An Open-source Bayesian Atmospheric Radiative Transfer (BART) Code. III. Initialization, Atmospheric Profile Generator, Post-processing Routines

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Abstract

This and companion papers by Harrington et al. and Cubillos et al. describe an open-source retrieval framework, Bayesian Atmospheric Radiative Transfer (BART), available to the community under the reproducible-research license via https://github.com/exosports/BART. BART is a radiative transfer code (transit; https://github.com/exosports/transit; Rojo et al.), initialized by the Thermochemical Equilibrium Abundances (TEA; https://github.com/dzesmin/TEA) code (Blecic et al.), and driven through the parameter phase space by a differential-evolution Markov Chain Monte Carlo (MC3; https://github.com/cubillos/mc3) sampler (Cubillos et al.). In this paper we give a brief description of the framework and its modules that can be used separately for other scientific purposes; outline the retrieval analysis flow; present the initialization routines, describing in detail the atmospheric profile generator and the temperature and species parameterizations; and specify the post-processing routines and outputs, concentrating on the spectrum band integrator, the best-fit model selection, and the contribution functions. We also present an atmospheric analysis of WASP-43b secondary eclipse data obtained from space- and ground-based observations. We compare our results with the results from the literature and investigate how the inclusion of additional opacity sources influences the best-fit model.

Unified Astronomy Thesaurus concepts: Planetary atmospheres (1244); Uncertainty bounds (1917); Astrostatistics techniques (1886); Open source software (1866); Exoplanet systems (484); Exoplanet atmospheric composition (2021)

1. Introduction

The rapid increase of detected extrasolar planets in the past decade (4375 confirmed and 2614 candidates as of 2021 April; https://exoplanetarchive.ipac.caltech.edu) and the number of novel techniques employed to analyze their data (e.g., Swain et al. 2008; Knutson et al. 2009a; Carter & Winn 2010; de Wit et al. 2012; Stevenson et al. 2012; Deming et al. 2013, 2015; May & Stevenson 2020; Challener et al. 2021) have prompted theorists to develop different approaches to model their atmospheres. To get insights into their thermal structures and chemical compositions, initial methods started from first principles in a one-dimensional (1D) scheme (e.g., Fortney et al. 2005) and later developed into complex three-dimensional (3D) models that studied the atmospheric dynamics and circulations (e.g., Showman et al. 2009; Dobbs-Dixon & Agol 2013).

Today, we have several major approaches to atmospheric modeling. One applies a direct, forward-modeling technique that provides a set of parameters to generate the observed spectra (e.g., Burrows et al. 2008; Fortney et al. 2008a; Sing et al. 2016); another utilizes observations to determine the model’s best-fit parameters and their uncertainties; and the most recent one applies machine-learning methods that use a precomputed grid of atmospheric models to retrieve the full posterior distribution of parameters (Márquez-Neila et al. 2018; Zingales & Waldmann 2018; Cobb et al. 2019; Oreshenko et al. 2020).

The inverse, retrieval approach, such as the one implemented in the framework we present here, determines the properties of the planetary atmosphere based on the available observations. It uses a statistical algorithm, usually a Markov Chain Monte Carlo (MCMC) method, or nested sampling (e.g., Ford 2005; Skilling 2006, and references within) to estimate the posterior distribution of the model given the data. By searching for the regions of space that fit data the best, this approach also determines the uncertainties in the model parameters.

Today, we have more than a handful of retrieval frameworks used in the exoplanetary field that implement various complexities of physical phenomena, statistical criteria, and optimization techniques. In the study of exoplanetary atmospheres, the retrieval approach was first introduced by Madhusudhan & Seager (2009). They used a multidimensional grid-optimization scheme within a radiative transfer model to explore the phase...
space of model parameters. In their following paper, Madhusudhan & Seager (2010) utilized the first application of an MCMC algorithm. Soon after, Lee et al. (2012) introduced a nonlinear estimation algorithm NEMESIS (Irwin et al. 2008; Rodgers 2000) that applied the correlated-k technique, allowing for a rapid description of the model spectra and an order-of-magnitude-faster exploration of the phase space than previous line-by-line algorithms. Their method also required fewer model evaluations, attributed to the assumption that the parameter error distributions are Gaussians, and offered a single best-fit solution calculated using the Levenberg–Marquardt algorithm (Levenberg 1944; Marquardt 1963). The same year, Benneke & Seager (2012) released another Bayesian retrieval algorithm (later called SCARLET; Fraine et al. 2014). This framework introduced the parameter credible regions, considered non-Gaussian uncertainties of the model parameters, employed a radiative-convective model to calculate the temperature profile, and allowed for the presence of a cloud deck or solid surface. The following year, Benneke & Seager (2013) went a step further and introduced, for the first time, the nested-sampling algorithm for efficient parameter exploration (Skilling 2004; Feroz & Hobson 2008) and a Bayesian model comparison via Bayesian evidence (Gregory 2007; Trotta 2008). In 2013, Line et al. (2013) presented CHIMERA and tested three retrieval exploration algorithms: optimal estimation, differential-evolution MCMC (DEMC), and bootstrap Monte Carlo.

Several years later, Waldmann et al. (2015) introduced the \( \tau \)-REx code that utilized the molecular line lists from the ExoMol project and a custom-built software that identifies likely absorbers/emitters in the spectra. In 2017, Lavie et al. (2017) released the HELIOS-R open-source code that uses the PyMultiNest package (Buchner et al. 2014) and can apply free or self-consistent equilibrium chemistry retrieval. The same year, Wakeford et al. (2017) and Evans et al. (2017) published a Bayesian framework based on the 1D forward model ATMO (Tremblin et al. 2015), and MacDonald & Madhusudhan (2017b) introduced POSEIDON, a two-dimensional (2D) atmospheric retrieval algorithm that includes inhomogeneous cloud prescription. A year after, the same group (Gandhi & Madhusudhan 2018) presented a new disequilibrium retrieval framework, HYDRA, that introduced a self-consistent model to constrain layer-by-layer deviations from chemical and radiative-convective equilibrium. Since then, two open-source codes have been published: petitRADTRANS, which uses the correlated-k method and implements various cloud parameterizations (Mollière et al. 2019), and PLATON (Zhang et al. 2019), which implements a two-parameter, equilibrium chemistry model and includes a Mie-scattering cloud model and unocculted starspot corrections. Also, most of the previous frameworks got upgraded: the NEMESIS framework (Barstow et al. 2020) now includes the PyMultiNest algorithm (Buchner et al. 2014; Krissansen-Totton et al. 2018) and multiple parameterized cloud models (Barstow 2020), and the HELIOS-R code implemented the first hybrid CPU-GPU approach (Kitzmann et al. 2020). Very recently, Min et al. (2020) presented the ARCIS retrieval framework, which combines a self-consistent physical modeling with a parameterized approach.

Here we present another open-source framework, the Bayesian Atmospheric Radiative Transfer (BART) code for forward and retrieval modeling. This paper is one of three papers that describe the architecture, individual modules and packages, and theory implemented in this code. Figure 1 shows a simplified flow of the BART code. The underlying theory and the code structure of the modules and packages marked by the stars will be covered in more detail in this paper. The radiative transfer module is described in the collaborative paper by Cubillos et al. (2022). The overall design of the code, validation tests, performance, and optimization are described in the collaborative paper by Harrington et al. (2022). In addition, each paper presents an atmospheric analysis of a hot exoplanet using BART, showing its diverse features.

**Figure 1.** Simplified BART flow chart. In purple are the three major BART modules. TEA and MC3 are written in Python, while transit is written in C. Other supporting modules are written in Python and given in yellow. In white are the inputs/outputs of each module. In green are the input files. In blue are transit and eclipse ray-path-solution submodules. Stars denote modules and packages that will be described in more detail in this paper.
In Section 2, we present BART and describe the implementation of the initialization routines, atmospheric profile generator, spectrum integrator, best-fit routines, and contribution function module. We also briefly outline the characteristics of the three major modules: TEA, \texttt{transit}, and MC3, which are described in detail in Blecic et al. (2016), Cubillos et al. (2022), and Cubillos et al. (2017), respectively. In Section 3, we present an atmospheric analysis of WASP-43b secondary eclipse data using BART. In Section 4, we give a short summary and our conclusions.

2. The Bayesian Atmospheric Radiative Transfer Code

BART is an open-source Bayesian, thermochemical, radiative transfer code written in Python and C available to the community under the Reproducible-Research Software License via https://github.com/exosports/BART. It consists of three major parts (Figure 1, purple boxes): the Thermochemical Equilibrium Abundances module (TEA; see Section 2.3), a radiative transfer module (\texttt{transit}; see Section 2.5), and the Multicore Markov Chain Monte Carlo statistical module (MC3; see Section 2.4). Each of the modules works independently and can be used for other scientific purposes. TEA is an open-source thermochemical equilibrium abundances code that calculates the volume mixing fraction of gaseous molecular species (Blecic et al. 2016, https://github.com/dzesmin/TEA). \texttt{Transit} is an open-source radiative transfer code that applies a 1D opacity-sampling computation to generate model spectra (see the collaborative paper by Cubillos et al. 2022, https://github.com/exosports/transit). MC3 is an open-source Bayesian framework that estimates a posterior distribution and the best-fit model (Cubillos et al. 2017; https://github.com/pcubillos/mc3).

To start off retrieval (Figure 1), BART generates an initial atmospheric model (see Section 2.1). Given a range of pressures, BART evaluates the temperature profile by using one of several parameterization schemes (see Section 2.2). Then, for given elemental and molecular species, the species volume mixing ratios are calculated using the TEA module (see Section 2.3) or a routine that produces vertically uniform abundance profiles. Arbitrary abundance profiles may also be used. The terms of the temperature–pressure, $T(p)$, profile and species abundances are free parameters.

Given an initial guess, the atmospheric generator produces the atmospheric model, passes it to \texttt{transit} (see Section 2.5) to calculate the transit or eclipse spectrum, and integrates the spectrum over the observational bandpasses (see Section 2.6). The band-integrated values are sent to MC3 to compare them against the observations and calculate $\chi^2$. Then, MC3 generates a new set of free parameters, repeating the process until the phase space of all parameters is fully explored, and two convergence criteria, the Gelman and Rubin convergence test (Gelman & Rubin 1992) and the desired number of effectively independent samples (ESS), are satisfied (see Harrington et al. 2022, Section 5 and Appendix C for more details on the ESS criterion).

The best-fit parameters are then used to run the \texttt{transit} module once more to reproduce the spectrum of the best-fit model atmosphere (see Section 2.7). In this run, \texttt{transit} generates a file with the optical depth values for each atmospheric layer and wavelength, which is used to calculate the contribution functions of each observation (see Section 2.8).

Finally, BART returns the best-fit parameters’ values and credible regions and plots the best-fit spectrum, the $T(p)$ and abundance profiles, and the contribution functions. In addition, MC3 plots the parameters’ traces, pairwise posterior distributions, and marginal posterior histograms.

In the following sections, we describe in more detail the implementation of the initialization routines (Section 2.1), the atmospheric profile generator (Section 2.2), the spectrum integrator (Section 2.6), the best-fit routines (Section 2.7), and the contribution function module (Section 2.8). In Sections 2.3, 2.4, and 2.5 we briefly describe TEA, MC3, and \texttt{transit} modules for completeness, but we refer the reader to Blecic et al. (2016), Cubillos et al. (2017), and Cubillos et al. (2022), respectively, where we describe these codes in detail.

2.1. BART Initialization

BART configures an initial model atmosphere following the user’s educated guess about the planetary temperature, pressure, and species volume mixing ratios (abundances) at each atmospheric layer. The choice of this initial model atmosphere does not influence the final result (but could speed up the convergence), in the case when, as assumed in BART, one retrieves constant-with-altitude abundance profiles. The $T(p)$ profile can be generated using either parameterized or isothermal schemes, while the chemical species can be calculated either using the TEA code or assuming vertically uniform profiles. The initial configuration parameters are set in an ASCII file, BART.cfg, that carries, in addition, the full set of other parameters to run retrieval. BART driver, BART.py, accepts this file and executes all modules and subroutines. It communicates the initial parameters to MC3 for reference but also runs the initialization instead of the Atmospheric Profile Generator on the first iteration. Figure 2 shows a simplified execution order of the routines called in BART.py. Section \texttt{Init} outlines steps executed to generate the initial atmospheric profile based on the user’s choice of the elemental and molecular species, elemental volume mixing ratios, C/O ratio, metallicity, and whether chemical equilibrium or uniform abundances are assumed. Section \texttt{Run MCMC Loop} is described in the collaborative paper by Cubillos et al. (2022), and Section \texttt{Run Best Fit} is described in Section 2.7 of this paper.

2.2. Atmospheric Profile Generator

Once the initial atmospheric model is generated and compared to the observations using a radiative transfer algorithm (\texttt{transit}), any subsequent atmospheric models are generated using the atmospheric profile generator (see Figure 1).

This submodule generates models based on the parameters passed by a statistical algorithm (MC3). To calculate the abundances of free chemical species, BART changes the initial abundance profiles using one scaling factor per species. To create a $T(p)$ profile, BART can currently use one of four parameterized temperature profile schemes: isothermal, adiabatic, one originally developed by Guillot (2010), and one based on the parameterization described in Madhusudhan & Seager (2009).

The isothermal parameterization scheme, often utilized in transmission geometry, uses one free parameter, $T_{\text{iso}}$, assuming the same temperature across all altitudes. The adiabatic parameterization scheme, originally developed for brown dwarf atmospheres, assumes that an adiabat is driven
by the relationship \( p^{1-\gamma}T^\gamma = \text{constant} \), where \( \gamma \) is the ratio of specific heats at constant pressure and constant volume. The temperature as a function of pressure \( p \) is then given as

\[
T = T_0\left[ 1 + \frac{\gamma - 1}{\gamma}\ln\left(\frac{p_0}{p}\right) \right]
\]

and has three free parameters: reference temperature \( T_0 \), reference pressure \( p_0 \), and \( \gamma \).

The last two parameterization schemes, utilized most often in the eclipse geometry, allow for more complex temperature profiles to be explored in retrieval. We denote them as T-Parameterization schemes I and II, and in the following Sections 2.2.1 and 2.2.2 we outline their basic equations implemented in BART. More details about the parameters and physics behind these models can be found in Line et al. (2013) and Madhusudhan & Seager (2009), respectively, while details on the limitations of these approaches are discussed in Heng et al. (2014), Blecic et al. (2017), and Parmentier & Guillot (2014).

### 2.2.1. T-Parameterization Scheme I

This parameterization scheme was originally formulated by Guillot (2010) and subsequently modified by Heng et al. (2012), Line et al. (2013), and Parmentier & Guillot (2014). In this approach the planet’s temperature is given as

\[
T^4(\tau) = \frac{3T^4_{\text{int}}}{4}\left(\frac{2}{3} + \tau\right) + \frac{3T^4_{\text{irr}}}{4}(1 - \alpha)\xi_\gamma(\tau) + \frac{3T^4_{\text{irr}}}{4}\alpha \xi_{\gamma_2}(\tau),
\]

where \( \xi_\gamma \) is

\[
\xi_\gamma = \frac{2}{3} + \frac{2}{3\gamma_1}\left[ 1 + \left(\frac{\gamma_1 \tau}{2} - 1\right)e^{-\gamma_1 \tau} \right] + \frac{2\gamma_1}{3}\left( 1 - \frac{\tau^2}{2} \right)E_2(\gamma_1 \tau).
\]

Parameters \( \gamma_1 = \kappa_{\nu_1}/\kappa_{\text{IR}} \) and \( \gamma_2 = \kappa_{\nu_2}/\kappa_{\text{IR}} \) are ratios of the mean opacities in the visible to the infrared. The parameter \( \alpha \) ranges between 0 and 1 and describes the partition between the two visible streams, \( \kappa_{\nu_1} \) and \( \kappa_{\nu_2} \): \( E_2(\gamma_1 \tau) \) is the exponential integral function. The planet internal flux is given as

\[
T_{\text{int}} = \beta \left( \frac{R_s}{2a} \right)^{1/2} T_*,
\]

where \( R_s \) and \( T_* \) are the stellar radius and temperature, respectively, and \( a \) is the semimajor axis. The incident solar flux is denoted as \( T_{\text{irr}} \). Both \( T_{\text{int}} \) and \( T_{\text{irr}} \) variables have fixed values. The parameter \( \beta \) accounts for albedo, emissivity, and day–night redistribution and has a value around 1 for zero albedo and unit emissivity. The parameter \( \tau \) is the optical depth, and it is calculated using the mean infrared opacity \( \kappa_{\text{IR}} \), pressure \( P \), and planet surface gravity \( g \) at the 1 bar level:

\[
\tau = \frac{\kappa_{\text{IR}} P}{g}.
\]
and one noninverted temperature profile generated using Equation (1). We note that this parameterization suffers from the artifact that the upper atmosphere is artificially isothermal (Parmentier & Guillot 2014). Figure 21 of Blecic et al. (2017) shows an exploration of all parameters.

### 2.2.2. T-Parameterization Scheme II

Our second option for the temperature profile generator is a parameterization scheme similar to the one developed by Madhusudhan & Seager (2009). We made some minor changes to this method, which we describe below.

In this scheme, the profiles are generated for inverted and noninverted atmospheres separately. The atmosphere is divided into three layers based on the physical constraints expected in hot Jupiters (Figure 4). For more details on each of those layers see Section 2.1 in Madhusudhan & Seager (2009). The following set of equations mimics the behavior in each atmospheric layer

\[
P_0 < P < P_1 = P_0 e^{\alpha_1(T - T_0) / T_0} \text{ layer 1} \\
P_1 < P < P_2 = P_2 e^{\alpha_2(T - T_3) / T_3} \text{ layer 2} \\
P > P_2 T = T_3 \text{ layer 3.} 
\]

(5)

The set contains 12 variables: \( P_0, P_1, P_2, P_3, T_0, T_1, T_2, T_3, \alpha_1, \alpha_2, \beta_1, \) and \( \beta_2. \) To decrease the number of free parameters, we first set \( P_0 \) to the pressure at the top of the atmosphere. The parameters \( \beta_1 \) and \( \beta_2 \) are empirically determined to be \( \beta_1 = \beta_2 = 0.5 \) (see Section 2.3 in Madhusudhan & Seager 2009).

Two of the parameters can be eliminated based on the two constraints of continuity at the two layer boundaries. The temperature \( T_3 \) can be estimated based on the effective (surface) temperature of the planet, or by taking the limit of Equation (1) when \( T_{\text{int}} = 0 \) as the optical depth goes to infinity. When a planet total emissivity in the observed wavelength band is less than 1, due to the presence of an atmosphere, its emissivity is less than that of a blackbody and the actual temperature of the object is higher than the effective temperature. Thus, to account for the presence of an atmosphere and spectral features, we use a scaling factor of 1–1.5 to constrain the maximum range of the \( T_3 \) temperature.

The effective temperature of the planet is calculated based on the energy balance equation as

\[
T_{\text{eff}}^4 = f T_{\text{star}}^4 \left( \frac{R}{a} \right)^2 (1 - A),
\]

(6)

where factor \( f \) describes the energy redistribution from the day to the night side, and \( T_{\text{star}} \) is the temperature of the star. \( f = 1/4 \) defines the uniform redistribution of energy between the day and the night side of the planet. In the case where the energy received is uniformly redistributed on the planet’s dayside, and none of the energy is transferred to the night side, \( f = 1/2. \) Our choice of these values for \( f \) is not universal. As noted by Cowan & Agol (2011), any single-parameter implementation of advection is incapable of capturing the real complexities involved (see also the discussion in the Appendix of Spiegel & Burrows 2010). For zero albedo, Equation (6) becomes

\[
T_{\text{eff}}^4 = \frac{1}{2} T_{\text{star}}^4 \left( \frac{R}{a} \right)^2.
\]

(7)

To remove one more free parameter, we rewrite Equation (5) to distinguish the increasing and decreasing part of the Layer 2 curve

\[
P_0 < P < P_1 = P_0 e^{\alpha_1(T - T_0) / T_0} \\
P_1 < P < P_2 = P_2 e^{\alpha_2(T - T_3) / T_3} \\
P > P_2 T = T_3.
\]

(8)

### 2.2.2.1. Inverted \( T(p) \) Profile

The parametric profile for the inverted atmosphere has six free parameters: \( P_1, P_2, P_3, T_3, \alpha_1, \) and \( \alpha_2. \) We calculate the \( T_0, \)
$T_1$, and $T_2$ temperatures as

$$T_2 = T_3 - \frac{\left(\log\left(P_3/P_2\right)\right)^2}{\alpha_2}$$

$$T_0 = T_2 - \frac{\left(\log\left(P_1/P_0\right)\right)^2}{\alpha_1} + \frac{\left(\log\left(P_1/P_2\right)\right)^2}{-\alpha_2}$$

$$T_i = T_0 + \frac{\left(\log\left(P_i/P_0\right)\right)^2}{\alpha_1}.$$  \hfill (9)

An example of an inverted $T(p)$ profile is shown in the left panel of Figure 4. To remove sharp kinks on the layer boundaries (between Layers 1–2 and Layers 2–3), we again followed the Madhusudhan & Seager (2009) approach and used a SciPy smoothing function with the nearest neighbor and the lowest standard deviation settings, smoothing only a few points around the boundaries. Such an approach does not cause any correlation between distant atmospheric layers and mimics the smooth transitions observed in temperature profiles of solar system planets (see Figure 2 in Madhusudhan & Seager 2009). Recently, Kitzmann et al. (2020) developed a more advanced temperature profile that avoids a need for any smoothing.

2.2.2.2. Noninverted $T(p)$ Profile

For the noninverted atmosphere, we assume that Layer 2 follows an adiabatic temperature profile and exclude $P_2$ as a free parameter. Thus, the parametric profile for the inverted atmosphere has five free parameters: $P_1, P_3, T_3, \alpha_1, \alpha_2$. We calculate $T_0$ and $T_1$ as

$$T_i = T_3 - \frac{\left(\log\left(P_3/P_i\right)\right)^2}{\alpha_2}$$

$$T_0 = T_1 - \frac{\left(\log\left(P_1/P_0\right)\right)^2}{\alpha_1}.$$  \hfill (10)

An example of a noninverted $T(p)$ profile is shown in the right panel of Figure 4. Figure 19 of Blecic et al. (2017) shows an exploration of all parameters.

2.2.3. Species Factors

In addition to the temperature profile parameters, the atmospheric generator accepts free parameters for the molecular species scaling factors. For each selected free species, we modify its initial volume mixing ratio profile by multiplying it by a scaling factor. As commonly seen in the literature, in retrieval we adopt constant-with-altitude initial abundance profiles, assuming that eddy diffusion causes vertically quenched species abundances (Prinn & Barshay 1977; Moses et al. 2013). We, however, note that it has been shown (e.g., Tsai et al. 2017) that, for some species, disequilibrium processes may play a more dominant role than transport-induced quenching.

We allow the species volume mixing ratios between a maximum value of 1 and a minimum value low enough that the species does not affect the absorption spectrum (e.g., $10^{-12}$). Such an approach allows for nonequilibrium conditions in the planetary atmosphere to occur. Additionally, one can impose a maximum value for the sum of the fitting volume mixing ratios (e.g., to ensure an H$_2$/He-dominated atmosphere).

We have as many free parameters as species we want to fit in our model. Our scaling factors apply to the entire initial profile for a species, and we are retrieving the log of the species abundances to prevent negative and physically implausible mixing ratios and to allow them to vary over several orders of magnitude. This code can easily be modified to use abundance profiles with multiple free parameters, as with $T(p)$.

2.3. TEA Module

To calculate the equilibrium abundances for the species of interest, we use the Thermochemical Equilibrium Abundances (TEA) code (Blecic et al. 2016). This calculation allows us to estimate the initial constant-with-altitude species abundances for retrieval. TEA calculates the volume mixing fractions of gaseous molecular species following the methodology of White et al. (1958) and Eriksson (1971). Given a $T(p)$ profile and elemental abundances, TEA determines the volume mixing fractions of the desired molecular species by minimizing the total Gibbs free energy of the system (Zeleznik & Gordon 1960). The minimization is done using an iterative Lagrangian steepest-descent method that minimizes a multivariate function under constraint. In addition, to guarantee physically plausible results, i.e., positive volume mixing fractions, TEA implements the Lambda Correction algorithm (White et al. 1958).

This approach requires a knowledge of the free energy of the species as a function of temperature. These are obtained from the JANAF (Joint Army Navy Air Force) tables (http://kinetics.nist.gov/janaf/; Chase et al. 1982; Chase 1986). Thus, TEA has an access to 84 elemental species and the thermodynamical data for more than 600 gaseous molecular species (valid between 100 and 6000 K for the species of our interest here). We use the reference table containing elemental solar abundances given in Asplund et al. (2009, Table 1).

TEA is tested against the original method developed by White et al. (1958), the analytic method developed by Burrows & Sharp (1999), and the Newton-Raphson method implemented in the free Chemical Equilibrium with Applications code (CEA; http://www.grc.nasa.gov/WWW/CEAWeb/). Using the free energies listed in White et al. (1958, their Table 1) and derived free energies based on the thermodynamic data provided in CEA’s thermo.inp file, TEA produces identical final abundances for both approaches, but with a higher numerical precision. TEA is also benchmarked against the analytical codes developed by Heng & Tsai (2016), Heng & Lyons (2016), and Cubillos et al. (2019) and the numerical code developed by Woitke et al. (2018), GGchem.

The thermochemical equilibrium abundances obtained with TEA can be used in static atmospheres as well as a starting point in models of gaseous chemical kinetics and abundance retrievals. TEA is written in Python in a modular way; it is documented (the start guide, the user manual, the code document, and the theory paper are provided with the code), actively maintained, and available to the community via the open-source development site https://github.com/dzesmin/TEA.

The thermochemical equilibrium abundances of the desired chemical species to be used in BART could also be calculated using any other available equilibrium abundances code like GGChem (Woitke et al. 2018), FastChem (Stock et al. 2018), and CEA (Gordon & McBride 1994), providing the same input format as BART requires.
2.4. Statistical Module

BART explores the parameter space of thermal profiles and species abundances using the MC3 module (Cubillos et al. 2017). MC3 is an open-source general-purpose statistical package for model fitting. Using Bayesian inference through an MCMC algorithm, MC3 provides three routines to sample the parameters’ posterior distributions: differential evolution (DEMC, Ter Braak C., 2006), Snookey DEMC (Ter Braak & Vrugt 2008), and Metropolis Random Walk (using multivariate Gaussian proposals). The key aspect of the DEMC algorithm is that it automatically adjusts the scale and orientation of the proposal distribution, therefore optimizing acceptance rates and efficiency. MC3 handles Bayesian priors (uniform, Jeffrey’s, or informative) and implements the Gelman–Rubin convergence test (Gelman & Rubin 1992) together with ESS (see Section 2), which defines the accuracy of credible regions. It utilizes single-CPU and multicore computation, supported through Message Passing Interface (MPI). The code, written in Python with several C-routines, is documented and available to the community via https://github.com/pccubillos/mc3.

There are two versions of MC3, both written in Python 3. The main repo uses Python’s multiprocessing module, while a branch uses MPI. BART uses the MPI branch of MC3 for concurrent processing. The MC3 code consists of a central routine that coordinates the MCMC run and multiple worker routines that evaluate the transmission model. On initialization, the central routine creates one worker for each MCMC chain, which remain instantiated throughout the run for efficiency. The central routine communicates with the workers via MPI by sending sets of model parameters and receiving back the corresponding \( \chi^2 \) for each iteration. These instances use shared memory to store the large opacity table and other objects used in the calculation, vastly reducing memory use.

2.5. Transit

The transit module solves the radiative transfer equation to generate planetary spectra. It is an open-source radiative transfer code originally developed by Rojo et al. (2009) that applies a 1D opacity-sampling computation in local thermodynamic equilibrium to generate model spectra. This code, written in C, was built specifically to attempt to detect water in the extrasolar planet HD 209458b using transit spectroscopy. Since then, transit has been significantly improved to handle eclipse geometry and multiple line-list and collision-induced absorption (CIA) sources and to perform opacity grid and Voigt profile calculations (see the collaborative paper by Cubillos et al. 2022). The BART project also added user and programmer documentation to the package. The code is available via https://github.com/exosports/transit.

2.6. Spectrum Band Integrator

To compare the model spectra to the data, BART integrates the spectra over the spectral response curve for each observing band. For transit geometry, the observed transit depths are directly compared to the band-integrated transmission spectra. For eclipse geometry, the observed eclipse depths correspond to the planet-to-star flux ratio

\[
\frac{F_p}{F_{\text{star}}} = \frac{F_p^{\text{surf}}}{F_{\text{star}}^{\text{surf}}} \left( \frac{R_p}{R_{\text{star}}} \right)^2,
\]

where \( F_p^{\text{surf}} \) is the surface flux spectrum of the planet and \( F_{\text{star}}^{\text{surf}} \) is the surface flux spectrum of the star. BART incorporates the Kurucz models for the stellar spectra (Castelli & Kurucz 2004).

2.7. Best Fit

Upon running the required number of MCMC iterations to satisfy both convergence criteria (see Section 2), MC3 generates the best-fit parameters file that we use to run the transit module one more time. This produces the final BART outputs, the best-fit atmospheric file, and the best-fit spectrum file. In addition, the MC3 module generates a file with parameters’ best-fit values and 68% credible regions, trace plots showing the sequence of parameters’ values for each MCMC iteration, 1D plots showing the parameters’ marginalized posterior probability distributions, and 2D plots showing pairwise posterior marginalizations for all the combinations of free-parameter pairs. These plots help identify possible nonconvergence, multimodal posteriors, correlations, or incorrect priors. Using this information, BART plots the best-fit spectrum, the \( T \) (\( p \)) profiles, the abundances profiles, and the contribution functions.

2.8. Contribution Functions

The contribution functions provide information on where the emission measured by the telescope originates (Chamberlain 1978; Griffith et al. 1998; Knutson et al. 2009b). To assess the contribution from a certain layer to the observed intensity, we calculate two quantities: the transmission weighting function and the Planck function at a given temperature. The weighting function, which describes how transmission is changing with altitude, is the kernel of the radiative transfer integral. It weights the contribution to the intensity from the Planck functions at different log-pressure altitudes. The contribution function, the product of the weighting function and the Planck function, is the integrand of the radiative transfer integral.

The weighting function, \( W \), is defined as a derivative of the transmission function, \( T(\tau = e^{-\tau/\mu}) \), as \( W = \frac{\partial T}{\partial \tau} \), where \( \tau \) is the optical depth, \( z \) is the altitude, and \( \mu \) is the cosine of the ray path’s angle to the normal. The altitude where the peak of the weighting function is found depends on the opacity at that wavelength. In other words, it is sensitive to the atmospheric thermal structure and composition (volume mixing fractions). The contribution function assesses vertical sensitivity of the emission spectrum by giving the pressure level at which thermal emission from the atmosphere contributes most to the intensity observed at the top of the atmosphere in each wavelength.

To investigate the contribution from a certain atmospheric layer to the observed intensity, we start with the equation that defines the intensity at the top of the atmosphere,

\[
I_0(\tau = 0) = \int_0^\tau \frac{B_\nu}{\mu} e^{-\tau/\mu} d\tau',
\]

and by using the hydrostatic balance equation and the equation of state, we rewrite it in terms of pressure,

\[
I_p(p) = \int_{p_b}^{p_t} B_\nu \frac{d T}{d (\log p)} d (\log p),
\]

where \( p_b \) and \( p_t \) are pressures at the bottom and top of the atmosphere, respectively. The weighting function is then given
as

\[ W(p) = \frac{dT}{d(\log p)} \],

and the contribution function as

\[ CF(p) = B_{r} \frac{dT}{d(\log p)} \]  \hspace{1cm} (15)

Since the weighting function is the convolution of the rising transmission and falling density, it will have a roughly Gaussian shape for all wavelengths that do not sense the surface. When the atmosphere is more transparent, the peak of the weighting function moves toward larger pressures (lower altitudes). For wavelengths where the atmosphere is completely transparent, the weighting function is below the surface and the shape becomes exponential. Above the peak, the telescope does not sense the atmosphere that well, due to the low atmospheric density and few emitting molecules. Below the peak, the emitted radiation is mostly absorbed by the atmosphere above.

The weighting and contribution functions are key quantities in temperature retrievals, and they strongly depend on the best-fitting models. BART calculates the contribution functions after MC3 has determined the best-fit parameters. Using the best-fit parameters, we run the transit module again and reproduce the optical depth array of the best-fit model. The optical depths are used to calculate contribution functions at each wavelength across the planet’s spectrum. The band-averaged contribution functions are obtained by integrating the calculated contribution functions across the filter bandpasses of our observations (the transmission response functions) at every pressure layer.

### 3. Atmospheric Analysis of WASP-43b

WASP-43b (Hellier et al. 2011) is one of the closest-orbiting hot Jupiters, revolving around one of the coldest stars (4400 ± 200 K) that hosts hot Jupiters. Attributed to the small radial distance of the host star (0.667 ± 0.011 \( R_{\odot} \); Gillon et al. 2012), its cool temperature, and its small semimajor axis (0.01526 ± 0.00018 au), the system produces significant dips in both transit and eclipse. This makes WASP-43b one of the most favorable targets today for space and ground observations and a perfect exoplanet for atmospheric characterization.

Previous WASP-43b atmospheric analyses suggest a carbon-rich composition (Zhou et al. 2014) with C/O ratio larger than solar but smaller than 1 (Line et al. 2014; Benneke 2015), water abundance consistent with solar composition (Stevenson et al. 2014b; Benneke 2015; Kataria et al. 2015), supersolar metallicity (Stevenson et al. 2014b; Kataria et al. 2015; Stevenson et al. 2017), and the possible existence of high-altitude clouds or hazes (Chen et al. 2014; Stevenson et al. 2017). The presence of thermal inversion was initially ruled out by Gillon et al. (2012), Line et al. (2014) and Blecic et al. (2014) but found to be localized on the dayside of the planet by Kataria et al. (2015). The planet energy budget and redistribution were analyzed by many groups, initially suggesting a poor day-to-night redistribution (Gillon et al. 2012; Blecic et al. 2014; Stevenson et al. 2014b, 2017). However, the inclusion of the reflected light in models by Keating & Cowan (2017) revealed a much hotter nightside. This result was subsequently confirmed by Mendonça et al. (2018) utilizing their improved data reduction technique and assuming clouds on the planet’s night side. A cloudy nightside was also hypothesized by Venot et al. (2020), who performed phase-curve retrieval analysis of WASP-43b synthetic James Webb Space Telescope/Mid-Infrared Instrument (JWST/MIRI) observations. Very recently, Irwin et al. (2020) performed a multidimensional “2.5D retrieval” of all WASP-43b orbital phases simultaneously, using an optimal estimation algorithm, confirming again thick clouds on the nightside of WASP-43b.

In this paper, we performed an atmospheric analysis of WASP-43b secondary eclipse data from space- and ground-based observations using BART (see Table 1). Our goal was to compare our results with the results from the literature (Kreidberg et al. 2014; Line et al. 2014) and in this way validate our framework, as well as to investigate several cases previously unexplored for WASP-43b.

#### 3.1. BART Setup

The pressure range for all of our models was constrained between 10^{-2} and 10^{-5} bars and sampled 100 times uniformly in log space. We used the parameterization from Section 2.2.1 to generate our \( T(p) \) profile. We performed several trial runs including all five \( T(p) \) profile parameters and concluded that we can fix \( \gamma_2 \) and \( \alpha \) to zero. Parameter \( \gamma_2 \) is redundant when

### Table 1

| Source and Instrument | Wavelength (\( \mu \text{m} \)) | Eclipse Depth (%) |
|-----------------------|-------------------------------|-------------------|
| Gillon et al. (2012), VLT/HAWK | 1.19 | 0.079 ± 0.032 |
| | 2.09 | 0.156 ± 0.014 |
| Wang et al. (2013), CFHT/WIRCam | 1.65 | 0.103 ± 0.017 |
| | 2.19 | 0.194 ± 0.029 |
| Chen et al. (2014), MPG/ESO/GROND | 0.806 | 0.037 ± 0.022 |
| | 2.19 | 0.197 ± 0.042 |
| Blecic et al. (2014), Spitzer | 3.6 | 0.347 ± 0.013 |
| | 4.5 | 0.382 ± 0.015 |
| Zhou et al. (2014), IRIS | 2.15 | 0.181 ± 0.027 |
| Stevenson et al. (2014b), HST | 1.1425 | 0.0365 ± 0.0045 |
| | 1.1775 | 0.0431 ± 0.0039 |
| | 1.2125 | 0.0414 ± 0.0038 |
| | 1.2475 | 0.0482 ± 0.0036 |
| | 1.2825 | 0.0460 ± 0.0037 |
| | 1.3175 | 0.0473 ± 0.0033 |
| | 1.3525 | 0.0533 ± 0.0034 |
| | 1.3875 | 0.0313 ± 0.0030 |
| | 1.4225 | 0.0320 ± 0.0036 |
| | 1.4575 | 0.0394 ± 0.0036 |
| | 1.4925 | 0.0439 ± 0.0033 |
| | 1.5275 | 0.0458 ± 0.0035 |
| | 1.5625 | 0.0595 ± 0.0036 |
| | 1.5975 | 0.0614 ± 0.0037 |
| | 1.6325 | 0.0732 ± 0.0042 |
| Stevenson et al. (2017), Spitzer | 3.6 | 0.3300 ± 0.0089 |
| | 4.5 | 0.3827 ± 0.0084 |

Notes.

a Cryogenic near-IR imager HAWK at the Very Large Telescope.

b WIRCam on the Canada–France–Hawaii Telescope.

c Gamma Ray Burst Optical and Near-Infrared Detector on the MPG 2.2 m telescope at La Silla Observatory, Chile.

d Very Large Telescope Infrared Image Sensor.

e Hubble Space Telescope.

### Notes.

b Cryogenic near-IR imager HAWK at the Very Large Telescope.

c Gamma Ray Burst Optical and Near-Infrared Detector on the MPG/ESO 2.2 m telescope at La Silla Observatory, Chile.

d Very Large Telescope Infrared Image Sensor.

e Hubble Space Telescope.
We used the ExoMol\textsuperscript{11} database for H$_2$O, CO$_2$, NH$_3$, C$_2$H$_2$, C$_2$H$_4$, H$_2$S, TiO, and VO and the HITTEMP\textsuperscript{12} database for CO and CH$_4$ species as our sources for the molecular line-list data. For H$_2$O, we used the molecular line-list data from Polyansky et al. (2018) for CO$_2$, Rothman et al. (2010) for HCN, Harris et al. (2006, 2008), for NH$_3$, Yurchenko et al. (2011) and Yurchenko (2015) for C$_2$H$_2$, Wilzewski et al. (2016) and Gordon et al. (2017) for C$_2$H$_4$, Mant et al. (2018) for TiO, McKemnish et al. (2019) for H$_2$S, Azzam et al. (2016) and for VO, McKemnish et al. (2016). For CH$_4$ we used the newly available HITTEMP line list from Hargreaves et al. (2020), shown to provide more accurate line-list information than ExoMol, and for CO we used the HITTEMP line list from Li et al. (2015). Since many ExoMol databases consist of billions of line transitions, we used the REPACK package (Cubillos 2017) to extract only the strongest line transitions that dominate the opacity spectrum. The partition functions for the HITTEMP opacity sources were calculated based on Laraia et al. (2011), and for ExoMol we used the tabulated values provided with the line lists. In addition to the molecular line lists, we included the H$_2$–H$_2$ collision-induced opacities from Borysow et al. (2001) and Borysow (2002) and H$_2$–He collision-induced opacities from Richard et al. (2012). For this analysis, when calculating opacities, we sampled the Voigt profiles uniformly in wavenumber space, at the resolution of 1 cm$^{-1}$ (see Cubillos et al. 2022, for details on the appropriate choice for resolution).

We used uniform priors for $\beta$ (the temperature profile parameter; see Section 2.2.1) and log-uniform priors for all other temperature profile parameters and molecular species, with boundary limits set wide enough to allow MC3 to explore the parameter phase space thoroughly. On each iteration, we rescaled the mixing ratios of H$_2$ and He, preserving their original ratio such that the total sum of all species’ abundances is unity. To be able to compare our results with Line et al. (2014), we impose the same constraint as they do, that the sum of the fitted molecular species abundances must not exceed 15%. Prior to proceeding with this approach, we performed tests confirming that our conclusions are not changed by imposing this limit. This constraint is bounding the atmospheric compositions to a hydrogen-dominated atmosphere, roughly restricting the metallicity to less than 200 solar. A similar approach has been applied recently by Tsiaras et al. (2018).

We generated the line-list data files for the species and the wavelength range of interest, and from them we generated the opacity tables with the opacity grid between 300 and 3000 K in 100 K intervals and between 0.6 and 5.5 $\mu$m in 1 cm$^{-1}$ intervals in the wavenumber space. The maximum optical depth was set to 10 for all models (\textit{transit} stops the extinction calculation at each wavelength when the optical depth reaches the user-defined value $\tau_{\text{max}}$; see collaborative paper by Cubillos et al. 2022).

We ran 10 independent chains and enough iterations until the Gelman–Rubin convergence test for all free parameters drops...
Figure 5. Opacities of the species used in WASP-43b atmospheric retrieval, calculated at temperature of 1500 K and pressure of 1 bar, and their influence on the equilibrium spectra of WASP-43b. The spectrum model includes the corresponding molecular and CIA opacities (see Section 3.1). The gaps in the opacity figures come from the limited y-axis range (the values not shown are well below $10^{-12}$ cm$^2$ g$^{-1}$). The $T(p)$ profile and species abundances used to generate WASP-43b spectra are given in the inset figures. Black dots represent the data points with uncertainties. At the bottom of the figures, we show the bandpasses for each of the observations used in the analysis. From the individual equilibrium WASP-43b models, we see that H$_2$O, CO, NH$_3$, and potentially HCN are the only absorbers that significantly influence the WASP-43b emission spectra in the wavelength range of the available observations, with H$_2$O being the most apparent.
Figure 6. Best-fit model and $T(p)$ profile for Case 1, four fitted species. The left panel shows the best-fit spectrum. In red are the data points (eclipse depths) with uncertainties, and in black are the integrated points of our model over the bandpasses of our observations shown at the bottom. The models are generated with the four major molecular species and their opacities. The right panel shows the median temperature and pressure profile with the 1σ confidence region.

Inclusion of additional opacity sources, assuming equilibrium and nonequilibrium chemical composition.

To assess different models quantitatively, we used two statistical factors: the reduced $\chi^2$, $\chi^2_{\text{red}} = \chi^2 / N - k$, where $N$ is the number of data points and $k$ is the number of free parameters, and the BIC, $\chi^2 + k \ln(N)$. We consider BIC to be one of the most important factors. It allows us to compare goodness of fit for the models generated on the same data set. Although, in general, models with more free parameters improve the fit, BIC adds a penalty for any additional parameters in the system by increasing its value. A lower BIC value indicates a better fit.

BART is also able to estimate the Bayes factor, i.e., the ratio of Bayesian evidences (marginal probabilities) of the two competing models (Gregory 2007; Trotta 2008; Benneke & Seager 2012), as this ratio is calculated, in the first approximation, using BIC (see Equations (20)–(22) in Raftery 1995). Since both statistical criteria lead to the same conclusions, in our analysis we use BIC for model comparison.

3.3. Results—Four Fitted Species

In this section, we describe cases where we fit four major molecular species, $\text{H}_2\text{O}$, $\text{CO}_2$, $\text{CO}$, and $\text{CH}_4$, and then we investigate how the inclusion of additional species and their opacities affects the best-fit model.

The initial $T(p)$ parameters were set to the values that reproduce the best-fit temperature profile from Line et al. (2014). The initial species abundances were set to the equilibrium solar composition values at 0.1 bar level, assuming constant-with-altitude abundances, calculated using TEA.

We generated three different cases (see Table 2):

1. We reproduced the setup from Line et al. (2014) and retrieved the $T(p)$ profile with four major molecular species. We thus included only the four major molecular species and their opacities in the mean molecular mass and opacity calculations.
2. We tested the statistical significance when additional molecules and their opacity sources were included in the calculation, assuming thermodynamical equilibrium and solar composition. In this case, in addition to $\text{H}_2\text{O}$, $\text{CO}_2$, $\text{CO}$, and $\text{CH}_4$, we included nitrogen species $\text{NH}_3$, HCN, and HCN.

Atmospheric Cases

| Case  | Fitted Species | Opacity Sources |
|-------|----------------|-----------------|
| Case 1 | 4$^a$          | 4$^a$           |
| Case 2 | 4$^a$          | 7$^b$           |
| Case 3 | 4$^a$          | 11$^c$          |
| Case 4 | 7$^b$          | 7$^b$           |
| Case 5 | 7$^b$          | 11$^c$          |

Notes.

$^a$ $\text{H}_2\text{O}$, $\text{CO}_2$, $\text{CO}$, $\text{CH}_4$,

$^b$ $\text{H}_2\text{O}$, $\text{CO}_2$, $\text{CO}$, $\text{NH}_3$, HCN, $\text{C}_2\text{H}_2$.

$^c$ $\text{H}_2\text{O}$, $\text{CO}_2$, $\text{CO}$, $\text{NH}_3$, HCN, $\text{C}_2\text{H}_2$, $\text{C}_2\text{H}_4$, $\text{H}_2\text{S}$, TiO, VO.

Notes. (Gelman & Rubin 1992), and until we reach a satisfactory ESS value (see Section 5 and Appendix C of Harrington et al. 2022).

3.2. Retrieved Models

It is well known in the retrieval community that the retrieval results can be biased depending on the atmospheric setup, assumed chemical species and their opacities included in the model, model selection, and physical and chemical processes assumed (e.g., Madhusudhan et al. 2011; Crossfield et al. 2012; Stevenson et al. 2014; Barstow 2020; Barstow & Heng 2020).

In an attempt to test this and the conclusions from, for example, Hansen et al. (2014) and Swain et al. (2013) on how the inclusion of additional opacity sources influences the best-fit model, we generated five atmospheric cases and compared them using statistical factors (Table 2). We present cases where we fit four major molecular species, $\text{H}_2\text{O}$, $\text{CO}_2$, $\text{CO}$, and $\text{CH}_4$, and seven molecular species, $\text{H}_2\text{O}$, $\text{CO}_2$, $\text{CO}$, $\text{CH}_4$, $\text{NH}_3$, HCN, and $\text{C}_2\text{H}_2$. We also include additional cases with nonfit opacities, assuming solar equilibrium composition. These exercises were performed to investigate whether the most often used basic approach for hot Jupiters, which includes only four major molecular species in the model and fits them in retrieval, is lacking some major spectral features from other relevant species and to test how sensitive the data are on the
and the most abundant species occurring in the conditions when the atmospheric C/O ratio is larger than 1, C$_2$H$_2$, testing whether their spectral features are present in the model (Madhusudhan 2012).

3. Same as Case 2 with the inclusion of the species that are considered to be responsible for thermal inversions in hot-Jupiter atmospheres, TiO, VO, and H$_2$S, together with C$_2$H$_4$, the second most abundant species when C/O ratio is larger than 1.

Table 3 lists $\chi^2_{\text{red}}$ and BIC values for Cases 1, 2, and 3. We provide $\chi^2_{\text{red}}$ as a figure of merit but use only BIC to perform model comparison. According to BIC, Case 1 is slightly favored compared to Case 2 by a probability ratio ($e^{\Delta \text{BIC}/2}$) of 3.5 and to Case 3 by a probability ratio of 4.0. Figure 6 shows the Case 1 best-fit spectrum and $T(p)$ model. In the inset, we give the wavelength range covered by the HST data. Figure 7 shows the influence of the individual species on the best-fit model for Case 1, while Figure 8 shows the histograms of the posterior distribution of the retrieved molecular species with their best-fit values. In Figure 9, we show the pairwise correlation plots, where we see a strong correlation between the mean infrared opacity $\kappa$$_{IR}$ and the water abundance. As pointed out by Heng et al. (2014, their Section 4), this degeneracy could come from a nonexplicit definition of the term “mean.”

The best-fit model, $T(p)$ profile, histograms, pairwise correlation plots, and influence of each species on the best-fit spectra for Cases 2 and 3 are almost identical to those for Case 1. Table 3 compares the goodness of fit for all three cases. According to BIC, the inclusion of additional opacity sources does not improve the fit, as their effect on the WASP-43b best-fit model is negligible.

As seen, water features dominate the spectrum, and thus water is constrained the best in this analysis. There is some evidence for CO$_2$, showing a soft upper limit, and we also see a more pronounced upper limit of CH$_4$. CO appears abundant, hitting the set limit and peaking just below it.

These conclusions agree well with the results from Line et al. (2014). In particular, our retrieved $T(p)$ profile is fully consistent with theirs.

### 3.4. Results—Seven Fitted Species

We continued our analysis by fitting seven molecular species: H$_2$O, CO$_2$, CO, CH$_4$, NH$_3$, HCN, and C$_2$H$_2$. Again,
we tested the effect of including additional opacity sources, and we generated two different cases:

1. Using the same initial $T(p)$ profile and vertically uniform species abundances as in our previous cases, we modeled the atmosphere of WASP-43b including the opacity sources for all seven molecules.

2. Same as Case 4 with the inclusion of all 11 species and their opacities in the calculation (C$_2$H$_4$, H$_2$S, TiO, and VO in addition to the species from Case 4), assuming equilibrium and solar composition.

Figure 10 shows the best-fit spectrum and $T(p)$ profile for Case 4, seven fitted species. The left panel shows the best-fit spectrum. In red are the data points (eclipse depths) with uncertainties, and in black are the integrated points of our model over the bandpasses shown in gray. The models are generated with the seven molecular species and their opacities. The right panel shows the median temperature and pressure profile with 1σ and 2σ confidence regions.

Figure 11 shows the influence of the NH$_3$, HCN, and C$_2$H$_2$ species on the best-fit model for Case 4, seven fitted species. H$_2$O, CO$_2$, CO, and CH$_4$ have similar influence on the spectra to that seen in Figure 7.

Figure 12 shows the histograms for Case 4, seven fitted species. The figure shows the species’ abundances (X), expressed as log$_{10}(X)$, with their best-fit values shown as dashed lines.

Table 4 Goodness of Fit, Seven Species

| Species | $\chi^2_{red}$ | BIC  |
|---------|---------------|------|
| Case 4, 7 opacities | 2.4754 | 72.1866 |
| Case 5, 11 opacities | 2.5070 | 72.6932 |

According to BIC values (Table 4), Case 4 is favored over Case 5 for a probability ratio of 6.3. However, Case 1 is favored over Case 4 for a probability ratio of 129. The inclusion of any additional opacity sources does not improve the fit. We also see that BIC values are generally larger when we fit seven species (Table 4) than when we fit four species. In Table 5, we list the best-fit species abundances for Cases 1 and...
credible regions calculated following Harrington et al. Case 1 and Case 4 posterior accuracy, i.e., 14 and their corresponding confidence regions. Table 6 lists Case 1 and Case 4 posterior accuracy, i.e., 1σ errors on our credible regions calculated following Harrington et al. (2022, Section 5 and Appendix C).

3.5. WASP-43b Contribution Functions

Figure 14 shows the $T(p)$ profile and normalized contribution functions for HST, Spitzer, and ground-based observations, for the best-fit model from Section 3.3, Case 1, our lowest BIC model. The right panel shows the pressures where the maximum optical depth is reached. We see that the best-fit atmospheric model probes mostly the thermal structure around 1 bar. The observations done by Spitzer’s channel 2 (4.5 μm) probe lower pressures, around 0.1 bars, explained by the presence of several opacity sources in this bandpass. Figure 7 shows that most of the spectral features from CO are concentrated in this region, in addition to H₂O features.

4. Summary and Conclusions

This paper is one of three papers that present a novel retrieval framework, the BART code. BART is an open-source, open-development, Bayesian, thermochemical, radiative transfer code under a Reproducible Research license available at https://github.com/exosports/BART. In this paper, we presented the implementation and the underlying theory of the initialization routines, TEA module, atmospheric profile generator, best-fit routines, and contribution functions module. Other modules and packages are described in Cubillos et al. (2022), while Harrington et al. (2022) describe the overall framework, tests, and Bayesian best practices.

We also present forward and retrieval analyses of space- and ground-based secondary eclipse data, in an attempt to compare our results with some previous analyses and validate our framework, and to investigate several new scenarios. We find that the temperature decreases with increasing altitude for all cases, in agreement with previous studies from Stevenson et al. (2014b), Line et al. (2014), and Blecic et al. (2014). The data are best fit with the model including only four major molecular species (H₂O, CO₂, CO, and CH₄). We do not find the signatures of HCN, C₂H₂, and C₂H₄ in any of our models, inferring that it is unlikely that the atmosphere of WASP-43b has high C/O ratio or high metallicity. We also find that the inclusion of TiO, VO, and H₂S opacities does not improve the fit, suggesting that there is no indication of strong absorbers in the visible that could lead to thermal inversions in WASP-43b. Our results are in agreement with the conclusions made by Line et al. (2014) and Kreidberg et al. (2014). Overall, the inclusion of additional opacity sources does not change the shape of the best-fit spectrum, only marginally influences the best-fit species abundances, and does not improve the fit. According to BIC, the atmospheric model with only four major opacity sources is the best match to the data.

The spectrum is dominated primarily by H₂O, and to some extent by CO at specific wavelengths, showing spectral features in the bandpasses of our observations, with water being the most dominant. CO₂, CH₄, NH₃, and HCN are detected giving an upper limit, while C₂H₂ is unconstrained. We also see a degeneracy between CO and CO₂, with CO being preferred over CO₂. Both species have spectral features around 4.5 μm, but the broad band and sparse coverage do not allow us to entirely distinguish between them. Finally, we calculate the
water abundance using our best-fit model. Assuming the same solar water abundance of $6.1 \times 10^{-6}$ as Kreidberg et al. (2014), we constrain the water abundance on the dayside of WASP-43b to $2 - 6 \times 10^{-6}$, similar to the conclusions made by Blecic et al. (2014) and Kreidberg et al. (2014).

The Reproducible Research compendium for this paper including all codes, inputs, and outputs is available on GitHub (https://github.com/dzesmin/RRC-BlecicEtal-2021-ApJ-BART3), and a copy is preserved on Zenodo: https://doi.org/10.5281/zenodo.5560306.

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**Figure 14.** Left: contribution functions for the lowest BIC atmospheric model, Case 1, Section 3.3. The first panel shows the median temperature and pressure profile with 1σ and 2σ confidence regions, while the second panel shows the individual normalized contribution function of each observation. Right: pressures where the maximum optical depth is reached for each wavelength.

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