abundances. These can range any where from “stellar composition” to high metallicity (>100 $\times$ Solar, (e.g., Fortney et al. 2013; Mordasini et al. 2016)) or high carbon-to-oxygen ratios (C/O > 1, (e.g., Öberg et al. 2011; Helling et al. 2014; Madhusudhan et al. 2014; Eistrup et al. 2016)). Identifying at what mass, in general, the diversity in composition substantially increases can ultimately assist us in truly bridging the gap between stars and planets.

Because brown dwarfs sit between these mass limits, determining elemental abundances for a large number of substellar objects can help us to accomplish that goal.

There are several challenging aspects to determining the elemental abundance of a brown dwarf. First, at these cooler temperatures, the chemical inventory is largely in the form of molecular (rather than elemental) species. Molecules have
much more complex spectroscopic features than atomic species with broad and deep roto-vibrational bands that overwhelm the spectral continuum, an oft-used handle to obtain basic bulk parameters for hotter stars (e.g., Bean et al. 2006). Additionally, some molecular species are thought to be affected by both equilibrium condensate rainout and vertical disequilibrium mixing, while others can retain uniform chemical abundance profiles throughout the atmosphere (e.g., Burrows et al. 2001; Sharp & Burrows 2007). Therefore, in order to accurately characterize the atmospheres of brown dwarfs, one must include the key molecular components covered over their bandpass, as well as the relevant chemical and dynamical processes that could affect such constituents.

Here, we focus our elemental abundance results only on the metallicity and C/O ratios, as these are the most readily determinable elemental ratios for objects at these temperatures. Water and methane contain a bulk of the atmospheric metal content (C and O) for atmospheres cooler than ≤1000 K. We determine the metallicity and C/O directly from the retrieved molecular abundances. The metallicity is computed by summing the molecular metal content (e.g., M = H2O+2CO+3CO2+NH3+Na+K+CH4+H2S), then dividing by the background hydrogen content (H = 2H2+4CH4+3NH3+2H2O+2H2S), and finally normalizing by the solar M/H fraction to obtain our final “metallicity” ([M/H] = log((M/H)/(M/H)_{solar})). The C/O is determined by dividing the total carbon (CO+CO2+CH4) by the total oxygen (H2O+CO+2CO2).

For both the metallicity and C/O, really, it is the water and methane that dominate. We point out, as in Parts I and II, that this is a measure of the atmospheric elemental abundance inventory. The bulk abundances can only be determined via chemical assumptions. Specifically, it is predicted that condensate rain out by silicates (enstatite, forsterite) can sequester oxygen by effectively locking it into condensates that “rain” out of the atmosphere and no longer react with the surrounding gas (e.g., Fegley & Lodders 1994). As in Part I, we apply a correction factor to the C/O and metallicity by weighting the water abundance by a factor of 1.3 to accommodate for the lost O.

Figure 4 shows the results of our retrieved metallicity and C/O constraints (circles) compared to the results for late-T dwarfs in Part II (squares), as well as a representative sample of these parameters from nearby FGK stars (gray circles) (Hinkel et al. 2014). Overplotted (triangles) are the results for W2212, W1639, W1405, and W1541, for which the retrieved abundances—and thus, C/O and metallicities—are dependent upon the choice of priors for evolutionary parameters and should be interpreted with caution (Section 4.2). Plotted here are the results under the “free” retrieval assumption, to be consistent with the objects in Part II.

If we find that our metallicities are slightly enhanced, but overall broadly consistent with the local FGK stellar population. Our C/O values are consistent with the results of both Part II and the stellar population. We note that there appears to be no correlation between the effective temperature and metallicity or C/O for our sample. In Part II, we discussed an apparent trend of increasing C/O with increasing metallicity for the late-Ts that could potentially be explained by supersolar [Si/O] ratios affecting the efficiency of oxygen rainout into silicates. We find no such trend when our new late-T and early-Y sample is included, even if one were to discount the objects with questionable constraints.

4.3.2. Chemical Trends

One of the defining features of a classic retrieval is its ability to directly constrain atmospheric molecular abundances from the spectra, free from the a priori assumptions commonly made in self-consistent models. Molecular abundance trends with other properties provide insight into the chemical and physical processes operating in the atmospheres. The retrieved molecular abundances for the ensemble of HST WFC3 late-T and early-Y dwarf are given in Table 4. Here, we focus on how these abundances vary with effective temperature as this is predicted to be the dominant abundance controlling factor through equilibrium chemistry (Burrows & Sharp 1999; Lodders & Fegley 2002; Sharp & Burrows 2007).

Figure 5 summarizes these trends (red, yellow points) in comparison to predictions from a self-consistent grid model (black curves) and to those derived for the warmer T-dwarfs from Part II (blue points). Our chosen grid model was introduced and validated in Piskorz et al. (2018) and Bonnefoy et al. (2018). We produce a grid of models given T_{eff}, log(g), metallicity, and assuming radiative-convective thermochemical equilibrium. The molecular abundance curves here represent the column-weighted mixing ratio over the photosphere.

We find that the H2O and CH4 abundances show a systematic offset between the late-T and early-Y sample. For context, we have also plotted column-integrated abundance trends from our grid model, showing that the variation we see between the two samples is largely reproducible by variations in both the C/O ratio and the metallicity of the system. This falls in line with predictions from equilibrium chemistry: namely, that H2O and CH4 remain relatively constant for a given set of elemental abundance assumptions, and neither molecule should be sensitive to other chemical processes such as vertical disequilibrium mixing (Burrows & Sharp 1999; Sharp & Burrows 2007).

Part II found no systematic trend in the ammonia abundance with effective temperature, despite thermochemical equilibrium.
predicting a ∼0.5 dex increase over the 800–600K temperature range for a given metallicity. Ammonia is well-known to be influenced by vertical mixing at these cool temperatures. Vertical mixing is expected to quench the ammonia abundance to one order of magnitude lower than the equilibrium abundance over the photospheric layers (Saumon et al. 2006; Marley & Robinson 2015).

However, we note that, with the addition of our sample, we see a slight trend of increasing ammonia that is largely consistent with thermochemical equilibrium assumptions at a range of metallicities and gravities. Note that we have not included the yellow points in this analysis, given the complications (highlighted in Section 4.2) with these objects. Though it is possible that the ammonia in the atmospheres of these objects is being affected by disequilibrium mixing at varying strengths, the ability to test such ideas quickly becomes limited by both the sparse number of retrieved NH$_3$ abundances and the precision of our retrieval constraints.

A more striking compositional trend, extending far beyond the results in Part II, is that of the alkali metals with temperature. The retrieved Y-dwarf alkali abundances fall off substantially with temperature relative to the warmer T-dwarfs. In all but two cases (W0325, W0335), we only obtain upper limits on the alkali abundances, due to the lack of detectability. These results are consistent with predictions from equilibrium rainout chemistry (blue, solid) and strongly disfavor pure equilibrium (blue-dashed, from Burrows et al. 2001). Pure equilibrium permits the existence of aluminum and silicates in the middle atmosphere; they achieve equilibrium with the Na and K to form sanidine (KAlSi$_3$O$_8$) and albite (NaAlSi$_3$O$_8$) (Burrows et al. 2001), resulting in a rapid depletion of gaseous Na and K at ∼1300 K. In contrast, rainout rapidly removes aluminum/silicates, leaving behind the gas-phase alkalis until ∼700 K, where they begin to condense into KCl and Na$_2$S (e.g., Burrows et al. 2001). These results are the first to show that a number of indirect lines of evidence for rainout from both precomputed grid models (e.g., Marley et al. 2002; Morley et al. 2012, 2014) and observations of reddening Y–J colors (e.g., Liu et al. 2012; Schneider et al. 2015) are directly owed to the depletion of Na and K.

Figure 5. Constraints on our retrieved molecular abundances for H$_2$O (upper left), CH$_4$ (upper right), NH$_3$ (lower left), and Na+K (lower right) in units of Volume Mixing Ratio (VMR). Blue points are results from the hotter late-T sample in Part II. Red points are objects of this study whose abundances do not strongly depend on our assumptions of evolutionary priors (log(g), radius, mass), while yellow points are objects whose abundances are sensitive to these assumptions and should be interpreted with caution (see Section 4.2). Overlaid are grid model profiles for various metallicites, C/O ratios, and rainout assumptions. Unless stated otherwise, curves are 1x solar composition with assumed thermochemical equilibrium. Pure equilibrium trend from Burrows et al (2001).
We obtain two bound constraints for W0325 and W0335, and only lower limits for cooler targets, as the alkalis deplete below retrievable abundances. We note that the one anomalous lower limit at roughly 650K is W1639, whose temperature structure strongly deviates from the typical radiative-convective equilibrium. As a result, it is not surprising to structure strongly deviates from the typical radiative-convective equilibrium. As a result, it is not surprising to lower limit at roughly 650K is W1639, whose temperature below retrievable abundances. We note that the one anomalous constraints for our three other objects with questionable abundance shifted from the remainder of our curve. Additionally, the upper limit for the abundance of this target is systematically result of only obtaining upper limits for these targets.

Improved S/N and spectral resolution with JWST, particularly at the blue end of the Y band and near roughly 1.2 μm where the resonance features for Na and K peak, should allow us to probe cooler objects with far more depleted alkali abundances or uniquely constrain both Na and K independent of each other. In addition, improved NH3 constraints on a larger number of Y dwarfs may also allow us to directly confirm the presence of vertical disequilibrium mixing in the future.

4.4. Grid Model Fitting

While it is helpful that the retrieval-based approach places as little a priori information as possible into the atmospheric model, it is still prudent to compare such results against a grid-based model. Grid models incorporate more assumptions and are presumably more self-consistent, in that they often treat the atmosphere under radiative-convective-thermochemical equilibrium whereas our retrieval method makes no such assumptions. This is useful in the investigation of both missing model physics within the established grid models and any possible nonphysical results from the retrieval method, as we have seen with our evolutionary parameters.

We use a newly developed grid of self-consistent, cloud-free atmospheric models called Self-consistent CHIMERA (ScCHIMERA) (Bonnefoy et al. 2018; Piskorz et al. 2018). ScCHIMERA utilizes the same underlying radiative transfer and opacity sources as the retrieval forward model. Briefly, the self-consistent model solves for layer midpoint fluxes using the Toon et al. (1989) two-stream source function approach. The model is iterated to radiative equilibrium via the Newton-Raphson method until there is zero net flux divergence throughout the column. Convection is implemented through a mixing length flux (e.g., Marley & Robinson 2015). Line-by-line cross sections are converted to \( R = 100 \) correlated-K coefficients between 0.3 and 100 μm (using 20 Gauss quadrature points per wavenumber bin) via the "resort-rebin" (Amundsen et al. 2017) optical depth approach, in order to speed up efficiency while maintaining accurate flux computations. The converged models are "post-processed" to an \( R = 1000 \) (again with correlated-K). These moderate-resolution spectra are then convolved and binned to the data wavelength grid when undergoing fitting. The grid is generated as a function of \( T_{\text{eff}} \), \( \log(g) \), [M/H], the C/O ratio, and the vertical eddy diffusion \( K_{\text{v}} \) (through the Zahnle & Marley (2014) quench-timescale framework). The grid model parameter ranges and step sizes are given in Table 5. We fit each object with this five-dimensional grid using emcee and an interpolating function (a variant of Python’s griddata routine). We have also experimented with different subsets of parameters (e.g., fitting for only \( \log(g) \) and \( T_{\text{eff}} \) while fixing composition to solar).

4.4. Grid Model Fitting

While it is helpful that the retrieval-based approach places as little a priori information as possible into the atmospheric model, it is still prudent to compare such results against a grid-based model. Grid models incorporate more assumptions and are presumably more self-consistent, in that they often treat the atmosphere under radiative-convective-thermochemical equilibrium whereas our retrieval method makes no such assumptions. This is useful in the investigation of both missing model physics within the established grid models and any possible nonphysical results from the retrieval method, as we have seen with our evolutionary parameters.

We use a newly developed grid of self-consistent, cloud-free atmospheric models called Self-consistent CHIMERA (ScCHIMERA) (Bonnefoy et al. 2018; Piskorz et al. 2018). ScCHIMERA utilizes the same underlying radiative transfer and opacity sources as the retrieval forward model. Briefly, the self-consistent model solves for layer midpoint fluxes using the Toon et al. (1989) two-stream source function approach. The model is iterated to radiative equilibrium via the Newton-Raphson method until there is zero net flux divergence throughout the column. Convection is implemented through a mixing length flux (e.g., Marley & Robinson 2015). Line-by-line cross sections are converted to \( R = 100 \) correlated-K coefficients between 0.3 and 100 μm (using 20 Gauss quadrature points per wavenumber bin) via the "resort-rebin" (Amundsen et al. 2017) optical depth approach, in order to speed up efficiency while maintaining accurate flux computations. The converged models are "post-processed" to an \( R = 1000 \) (again with correlated-K). These moderate-resolution spectra are then convolved and binned to the data wavelength grid when undergoing fitting. The grid is generated as a function of \( T_{\text{eff}} \), \( \log(g) \), [M/H], the C/O ratio, and the vertical eddy diffusion \( K_{\text{v}} \) (through the Zahnle & Marley (2014) quench-timescale framework). The grid model parameter ranges and step sizes are given in Table 5. We fit each object with this five-dimensional grid using emcee and an interpolating function (a variant of Python’s griddata routine). We have also experimented with different subsets of parameters (e.g., fitting for only \( \log(g) \) and \( T_{\text{eff}} \) while fixing composition to solar).

### Table 5

| Parameter   | Range  | Step Size |
|-------------|--------|-----------|
| \( T_{\text{eff}} \) [K] | 300–950 | 50        |
| \( \log(g) \) (cgs) | 3.0–5.5 | 0.5       |
| [M/H]       | –1–1   | 0.5       |
| C/O         | 0.1–0.7 | 0.2       |
| \( \log(K_{\text{v}}) \) | 0.7–0.9 | 0.05      |

**Figure 6.** Top: best-fit grid-model (blue) and retrieval (red) results for W0404. With only four free parameters \( T_{\text{eff}}, \log(g), [\text{M/H}], \) and \( R, \) the grid model struggles to well-fit the entire \( YJK \)-band spectra with systematic offsets in each band. Comparing the Bayesian Information Criterion (BIC) between both models suggests the retrieval method is highly preferred. Bottom: marginalized posteriors for the relevant free parameters in each model. The poor fit of the grid model often disagrees with the retrieval model and obtains nonphysical constraints.

Figure 6 shows an example comparison (for W0404) between the grid model solutions and the retrieval solutions. In this specific instance, \( T_{\text{eff}}, \log(g), [\text{M/H}], \) and the radius-to-distance scaling are the free parameters of the grid with no quenching. From a visual standpoint, there are noticeable differences between the grid model fit and the retrieval fit. The best-fitting grid model underfits the \( Y \)-band peak and overestimates the \( J \)-band peak by \( \sim 10\%–20\% \), as well as the entire blue edge of the \( H \)-band. This issue of overestimating the \( J \) band, underestimating the \( Y \) and \( H \) bands, or both, is consistent across all of our objects. This result is also not unique to our
grid model, as previous works using other cloud-free grid models have had similar issues (Schneider et al. 2015; Leggett et al. 2017).

The best grid model fit produces a $\chi^2/N = 4.05$, compared to the retrieval’s $\chi^2/N = 1.36$. We utilize the Bayesian information criterion (BIC) to determine the balance between improved fit and increased parameters, as well as whether the retrieval parameters are indeed justified. The retrieval forward model includes 31 free parameters and 175 data points (we stop at 1 $\mu$m, due to constraints on the molecular cross sections), giving a BIC = 379. The self-consistent grid fit has only four free parameters (in this example) and 212 data points (the grid model goes down to 0.9 $\mu$m), resulting in a BIC = 880. The $\Delta$ BIC = 501 overwhelmingly favors the retrieval fit according the Jeffery’s Scale (Kass & Raftery 1995). Regardless of the number of free parameters we include in our grid model (including the vertical mixing and C/O ratio dimensions), we often find similar misfits.

Figure 6 also compares the retrieval and grid-model constraints on effective temperature, gravity, metallicity, and radius. We find (consistent among our other objects) that the retrieval and grid models often disagree by at least several sigma in almost all model parameters. In the specific example of W0404, the effective temperature derived from the grid model disagrees with our retrieval result by over 100K, the gravity estimate is inconsistent by almost a full order of magnitude, the metallicity is subsolar for the grid model yet supersolar for our retrieval, and the radius is inflated in the grid model fit.

For our other targets, the grid model often requires either unphysically high or low radii, masses, and gravities for typical field brown dwarfs, as well as effective temperatures inconsistent with previously measured spectral types. A full database of all fits, along with resulting model parameters, is available at our previously linked Zenodo site. This highlights the need for a retrieval methodology to fully utilize the information content contained in substellar atmospheric spectra in order to accurately characterize both current and future data sets.

5. JWST Simulation Constraints

JWST promises to revolutionize our knowledge of brown dwarf atmospheres, due to a vastly improved wavelength coverage across the near- and mid-infrared, combined with improved S/N and spectral resolution (Marley & Leggett 2009). Here, we take a preliminary look at the potential improvement in our retrieval parameters with JWST for a representative T9 object (W0404).

We take the model that best fits the HST data for W0404 (i.e., our best-fit model with the parameters specified in Tables 3, 4, and associated figures) and simulate both Near-InfraRed Spectrometer (NIRSpec) PRISM and Mid-InfraRed Instrument, Low-Resolution Spectroscopy (MIRI LRS) observations using the JWST Exposure Time Calculator (ETC) v1.3. We chose the largest 1.6′′ slit for the PRISM/CLEAR configuration and a slitless spectroscopy mode for MIRI LRS, in order to minimize potential systematic slit losses from the instrument. We set the integration time to obtain, somewhat arbitrarily, S/N $\approx$ 200 at the J-band peak within the PRISM mode and S/Ns $\approx$ 10 over MIRI LRS. We found this to be achievable with respective exposure times of 15 minutes and 1 hr on NIRSpec and MIRI.

We then applied the same retrieval tools to this simulated data set, under the same exact model assumptions, comparing three cases: WFC3 only (this work), WFC3+MIRI LRS, and NIRSpec PRISM only (Figure 7). Figure 8 summarizes the constraints (red = WFC3 only, blue = WFC3+MIRI, green = NIRSpec only). It is clear that JWST will provide astounding improvements on the molecular abundances, gravity, and temperature profile. For example, we find that the H$_2$O abundance constraint improves from $\pm$0.1 dex for WFC3 to roughly $\pm$0.06 dex for WFC3 combined with an hour of MIRI LRS integration time, and better than $\pm$10% for only 15 minutes of NIRSpec integration time. These extremely tight constraints approach the precision of remote solar system–quality science on brown dwarfs, and speak to the utility of JWST to well-characterize nearby substellar atmospheres in the future.

One caveat here is that this analysis makes the assumption that our model that best fits the YJH bands of WFC3 is an accurate representation of the object’s spectra at both longer wavelengths and higher spectral resolutions. Additionally, such an analysis does not account for any potential systematics, currently known or unknown, that will impact the future performance of JWST but are not properly accounted for in the JWST ETC. These systematic biases between instruments, or within JWST itself, will lower the precision of constraints shown here. Despite these limitations, such an analysis provides a first step toward understanding how well JWST will be able to constrain atmospheric properties of cool brown dwarfs.

6. Conclusions

We have extended the work of previous investigations, using a well-vetted atmospheric retrieval approach into the cooler Y-dwarf spectral class. This is done by comparing our model to a set of uniformly reduced, low-resolution WFC3 measurements for an ensemble of late-T and early-Y dwarfs. Such a methodology has provided the first direct constraints on the chemical composition of cool Y dwarfs and provides a foundational data set that can be compared to future low-mass characterization work. Our main scientific results are as follows:

1. We are able to well-fit our ensemble of late-T and early-Y dwarfs with our retrieval model across the YJH bands as shown in Figure 1, Section 4. We find no systematic deviations from the data in our residuals. This is in contrast to typical grid modeling efforts, which often miss key spectral features of these cooler objects.

2. Overall, the retrieved temperature structures are consistent with radiative-convective equilibrium, except in the marked case of W1639, whose peculiar Y-band structure may be indicative of a non-radiative–convective equilibrium structure in Figure 1, Section 4.1. However, inconsistencies in derived evolutionary parameters may also indicate that our model is not well-adapted to explaining the odd Y-band structure.

3. For most of our objects, we obtain mass estimates that are consistent with field-age brown dwarfs, but systematically smaller radii and higher gravities than allowable with evolutionary models (see Figure 3, Section 4.2). We attempted a myriad of tests on both the observational data and our retrieval model, in an effort to discover the cause
Figure 7. Top: best-fit spectrum (blue) for a combined WFC3 observation (1–1.7 \( \mu m \), red) and JWST MIRI LRS simulation (5–14 \( \mu m \), gray). Bottom: best-fit spectrum (green) for a simulated JWST NIRSpec PRISM spectrum (gray). NIRSpec provides a vastly improved S/N (200 vs. 10) with a much shorter exposure time (15 minutes vs. 1 hr) as compared to MIRI LRS.

Figure 8. Best-fitting model parameters from our analysis of WFC3 spectra (red). Overlaid are the resulting JWST NIRCam PRISM data points and error estimates from the ETC (green). An additional retrieval using a combined WFC3 and MIRI LRS spectrum is also shown for comparison (blue). A NIRCam PRISM observation provides substantially higher precision on molecular abundances and atmospheric structure than a combined WFC3 and MIRI LSR spectrum, for about a quarter of the JWST exposure time.
of this deviation. Using a distance estimate from another parallax program, we found that W2056’s anomalously high gravity could be explained by a systematic bias in the distance estimate. If the distances are all systematically underestimated, this would explain both our high gravities and the lower radii for the majority of our objects. More importantly, this indicates how sensitive our retrieved results can be to small changes in distance estimates. The results of the coldest Y dwarfs, W1405 and W1541, are speculative at best, given that the retrieved masses and radii are inconsistent with known limits for field-age brown dwarfs.

4. We obtain the first direct bound constraints or upper limits on H₂O, CH₄, CO, CO₂, H₂S, NH₃, and Na+K for an ensemble of cool Y dwarfs (see Section 4.3). From these measurements, we drive preliminary C/O and metallicity estimates that, when oxygen sequestering via chemical rainout of silicates is taken into account, are broadly consistent with the local FGK stellar population, albeit at slightly enhanced metallicity.

5. On the basis of these measurements, we investigate chemical trends with $T_{\text{eff}}$ that are diagnostic of the chemical mechanisms at work in the atmospheres of brown dwarfs. We find that H₂O and CH₄ are consistent with expected chemical equilibrium predictions and are not subject to either chemical rainout or vertical disequilibrium mixing. NH₃ may show a tentative trend with either pure chemical equilibrium or disequilibrium vertical mixing. Improved constraints from JWST would be more diagnostic of this trend, and may be able to constrain the strength of mixing. Finally, Na+K shows a trend consistent with both chemical rainout and the results in Part II, as opposed to pure chemical equilibrium. This result confirms that the blueshift in the Y–J color photometry across the T/Y boundary is owed to the depletion of alkali metals.

6. We make predictions for future JWST observations for cool late-T and early-Y dwarf targets. We find that NIRSpec offers the best observing mode for high-precision abundance measurements of nearby brown dwarfs, approaching that of current bulk solar system–quality measurements. Such high-precision abundance measurements provide a useful diagnostic for future modeling efforts to understand cool, substellar atmospheres.

We thank Roxana Lupu and Richard Freedman for continued development and support of their extensive opacity database, which makes much of this work possible. We also thank Dan Foreman-Mackey for his publicly available EMCEE code and the useful plotting routine corner.py. We thank Adam Schenider, Mark Marley, Jennifer Patience, Laura Kreidberg, Michael Cushing, Jackey Faherty, Trent Dupuy, and Wanda Feng for the many comments, discussions, and tools they provided, which have improved this work. This research has benefited from the Y Dwarf Compendium maintained by Michael Cushing at https://sites.google.com/view/ydwarfcompendium/. This material is based upon work supported by the National Science Foundation under grant No. AST-1615220.
