

# ASTROPHYSICAL S-FACTORS, THERMONUCLEAR RATES, AND ELECTRON SCREENING POTENTIAL FOR THE ${}^3\text{He}(\text{d},\text{p}){}^4\text{He}$ BIG BANG REACTION VIA A HIERARCHICAL BAYESIAN MODEL

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## ABSTRACT

We developed a hierarchical Bayesian framework to estimate S-factors and thermonuclear rates for the  ${}^3\text{He}(\text{d},\text{p}){}^4\text{He}$  reaction, which impacts the primordial abundances of  ${}^3\text{He}$  and  ${}^7\text{Li}$ . The available data are evaluated and only those direct measurements are taken into account in our analysis for which we can estimate separate uncertainties for systematic and statistical effects. For the nuclear reaction model we adopt a single-level, two-channel approximation of R-matrix theory, suitably modified to take electron screening at low energies into account. Apart from the usual resonance parameters (resonance location and partial widths for the incoming and outgoing reaction channel), we include for the first time the channel radii and boundary condition parameters in the model evaluation. Our new analysis of the  ${}^3\text{He}(\text{d},\text{p}){}^4\text{He}$  S-factor data results in improved estimates for the thermonuclear rates and associated uncertainties. This work represents the first data evaluation using R-matrix theory embedded into a hierarchical Bayesian framework, hence representing a testbed for future studies of more complex reactions.

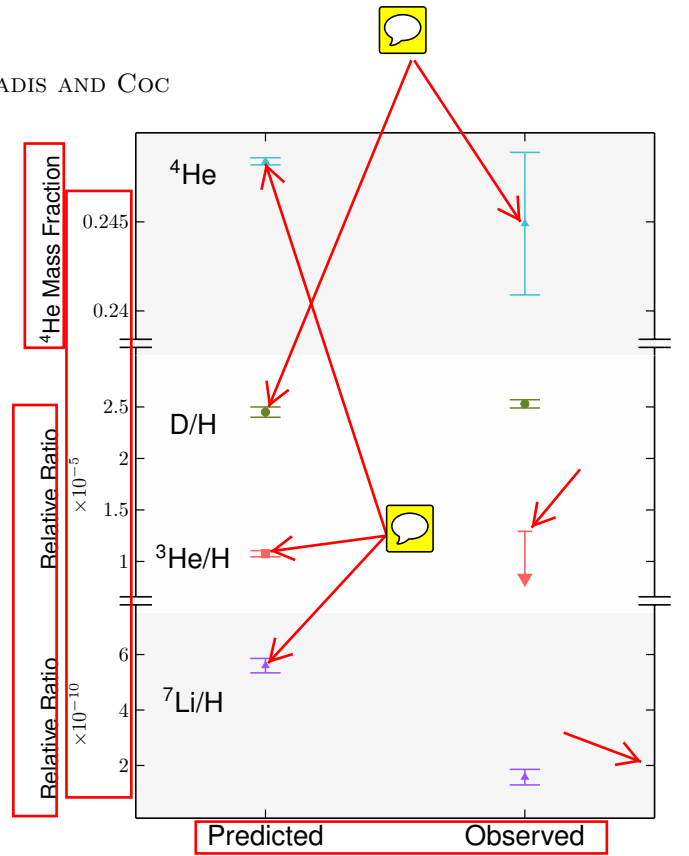
*Keywords:* Bayesian

## 1. INTRODUCTION

The big-bang theory rests on three observational pillars: **primordial big-bang nucleosynthesis** (BBN; Gamow 1948; Cyburt et al. 2016), the cosmic expansion (Riess et al. 1998; Peebles & Ratra 2003), and the cosmic microwave background radiation (Spergel et al. 2007; Planck Collaboration et al. 2016). The BBN takes place during the first 20 minutes after the big bang, at temperatures and densities near 1 GK and  $10^{-5}$  g/cm<sup>3</sup>, and is responsible for the production of the light nuclides, which play a major role in the subsequent history of cosmic evolution.

Primordial nucleosynthesis provides a sensitive test of the big bang model if the uncertainties in the predicted abundances can be reduced to the uncertainty level of the observed values. The uncertainties for the observed primordial abundances of <sup>4</sup>He, <sup>2</sup>H (or d), and <sup>7</sup>Li have been greatly reduced in recent years and amount to 1.6%, 1.6%, and 20%, respectively (Coc et al. 2015). For the observed primordial <sup>3</sup>He abundance, only an upper limit<sup>1</sup> is available ( $^3\text{He}/\text{H} \leq 1.3 \times 10^{-5}$ ; Bania et al. 2002). At present, the uncertainties in the predicted abundances of <sup>4</sup>He, <sup>2</sup>H (or d), <sup>3</sup>He, and <sup>7</sup>Li amount to 0.08%, 2.0%, 2.8%, and 4.6%, respectively (Coc et al. 2015). The primordial abundances predicted by the big bang model are in reasonable agreement with observations, as shown in Figure 1, except for the <sup>7</sup>Li/H ratio, where the predicted value (Cyburt et al. 2016) exceeds the observed one (Sbordone et al. 2010) by a factor of  $\approx 3$ . This long-standing “lithium problem” has not found a satisfactory solution yet.

Twelve nuclear processes of interest take place during big bang nucleosynthesis, (Figure 2). Among these are the weak interactions that transform neutrons into protons, and vice versa, and the  $p(n,\gamma)d$  reaction whose cross section can be calculated precisely using effective field theories (Savage et al. 1999). The ten remaining reactions,  $d(p,\gamma)^3\text{He}$ ,  $d(d,n)^3\text{He}$ ,  $d(d,p)t$ ,  $t(d,n)^4\text{He}$ ,  $t(\alpha,\gamma)^7\text{Li}$ ,  $^3\text{He}(d,p)^4\text{He}$ ,  $^3\text{He}(n,p)t$ ,  $^3\text{He}(\alpha,\gamma)^7\text{Be}$ ,  $^7\text{Li}(p,\alpha)^4\text{He}$ , and  $^7\text{Be}(n,p)^7\text{Li}$ , have been measured directly in the laboratory at the energies of astrophysical interest. Nevertheless, the estimation of thermonuclear reaction rates from the measured cross section (or S-factor) data remains challenging. Results obtained using traditional  $\chi^2$  minimization are plagued by a number of problems, including the treatment of systematic uncertainties and the implicit assumption

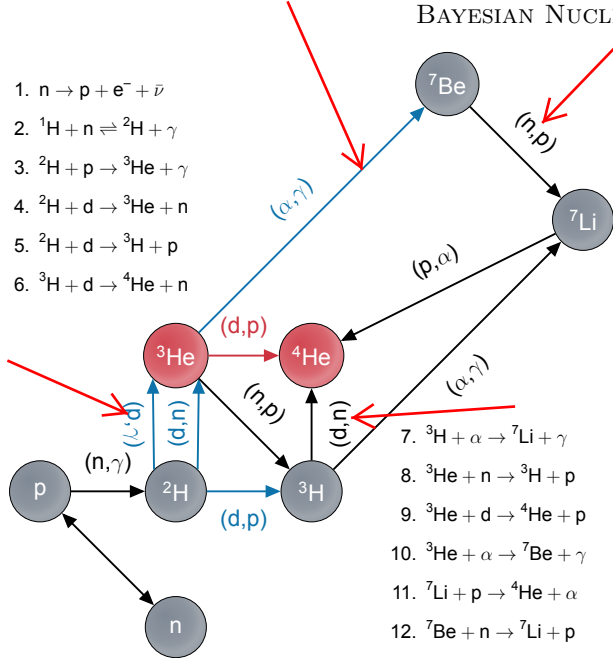


**Figure 1.** Predicted (left) versus observed (right) primordial abundances. For the primordial <sup>3</sup>He abundance only an upper limit is available, which we depict by a vertical arrow.

of normal likelihoods. Therefore, we have started a program to derive statistically sound big bang nucleosynthesis reaction rates using a hierarchical Bayesian model. Bayesian rates have recently been derived for  $d(p,\gamma)^3\text{He}$ ,  $^3\text{He}(\alpha,\gamma)^7\text{Be}$  (Iliadis et al. 2016),  $d(d,n)^3\text{He}$ , and  $d(d,p)^3\text{H}$  (Gómez Iñesta et al. 2017). These studies adopted the cross section energy dependence from the microscopic theory of nuclear reactions, while the absolute cross section normalization was found from a fit to the data within the Bayesian framework.

We report here on Bayesian reaction rates for a fifth big bang reaction,  $^3\text{He}(d,p)^4\text{He}$ . This reaction marginally impacts the primordial deuterium abundance, but sensitively influences the primordial abundances of <sup>3</sup>He and <sup>7</sup>Li (Coc & Vangioni 2010). Because of its low abundance, <sup>3</sup>He has not been observed yet outside of our Galaxy. However, the next generation of large telescope facilities **may allow** for the determination of the <sup>3</sup>He/<sup>4</sup>He ratio from observations of extragalactic metal-poor HII regions (Cooke 2015). Therefore, although a revised  $^3\text{He}(d,p)^4\text{He}$  reaction rate is not expected to solve the <sup>7</sup>Li problem, a new rate is nevertheless desirable for improving the predicted big bang nucleosynthesis abundances.

<sup>1</sup> Notice that the upper limit in Bania et al. 2002 is reported as “ $(1.1 \pm 0.2) \times 10^{-5}$ ” and, unfortunately, is frequently misinterpreted as an actual mean value with an error bar.



**Figure 2.** Nuclear reactions important for big bang nucleosynthesis. Reactions for which the rates have been obtained previously using Bayesian models are shown as blue arrows. The  $^3\text{He}(d,p)^4\text{He}$  reaction, which is subject of the present work, is shown in red.

The  $^3\text{He}(d,p)^4\text{He}$  reaction has been studied extensively during the past few decades, not only because of its importance to primordial nucleosynthesis, but also because it is relevant to the understanding of the electron screening effect and ~~the role of electrons in favoring deuteron induce reactions, relevant for~~ design of future nuclear fusion reactors for energy production (e.g. La Cognata et al. 2005). At the lowest energies, the measured astrophysical S-factor shows a marked increase caused by electron screening effects. The data at those energies were used to derive the electron screening potential, but the results depended strongly on the data sets analyzed and the nuclear model applied.

In the present work, we first evaluate the available cross section data and take only those experiments into account for which we can quantify the separate contributions of statistical and systematic effects to the total uncertainty. This leaves us with seven data sets to be analyzed. For the underlying nuclear model we assume a single-level, two-channel approximation of R-matrix theory. As will be discussed below, we introduce for the first time the channel radii and boundary conditions as parameters into the statistical model. Compared to previous work (Iliadis et al. 2016; Gómez Iñesta et al. 2017), the present Bayesian study is more complicated and, therefore, represents an important testbed for future studies of even more complex systems.

In Section 2, we summarize the reaction formalism. Our Bayesian model is discussed in Section 3, including likelihoods, model parameters, and priors. In Section 4.4, we present Bayesian S-factors and thermodynamic reaction rates. A summary and conclusions are given in Section 5. Appendix A lists the data we adopted in our analysis.

## 2. REACTION FORMALISM

Cross section (or S-factor) data for the  $^3\text{He}(d,p)^4\text{He}$  reaction have been fitted in the past using various assumptions, including polynomials (Krauss et al. 1987), a Padé expansion (Barbui et al. 2013), R-matrix expressions (Barker 2007), and hybrid models (Prati et al. 1994). See also Barker (2002) for a summary. Since we are mostly interested in the low-energy region where the s-wave contribution dominates the cross section, we follow Barker (1997) and describe the theoretical energy dependence of the cross section (or S-factor) using a one-level, two-channel R-matrix approximation, suitably modified to take electron screening at low energies into account.

The integrated cross section of the  $^3\text{He}(d,p)^4\text{He}$  reaction is given by

$$\sigma_{dp}(E) = \frac{\pi}{k_d^2} \frac{2J+1}{(2j_1+1)(2j_2+1)} |S_{dp}|^2 \quad (1)$$

where  $k_d$  and  $E$  are the deuteron wave number and center-of-mass energy, respectively,  $J = 3/2$  is the resonance spin,  $j_1 = 1/2$  and  $j_2 = 1$  are the ground-state spins of  $^3\text{He}$  and deuteron, respectively, and  $S_{dp}$  is the scattering matrix element. The corresponding bare nucleus astrophysical S-factor of the  $^3\text{He}(d,p)^4\text{He}$  reaction, which is not affected by electron screening, is given by

$$S_{bare}(E) = E e^{2\pi\eta} \sigma_{dp}(E), \quad (2)$$

where  $\eta$  is the Sommerfeld parameter. The scattering matrix element can be expressed as (Lane & Thomas 1958)

$$|S_{dp}|^2 = \frac{\Gamma_d \Gamma_p}{(E_0 + \Delta - E)^2 + (\Gamma/2)^2}, \quad (3)$$

where  $E_0$  represents the level eigenenergy. The partial widths of the  $^3\text{He} + d$  and  $^4\text{He} + p$  channels ( $\Gamma_d$ ,  $\Gamma_p$ ), the total width ( $\Gamma$ ), and the level shift ( $\Delta$ ) are given by

$$\Gamma = \sum_c \Gamma_c, \quad \Gamma_c = 2\gamma_c^2 P_c, \quad (4)$$

$$\Delta = \sum_c \Delta_c, \quad \Delta_c = -\gamma_c^2 (S_c - B_c), \quad (5)$$

where  $\gamma_c^2$  is the reduced width, and  $B_c$  is the boundary condition parameter. The energy-dependent quantities

$P_c$  and  $S_c$  denote the penetration factor and shift factors, respectively, for channel  $c$  (either  $d + {}^3\text{He}$  or  $p + {}^4\text{He}$ ), which are computed from the Coulomb wave functions,  $F_\ell$  and  $G_\ell$ , according to:

$$P_c = \frac{k_d a_c}{F_\ell^2 + G_\ell^2}, \quad S_c = \frac{k_d a_c (F_\ell F'_\ell + G_\ell G'_\ell)}{F_\ell^2 + G_\ell^2}. \quad (6)$$

The Coulomb wave functions and their derivatives are evaluated at the channel radius,  $a_c$ ;  $\ell$  denotes the orbital angular momentum for a given channel.

The R-matrix channel radius is usually expressed as

$$a_c = r_0 (A_1^{1/3} + A_2^{1/3}) \quad (7)$$

where  $A_1$  and  $A_2$  are the mass numbers of the two interacting nuclei;  $r_0$  denotes the radius parameter, with a value customarily chosen between 1 fm and 2 fm. For the  ${}^3\text{He}(d,p){}^4\text{He}$  reaction, previous choices for the channel radii ranged between 3 fm and 6 fm (e.g., Barker 2002; Descouvemont et al. 2004). R-matrix parameters and cross sections derived from data have a well-known dependence on the channel radii, which arises from the truncation of the R-matrix to a restricted number of poles (i.e., a finite set of eigenenergies). The radius of a given channel has no rigorous physical meaning, except that the chosen values should exceed the sum of the radii of the colliding nuclei (e.g. Descouvemont & Baye 2010). We will discuss the impact of varying the channel radii on our derived S-factors in Section 4.

For a narrow resonance, the observed resonance energy,  $E_r$ , i.e., the peak of the observed cross section or S-factor, can be defined as:

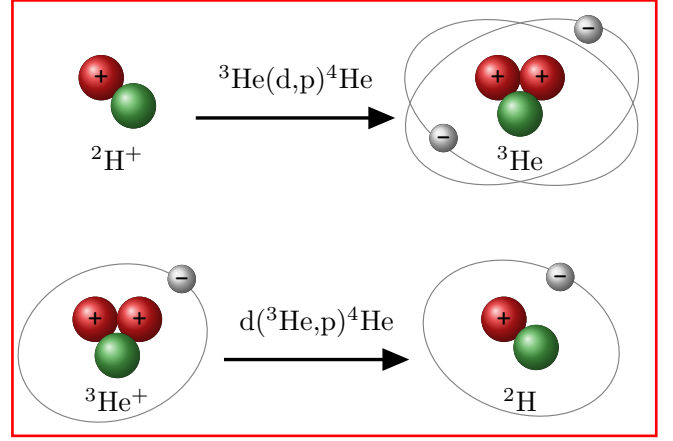
$$E_0 + \Delta(E_r) - E_r = 0. \quad (8)$$

The boundary condition parameter is then chosen as:

$$B_c = S_c(E_r), \quad (9)$$

so that the level shift becomes zero at the observed resonance energy ( $E_r = E_0$ ). This assumption, corresponding to setting the eigenenergy ( $E_0$ ) equal to the observed resonance energy ( $E_r$ ) in the data fitting, has been adopted in most previous studies (e.g. Barker 2007). However, it does not necessarily apply to broad resonances, where the maximum of the scattering matrix element, cross section, and S-factor peak at different energies. Indeed, for the low-energy  ${}^3\text{He}(d,p){}^4\text{He}$  resonance, the total observed width is approximately equal to the observed resonance energy. We will investigate in Section 4 the impact of varying the boundary condition parameters on our results.

In laboratory experiments, electrons are usually bound to the interacting projectile and target nuclei.



**Figure 3.** Illustration of the different processes involved in the  ${}^3\text{He}(d,p){}^4\text{He}$  and  $d({}^3\text{He},p){}^4\text{He}$  reactions. (Top) Deuterium ion beam (with no atomic electron) incident on a neutral  ${}^3\text{He}$  target atom (two atomic electrons). (Bottom)  ${}^3\text{He}$  ion (with one atomic electron) incident on a neutral deuterium target atom (one atomic electron). The electron screening effect is of different magnitude in these two situations.

These electron clouds effectively reduce the Coulomb barrier of the interaction nuclei and give rise to an increasing transmission probability. We perform the S-factor fit to the data using the expression (Assenbaum et al. 1987; Engstler et al. 1988):

$$S(E) \approx S_{bare}(E) e^{\pi\eta(U_e/E)}, \quad (10)$$

where  $U_e$  is the energy-independent electron screening potential.

Notice that the measurement can be performed in two ways, depending on the identity of the projectile and target. The situation is shown in Figure 3. The notation  ${}^3\text{He}(d,p){}^4\text{He}$  refers to a deuterium ion beam (without atomic electrons) directed onto a neutral  ${}^3\text{He}$  target (two electrons), while  $d({}^3\text{He},p){}^4\text{He}$  refers to a  ${}^3\text{He}$  ion beam (one electron) directed onto a neutral deuterium target (one electron). These two situations result in different electron screening potentials,  $U_e$ . The distinction is particularly important at center-of-mass energies below 50-keV, as will be shown below.

### 3. BAYESIAN MODEL

#### 3.1. General aspects

Bayesian probability theory provides a mathematical framework to infer, from the measured data, the degree of plausibility of model parameters. (Jaynes & Bretthorst 2003). It allows to update a current state of knowledge about a set of model parameters,  $\theta$ , in view of newly available information. The updated state of knowledge about  $\theta$  is described by the posterior distributions,  $p(\theta|y)$ , i.e., the probability of the parameters,

$\theta$ , given the data,  $y$ . At the foundation of the theory lies the Bayes' theorem:

$$p(\theta|y) = \frac{\mathcal{L}(y|\theta)\pi(\theta)}{\int \mathcal{L}(y|\theta)\pi(\theta)d\theta}. \quad (11)$$

The right term of Equation 11 represents the product of the model likelihood,  $\mathcal{L}(y|\theta)$ , i.e., the probability that the data,  $y$ , were obtained given the model parameters,  $\theta$ , and the prior distribution,  $\pi(\theta)$ , which represents our state of knowledge before considering the new data. The normalization factor appearing in the denominator, called the evidence, describes the probability of obtaining the data considering all possible parameter values.

In the Bayesian framework, the concept of hierarchical Bayesian models is of particular interest when accounting for different effects and processes that impact the measured data (Parent & Rivot 2012; de Souza et al. 2015, 2016; Hilbe et al. 2017). The underlying idea is to decompose higher-dimensional problems into a number of probabilistically linked lower-dimensional substructures. Hierarchical Bayesian models enable us to include in a coherent fashion the different types of uncertainties into the model, thereby solving inferential problems that are not amenable to traditional statistics (Trotta 2017).

### 3.2. An example

Figure 4 depicts a simple example for a nuclear counting experiment to illustrate an inherently hierarchical statistical structure. The vertical axis shows the number of counts and the different layers of variabilities are indicated on the horizontal axis. The theoretical mean value of the number of counts,  $y$  (grey dot), is unknown. In statistical parlance,  $y$  is called a latent or hidden variable, representing the boundary between the theoretical and observable world. The actual number of decays,  $y'$  (blue dot), differs from the theoretical mean value because of the stochastic nature of a nuclear decay or reaction processes. We can write

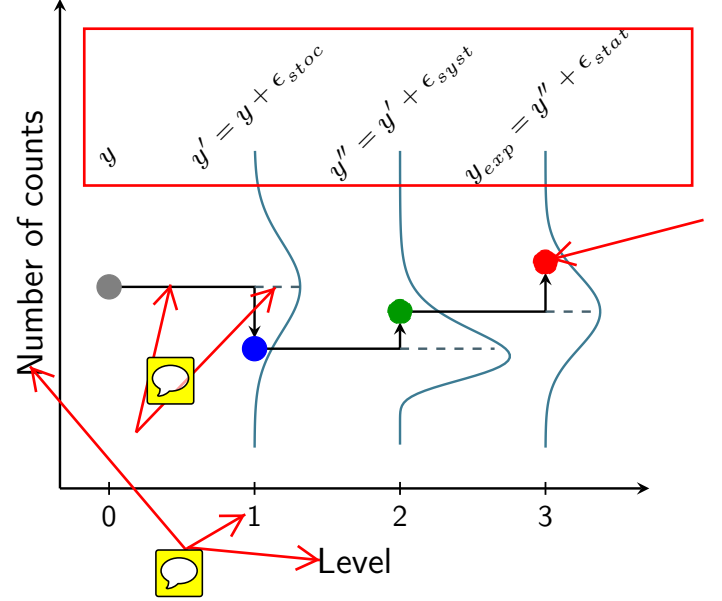
$$y' = y + \epsilon_{stoc}, \quad (12)$$

where  $\epsilon_{stoc}$  quantifies the stochastic contribution that perturbs  $y$ . The quantity  $y'$  is also unobservable since we have not considered experimental effects yet. Typically, data are subject to systematic and statistical effects.

The systematic contribution,  $\epsilon_{syst}$ , which affects all data points of a given experiment equally, perturbs the number of counts (blue dot) and gives rise to the green dot. We can write

$$y'' = y' + \epsilon_{syst}, \quad (13)$$

Finally, the statistical contribution,  $\epsilon_{stat}$ , which differs for each data point of a given experiment, also perturbs



**Figure 4.** Example of a counting experiment. The true (but unknown) value of the quantity,  $y$  (here the mean number of counts; gray circle) is perturbed at each level by different effects: (i) intrinsic stochasticity ( $\epsilon_{stoc}$ ; blue circle), (ii) experimental systematic effects ( $\epsilon_{syst}$ ; green circle), (iii) experimental statistical effects ( $\epsilon_{stat}$ ; red circle). The Bayesian model is constructed to estimate the posterior density for the true value of  $y$  (gray circle) from the actual measurement (red circle). The probability densities at each level are shown as solid blue lines.

the number of counts (green dot) and gives rise to the measured value (red dot), according to

$$y_{exp} = y'' + \epsilon_{stat}. \quad (14)$$

It is straightforward to construct the hierarchical Bayesian model that incorporates all of these different layers of variability, as explained in the next section. The goal is to estimate the posterior density for the unobservable theoretical mean,  $y$ , based on the measured value of  $y_{exp}$ .

### 3.3. Likelihoods and priors

We will next discuss how to construct likelihoods to quantify the different layers of uncertainty affecting the  ${}^3\text{He}(\text{d,p}){}^4\text{He}$  and  $\text{d}({}^3\text{He,p}){}^4\text{He}$  data. Throughout this work, we evaluate the Bayesian models using JAGS (“Just Another Gibbs Sampler”), a program for analysis of Bayesian hierarchical models using a Markov chain Monte Carlo framework (Plummer 2003). Specifically, we used the RJAGS package to interface JAGS with the R language (Team 2010).

Running a Bayesian model in JAGS refers to generating random samples from the posterior distribution of model parameters. This requires the definition of



the model, likelihoods, and priors, as well as the initialization, adaptation, and monitoring of the Markov chain. We implemented a new JAGS module to allow for sampling of a theoretical S-factor model for the  $^3\text{He}(\text{d,p})^4\text{He}$  reaction based on the R-matrix formalism (Section 2), including the effect of electron screening.

### 3.3.1. Stochastic effects

We will first discuss the treatment of a stochastic process. Suppose an experimental S-factor,  $S_{exp}$ , is free of systematic and statistical measurement uncertainties ( $\epsilon_{syst} = 0$ , and  $\epsilon_{stat} = 0$ ), but is subject to an unknown stochastic effect ( $\epsilon_{stoc} \neq 0$ ). If the variable under study is continuous, one can assume in the simplest case a Gaussian noise, with standard deviation of  $\sigma_{stoc}$ . The model likelihood connecting experiment with theory, assuming a vector of model parameters,  $\theta$ , is then given by:

$$\mathcal{L}(S_{exp}|\theta) = \prod_{i=1}^N \frac{1}{\sqrt{2\pi\sigma_{stoc}^2}} \exp \left[ -\frac{(S_{exp;i} - S_i(\theta))^2}{2\sigma_{stoc}^2} \right], \quad (15)$$

where  $S_i(\theta)$  is the model S-factor (obtained from R-matrix theory), and the product runs over all data points,  $N$ , labeled by  $i$ . In symbolic notation, this expression can be written as:

$$S_{exp;i} \sim \text{Normal}(S_i(\theta), \sigma_{stoc}^2) \quad (16)$$

implying that the experimental S-factor datum,  $i$ , is sampled from a normal distribution, with a mean equal to the true value,  $S_i(\theta)$ , and a variance of  $\sigma_{stoc}^2$ .

### 3.3.2. Statistical effects

Any experiment is subject to measurement uncertainties, which are the consequence of an inherent imperfection of the data taking process. Suppose the measurement uncertainties are solely given by statistical effects and that the likelihood can be described, in the simplest case, by a normal probability density. The likelihood for such model can be written symbolically as:

$$S_{exp;i} \sim \text{Normal}(S_i(\theta), \sigma_{stat;i}^2). \quad (17)$$

where  $\sigma_{stat;i}^2$  represents the variance of the normal density for datum  $i$ . Unlike the uncertainty caused by the effect of stochasticity (Section 3.3.1), statistical uncertainties can be reduced by improving the data collection procedure and by collecting more data.

When both statistical and stochastic uncertainties are present, the model can be easily extended to accommodate both effects. The likelihood for such model is given by the nested expressions:

$$S'_i \sim \text{Normal}(S_i(\theta), \sigma_{stoc}^2) \quad (18)$$

$$S_{exp;i} \sim \text{Normal}(S'_i, \sigma_{stat;i}^2) \quad (19)$$

These expressions provide an intuitive view of how a chain of probabilistic disturbances can be combined into a hierarchical structure. First, stochastic effects, quantified by the standard deviation  $\sigma_{stoc}$  of a normal probability density, perturb the theoretical value of a given S-factor datum,  $S_i(\theta)$ , to produce a value of  $S'_i$ ; second, the latter value is in turn perturbed by the statistical uncertainty, quantified by standard deviation  $\sigma_{stat;i}$  of a normal probability density, to produce the measured value  $S_{exp;i}$ . The above demonstrates how any effect impacting the data can be implemented in a straightforward manner into a Bayesian data analysis.

### 3.3.3. Systematic effects

Systematic uncertainties are usually not reduced by combining the results from different measurements or by collecting more data. Reported systematic uncertainties are based on assumptions made by the experimenter, are model-dependent, and follow vaguely known probability distributions (Heinrich & Lyons 2007). In a nuclear counting experiment, systematic effects impact the overall normalization by shifting all points of a given data set into the same direction, and they are often quantified by a multiplicative factor.

For example, if the systematic uncertainty for a given data set is reported as  $\pm 10\%$  (i.e.,  $\sigma_{syst} = 0.10$ ), the factor uncertainty amounts to 1.10. A useful distribution for normalization factors is the lognormal probability density:

$$f(x) = \frac{1}{\sigma_L x \sqrt{2\pi}} \exp \left[ -\frac{(\ln x - \mu_L)^2}{2\sigma_L^2} \right], \quad (20)$$

which is characterized by two quantities, the location parameter,  $\mu_L$ , and the shape parameter,  $\sigma_L$ . The median value of the lognormal distribution is given by  $e^{\mu_L}$ , while the factor uncertainty, for a coverage probability of 68%, is  $e^{\sigma_L}$ . In our model, we include a systematic effect as an informative lognormal prior with a median of 1.0, i.e.,  $\mu_L = 0$ , and a factor uncertainty given by the systematic uncertainty, i.e., in the above example,  $\sigma_L = \ln(1.10)$ . In our above model, we can include systematic uncertainties using the nested expressions:

$$S'_i \sim \text{Normal}(S_i(\theta), \sigma_{stoc}^2) \quad (21)$$

$$S_{exp;i,j} \sim \text{Normal}(\xi_j S'_i, \sigma_{stat;i}^2), \quad (22)$$

where  $\xi_j$  denotes the normalization factor for data set  $j$ .

### 3.3.4. Priors

To test the effects of different priors on our results, we consider two scenarios. In the first scenario ("case I"),

**Table 1.** Priors choices for Case I (moderately informative) and II (weakly informative)<sup>a</sup>.

|              | Case I                                   | Case II                                  |
|--------------|--|--|
| $E_0$        | HalfNormal(0,1)                          | HalfNormal(0, 1)                         |
| $E_r$        | $E_0$                                    | HalfNormal(0, 1)                         |
| $\gamma_d^2$ | HalfNormal(0,1)                          | HalfNormal(0,1)                          |
| $\gamma_p^2$ | HalfNormal(0,1)                          | HalfNormal(0,1)                          |
| $a_d$        | 6  | HalfNormal(6,1)                          |
| $a_p$        | 5  | HalfNormal(5,1)                          |
| $U_e$        | HalfNormal(0, 0.1 <sup>2</sup> )         | HalfNormal(0, 0.1 <sup>2</sup> )         |
| $\xi$        | LogNormal(0, $\sigma_L^2$ ) <sup>b</sup> | LogNormal(0, $\sigma_L^2$ ) <sup>b</sup> |

<sup>a</sup>Units for energies are in MeV, while those for the channel radii are in fm.

<sup>b</sup> $\sigma_L \equiv \ln(1 + \sigma_{\text{sys}}^2)$ .

we employ moderately informative priors for the eigenvalue ( $E_0$ ) and reduced widths ( $\gamma_d^2, \gamma_p^2$ ), and fixed values for the channel radii ( $a_d = 6$  fm,  $a_p = 5$  fm), consistent with Barker (2007). We will also set the eigenvalue,  $E_0$ , equal to the observed resonance energy,  $E_r$ , in the data fitting. In the second scenario (“case II”), we adopt weakly informative priors for  $E_0$ ,  $E_r$ ,  $\gamma_d^2$ ,  $\gamma_p^2$ ,  $a_d$ , and  $a_p$ .

As for the electron screening potential, Aliotta et al. (2001) obtained values of  $U_e = 146 \pm 5$  eV for the  $d(^3\text{He}, p)^4\text{He}$  reaction, and  $U_e = 201 \pm 10$  eV for the  $^3\text{He}(d, p)^4\text{He}$  reaction. Since  $U_e$  is a positive quantity, we will adopt a weakly informative prior given by a half-normal distribution (i.e., a normal distribution left-truncated at zero) with a standard deviation of 100 keV.

As already pointed out above, lognormal priors are adopted for the normalization factors,  $\xi_j$ , of each experiment,  $j$ . They are given by:

$$\xi_j \sim \text{LogNormal}(0, \ln(1 + \sigma_{\text{sys};j}^2)), \quad (23)$$

where  $\sigma_{\text{sys};j}$  denotes the systematic uncertainty for data set  $j$ . Table 1 summarizes our choices of priors for the two scenarios.

#### 4. ANALYSIS OF $^3\text{He}(d, p)^4\text{He}$ AND DATA

The current status of the available data for the  $^3\text{He}(d, p)^4\text{He}$  and  $d(^3\text{He}, p)^4\text{He}$  reactions is discussed in detail in Appendix A. For the present analysis, we adopt the results of Zhichang et al. (1977); Krauss et al. (1987); Möller & Besenbacher (1980); Geist et al. (1999); Costantini et al. (2000); Aliotta et al. (2001), because

only these data sets allow for a separate estimation of statistical and systematic uncertainties. In total, our analysis includes 214 data points at center-of-mass energies between 4.2 keV and 471 keV.

##### 4.1. Case I

The hierarchical Bayesian model, using case I as an example, can be summarized as:

Likelihoods

$$\begin{aligned} S'_i &\sim \text{Normal}(S_i(\theta) e^{\pi \eta(U_{e;k}/E_{exp;i})}, \sigma_{\text{stoc}}^2) \\ S_{exp;i,j} &\sim \text{Normal}(\xi_j S'_i, \sigma_{\text{stat};i}^2) \end{aligned} \quad (24)$$

Parameters

$$\theta \equiv (E_r, \gamma_d^2, \gamma_p^2, U_{e;k}, \xi_j)$$

Priors

$$\begin{aligned} \xi_j &\sim \text{LogNormal}(0, \ln(1 + \sigma_{\text{sys};j}^2)) \\ (E_0 \equiv E_r, \gamma_d^2, \gamma_p^2) &\sim \text{HalfNormal}(0, 1) \\ U_{e;k} &\sim \text{HalfNormal}(0, 0.01) \end{aligned}$$

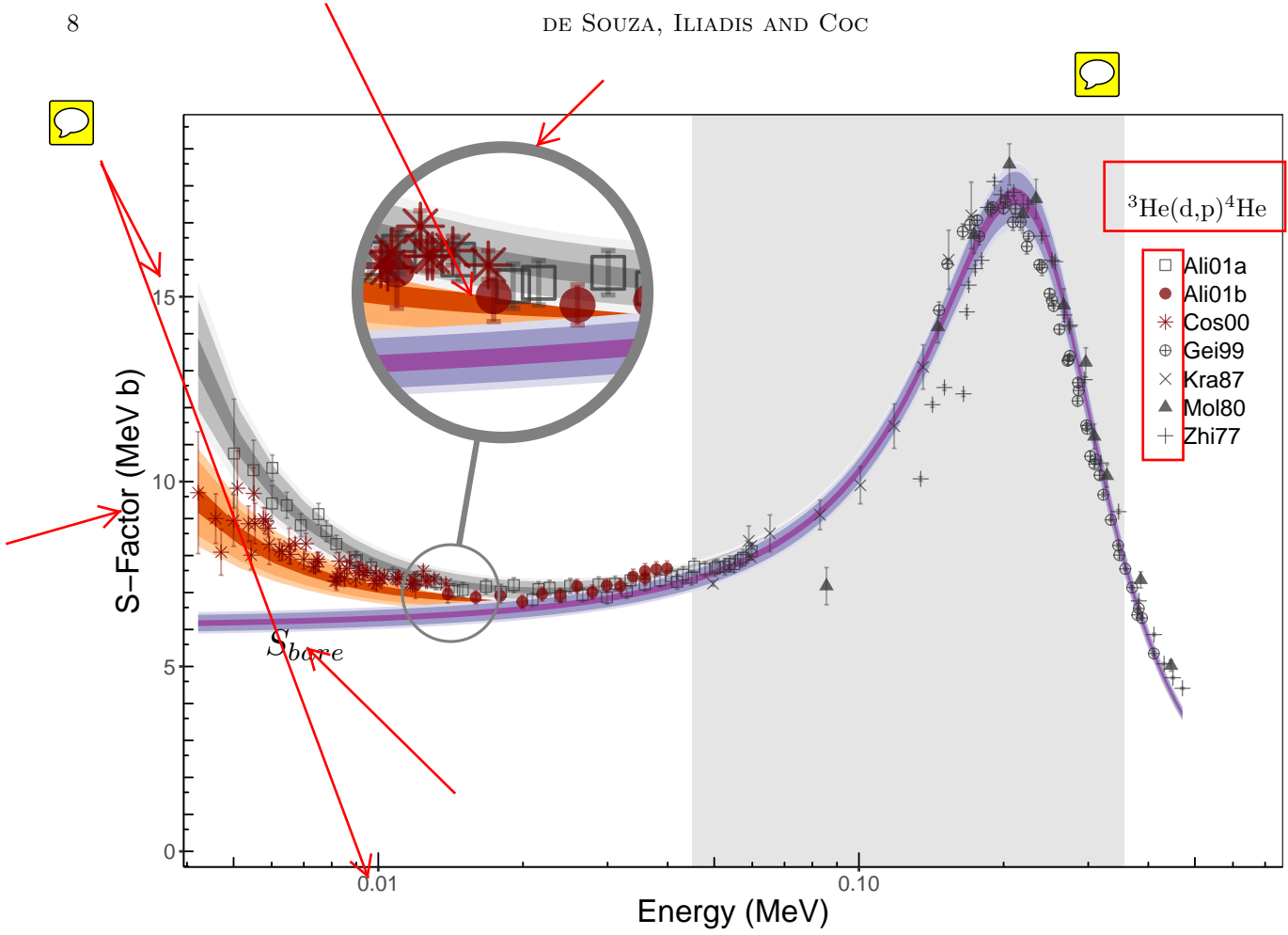
Indices

$$j = 1, \dots, 7; \quad k = 1 \text{ or } 2; \quad i = 1, \dots, 214$$

The first layer accounts for the effects of an inherent stochastic uncertainty and electron screening, while the second layer describes the effects of systematic and statistical uncertainties. The indices denote the number of data sets ( $j$ ), data points ( $i$ ), and the two possibilities for electron screening depending on the kinematics of the experiment ( $k$ ).

The MCMC sampling will provide the posteriors for all 12 parameters. We generate random samples using three independent Markov chains, each of length 20,000 (without burn-in). This ensures that the Monte Carlo fluctuations are negligible compared to the statistical and systematic uncertainties. The lengths of the initial adapting and burn-in phases were set to 5,000 steps. The fitted model is displayed at figure 5. The plot shows three solutions and their respective credible intervals: The bare S-factor (purple intervals), i.e. the estimated S-factor free from the effects of electron screening, and the solution for  $d(^3\text{He}, p)^4\text{He}$  (red intervals) and  $^3\text{He}(d, p)^4\text{He}$  (gray intervals) datasets. The inset highlights the region which the effects of electron screening starts to be non-negligible.

For Case I, the one- and two-dimensional marginalized posterior densities of the R-matrix parameters  $E_0$ ,  $\gamma_d$ ,  $\gamma_p$ ,  $U_e$  are shown in Figure 6, in addition we included the posteriors for the estimated S-factor at zero energy. The contours in the panels for the two-dimensional densities depict 68%, 95%, and 99.7% credible intervals around the marginal posterior mean.



**Figure 5.** Bayesian Astrophysical S-factor for the bare and screened nuclei versus  ${}^3\text{He} + \text{d}$  center-of-mass energy for the  ${}^3\text{He}(\text{d},\text{p}){}^4\text{He}$  reaction. The symbols show the data of each independent generated group. The error bars refer to statistical uncertainties only. The shaded areas depicts 50%, 95%, and 99% credible intervals around the mean S-factor.

#### 4.2. Case II

The hierarchical Bayesian model for case II, can be easily extended from the model 24 by replacing the priors on  $E_r$ ,  $a_d$ , and  $a_p$  following 1. The one- and two-dimensional marginalized posterior densities for its R-matrix parameters in addition to the estimated S-factor at zero energy, are shown in Figure 7. The contours in the panels for the two-dimensional densities depict 68%, 95%, and 99.7% credible intervals around the marginal posterior mean.

The inclusion of the channels radii  $a_d$ , and  $a_p$  as additional free parameters induces highly degeneracy and multi-modality in the posteriors. The weakly constrained capability have been previously identified in e.g. Descouvemont & Baye (2010). The screening-potential and the S-factor at zero energy are marginally affected by the prior choices or assumed values of the channel radii. In what follows, we compare our estimated pa-

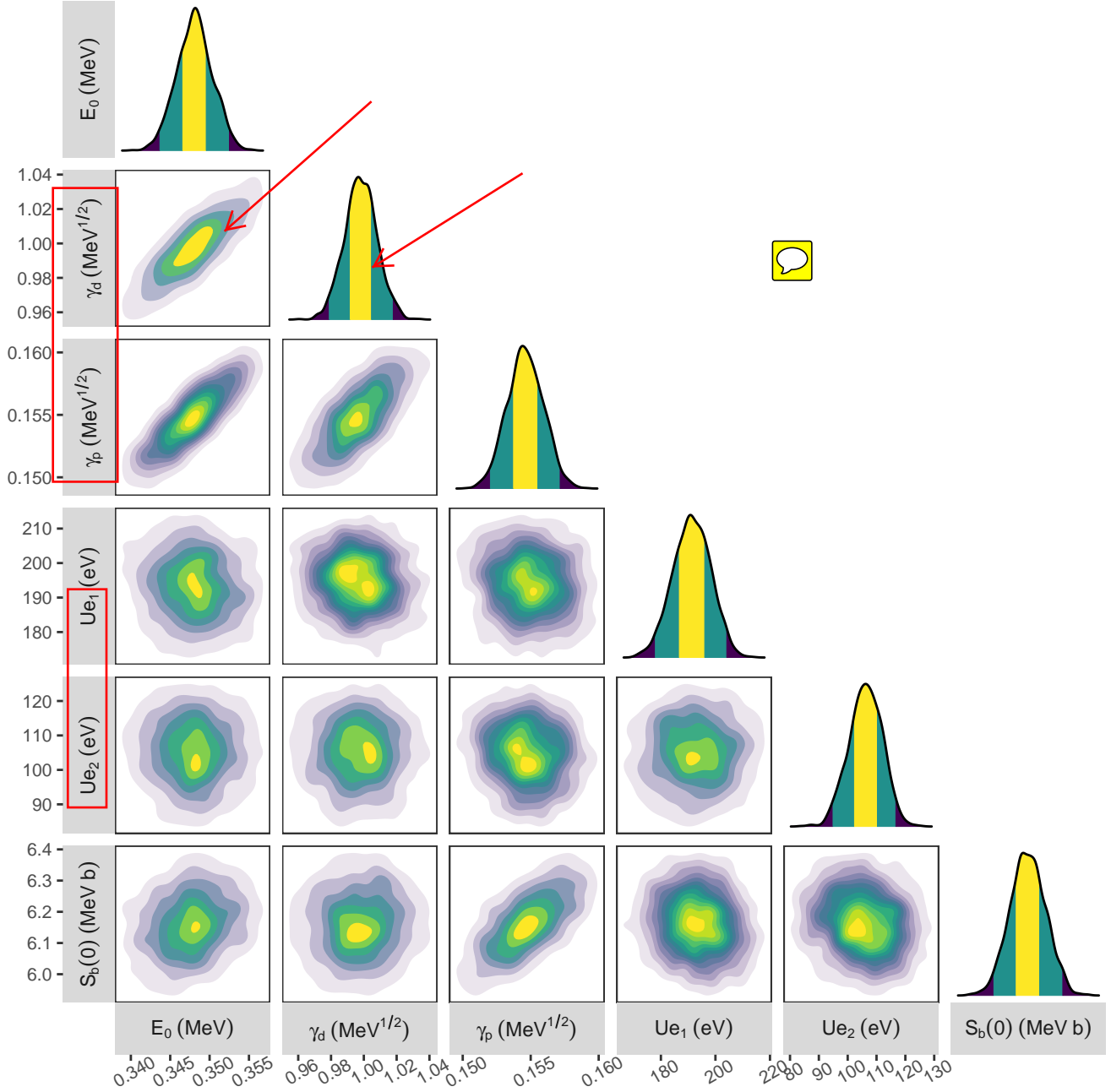
rameters with previous estimates and their subsequent impact in the thermonuclear reaction rates.

#### 4.3. Previous results

Previous estimates based on  $\chi^2$  optimization have been applied to the calculation of  ${}^3\text{He}(\text{d},\text{p}){}^4\text{He}$  R-matrix parameters (Barker 2007), screening effects (Descouvemont et al. 2004) and reaction rates Descouvemont et al. (2004); Xu et al. (2013).

A summary statistics of our analysis, means and standard errors of the mean estimate, are compared to previous analyses in Tables 2 and 3. For fixed values of channel radii our results for the other R-matrix parameters are somewhat close to the ones from Barker (2007). When fitted altogether, the strong correlation between partial widths and the channel radii leads to multi-modal posteriors and rather different estimated values of channel radii and partial widths. On the other



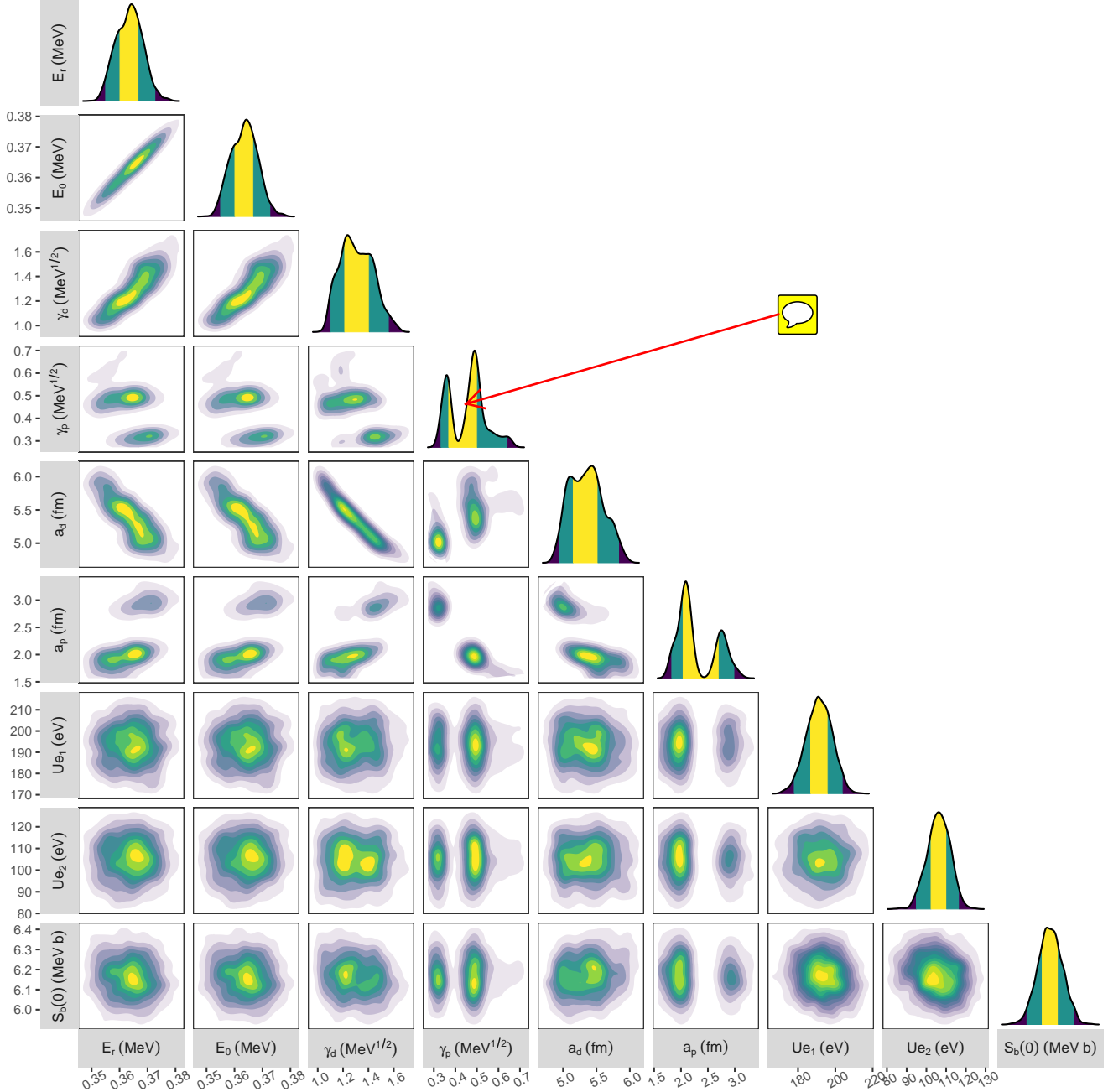


**Figure 6.** One- and two-dimensional marginalized posterior densities for the R-matrix parameters ( $E_0$ ,  $\gamma_d$ ,  $\gamma_p$ ,  $U_e$ , and  $S_b(0)$ ); see Section 2. The results were obtained for “case I” (see Section 3.3.4). The contours in the panels for the two-dimensional densities represent 68% and 96% credible intervals.

hand,  $E_r$  show resilience against different prior choices and channel radii assumptions.

Table 3 highlights the summary information of the electron screening potentials for  $d(^3\text{He},p)^4\text{He}$  and  $^3\text{He}(d,p)^4\text{He}$  reactions. Our estimates  $U_e = 105 \pm 10$  eV for  $d(^3\text{He},p)^4\text{He}$ , and  $U_e = 193 \pm 10$  eV for the  $^3\text{He}(d,p)^4\text{He}$ . The values for  $^3\text{He}(d,p)^4\text{He}$  are consistent with previous estimates from Barker (2007), and Descouvemont et al. (2004) within the uncertain-

ties, but slightly lower than Aliotta et al. (2001), unlike the  $d(^3\text{He},p)^4\text{He}$ , which shows a fair agreement with Aliotta et al. (2001), but is lower than Descouvemont et al. (2004). The S-factor at zero energy are overall consistent with previous estimates, although lower than Aliotta et al. (2001). We shall note that the current and previous estimated values are still larger than the so-called adiabatic limit – the difference in electron binding energies between the colliding atoms and the compound



**Figure 7.** One- and two-dimensional marginalized posterior densities for the R-matrix parameters ( $E_0$ ,  $E_r$ ,  $\gamma_d^2$ ,  $\gamma_p^2$ ,  $a_d$ , and  $a_p$ ); see Section 2. The results were obtained for “case I” (see Section 3.3.4). The contours in the panels for the two-dimensional densities represent 68% and 96% credible intervals.

atom –  $U_e = 65$  eV for  $d(^3\text{He}, p)^4\text{He}$ , and  $U_e = 120$  eV for  $^3\text{He}(d, p)^4\text{He}$  (e.g., Aliotta et al. 2001), and such discrepancy are yet to be explained.

Finally, we show the probability distributions for the normalization factors in Figure 3 for each data set. The vertical dashed red line represents zero systematic effects (i.e., a normalization factor of unity). The normaliza-

tion factors are mostly below 5% with 95% probability, indicating the absence of problematic experiments. A summary statistics of the normalization factors are given in table 4

#### 4.4. Bayesian Reaction Rates

The non-resonant thermonuclear reactions rates per particle pair is given by the Maxwellian-averaged rate times the Avogadro’s number  $N_A$ :

**Table 2.** Parameter values for R-matrix fit

|                            | $E_r$         | $\gamma_p$         | $\gamma_d$         | $a_d$       | $a_p$       |
|----------------------------|---------------|--------------------|--------------------|-------------|-------------|
|                            | MeV           | MeV <sup>1/2</sup> | MeV <sup>1/2</sup> | fm          | fm          |
| Barker (2007) <sup>b</sup> | 0.386         | 0.177              | 0.879              | 6           | 5           |
| Case I                     | 0.347 ± 0.004 | 0.155 ± 0.002      | 0.997 ± 0.020      | 6           | 5           |
| Case II                    | 0.363 ± 0.007 | 0.446 ± 0.107      | 1.307 ± 0.173      | 5.37 ± 0.32 | 2.27 ± 0.51 |

**Table 3.** Electron-screening potential and S-factors at zero-energy

|                                | Ue <sub>1</sub> | Ue <sub>2</sub> | S <sub>b</sub> (0) |
|--------------------------------|-----------------|-----------------|--------------------|
|                                | eV              | eV              | MeV b              |
| NACRE II <sup>a</sup>          | ×               | ×               | 5.9 ± 0.5          |
| Descouvemont et al. (2004)     | 201 ± 10        | 146 ± 5         | 5.9 ± 0.3          |
| Barker (2007) <sup>b</sup>     | 194             | ×               | 6.05               |
| Aliotta et al. (2001)          | 219 ± 7         | 109 ± 9         | 6.7                |
| Case I                         | 193.28 ± 10.17  | 105.23 ± 10.19  | 6.160 ± 0.106      |
| Case II                        | 193.28 ± 10.17  | 105.23 ± 10.19  | 6.126 ± 0.106      |
| <sup>a</sup> Xu et al. (2013). |                 |                 |                    |

**Table 4.** Systematic uncertainties

| Data   | Normalization factor |
|--------|----------------------|
| Ali01a | 0.993 ± 0.017        |
| Ali01b | 1.018 ± 0.017        |
| Cos00  | 1.045 ± 0.023        |
| Gei99  | 0.971 ± 0.017        |
| Kra87  | 1.004 ± 0.019        |
| Mol80  | 1.015 ± 0.01         |
| Zhi77  | 0.973 ± 0.017        |

$m_b$ ) is the reduced mass with  $m_A$  and  $m_a$  standing for the masses of target (a) and projectile (b) nuclei,  $k_B$  is the Boltzmann constant,  $T$  the temperature,  $\sigma$  the cross section.

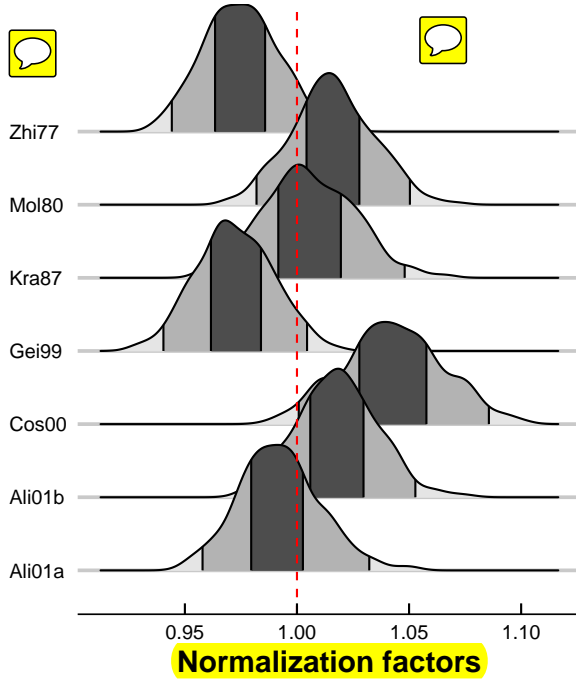
We estimate the reaction rates on a grid of temperatures from 1 MK to 10 GK, providing their mean values and uncertainties for both Cases I and II. The temperature grid, of 60 bins, is chosen to be consistent with previous works (Descouvemont et al. 2004), and to allow a seamless incorporation into the STARLIB library (Sallaska et al. 2013). Numerical reaction rate values are listed in Tables B, and 11. The recommended rates are computed as the 50th percentile of the probability density, while the rate factor uncertainty, f.u. =  $e^{\sigma_L}$ , with  $\sigma_L$  being the standard deviation of the lognormal posterior.

To illustrate the sensitivity of our results against the prior choice, figure 8 shows the ratio the nuclear rates between cases I and II. The agreement remains below 3% for the entire range of BBN interest with 99% probability.

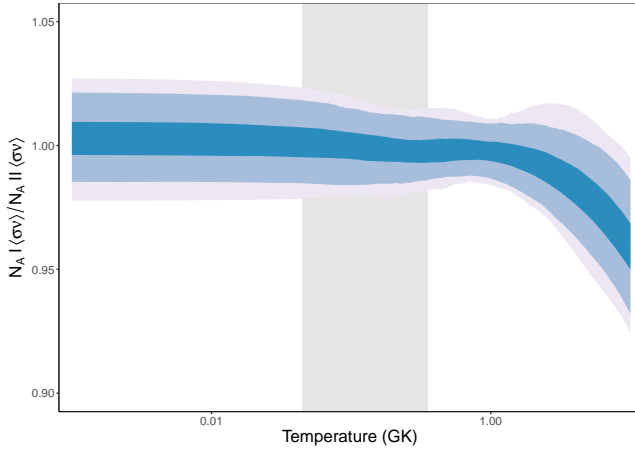
$$N_A \langle \sigma v \rangle = N_A \frac{(8/\pi)^{1/2}}{\mu_0^{1/2} (k_B T)^{3/2}} \int_0^\infty E \sigma(E) e^{-E/k_B T} dE$$

where  $\sigma(E) \equiv S(E) e^{-2\pi\eta}/E$  is the reaction cross section at the center-of-mass incident energy  $E = \mu v^2/2$  with  $v$  being the relative velocity. The term  $\mu_0 = m_a m_b / (m_a +$

## 5. SUMMARY AND CONCLUSIONS



Posterior densities of the normalization factors,  $\xi_i$ , for each of the seven datasets. The shaded gray areas depicts 68% 95% and 99.5% credible intervals, respectively. For the data set labels, see Figure 5.



**Figure 8.** Ratios of the present reaction rates for Cases I and II. The shaded areas depicts 50%, 95%, and 99% credible intervals around the mean ratio.

The Big-Bang nucleosynthesis represents a milestone in the Universe evolution, being responsible for the production of the first light nuclides. Accurate measurements of the nuclear reaction rates occurring on this epoch are paramount to calibrate models chemical evolution. The connection between the theoretical cross-section, subsumed by the Astrophysical S-factor, and the laboratory data, not without issues, as the data is subject to several sources of uncertainty, including intrinsic scatter, error-in-measurements and the effects of electron screening potential. Such stratified error-structure is not amenable by standard approaches such as  $\chi^2$  minimization due to the normality deviation.

To overcome such limitation, we presented a framework to derive statistically sound reaction rates from  $d(^3\text{He},p)^4\text{He}$  and  $^3\text{He}(d,p)^4\text{He}$  data. The model was based on a hierarchical Bayesian framework. Our approach consistently accounts for stochastic uncertainties, errors-in-measurements, systematic effects, and the effects of the electron screening potential.

Here we presented the first statistically rigorous results for d+d reaction rate probability densities. These can be employed in future Monte Carlo studies of big bang nucleosynthesis.

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## APPENDIX

### A. NUCLEAR DATA FOR THE $^3\text{He}(d,p)^4\text{He}$ REACTION

#### A.1. The $^3\text{He}(d,p)^4\text{He}$ data of Zhichang et al. (1977)

The cross section data of Zhichang et al. (1977), as reported in EXFOR (2017), originate from a private communication by the authors and were adopted from Figure 2 of the original article. The derived experimental S-factors, together with their statistical errors ( $\approx 0.6\%$ ) are listed in Table 5. The estimated systematic uncertainty is 3.4%, including the effects of target, solid angle, and beam intensity.

**Table 5.** The  ${}^3\text{He}(d,p){}^4\text{He}$  data of [Zhichang et al. \(1977\)](#).

| $E_{c.m.} \pm \Delta E_{c.m.}$<br>(MeV) | $S \pm \Delta S_{\text{stat}}^a$<br>(MeVb) | $E_{c.m.} \pm \Delta E_{c.m.}$<br>(MeV) | $S \pm \Delta S_{\text{stat}}^a$<br>(MeVb) |
|---|--|---|--|
| 0.1344±0.0048                           | 10.074±0.060                               | 0.2559±0.0042                           | 15.950±0.095                               |
| 0.1422±0.0047                           | 12.080±0.072                               | 0.2676±0.0042                           | 14.505±0.087                               |
| 0.1506±0.0047                           | 12.544±0.075                               | 0.2736±0.0041                           | 14.194±0.085                               |
| 0.1650±0.0046                           | 12.375±0.074                               | 0.2748±0.0041                           | 14.231±0.085                               |
| 0.1677±0.0045                           | 14.590±0.087                               | 0.2949±0.0041                           | 12.757±0.076                               |
| 0.1692±0.0045                           | 15.314±0.092                               | 0.3186±0.0041                           | 10.505±0.063                               |
| 0.1746±0.0045                           | 15.760±0.095                               | 0.3468±0.0040                           | 9.188±0.055                                |
| 0.1800±0.0044                           | 15.987±0.096                               | 0.3822±0.0040                           | 6.773±0.040                                |
| 0.1854±0.0044                           | 17.415±0.104                               | 0.4110±0.0039                           | 5.863±0.035                                |
| 0.1914±0.0044                           | 18.116±0.109                               | 0.4314±0.0038                           | 5.071±0.030                                |
| 0.1974±0.0044                           | 17.763±0.107                               | 0.4500±0.0037                           | 4.695±0.028                                |
| 0.2040±0.0044                           | 17.728±0.106                               | 0.4710±0.0037                           | 4.411±0.026                                |
| 0.2100±0.0044                           | 17.825±0.107                               | 0.5070±0.0036                           | 3.761±0.022                                |
| 0.2247±0.0043                           | 17.502±0.105                               | 0.5466±0.0035                           | 3.002±0.018                                |
| 0.2400±0.0043                           | 16.640±0.099                               | 0.5772±0.0034                           | 2.999±0.018                                |
| 0.2520±0.0042                           | 15.987±0.096                               | 0.6135±0.0033                           | 2.364±0.014                                |

<sup>a</sup>Systematic uncertainty: 3.4%.

#### A.2. The ${}^3\text{He}(d,p){}^4\text{He}$ and $d({}^3\text{He},p){}^4\text{He}$ data of [Krauss et al. \(1987\)](#)

The [Krauss et al. \(1987\)](#) experiments took place at the ion accelerators in Münster and Bochum. Table 3 in [Krauss et al. \(1987\)](#) lists measured S-factors and statistical uncertainties. A normalization uncertainty of 6% originates from an absolute  ${}^3\text{He}(d,p){}^4\text{He}$  cross section measurement at a center-of-mass energy of 59.66 keV, to which a 5% uncertainty caused by variations in the alignment of beam and gas jet target profiles has to be added for the Münster data. Hence, we adopt a systematic uncertainty of 6.0% for the Bochum data and, following the authors, a value of 7.8% for the Münster data. Note that [Krauss et al. \(1987\)](#) do not report separately the results for  ${}^3\text{He}(d,p){}^4\text{He}$  and  $d({}^3\text{He},p){}^4\text{He}$ . Since this distinction is important below a center-of-mass energy of 50 keV, we disregard all of their data points in this energy range. The data ~~that were~~ adopted for our analysis are listed in Table 6.

#### A.3. The $d({}^3\text{He},p){}^4\text{He}$ data of [Möller & Besenbacher \(1980\)](#)

In this experiment, the  $d({}^3\text{He},p){}^4\text{He}$  differential cross section was measured at two angles, relative to the  $d(d,p){}^3\text{H}$  cross section. The total cross section was calculated using the angular distributions from [\(Yarnell et al. 1953\)](#). The statistical error is less than 3%, except at the lowest energy (7%). The systematic error, which arises from the normalization, the  $d(d,p){}^3\text{H}$  cross section, and the anisotropy coefficient, amounts to 3.9%. The EXFOR cross section data were presumably scanned from Fig. 3 of [\(Möller & Besenbacher 1980\)](#). Our adopted S-factors are listed in Table 7.

#### A.4. The ${}^3\text{He}(d,p){}^4\text{He}$ and $d({}^3\text{He},p){}^4\text{He}$ data of [Geist et al. \(1999\)](#)

The cross section data are presented in Figure 5 of [Geist et al. \(1999\)](#) and are available in tabular form from EXFOR, as communicated by the authors. Three data sets exist, one for the  ${}^3\text{He}(d,p){}^4\text{He}$  reaction and two for the  $d({}^3\text{He},p){}^4\text{He}$  reaction, ~~depending on the detected particle~~. The data are listed in Table 8, with statistical uncertainties only. We do



**Table 6.** The  ${}^3\text{He}(d,p){}^4\text{He}$  and  $d({}^3\text{He},p){}^4\text{He}$  data of Krauss et al. (1987)<sup>a</sup>.

| $E_{c.m.}$<br>(MeV)  | $S \pm \Delta S_{\text{stat}}^b$<br>(MeVb) | $E_{c.m.}^d$<br>(MeV) | $S \pm \Delta S_{\text{stat}}^b$<br>(MeVb) |
|----------------------|--|-----------------------|--|
| 0.04970 <sup>c</sup> | 7.24 $\pm$ 0.07                            | 0.0830                | 9.1 $\pm$ 0.4                              |
| 0.05369 <sup>c</sup> | 7.67 $\pm$ 0.08                            | 0.1007                | 9.9 $\pm$ 0.5                              |
| 0.05900 <sup>d</sup> | 8.4 $\pm$ 0.4                              | 0.1184                | 11.5 $\pm$ 0.6                             |
| 0.05952 <sup>c</sup> | 7.96 $\pm$ 0.08                            | 0.1360                | 13.1 $\pm$ 0.6                             |
| 0.05966 <sup>c</sup> | 8.26 $\pm$ 0.08                            | 0.1537                | 16.0 $\pm$ 0.8                             |
| 0.0653 <sup>d</sup>  | 8.6 $\pm$ 0.5                              | 0.1713                | 17.2 $\pm$ 0.9                             |

<sup>a</sup>We disregarded all data points below a center-of-mass energy of 50 keV (see text).

<sup>b</sup>For some data points without reported statistical uncertainty, we assumed a value of 1%.

<sup>c</sup>Bochum data; systematic uncertainty: 6.0%.

<sup>d</sup>Münster data; systematic uncertainty: 7.8%.

not distinguish between the  ${}^3\text{He}(d,p){}^4\text{He}$  and  $d({}^3\text{He},p){}^4\text{He}$  reactions because all data points were measured at center-of-mass energies above 50 keV and, therefore, electron screening effects can be disregarded. A systematic uncertainty of 4.3% is obtained by adding quadratically the contributions from the  $d(d,p){}^3\text{H}$  monitor cross section scale and fitting procedure (1.3% and 3%, respectively), the incident beam energy and energy loss (2%), and the beam integration (2%).

#### A.5. The $d({}^3\text{He},p){}^4\text{He}$ data of Costantini et al. (2000)

We adopted the  $d({}^3\text{He},p){}^4\text{He}$  results of Table 1 in Costantini et al. (2000), which lists the effective energy, S-factor, statistical uncertainty, and systematic uncertainty. The latter ranges from 8% at the lowest energy (4.22 keV) to 3.0% at the highest energy (13.83 keV). In our analysis, we assume an average systematic uncertainty of 5.5%. Table 9 lists the S-factors adopted in the present work.

#### A.6. The ${}^3\text{He}(d,p){}^4\text{He}$ and $d({}^3\text{He},p){}^4\text{He}$ data of Aliotta et al. (2001)

The S-factor data for the  ${}^3\text{He}(d,p){}^4\text{He}$  and  $d({}^3\text{He},p){}^4\text{He}$  reaction are taken from Tables 1 and 2, respectively, in Aliotta et al. (2001). The quoted uncertainties include only statistical (2.6%) effects. The systematic uncertainty arises from the target pressure, calorimeter, and detection efficiency, and amounts to 3.0%. The S-factor data adopted in the present work are listed in Table 10.

#### A.7. Other data

The following data sets were excluded from our analysis. Bonner et al. (1952) only present differential cross sections measured at zero degrees. The cross section data of Jarvis & Roaf (1953), obtained using photographic plates, are presented in their Table 1 for three bombarding energies. However, the origin of their quoted errors (6% – 14%) is not clear. Yarnell et al. (1953) report the differential cross section at 86° (see their Figure 6), but the bombarding energy uncertainty is large (3% – 14%) and the different contributions to the total cross section uncertainty cannot be estimated separately from the information provided. The latter argument also holds for the data of Freier & Holmgren (1954) (see their Figure 1). Arnold et al. (1954) provide cross section between 36 keV and 93 keV bombarding deuteron energy (see their Table 3), including a detailed error analysis. However it was suggested by Coc et al. (2015) that an unaccounted systematic error affected the  $d(d,n){}^3\text{He}$  cross section measured in the same experiment. For the data of Kunz (1955), we could not estimate separately the statistical and systematic uncertainty contributions. We

**Table 7.** The  $d(^3\text{He},p)^4\text{He}$  data of Möller & Besenbacher (1980).

| $E_{c.m.}$<br>(MeV) | $S$<br>(MeVb) | $\Delta S_{\text{stat}}$<br>(MeVb) | $\Delta S_{\text{sys}}$<br>(MeVb) |
|---------------------|---------------|------------------------------------|-----------------------------------|
| 0.0856              | 7.17          | 0.50                               | 0.28                              |
| 0.1460              | 14.18         | 0.42                               | 0.55                              |
| 0.1736              | 16.68         | 0.50                               | 0.65                              |
| 0.2056              | 18.58         | 0.56                               | 0.72                              |
| 0.2196              | 17.24         | 0.52                               | 0.67                              |
| 0.2336              | 17.65         | 0.53                               | 0.69                              |
| 0.2668              | 14.77         | 0.44                               | 0.58                              |
| 0.2964              | 13.22         | 0.40                               | 0.52                              |
| 0.3088              | 11.22         | 0.34                               | 0.44                              |
| 0.3280              | 10.16         | 0.30                               | 0.40                              |
| 0.3856              | 7.34          | 0.22                               | 0.29                              |
| 0.4460              | 5.02          | 0.15                               | 0.20                              |
| 0.5064              | 3.87          | 0.12                               | 0.15                              |
| 0.5648              | 2.885         | 0.086                              | 0.11                              |
| 0.6256              | 2.337         | 0.070                              | 0.090                             |
| 0.6836              | 2.011         | 0.060                              | 0.080                             |
| 0.7504              | 1.681         | 0.050                              | 0.070                             |
| 0.8068              | 1.553         | 0.046                              | 0.060                             |

disregarded the data of La Cognata et al. (2005) because their indirect method does not provide absolute cross section values. They normalized their results to cross sections obtained in other experiments, mainly the data of Geist et al. (1999). See also the discussion in Barker (2007) regarding the absolute cross section normalization of La Cognata et al. (2005). We did not include the data of Engstler et al. (1988) and Prati et al. (1994) in our analysis because these results are biased by stopping-power problems. Finally, we also did not take into account the results of Barbui et al. (2013), who reported the plasma $^3\text{He}(d,p)^4\text{He}$  S-factor using intense ultrafast laser pulses. The derivation of the S-factor versus center of mass energy from the measured Maxwellian-averaged cross section at different plasma temperatures is complicated and the systematic effects are not apparent to us.

B. REACTION RATES



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**Table 8.** The  ${}^3\text{He}(\text{d},\text{p}){}^4\text{He}$  and  $\text{d}({}^3\text{He},\text{p}){}^4\text{He}$  data of Geist et al. (1999).

| $E_{c.m.}$<br>(MeV) | $S \pm \Delta S_{\text{stat}}^a$<br>(MeVb) | $E_{c.m.}$<br>(MeV) | $S \pm \Delta S_{\text{stat}}^a$<br>(MeVb) |
|---------------------|--|---------------------|--|
| 0.1527              | 15.89 $\pm$ 0.11                           | 0.3344              | 8.965 $\pm$ 0.033                          |
| 0.1645              | 16.76 $\pm$ 0.21                           | 0.3463              | 8.273 $\pm$ 0.046                          |
| 0.1762              | 17.07 $\pm$ 0.14                           | 0.3583              | 7.640 $\pm$ 0.041                          |
| 0.1880              | 17.36 $\pm$ 0.20                           | 0.3702              | 7.134 $\pm$ 0.045                          |
| 0.1899              | 17.418 $\pm$ 0.067                         | 0.3821              | 6.571 $\pm$ 0.037                          |
| 0.1999              | 17.40 $\pm$ 0.15                           | 0.3880              | 6.309 $\pm$ 0.036                          |
| 0.2017              | 17.562 $\pm$ 0.094                         | 0.1468              | 14.64 $\pm$ 0.22                           |
| 0.2117              | 17.38 $\pm$ 0.23                           | 0.1702              | 16.94 $\pm$ 0.23                           |
| 0.2236              | 16.36 $\pm$ 0.21                           | 0.1779              | 16.64 $\pm$ 0.23                           |
| 0.2255              | 16.635 $\pm$ 0.070                         | 0.2092              | 17.02 $\pm$ 0.22                           |
| 0.2374              | 15.86 $\pm$ 0.12                           | 0.2170              | 17.02 $\pm$ 0.22                           |
| 0.2493              | 15.08 $\pm$ 0.12                           | 0.2404              | 15.79 $\pm$ 0.21                           |
| 0.2612              | 14.12 $\pm$ 0.10                           | 0.2522              | 14.903 $\pm$ 0.081                         |
| 0.2732              | 13.300 $\pm$ 0.045                         | 0.2542              | 14.747 $\pm$ 0.059                         |
| 0.2746              | 13.399 $\pm$ 0.052                         | 0.2717              | 13.27 $\pm$ 0.11                           |
| 0.2851              | 12.181 $\pm$ 0.077                         | 0.2855              | 12.68 $\pm$ 0.11                           |
| 0.2866              | 12.464 $\pm$ 0.083                         | 0.3029              | 10.69 $\pm$ 0.14                           |
| 0.2971              | 11.520 $\pm$ 0.079                         | 0.3169              | 10.17 $\pm$ 0.11                           |
| 0.2985              | 11.428 $\pm$ 0.064                         | 0.3482              | 8.012 $\pm$ 0.083                          |
| 0.3089              | 10.474 $\pm$ 0.090                         | 0.3795              | 6.394 $\pm$ 0.074                          |
| 0.3105              | 10.598 $\pm$ 0.055                         | 0.4108              | 5.351 $\pm$ 0.060                          |
| 0.3224              | 9.6450 $\pm$ 0.053                         |                     |  |

<sup>a</sup>Systematic uncertainty: 4.3%.

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**Table 9.** The  $d(^3\text{He},p)^4\text{He}$  data of Costantini et al. (2000).

| $E_{c.m.}$<br>(MeV) | $S \pm \Delta S_{\text{stat}}^a$<br>(MeVb) | $E_{c.m.}$<br>(MeV) | $S \pm \Delta S_{\text{stat}}^a$<br>(MeVb) |
|---------------------|--|---------------------|--|
| 0.00422             | 9.7 $\pm$ 1.7                              | 0.00834             | 7.51 $\pm$ 0.22                            |
| 0.00459             | 9.00 $\pm$ 0.67                            | 0.00851             | 7.38 $\pm$ 0.22                            |
| 0.00471             | 8.09 $\pm$ 0.62                            | 0.00860             | 7.65 $\pm$ 0.23                            |
| 0.00500             | 8.95 $\pm$ 0.70                            | 0.00871             | 7.82 $\pm$ 0.28                            |
| 0.00509             | 9.8 $\pm$ 1.0                              | 0.00898             | 7.36 $\pm$ 0.19                            |
| 0.00537             | 8.86 $\pm$ 0.48                            | 0.00908             | 7.66 $\pm$ 0.17                            |
| 0.00544             | 8.01 $\pm$ 0.39                            | 0.00914             | 7.60 $\pm$ 0.24                            |
| 0.00551             | 9.68 $\pm$ 0.70                            | 0.00929             | 7.54 $\pm$ 0.23                            |
| 0.00554             | 8.87 $\pm$ 0.55                            | 0.00938             | 7.47 $\pm$ 0.14                            |
| 0.00577             | 8.99 $\pm$ 0.31                            | 0.00948             | 7.59 $\pm$ 0.13                            |
| 0.00583             | 8.93 $\pm$ 0.36                            | 0.00978             | 7.32 $\pm$ 0.22                            |
| 0.00590             | 8.74 $\pm$ 0.25                            | 0.00987             | 7.52 $\pm$ 0.19                            |
| 0.00593             | 8.31 $\pm$ 0.55                            | 0.00991             | 7.24 $\pm$ 0.18                            |
| 0.00623             | 8.15 $\pm$ 0.29                            | 0.01007             | 7.39 $\pm$ 0.19                            |
| 0.00631             | 8.10 $\pm$ 0.23                            | 0.01018             | 7.35 $\pm$ 0.14                            |
| 0.00652             | 8.26 $\pm$ 0.48                            | 0.01029             | 7.44 $\pm$ 0.17                            |
| 0.00657             | 8.03 $\pm$ 0.26                            | 0.01087             | 7.38 $\pm$ 0.16                            |
| 0.00672             | 8.32 $\pm$ 0.16                            | 0.01096             | 7.35 $\pm$ 0.13                            |
| 0.00700             | 7.90 $\pm$ 0.27                            | 0.01105             | 7.41 $\pm$ 0.17                            |
| 0.00707             | 8.32 $\pm$ 0.28                            | 0.01165             | 7.24 $\pm$ 0.14                            |
| 0.00734             | 7.70 $\pm$ 0.16                            | 0.01178             | 7.21 $\pm$ 0.12                            |
| 0.00740             | 7.69 $\pm$ 0.15                            | 0.01185             | 7.35 $\pm$ 0.11                            |
| 0.00746             | 7.90 $\pm$ 0.18                            | 0.01241             | 7.58 $\pm$ 0.14                            |
| 0.00752             | 7.83 $\pm$ 0.26                            | 0.01255             | 7.31 $\pm$ 0.13                            |
| 0.00812             | 7.31 $\pm$ 0.11                            | 0.01265             | 7.31 $\pm$ 0.14                            |
| 0.00819             | 7.31 $\pm$ 0.25                            | 0.01307             | 7.36 $\pm$ 0.13                            |
| 0.00822             | 7.43 $\pm$ 0.24                            | 0.01383             | 7.23 $\pm$ 0.13                            |
| 0.00829             | 7.85 $\pm$ 0.24                            |                     |  |

<sup>a</sup> Average systematic uncertainty: 5.5%.

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**Table 10.** The  ${}^3\text{He}(\text{d},\text{p}){}^4\text{He}$  and  $\text{d}({}^3\text{He},\text{p}){}^4\text{He}$  data of Aliotta et al. (2001)<sup>a</sup>.

| $E_{c.m.}$<br>(MeV)  | $S \pm \Delta S_{\text{stat}}^c$<br>(MeVb) | $E_{c.m.}$<br>(MeV)  | $S \pm \Delta S_{\text{stat}}^c$<br>(MeVb) |
|----------------------|--|----------------------|--|
| 0.00501              | 10.8±1.5                                   | 0.02508              | 7.18±0.20                                  |
| 0.00550              | 10.31±0.81                                 | 0.02592 <sup>b</sup> | 7.17±0.19                                  |
| 0.00601              | 9.41±0.48                                  | 0.02662              | 6.93±0.18                                  |
| 0.00602              | 10.37±0.35                                 | 0.02788 <sup>b</sup> | 7.01±0.19                                  |
| 0.00645              | 9.36±0.35                                  | 0.02873              | 7.22±0.20                                  |
| 0.00690              | 8.82±0.31                                  | 0.02988 <sup>b</sup> | 7.19±0.19                                  |
| 0.00751              | 9.12±0.29                                  | 0.02991              | 6.87±0.18                                  |
| 0.00780              | 8.66±0.28                                  | 0.03110              | 7.24±0.20                                  |
| 0.00818              | 8.31±0.24                                  | 0.03190 <sup>b</sup> | 7.17±0.19                                  |
| 0.00896              | 7.85±0.26                                  | 0.03289              | 7.04±0.20                                  |
| 0.00902              | 7.88±0.22                                  | 0.03349              | 7.33±0.20                                  |
| 0.00966              | 7.68±0.22                                  | 0.03389 <sup>b</sup> | 7.43±0.20                                  |
| 0.01072              | 7.48±0.20                                  | 0.03586              | 7.22±0.18                                  |
| 0.01144              | 7.29±0.20                                  | 0.03589 <sup>b</sup> | 7.39±0.19                                  |
| 0.01195 <sup>b</sup> | 7.19±0.35                                  | 0.03589 <sup>b</sup> | 7.58±0.20                                  |
| 0.01199              | 7.35±0.20                                  | 0.03788 <sup>b</sup> | 7.63±0.20                                  |
| 0.01318              | 7.28±0.20                                  | 0.03858              | 7.33±0.18                                  |
| 0.01395 <sup>b</sup> | 6.95±0.23                                  | 0.03987 <sup>b</sup> | 7.65±0.20                                  |
| 0.01439              | 7.04±0.20                                  | 0.04067              | 7.44±0.22                                  |
| 0.01499              | 7.07±0.20                                  | 0.04187              | 7.29±0.20                                  |
| 0.01595 <sup>b</sup> | 6.87±0.18                                  | 0.04306              | 7.48±0.22                                  |
| 0.01675              | 7.16±0.20                                  | 0.04485              | 7.40±0.20                                  |
| 0.01794 <sup>b</sup> | 6.91±0.19                                  | 0.04544              | 7.70±0.22                                  |
| 0.01799              | 7.02±0.20                                  | 0.04786              | 7.63±0.20                                  |
| 0.01914              | 7.20±0.20                                  | 0.05021              | 7.66±0.22                                  |
| 0.01993 <sup>b</sup> | 6.75±0.18                                  | 0.05083              | 7.70±0.20                                  |
| 0.02094              | 6.81±0.18                                  | 0.05265              | 7.70±0.22                                  |
| 0.02155              | 7.09±0.20                                  | 0.05382              | 7.77±0.22                                  |
| 0.02192 <sup>b</sup> | 6.96±0.19                                  | 0.05504              | 7.77±0.22                                  |
| 0.02271              | 7.13±0.20                                  | 0.05681              | 7.88±0.20                                  |
| 0.02392 <sup>b</sup> | 6.92±0.19                                  | 0.05741              | 7.94±0.22                                  |
| 0.02393              | 6.91±0.18                                  | 0.05980              | 8.12±0.22                                  |

<sup>a</sup>S-factors obtained from  ${}^3\text{He}(\text{d},\text{p}){}^4\text{He}$  measurement, unless noted otherwise.

<sup>b</sup>S-factors obtained from  $\text{d}({}^3\text{He},\text{p}){}^4\text{He}$  measurement.

<sup>c</sup>Systematic uncertainty: 3.0%.



**Table 11.** Case I: Recommended reaction rates.<sup>a</sup>

| T (GK) | Rate       | Low Rate <sup>b</sup> | High Rate <sup>b</sup> | f.u.  | T (GK) | Rate       | Low Rate <sup>b</sup> | High Rate <sup>b</sup> | f.u.  |
|--------|------------|-----------------------|------------------------|-------|--------|------------|-----------------------|------------------------|-------|
| 0.001  | 3.6015E-19 | 3.6698E-19            | 3.7307E-19             | 1.019 | 0.14   | 2.8718E+05 | 2.9214E+05            | 2.9685E+05             | 1.018 |
| 0.002  | 6.2037E-13 | 6.3216E-13            | 6.4264E-13             | 1.019 | 0.15   | 3.8441E+05 | 3.9101E+05            | 3.9747E+05             | 1.018 |
| 0.003  | 6.4102E-10 | 6.5324E-10            | 6.6408E-10             | 1.019 | 0.16   | 5.0235E+05 | 5.1092E+05            | 5.1946E+05             | 1.018 |
| 0.004  | 5.0455E-08 | 5.1415E-08            | 5.2270E-08             | 1.019 | 0.18   | 8.0886E+05 | 8.2236E+05            | 8.3594E+05             | 1.017 |
| 0.005  | 1.1181E-06 | 1.1392E-06            | 1.1582E-06             | 1.018 | 0.2    | 1.2221E+06 | 1.2424E+06            | 1.2629E+06             | 1.017 |
| 0.006  | 1.1825E-05 | 1.2048E-05            | 1.2250E-05             | 1.018 | 0.25   | 2.8097E+06 | 2.8564E+06            | 2.9023E+06             | 1.017 |
| 0.007  | 7.7515E-05 | 7.8974E-05            | 8.0296E-05             | 1.018 | 0.3    | 5.3030E+06 | 5.3905E+06            | 5.4735E+06             | 1.017 |
| 0.008  | 3.6473E-04 | 3.7163E-04            | 3.7781E-04             | 1.018 | 0.35   | 8.7431E+06 | 8.8902E+06            | 9.0296E+06             | 1.017 |
| 0.009  | 1.3480E-03 | 1.3734E-03            | 1.3962E-03             | 1.018 | 0.4    | 1.3082E+07 | 1.3305E+07            | 1.3521E+07             | 1.017 |
| 0.01   | 4.1501E-03 | 4.2280E-03            | 4.2978E-03             | 1.018 | 0.45   | 1.8203E+07 | 1.8521E+07            | 1.8809E+07             | 1.017 |
| 0.011  | 1.1079E-02 | 1.1287E-02            | 1.1473E-02             | 1.018 | 0.5    | 2.3946E+07 | 2.4375E+07            | 2.4752E+07             | 1.017 |
| 0.012  | 2.6396E-02 | 2.6891E-02            | 2.7334E-02             | 1.018 | 0.6    | 3.6655E+07 | 3.7322E+07            | 3.7911E+07             | 1.017 |
| 0.013  | 5.7322E-02 | 5.8395E-02            | 5.9357E-02             | 1.018 | 0.7    | 5.0018E+07 | 5.0955E+07            | 5.1777E+07             | 1.017 |
| 0.014  | 1.1529E-01 | 1.1744E-01            | 1.1938E-01             | 1.018 | 0.8    | 6.3172E+07 | 6.4346E+07            | 6.5427E+07             | 1.017 |
| 0.015  | 2.1741E-01 | 2.2145E-01            | 2.2510E-01             | 1.018 | 0.9    | 7.5587E+07 | 7.6998E+07            | 7.8304E+07             | 1.018 |
| 0.016  | 3.8814E-01 | 3.9530E-01            | 4.0185E-01             | 1.018 | 1      | 8.6945E+07 | 8.8579E+07            | 9.0069E+07             | 1.018 |
| 0.018  | 1.0809E+00 | 1.1008E+00            | 1.1191E+00             | 1.018 | 1.25   | 1.1022E+08 | 1.1228E+08            | 1.1416E+08             | 1.018 |
| 0.02   | 2.6075E+00 | 2.6559E+00            | 2.7000E+00             | 1.018 | 1.5    | 1.2656E+08 | 1.2893E+08            | 1.3116E+08             | 1.018 |
| 0.025  | 1.5167E+01 | 1.5446E+01            | 1.5702E+01             | 1.018 | 1.75   | 1.3741E+08 | 1.4003E+08            | 1.4249E+08             | 1.018 |
| 0.03   | 5.7874E+01 | 5.8926E+01            | 5.9902E+01             | 1.018 | 2      | 1.4420E+08 | 1.4690E+08            | 1.4958E+08             | 1.018 |
| 0.04   | 4.0496E+02 | 4.1220E+02            | 4.1901E+02             | 1.018 | 2.5    | 1.4968E+08 | 1.5256E+08            | 1.5527E+08             | 1.018 |
| 0.05   | 1.6089E+03 | 1.6377E+03            | 1.6647E+03             | 1.018 | 3      | 1.4899E+08 | 1.5187E+08            | 1.5461E+08             | 1.018 |
| 0.06   | 4.6016E+03 | 4.6832E+03            | 4.7604E+03             | 1.018 | 3.5    | 1.4527E+08 | 1.4808E+08            | 1.5080E+08             | 1.018 |
| 0.07   | 1.0647E+04 | 1.0835E+04            | 1.1013E+04             | 1.018 | 4      | 1.4014E+08 | 1.4283E+08            | 1.4546E+08             | 1.018 |
| 0.08   | 2.1282E+04 | 2.1655E+04            | 2.2014E+04             | 1.018 | 5      | 1.2863E+08 | 1.3114E+08            | 1.3360E+08             | 1.019 |
| 0.09   | 3.8244E+04 | 3.8912E+04            | 3.9565E+04             | 1.018 | 6      | 1.1753E+08 | 1.1983E+08            | 1.2205E+08             | 1.019 |
| 0.1    | 6.3426E+04 | 6.4522E+04            | 6.5610E+04             | 1.018 | 7      | 1.0755E+08 | 1.0965E+08            | 1.1171E+08             | 1.019 |
| 0.11   | 9.8816E+04 | 1.0054E+05            | 1.0221E+05             | 1.018 | 8      | 9.8767E+07 | 1.0074E+08            | 1.0264E+08             | 1.019 |
| 0.12   | 1.4651E+05 | 1.4904E+05            | 1.5151E+05             | 1.018 | 9      | 9.1126E+07 | 9.2951E+07            | 9.4686E+07             | 1.019 |
| 0.13   | 2.0859E+05 | 2.1219E+05            | 2.1566E+05             | 1.018 | 10     | 8.4445E+07 | 8.6148E+07            | 8.7771E+07             | 1.02  |

<sup>a</sup>In units of  $cm^3 mol^{-1} s^{-1}$ . The values correspond to the median rate, i.e., the 50th percentile of the rate probability density. The rate factor uncertainty, f.u., corresponding to a coverage probability of 68%, is calculated from  $f.u. = e^\sigma$ , where  $\sigma$  denotes the spread parameter of the lognormal approximation to the rate probability density.

<sup>b</sup>Low Rate = 16th, and High Rate = 84th percentiles respectively.

**Table 12.** Case II: Recommended reaction rates.

| T (GK) | Rate       | Low Rate <sup>b</sup> | High Rate <sup>b</sup> | f.u.  | T (GK) | Rate       | Low Rate <sup>b</sup> | High Rate <sup>b</sup> | f.u.  |
|--------|------------|-----------------------|------------------------|-------|--------|------------|-----------------------|------------------------|-------|
| 0.001  | 3.5985E-19 | 3.6620E-19            | 3.7277E-19             | 1.018 | 0.14   | 2.8776E+05 | 2.9271E+05            | 2.9712E+05             | 1.017 |
| 0.002  | 6.1990E-13 | 6.3086E-13            | 6.4210E-13             | 1.018 | 0.15   | 3.8522E+05 | 3.9193E+05            | 3.9777E+05             | 1.017 |
| 0.003  | 6.4057E-10 | 6.5193E-10            | 6.6348E-10             | 1.018 | 0.16   | 5.0354E+05 | 5.1230E+05            | 5.1986E+05             | 1.017 |
| 0.004  | 5.0419E-08 | 5.1313E-08            | 5.2219E-08             | 1.018 | 0.18   | 8.1090E+05 | 8.2508E+05            | 8.3708E+05             | 1.016 |
| 0.005  | 1.1172E-06 | 1.1371E-06            | 1.1571E-06             | 1.018 | 0.2    | 1.2261E+06 | 1.2465E+06            | 1.2651E+06             | 1.016 |
| 0.006  | 1.1816E-05 | 1.2026E-05            | 1.2238E-05             | 1.018 | 0.25   | 2.8213E+06 | 2.8657E+06            | 2.9080E+06             | 1.016 |
| 0.007  | 7.7454E-05 | 7.8840E-05            | 8.0221E-05             | 1.018 | 0.3    | 5.3183E+06 | 5.4073E+06            | 5.4880E+06             | 1.016 |
| 0.008  | 3.6449E-04 | 3.7101E-04            | 3.7749E-04             | 1.018 | 0.35   | 8.7698E+06 | 8.9165E+06            | 9.0501E+06             | 1.016 |
| 0.009  | 1.3471E-03 | 1.3712E-03            | 1.3952E-03             | 1.018 | 0.4    | 1.3126E+07 | 1.3341E+07            | 1.3542E+07             | 1.016 |
| 0.01   | 4.1473E-03 | 4.2213E-03            | 4.2949E-03             | 1.018 | 0.45   | 1.8261E+07 | 1.8567E+07            | 1.8837E+07             | 1.016 |
| 0.011  | 1.1072E-02 | 1.1270E-02            | 1.1466E-02             | 1.018 | 0.5    | 2.4013E+07 | 2.4429E+07            | 2.4780E+07             | 1.016 |
| 0.012  | 2.6379E-02 | 2.6850E-02            | 2.7316E-02             | 1.018 | 0.6    | 3.6752E+07 | 3.7396E+07            | 3.7939E+07             | 1.016 |
| 0.013  | 5.7286E-02 | 5.8307E-02            | 5.9322E-02             | 1.018 | 0.7    | 5.0151E+07 | 5.1039E+07            | 5.1791E+07             | 1.016 |
| 0.014  | 1.1522E-01 | 1.1727E-01            | 1.1931E-01             | 1.018 | 0.8    | 6.3360E+07 | 6.4464E+07            | 6.5466E+07             | 1.016 |
| 0.015  | 2.1728E-01 | 2.2114E-01            | 2.2499E-01             | 1.018 | 0.9    | 7.5825E+07 | 7.7154E+07            | 7.8368E+07             | 1.016 |
| 0.016  | 3.8787E-01 | 3.9477E-01            | 4.0166E-01             | 1.018 | 1      | 8.7273E+07 | 8.8764E+07            | 9.0197E+07             | 1.017 |
| 0.018  | 1.0802E+00 | 1.0994E+00            | 1.1186E+00             | 1.018 | 1.25   | 1.1070E+08 | 1.1263E+08            | 1.1451E+08             | 1.017 |
| 0.02   | 2.6064E+00 | 2.6525E+00            | 2.6988E+00             | 1.018 | 1.5    | 1.2731E+08 | 1.2953E+08            | 1.3169E+08             | 1.017 |
| 0.025  | 1.5160E+01 | 1.5428E+01            | 1.5695E+01             | 1.018 | 1.75   | 1.3843E+08 | 1.4083E+08            | 1.4320E+08             | 1.017 |
| 0.03   | 5.7847E+01 | 5.8862E+01            | 5.9885E+01             | 1.018 | 2      | 1.4548E+08 | 1.4796E+08            | 1.5050E+08             | 1.017 |
| 0.04   | 4.0486E+02 | 4.1187E+02            | 4.1899E+02             | 1.017 | 2.5    | 1.5137E+08 | 1.5403E+08            | 1.5673E+08             | 1.017 |
| 0.05   | 1.6094E+03 | 1.6367E+03            | 1.6649E+03             | 1.017 | 3      | 1.5109E+08 | 1.5376E+08            | 1.5645E+08             | 1.017 |
| 0.06   | 4.6036E+03 | 4.6819E+03            | 4.7614E+03             | 1.017 | 3.5    | 1.4773E+08 | 1.5030E+08            | 1.5293E+08             | 1.018 |
| 0.07   | 1.0654E+04 | 1.0836E+04            | 1.1015E+04             | 1.017 | 4      | 1.4284E+08 | 1.4538E+08            | 1.4794E+08             | 1.018 |
| 0.08   | 2.1301E+04 | 2.1664E+04            | 2.2019E+04             | 1.017 | 5      | 1.3175E+08 | 1.3413E+08            | 1.3649E+08             | 1.018 |
| 0.09   | 3.8287E+04 | 3.8939E+04            | 3.9567E+04             | 1.017 | 6      | 1.2087E+08 | 1.2308E+08            | 1.2530E+08             | 1.018 |
| 0.1    | 6.3503E+04 | 6.4591E+04            | 6.5625E+04             | 1.017 | 7      | 1.1104E+08 | 1.1309E+08            | 1.1516E+08             | 1.019 |
| 0.11   | 9.8952E+04 | 1.0067E+05            | 1.0225E+05             | 1.017 | 8      | 1.0237E+08 | 1.0431E+08            | 1.0623E+08             | 1.019 |
| 0.12   | 1.4670E+05 | 1.4926E+05            | 1.5156E+05             | 1.017 | 9      | 9.4791E+07 | 9.6630E+07            | 9.8420E+07             | 1.019 |
| 0.13   | 2.0892E+05 | 2.1255E+05            | 2.1579E+05             | 1.017 | 10     | 8.8173E+07 | 8.9895E+07            | 9.1588E+07             | 1.019 |

<sup>a</sup>In units of  $cm^3 mol^{-1} s^{-1}$ . The values correspond to the median rate, i.e., the 50th percentile of the rate probability density. The rate factor uncertainty, f.u., corresponding to a coverage probability of 68%, is calculated from  $f.u. = e^\sigma$ , where  $\sigma$  denotes the spread parameter of the lognormal approximation to the rate probability density.

<sup>b</sup>Low Rate = 16th, and High Rate = 84th percentiles respectively.

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