

Improved lanthanide constraints for the kilonova AT 2017gfo

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ABSTRACT

Spectroscopic observations of the kilonova AT 2017gfo provide a unique opportunity to identify signatures from individual heavy elements freshly synthesized via the r -process, the nucleosynthetic channel responsible for producing \sim half of all trans-iron-group elements. Limitations in the available atomic data have historically hampered comprehensive line identification studies; however, renewed interest has led to the generation of improved (more complete and accurately calibrated) line lists for r -process species. Here we demonstrate the utility of such data, by exploiting newly generated line lists for the lanthanides to model the photospheric-phase 3.4 d X-shooter spectrum of AT 2017gfo with the radiative transfer tool TARDIS. We find the data can only be reproduced by invoking a substantially diminished lanthanide mass fraction (X_{LN}) than that proposed by previous studies. Specifically, our model necessitates $X_{\text{LN}} \approx 2.5 \times 10^{-3}$ in the line-forming region, a value $20\times$ lower than previously claimed. This substantial reduction in X_{LN} is driven by our inclusion of much more complete lanthanide line information that enables better estimation of their total contribution to the observations. We encourage future modelling works to exploit all atomic data advances, and also encourage continued efforts to generate the necessary data for the remaining r -process species of interest.

Key words: atomic data – line: identification – radiative transfer – neutron star mergers.

1 INTRODUCTION

For more than 50 yr, compact binary mergers have been postulated as an ideal site for the rapid neutron-capture process (r -process) to synthesize many of the heaviest elements (J. M. Lattimer & D. N. Schramm 1974; E. Symbalisty & D. N. Schramm 1982; D. Eichler et al. 1989; L.-X. Li & B. Paczyński 1998; C. Freiburghaus, S. Rosswog & F. K. Thielemann 1999; S. Rosswog et al. 1999). Simulations of a neutron star (NS) merging with another NS, or a stellar-mass black hole, have demonstrated that the conditions within the ejected material can plausibly support this extreme nucleosynthetic channel (e.g. S. Goriely, A. Bauswein & H.-T. Janka 2011; O. Korobkin et al. 2012; S. Goriely et al. 2013, 2015; A. Perego et al. 2014; S. Wanajo et al. 2014; 2015; O. Just et al. 2015). The radioactive decay of the ensemble of freshly synthesized unstable heavy elements produced via r -process nucleosynthesis can subsequently power a thermal ultraviolet–optical–infrared transient, dubbed a kilonova (KN; L.-X. Li & B. Paczyński 1998; B. D. Metzger et al. 2010; J. Barnes & D. Kasen 2013; B. D. Metzger 2019).

Since the observations of the first spectroscopically confirmed KN event (AT 2017gfo; B. P. Abbott et al. 2017), numerous works have attempted to model these data in an effort to identify spectral

features that can be linked to an individual (or a family of) r -process species, leading to direct tethering of r -process production to NS mergers. Initial work by S. J. Smartt et al. (2017) suggested Cs and Te were dominant contributors to the observed 0.7–0.85 μm absorption feature in the early spectra of AT 2017gfo. Further work by D. Watson et al. (2019) showed that this absorption was likely produced instead by the first r -process peak element Sr, and not Cs or Te. This Sr identification has since been independently corroborated by further quantitative analyses (e.g. N. Domoto et al. 2021; J. H. Gillanders et al. 2022; A. Perego et al. 2022). Further spectral identifications have been proposed for this (and other) features in the spectra; some examples include Y (A. Sneppen & D. Watson 2023), La and Ce (N. Domoto et al. 2022; J. H. Gillanders et al. 2024), Te (K. Hotokezaka et al. 2023; J. H. Gillanders et al. 2024), Rb (Q. Pognan et al. 2023), and He (A. Perego et al. 2022; Y. Tarumi et al. 2023). All feature identification studies have suffered from limitations in the available line transition data, with works typically focusing on the species that have reasonably complete data, or exploiting newly generated data.

The interpretation of KN spectra relies on atomic data that are both complete and accurate. These two qualities, however, do not always come from the same source. Theoretical atomic structure calculations are indispensable because they can, in principle, provide line lists that are essentially complete for a given ion (e.g. M. Tanaka et al. 2020). This completeness is crucial for opacity calculations; if important transitions are missing, the

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total opacity of the ejecta will be underestimated, resulting in misleading conclusions about the physical conditions and the elemental composition of the outflow. By contrast, experimental measurements of energy levels and transition wavelengths are limited in scope due to the wavelength range that can be sampled, but also by the sheer numbers of dense lines in the experimental spectra of open f -shell species that can lead to multiyear line identification studies for a single ion. As a result, these open f -shell species typically were not (until recently) studied in detail. Oscillator strengths are harder still, since they require radiative lifetime measurements combined with branching fractions, or calibrated absorption experiments. Thus, relying exclusively on the existing experimental data can severely underestimate the true opacity.

Theoretical calculations face their own limitations. While calculations optimized for generating large data sets provide completeness, the predicted wavelengths of transitions are often inaccurate. In extreme cases, uncalibrated calculations can deviate from laboratory measurements by as much as 50 per cent (see e.g. A. Flörs et al. 2023; L. J. Shingles et al. 2023). Even much smaller discrepancies are enough to make the reliable identification of individual spectral features very challenging. Consequently, data sets based solely on theoretical calculations can be used to compute opacities, but are inadequate for detailed line identification studies.

Taken together, these issues highlight the need for a combined approach. For reliable modelling of KN spectra, one requires the completeness of theoretical atomic structure calculations to capture the total opacity, alongside the accuracy of experimental measurements to allow confident line identifications for spectral features. Calibrating theoretical data against available experimental benchmarks is therefore essential, since it bridges the gap between completeness and accuracy. Only through this synthesis can we achieve the dual goals of computing reliable opacities and securely identifying the species responsible for the spectral feature(s) present in KNe.

Significant advances have been made in expanding the available atomic data needed for detailed KN studies. A recent example includes the publication of the *Japan–Lithuania Opacity Database for Kilonova*¹ (M. Tanaka et al. 2020; D. Kato et al. 2024), which contains uncalibrated line transition information for neutral to triply ionized Fe to Ra ($Z = 26$ –88, ions I–IV). These data are well-suited for capturing the general impact of these heavy elements to the opacity of KN ejecta, but transition wavelength uncertainties prevent precise spectral feature predictions. Other atomic physics groups have also been working towards generating the line transition information needed for r -process species; for example, calibrated line information now exists for some of the first (Sr, Y, and Zr; L. P. Mulholland et al. 2024a; D. J. Dougan et al. 2025; M. McCann et al. 2025), second (Te; L. P. Mulholland et al. 2024b, 2025), and third (W, Pt, and Au; R. T. Smyth et al. 2018; J. H. Gillanders et al. 2021; N. L. Dunleavy et al. 2022; M. McCann et al. 2022, 2024) r -process peak elements.

Recently, A. Flörs et al. (2026) presented calibrated line information for singly and doubly ionized lanthanide species ($_{57}\text{La}$ – $_{70}\text{Yb}$). This catalogue of atomic structure data comprises 146 856 bound energy levels and nearly 28.7 million transitions across 28 ions, all computed with the Flexible Atomic Code (FAC; M. F. Gu 2008). Of these, 66 591 transitions were experimentally calibrated

Table 1. Summary of the different atomic data sources incorporated into our TARDIS atomic data file, compared to that of J. H. Gillanders et al. (2022).

Species	This work	J. H. Gillanders et al. (2022)
^1H , ^2He	CHIANTI	CHIANTI
^3Li – ^{37}Rb	GFALL	GFALL
^{38}Sr – ^{40}Zr	ATOMS	ATOMS
^{41}Nb – ^{56}Ba	GFALL	GFALL
^{57}La – ^{70}Yb	GSI	DREAM and GFALL ^a
^{71}Lu	DREAM	DREAM
^{72}Hf – ^{77}Ir	GFALL	GFALL
^{78}Pt , ^{79}Au	QUB	QUB
^{80}Hg – ^{92}U	GFALL	GFALL

^aDREAM does not contain data for La II, Eu II, Gd II, Tb II, Dy II, and Ho II; J. H. Gillanders et al. (2022) default to GFALL for these ions.

and therefore provide highly reliable wavelengths. The strong electric dipole transitions with $\log(gf) > -1$ show good agreement with available experimental and semi-empirical data. Moreover, for ions with relatively extensive experimental information, the resulting opacities are consistent with previous models, while also capturing the wavelength accuracy of low-lying transitions where experimental data are available.

In this manuscript, we explore the effects of extending previous radiative transfer studies to make use of recent advances in atomic data. Specifically, this study aims to explore the inferences one can now make by utilizing the current state-of-the-art, publicly available atomic data presented by A. Flörs et al. (2026). To this end, we re-analyse the 3.4 day X-shooter spectrum of AT 2017gfo in a similar manner to that of J. H. Gillanders et al. (2022). We present similar models and focus specifically on the differences caused by incorporating new, more complete, line transition information.

2 ATOMIC DATA

For our radiative transfer modelling we utilize TARDIS, which we describe in Section 3. First, we outline the different atomic data sources that we combine for our modelling efforts.

In addition to the sources used to build the ‘default’ TARDIS atomic data file (the CHIANTI and Kurucz GFALL data; R. Kurucz & B. Bell 1995; K. P. Dere et al. 1997, 2019), we expand to include the Kurucz ATOMS (R. L. Kurucz 2018), DREAM (E. Biémont, P. Palmeri & P. Quinet 1999; P. Quinet & P. Palmeri 2020), QUB (J. H. Gillanders et al. 2021; M. McCann et al. 2022), and GSI atomic data (A. Flörs et al. 2026). We substitute the existing (or non-existent) ‘default’ TARDIS atomic data following a hierarchical preference of GSI and QUB \rightarrow DREAM and ATOMS_{Sr–Zr} and CHIANTI_{H,He} \rightarrow GFALL. A summary of which atomic data sources are included for $Z = 1$ –92 is presented in Table 1. We note that the atomic data compilation presented here is almost identical to that utilized by J. H. Gillanders et al. (2022); the only difference is that here, we have replaced the DREAM and GFALL data for $Z = 57$ –70 (ions II and III) with that of GSI, which represents an improvement in both completeness and accuracy (see A. Flörs et al. 2026).

These atomic data sources were combined and ingested into an atomic data file for use with TARDIS using the CARSUS tool.² We

¹<http://dpc.nifs.ac.jp/DB/Opacity-Database>

²<https://github.com/tardis-sn/carsus>

Table 2. Number of lines present in the GSI and J. H. Gillanders et al. (2022) (DREAM and GFALL) data sets that satisfy $\log(gf) \geq -3$.

Element	Ion	No. of lines			
		GSI		J. H. Gillanders et al. (2022)	
		All λ	> 1 μm	All λ	> 1 μm
$_{57}\text{La}$	II	15 961	5118	273	1
"	III	205	52	129	0
$_{58}\text{Ce}$	II	338 476	97 689	12 717	2
"	III	6230	644	2391	0
$_{59}\text{Pr}$	II	424 350	43 222	144	0
"	III	55 767	2746	12 986	0
$_{60}\text{Nd}$	II	2357 380	307 542	106	0
"	III	514 365	35 636	43	0
$_{61}\text{Pm}$	II	415 689	34 646	0	0
"	III	538 011	14 900	0	0
$_{62}\text{Sm}$	II	578 557	19 981	162	0
"	III	1134 068	36 465	73	0
$_{63}\text{Eu}$	II	385 059	48 152	159	6
"	III	734 893	24 168	788	0
$_{64}\text{Gd}$	II	1614 181	77 469	779	0
"	III	516 465	2759	44	0
$_{65}\text{Tb}$	II	3147 305	50 576	104	0
"	III	856 585	14 670	793	0
$_{66}\text{Dy}$	II	2435 744	49 310	790	0
"	III	207 615	128	1152	0
$_{67}\text{Ho}$	II	446 994	13 706	12	0
"	III	285 764	12 427	1068	0
$_{68}\text{Er}$	II	657 642	22 205	19	0
"	III	120 180	7391	1065	0
$_{69}\text{Tm}$	II	92 279	3659	6317	0
"	III	9088	605	1177	0
$_{70}\text{Yb}$	II	7486	606	5112	667
"	III	903	32	230	0
Total		17 897 242	926 504	48 633	676

truncate all line lists by discarding transitions with $\log(gf) < -3$ to reduce computational demand. These weak transitions have a negligible impact on our synthetic spectra, and so they can be safely discarded.³

After compiling our new atomic data set, we find that the total number of lines included has substantially increased relative to the atomic data set utilized by J. H. Gillanders et al. (2022). Given the only difference in these data compilations is the inclusion of GSI data over DREAM and ATOMS, we compare the number of lines in each (see Table 2). The GSI data set contains 17 897 242 lines for singly and doubly ionized $_{57}\text{La}$ – $_{70}\text{Yb}$, a $370\times$ increase in the number of lines contained in DREAM and ATOMS for the same species and for the same $\log(gf)$ cut (48 633).

3 MODEL SET-UP

As in J. H. Gillanders et al. (2022), we use TARDIS (W. E. Kerzen-dorf & S. A. Sim 2014), the one-dimensional, time-independent, Monte Carlo radiative transfer spectral synthesis tool for generating our synthetic spectra.⁴ While TARDIS was originally devel-

oped to model thermonuclear supernovae (SNe), the code has since been exploited to model a range of explosive transient phenomena, with multiple works utilizing the tool to generate synthetic KN spectra (e.g. S. J. Smartt et al. 2017; D. Watson et al. 2019; J. H. Gillanders et al. 2022, 2024; A. Perego et al. 2022; N. Vieira et al. 2023, 2024)

Here we extend the work of J. H. Gillanders et al. (2022), with vastly improved atomic data inputs (as outlined in Section 2). As in J. H. Gillanders et al. (2022), we reduce the parameter space we explore with our modelling by restricting ourselves to a limited set of composition profiles. In addition to consulting a Solar r -process composition abundance (e.g. those presented by S. Goriely 1999; N. Prantzos et al. 2020), we allow ourselves to also utilize the 13 abundance profiles presented by J. H. Gillanders et al. (2022), which were extracted from a nucleosynthetic post-processing calculation based on a realistic hydrodynamical simulation of a binary NS merger (as presented by S. Goriely et al. 2011, 2013, 2015; A. Bauswein, S. Goriely & H. T. Janka 2013). Despite this apparent restriction, this limited set of ‘realistic’ composition profiles successfully reproduced the 2.4–7.4 d X-shooter data of AT 2017gfo (specifically, J. H. Gillanders et al. 2022 were able to reproduce the observations invoking the $Y_e - 0.29$ a composition profile). For full details of model set-up and approach, see J. H. Gillanders et al. (2022); here we only outline updates and differences to this approach, for brevity.

As in J. H. Gillanders et al. (2022), we utilize the LTE treatment for ionization, dilute-LTE treatment for excitation, and macroatom line treatment to account for fluorescence effects – an important effect for spectral feature formation in KNe. These quasi-LTE approximations within our TARDIS simulations should be reasonable for modelling KN spectra at early times (see e.g. Q. Pognan, A. Jerkstrand & J. Grumer 2022; although see D. Brethauer et al. 2026 for a recent counterexample).

Since the work of J. H. Gillanders et al. (2022), the TARDIS code has been updated to correct the special relativistic treatment of C. Vogl et al. (2019).⁵ Specifically, a correction to the photon packet initialization properties was required, as, at the beginning of a simulation, packets were being initialized at the inner boundary with properties sampled from a single-temperature blackbody function with an incorrect temperature; it was a factor $(2\beta + 1)^{1/4}$ lower than expected (where $\beta = \frac{v}{c}$). Thus, re-running one of the ‘best-fitting’ models presented by J. H. Gillanders et al. (2022) with an updated version of the code returns a synthetic spectrum that is too luminous to match the observed data, as demonstrated in Fig. 1.⁶

A first-order fix to update the best-fitting TARDIS models of J. H. Gillanders et al. (2022) is to re-scale the input T values by this correction factor. New TARDIS models can be obtained that closely match those of J. H. Gillanders et al. (2022) from this approach. In Fig. 1, we present a model with T re-scaled from 3400 \rightarrow 3200 K (given $v_{\text{inner}} = 0.15c$, and thus $T_{\text{new}} = T_{\text{old}}/(2\beta + 1)^{1/4} \simeq 3200$ K). However, this updated inner boundary initialization temperature has knock-on effects on the plasma properties (specifically, on ionization and excitation). Thus, one should formally explore the full effects of this updated special relativistic treatment on the entire sequence of AT 2017gfo models presented by J. H. Gillanders et al. (2022). For now, we

³We ran test models with an extended line list including lines for $\log(gf) \geq -5$, and found that these additional lines had a negligible impact on the resultant synthetic spectrum.

⁴Specifically, we use TARDIS v2024.01.08.

⁵<https://github.com/tardis-sn/tardis/pull/2159>

⁶We note that this is also the source of a similar discrepancy between model and observation in the work of L. P. Mulholland et al. (2024a).

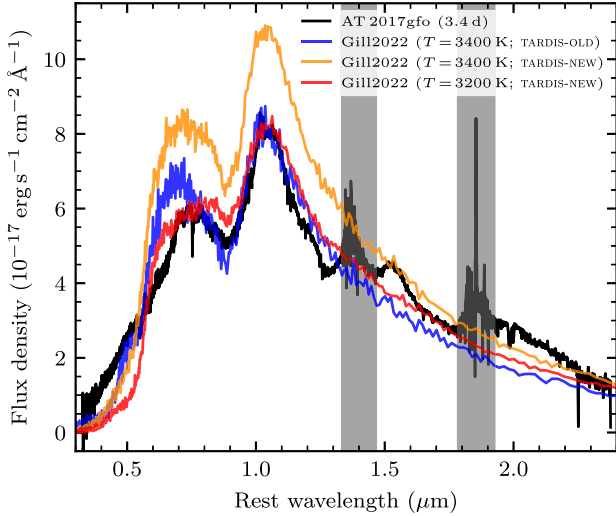


Figure 1. Comparison of the best-fitting TARDIS model from J. H. Gillanders et al. (2022) with the observed 3.4 d X-shooter spectrum of AT 2017gfo. Regions of strong telluric absorption are shaded. We also show the resultant spectrum obtained by regenerating this best-fitting model with the updated TARDIS code and its corrected relativistic treatment, to illustrate the impact this correction has on the synthetic spectrum. Finally, we present the same model, but with T re-scaled, to approximately account for this correction ($T = 3200$ K, versus the original $T = 3400$ K). We find that this re-scaled model closely resembles both the best-fitting model presented by J. H. Gillanders et al. (2022), and the observed data.

limit ourselves to re-analysing the 3.4 d X-shooter spectrum of AT 2017gfo (E. Pian et al. 2017), as the focus of this work is not on updates to the TARDIS code base, but instead on the impact of updated input atomic data (specifically the calibrated line transition information of A. Flörs et al. 2026). We utilize the flux-calibrated, de-reddened and de-redshifted spectral reduction from the ENGRAVE public data release,⁷ and convert the observational data to luminosity using $D_L = 40.4$ Mpc (J. Hjorth et al. 2017).

4 RESULTS AND DISCUSSION

We begin our analysis by exploring a like-for-like comparison between the two atomic data sets (J. H. Gillanders et al. 2022 versus this work). In Fig. 2, we compare the updated best-fitting TARDIS model⁸ for the 3.4 d X-shooter spectrum of AT 2017gfo to an identical model with our updated compilation of atomic data. The only difference between these two models is the input atomic data.

The spectral energy distribution (SED) of the new model is completely altered, and now no longer matches the observed spectrum. Inspecting the different model contributions (see Fig.

⁷<https://www.engrave-eso.org/AT2017gfo-Data-Release>

⁸Note that here, and throughout the rest of this manuscript, when we refer to the best-fitting model of J. H. Gillanders et al. (2022), we are referring to the synthetic spectrum presented in Fig. 1 which has been generated with a re-scaled T to account for corrections to the TARDIS code [dubbed ‘Gill2022 ($T = 3200$ K; TARDIS-NEW)’. This allows us to remove any discrepancy between old and new model fits that are due to updates to the code base; i.e. any changes between this model and our other presented models will be due to updates to our input model properties only.

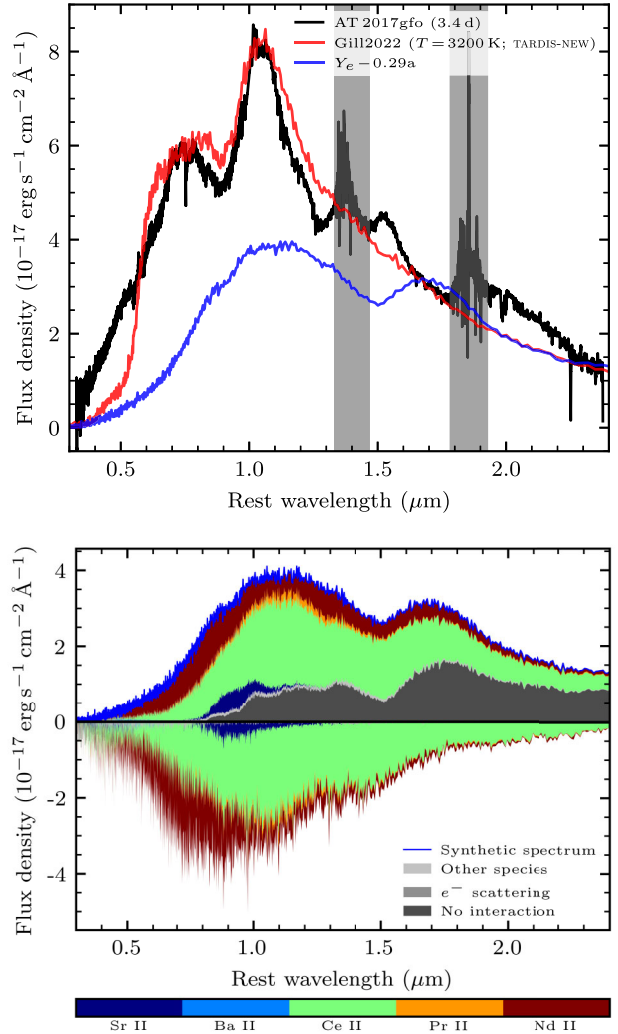


Figure 2. Top: Updated best-fitting models compared with the 3.4 d X-shooter spectrum of AT 2017gfo. Regions of strong telluric absorption in the observations are shaded. The re-scaled $T = 3200$ K model that closely matches that of J. H. Gillanders et al. (2022) is again shown. The same model generated with our updated atomic data set is plotted for comparison. Note how the entire SED has changed shape, due to the significantly increased lanthanide opacity. Bottom: Model decomposition plot to illustrate the strongest contributions to the new model SED. Contributions from specific species are colour-coded; absorption is represented by shaded regions below Flux = 0, while emission is represented by shaded regions above Flux = 0.

2), we see that this change is predominantly due to substantial line blanketing by the lanthanide species Ce II and Nd II. The old data set, which contained DREAM data for the lanthanides, has now been replaced by GSI data. In addition to a dramatic increase in the total number of transitions (see Table 2), this new atomic data extends to much longer wavelengths, allowing substantial deviation from the inner boundary continuum in the near-infrared compared with the previous model (see fig. 8 in J. H. Gillanders et al. 2022). As a specific example, Ce II (the ion that dominates our line-forming region; see Fig. 2) has 12 717 lines in the DREAM data set, whereas the GSI data contains 338 476 lines (a 27 \times increase; Table 2). While there is of course some variation in the oscillator strengths for common lines in DREAM and GSI

(A. Flörs et al. 2026), which may result in a small subset of lines contributing more (or less) to the opacity in this new model, this effect is vastly subdominant to the effect of increasing the sheer number of available transitions in the model.

The inclusion of these new, significantly improved, atomic data immediately reveals the true impact of lanthanide elements in KN ejecta. We can see from Fig. 2 that the lanthanide contribution has been substantially underestimated by all previous works that have employed TARDIS for modelling the spectra of AT 2017gfo, including J. H. Gillanders et al. (2022). This is a result of basing mass fraction estimates on vastly incomplete line transition information. Given the substantial impact of the lanthanides, we need to vastly reduce their total model contribution to better match the observed data. We can accomplish this by (i) lowering the density of the model ejecta, thereby reducing the amount of lanthanide material in the model or (ii) exploring other compositions with lower lanthanide mass fractions.

For (i), we explore a wide parameter space of input model parameters (e.g. by varying v_{inner} , T , ρ_0 , Γ),⁹ and find that updates to these model parameters alone are not sufficient; for example, while it is true that reducing the density in the model reduces the overly strong impact of lanthanides on the emergent spectrum, it also reduces the amount of Sr II, thereby destroying model agreement with the Sr II P-Cygni feature. For (ii), we find that none of the 13 composition profiles presented by J. H. Gillanders et al. (2022) – or a Solar r -process composition – can be invoked to reproduce the data. All models fail to reproduce the flux suppression at blue wavelengths ($\lesssim 0.7 \mu\text{m}$), while also producing a prominent P-Cygni feature to match the data between ~ 0.7 and $1.2 \mu\text{m}$. This is a result of all composition profiles containing incompatible composition ratios of Sr/lanthanides. This statement alone contains some interesting insight; perhaps this indicates that the previously published composition profiles are not representative of characteristic KN ejecta, or at least it may indicate that they are incompatible with this specific event. Further quantification of this, with parameter-space expansion including other proposed KN ejecta compositions, should be undertaken.

Given we are unable to reproduce the data, we allow ourselves to deviate from these fixed composition profiles, to explore what type of abundance profile can reproduce the data. Fundamentally, to match the data, we require two things – a source of flux suppression at blue ($\lesssim 0.7 \mu\text{m}$) wavelengths, and enough Sr II to replicate the prominent ~ 0.7 - $1.2 \mu\text{m}$ P-Cygni profile. Given the lanthanide species appear to be the cause of the largest discrepancy with the data, we opt to alter the best-fitting $Y_e - 0.29a$ composition profile from J. H. Gillanders et al. (2022) by re-scaling the lanthanide mass fractions.

From this approach, we find that we can recover a much more reasonable fit to the data; specifically, by invoking a $20\times$ reduction in the lanthanide ($Z = 57$ - 70) mass fraction.¹⁰ The input TARDIS model properties of this updated best-fitting model are summarized in Table 3, while the model spectrum is compared to the 3.4 d X-shooter spectrum of AT 2017gfo in Fig. 3. This

Table 3. Input properties invoked for our updated best-fitting TARDIS model, and those of the best-fitting model of J. H. Gillanders et al. (2022).

	This work	J. H. Gillanders et al. (2022)
t_{exp} (d)	3.4	3.4
v_{inner} (c)	0.15	0.15
v_{outer} (c)	0.35	0.35
ρ_0 (g cm^{-3})	4×10^{-15}	4×10^{-15}
Γ	-3	-3
Composition profile	$Y_e - 0.29a^a$	$Y_e - 0.29a$
T (K)	3200	3400 ^b

^aThis model utilizes a modified version of the $Y_e - 0.29a$ composition profile (the relative mass fractions of $_{57}\text{La}$ - $_{70}\text{Yb}$ have been re-scaled; see Fig. 4).

^bThis temperature is the best-fitting value derived from an older version of the TARDIS code (see Section 3).

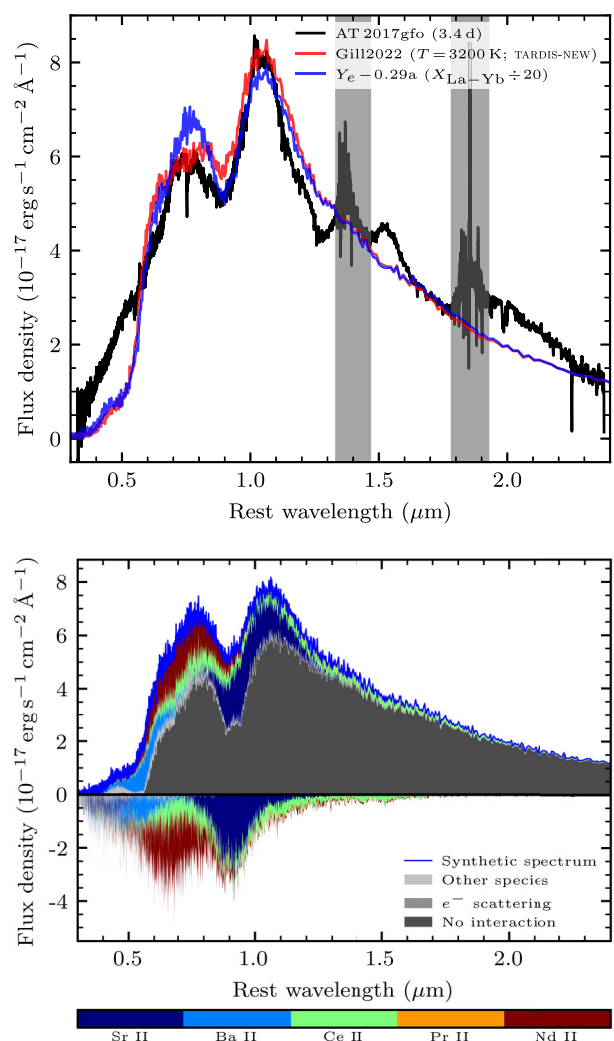


Figure 3. Top: Comparison between our new best-fitting model, our old best-fitting model, and the 3.4 d X-shooter spectrum of AT 2017gfo. Regions of strong telluric absorption are again shaded. This best-fitting model was obtained with a modified version of the $Y_e - 29a$ composition profile. Bottom: Model decomposition plot for our new best-fitting model.

⁹We invoke a power-law density structure with normalization parameters, $t_0 = 2$ d and $v_0 = 14000 \text{ km s}^{-1}$ (see J. H. Gillanders et al. 2022).

¹⁰Modelling of the 2.4–5.4 d X-shooter spectral sequence reveals that this modified composition profile can also reproduce those data; additionally, we find that a different composition is still required to model the earliest 1.4 d X-shooter spectrum (corroborating J. H. Gillanders et al. 2022).

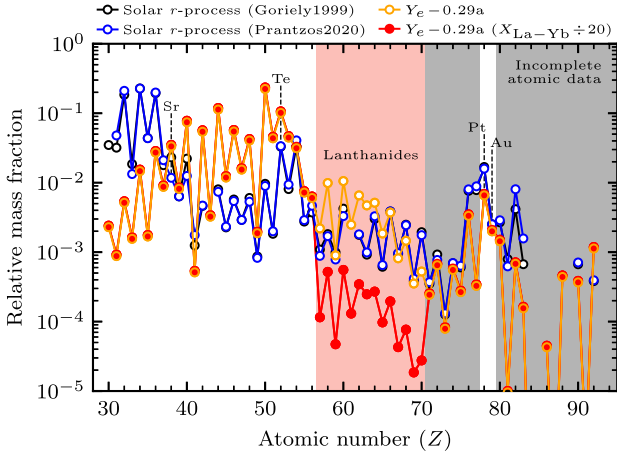


Figure 4. Comparison between the Solar r -process distributions of S. Goriely (1999) and N. Prantzos et al. (2020), the $Y_e - 29a$ composition profile of J. H. Gillanders et al. (2022), and our re-scaled composition profile invoked in this work. All distributions have been re-scaled such that relative mass fractions for $Z = 30-92$ sum to unity. Elements of interest have been labelled, and shaded regions highlight the lanthanide elements and elements with very incomplete atomic data.

model more closely resembles the SED of the observed spectrum for $\lambda \geq 0.6 \mu\text{m}$, but contains prominent absorption at shorter wavelengths, at odds with the observed data (but mirroring the previous best-fitting TARDIS model). This discrepancy is due to Ba II. Ba II appears to be able to create a prominent feature in the model if there is not some strong blanketing from other, heavier, r -process species. Ba is a Group 2 element, and thus Ba II is a homologue to both Ca II and Sr II; all three of these species have simple energy level structures, resulting in relatively few, but intrinsically very strong, permitted transitions. Ca II and Sr II have already been shown to produce strong imprints on KN spectra (N. Domoto et al. 2021), even while having modest abundances, and Ba II is no different (see also N. Domoto et al. 2022).

J. H. Gillanders et al. (2022) claim that the lanthanide mass fraction in the line-forming region of the ejecta > 2 d is $X_{\text{LN}} \simeq 0.05^{+0.05}_{-0.02}$. Here we find that this is a significant overestimate. Instead we find that, to reproduce the 3.4 d X-shooter spectrum of AT 2017gfo, we require $X_{\text{LN}} \approx 2.5 \times 10^{-3}$. Our new best-fitting composition profile is presented in Fig. 4, where we compare it to both the Solar r -process compositions of S. Goriely (1999) and N. Prantzos et al. (2020), as well as the unscaled $Y_e - 29a$ composition profile. The most striking result from this new fit to the observations (and evidenced most clearly in Fig. 4) is that the new inferred abundance of the lanthanide species is significantly lower than the Solar r -process distribution. Further study is needed to quantify the (somewhat arbitrary) composition profile we invoke here; but it, at least initially, appears to indicate that AT 2017gfo-like events may struggle to reproduce the heavy r -process elements to the degree needed to match the Solar r -process distribution. However, we caution that our modelling is only sensitive to the ejecta within the line-forming region; the dense inner regions of ejecta may contain heavier r -process species, potentially resolving this apparent conflict. Our finding of a sub-Solar r -process composition is in line with the compilation of X_{LN} values presented by A. P. Ji, M. R. Drout & T. T. Hansen (2019) ($X_{\text{LN}} = 2 \times 10^{-3} - 2 \times 10^{-2}$).

One point to note with regards to our new best-fitting composition profile, presented in Fig. 4, is that our model possesses

abundances for many trans-lanthanide (i.e. $Z \geq 71$) species that are higher than the lanthanide abundances. We are not claiming that our model necessitates this top-heavy composition profile, consisting of a high mass fraction of very heavy r -process species. Instead, our modelling inferences for species with $Z = 71-92$ (excluding $_{78}\text{Pt}$ and $_{79}\text{Au}$) are hampered by the extremely sparse atomic data (from GFALL) for these species. While we have very complete atomic data from QUB for Pt and Au (J. H. Gillanders et al. 2021; M. McCann et al. 2022), these species have already been shown to only weakly contribute to photospheric-phase KN spectra (J. H. Gillanders et al. 2021). Thus, our modelling is unable to probe abundances for species heavier than the lanthanides, and so the mass fractions for $Z = 71-92$, presented in Fig. 4, should not be overinterpreted.

5 CONCLUSIONS

In this manuscript, we have revisited previously published spectral modelling analysis of AT 2017gfo, with an emphasis on exploiting the newly published, and significantly more complete, line transition information for the lanthanide elements from A. Flörs et al. (2026). From our spectral modelling and analysis, we derive the following main conclusions:

(i) The previously inferred effects of lanthanide material on the emergent SED of the KN models presented by J. H. Gillanders et al. (2022) were significantly underestimated. The updated line transition information utilized here (GSI; A. Flörs et al. 2026) has shown that all previously utilized data sets were vastly incomplete, and that the number of transitions that were present in the previous data were not enough to quantitatively constrain lanthanide contribution.

(ii) It is no longer possible to reproduce the 3.4 d X-shooter spectrum of AT 2017gfo with one of the ‘realistic’ KN composition profiles presented by J. H. Gillanders et al. (2022). Whether this implies AT 2017gfo possessed an atypical composition, or that these profiles are not representative of the ejecta of KNe (or specifically AT 2017gfo) remains an open question.

(iii) We can reproduce the data with a modified version of these KN composition profiles (see Fig. 4). Our new best-fitting model suggests that the mass fraction of lanthanides in the line-forming region of AT 2017gfo at 3.4 d is $X_{\text{LN}} \approx 2.5 \times 10^{-3}$, $20\times$ lower than that reported by J. H. Gillanders et al. (2022) ($X_{\text{LN}} \simeq 0.05^{+0.05}_{-0.02}$). Further modelling works should be undertaken to determine whether this new lanthanide mass fraction estimate is compatible with the other epochs of observed spectra of AT 2017gfo, and/or whether a more physically motivated composition profile can satisfactorily reproduce the observed data.

(iv) We find that to match the data, we need to invoke a significantly sub-Solar abundance for the lanthanides. KNe likely possess stratified compositions as a result of their multiple distinct ejection mechanisms; thus, we cannot constrain the bulk ejecta composition (and total ejected lanthanide mass) from this analysis. The inference of a sub-Solar lanthanide abundance in the line-forming region of AT 2017gfo, while intriguing, does not necessarily mean that AT 2017gfo-like KNe are incapable of producing the Solar r -process distribution; further study should be undertaken to explore this more fully, in an effort to quantify lanthanide production in AT 2017gfo.

This study demonstrates that more complete, and crucially, accurately calibrated, line transition information is vital for spectroscopic studies such as that presented here. The recently pub-

lished GSI data from A. Flörs et al. (2026) provides a substantial step forward for this, and other similar studies. Accurately calibrated data now exist for a substantial number of relevant species across the first, second, and third r -process peaks, in addition to the lanthanides. Further atomic data advances in the coming years will enable iterative improvement towards understanding the composition of KNe, thus ultimately leading to an improved understanding of their role as (one of) the site(s) of r -process nucleosynthesis.

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DATA AVAILABILITY

The observational data presented are publicly available. All information needed to reproduce our modelling has been outlined.

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