Constraints on the presence of platinum and gold in the spectra of the kilonova AT2017gfo

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ABSTRACT

Binary neutron star mergers are thought to be one of the dominant sites of production for rapid neutron capture elements, including platinum and gold. Since the discovery of the binary neutron star merger GW170817, and its associated kilonova AT2017gfo, numerous works have attempted to determine the composition of its outflowing material, but they have been hampered by the lack of complete atomic data. Here, we demonstrate how inclusion of new atomic data in synthetic spectra calculations can provide insights and constraints on the production of the heaviest elements. We employ theoretical atomic data (obtained using GRASP0) for neutral, singly and doubly ionized platinum and gold, to generate photospheric and simple nebular nebular phase modelling, we place tentative upper limits on the platinum and gold mass of \( 10^{-3} \) M\(_\odot\), and \( 10^{-2} \) M\(_\odot\), respectively. This work demonstrates how new atomic data of heavy elements can be included in radiative transfer calculations, and motivates future searches for elemental signatures.

Key words: atomic data – line: identification – radiative transfer – stars: neutron – supernovae: individual: AT2017gfo – neutron star mergers.

1 INTRODUCTION

Mergers of binary neutron star (BNS) and neutron star–black hole (NSBH) systems have long been hypothesized to be an ideal location for the synthesis of the rapid neutron capture (r-process) elements (see discussion by Metzger 2017). Theoretical modelling has shown that the large neutron fraction in expelled material from these mergers is sufficient to generate these heavy elements (Lattimer & Schramm 1974; Eichler et al. 1989; Freiburghaus, Rosswog & Thielemann 2013, 2015; Perego et al. 2014; Just et al. 2015; Sekiguchi et al. 2016). However, spectrophotometric observations are needed to confirm the validity of the models. The first kilonova (KN; the optical counterpart of a BNS merger) was detected in 2017 (AT2017gfo; Andreoni et al. 2017; Arcavi et al. 2017; Chornock et al. 2017; Coulter et al. 2017; Cowperthwaite et al. 2017; Drout et al. 2017; Evans et al. 2017; Kasliwal et al. 2017; Lipunov et al. 2017; Nicholl et al. 2017; Pian et al. 2017; Smartt et al. 2017; Tanvir et al. 2017; Troja et al. 2017; Utsumi et al. 2017; Valenti et al. 2017; Abbott et al. 2017a). Early theoretical models (Kasen et al. 2017) predicted the overall shape of the spectra, and showed that it can be readily explained by the presence of r-process material, as the associated high opacities lead to a red, long-lived component.

Radiative transfer simulations for the spectra of AT2017gfo have taken two approaches. The first is to attempt direct identification of species contributing to apparent absorption features in the early spectra. Smartt et al. (2017) suggested attribution of spectral features to Te I and Cs I, elements from the second r-process peak. Further work by Watson et al. (2019) attributed the same absorption features to lighter r-process elements, specifically Sr II. Both works, however, rely on incomplete atomic data. Specifically, both use data from Kurucz (2017) for their models. This atomic line list provides data for the lowest few ionization stages for all elements up to Te I and Cs I, elements from the second r-process peak. However, due to the difficulties involved with generating this information for heavier elements, the line lists are mostly incomplete beyond this first peak. This makes any modelling, and subsequent conclusions difficult, as the elements without complete atomic data will be excluded from consideration.

The second approach is to calculate new atomic data for heavy elements, and to model the temporal evolution of the spectra in a broad sense. The models of Kasen et al. (2017) and Tanaka et al. (2018, 2020) calculate broad-band spectral energy distributions (SEDs) for low Y\(_\odot\) material, which can reproduce the rising near-infrared (NIR) flux observed in AT2017gfo. The main reason why these works have focused on modelling the broad spectral shapes is due to the accuracy of the atomic data used. Kasen et al. (2017)

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have used elements with complete and well-calibrated atomic data to represent their less well-sampled homologues (e.g. the atomic data for the elements with $Z = 21–28$ have been used as ‘surrogate’ data for the open d-shell $r$-process elements with $Z = 39–48$ and $Z = 72–80$). This allows them to approximate the general behaviour of these heavier open d-shell elements, but restricts them from predicting individual features. They also use new atomic data for the elements with $Z = 58–70$, but these data have not been calibrated. Therefore they cannot be used to accurately predict the locations of individual transitions, as these will be systematically offset from the true wavelengths. Similarly, the atomic data used by Tanaka et al. (2018, 2020) have not been calibrated, and so these results also cannot be used to accurately predict the locations of individual transitions. This will enable us to base our models on accurate atomic data, and allow us to make strong predictions about individual transitions of interest. To that end, the work presented here is a pilot study, focusing specifically on platinum and gold, to demonstrate the validity and usefulness of such a study.

Two of the most interesting heavy elements to search for signatures of are platinum (Pt) and gold (Au). We chose to focus our efforts on these elements for the following reasons. Pt is one of the most abundant third peak $r$-process elements predicted to be synthesized in BNS mergers (Bauswein, Goriely & Janka 2013; Goriely et al. 2013, 2015). We want to explore the presence of heavy elements from this peak, and so Pt was an obvious choice. Au is also among the more abundant elements produced in the third peak, and so this was one reason for selecting it. Another motivation for selecting Au was to explore how much variation there may be between similar elements. Pt and Au are next to each other on the periodic table, and we would like to explore how spectroscopically similar they are. From this, we can investigate the importance of having complete atomic data for all elements abundant in BNS merger synthesis calculations, as opposed to approximating the spectral properties of one element for a whole group of elements (e.g. using Pt to approximate the behaviour of all third peak $r$-process elements).

The cosmic origin of Pt and Au is currently unknown and Kobayashi, Karakas & Lugaro (2020) argue two sites of production may be needed, with a rapid injection of the elements to explain abundance patterns in metal-poor stars. The BNS channel may have a natural time delay that cannot account for the excess in Pt and Au observed. Collapsar accretion discs have been suggested as potential production sites of these elements, and could be the dominant source of heavy elements in the early Universe, as they do not suffer from as long a time delay (Siegel, Barnes & Metzger 2019).

Additionally, magnetorotational supernovae (MR-SNe) have been suggested to be a site of $r$-process nucleosynthesis (Winteler et al. 2012; Mösta et al. 2018), and could contribute to the production of Pt and Au in the early Universe. However, no distinct spectroscopic signature has yet been identified to corroborate this. For further information on potential $r$-process element production sites, see Cowan et al. (2021). No signature of any ion of Pt or Au has been identified in the spectra of AT2017gfo, and hence our motivation for this work is to employ recently calculated, high quality atomic data to predict possible spectral features in kilonova-type expanding ejecta.

We note that there have been previous reports of observations of Pt and Au lines in astrophysical objects. Ross & Aller (1972) report observations of the Au I 3122.8 Å line in the solar photospheric spectrum. Jaschek & Malaroda (1970) report detections of Pt and Au lines in the spectrum of the A-type star 73 Draconis; they observe seven Pt II lines, the strongest of which is the Pt II 4645 Å transition, and four lines belonging to Au I. There have been other observing efforts since, which have observed more Pt and Au lines in various different stars (see e.g. Fuhrmann 1989; Adelman 1994). Also, Castelli & Hubrig (2004) identify two Pt lines in the spectrum of HD 175640, a narrow lined, chemically peculiar star. They identify the Pt II 4061.6, 4514.1 Å transitions. They also identify two Au lines in the spectra; specifically, they detected the Au II 4016.7, 4052.8 Å transitions.

These line detections have all been made in the photospheric spectra of the different stars under investigation. These all have surface temperatures on the order of $\sim 4000–10000$ K, which is comparable to the temperature of KN ejecta at early times (see Shappee et al. 2017; Smartt et al. 2017, where at $0.5–1.5$ d post-merger, the characteristic blackbody temperature drops from $\sim 10000$ to $\sim 5000$ K). It is therefore expected that the strongest Pt and Au lines that have been observed in these stellar spectra could feasibly also appear in the spectra of KNe, at least while the KN exhibits similar temperatures.

All these observed Pt and Au features correspond to strong permitted transitions. To date, there have been no observations of forbidden Pt or Au transitions in astrophysical sources. Forbidden lines for other elements are routinely observed in the late-time spectra of SNe (Jerkstrand 2017). However, the lines observed correspond to elements that are abundant in the ejecta of these transients. Since typical SNe (with the exception of collapsars and MR-SNe) are not predicted to synthesize large masses of $r$-process material, the only $r$-process material in the ejecta will be present from the initial formation of the star. This results in abundances much lower than that required to produce any spectral features of Pt or Au, hence the lack of observations. However, the late-phase spectra of KNe may have promise for the detection of these elements, and other $r$-process elements, since the explosions are hypothesized to synthesize significant masses of $r$-process material. This will result in late-phase spectra dominated by emission features from $r$-process material, and, if Pt and Au are produced in significant quantities, then their spectral signatures could be identifiable.

Our work consists of two parts. First, we determine which strong features of Pt and Au are most likely to be prominent in the early, photospheric spectra of KNe. Secondly, we determine whether any forbidden transitions of Pt and Au could provide emission lines in the late time, nebular spectra of KNe. In both cases, we present predictions and compare to the spectra of AT2017gfo. In Section 2, we detail the sources of the AT2017gfo spectra we compare our models to. In Section 3, we summarize how the atomic data we use in this work was generated. Section 4 contains some motivation for the values we chose for ejecta mass in our work. In Section 5, we outline the steps taken to produce our photospheric phase spectral models, and we highlight our main results. Section 6 details how we generated our syntheic nebular phase spectra, and also contains our results. Finally, we summarize our work in Section 7.
2 SPECTRA

As well as providing model spectra and predictions for the features of Pt and Au, we compare our models with the one known kilonova with a spectroscopic sequence, AT2017gfo. The data we primarily use are the set of 10 X-shooter spectra originally published by Pian et al. (2017) and Smartt et al. (2017). As part of the ENGRAVE project, all the X-shooter spectra were flux-calibrated to a compiled set of photometric measurements taken from the published values of Andreoni et al. (2017), Arcavi et al. (2017), Chornock et al. (2017), Cowperthwaite et al. (2017), Drout et al. (2017), Evans et al. (2017), Kasliwal et al. (2017), Pian et al. (2017), Smartt et al. (2017), Tanvir et al. (2017), Troja et al. (2017), Utsumi et al. (2017), Valenti et al. (2017). This data set is publicly available, and can be accessed through the ENGRAVE webpage, along with release notes describing the calibration, extinction correction, rest-frame velocity correction, and smoothing.

We supplemented this set of spectra with data from two other sources, to extend its temporal coverage to earlier times, and to improve the spectral quality (where possible). Shappee et al. (2017) present early spectra for AT2017gfo. The spectrum taken at +0.5 d (obtained 0.9 d before the earliest X-shooter spectrum presented by Pian et al. 2017; Smartt et al. 2017) is useful for demonstrating the blue, featureless shape characteristic of early KN spectra, and so we use it here to compare with our early models. We flux-calibrated this spectrum (using the SmS code; see Inserza et al. 2018) to the same compiled set of photometric points as detailed above; we also corrected for extinction, and rest-frame velocity. Tanvir et al. (2017) present HST spectra of AT2017gfo, obtained at four separate epochs. The +9.4 d spectrum is particularly interesting as it contains a broad, emission-like feature at ~14 000 Å, which lies in the telluric region, and so it is not observable in our X-shooter spectrum at the same epoch. We merged this HST spectrum with the X-shooter spectrum at this epoch, replacing the pixels of X-shooter with the flux-calibrated HST pixels, within the telluric region.

3 ATOMIC DATA

For KN observations at times, t > 1 d, and ejecta temperatures, T < 20 000 K, the typical ionization stages of heavy elements are neutral up to triply ionized (t−iv); Tanaka et al. 2020). For AT2017gfo, after ~0.5 d, the ejecta temperature dropped to ~10 000 K, and so we expect that typical ionization stages of heavy elements in AT2017gfo are neutral up to doubly ionized (t−iii). Hence, for this work we focused on these ionization stages of Pt and Au.

The atomic structure for these first three ion stages of platinum and gold were calculated within a Dirac–Coulomb framework, employing the General Relativistic Atomic Structure Package (GRASP); Dyall et al. 1989). The orbitals were variationally determined using a multi-configurational Dirac–Fock approach for each of the six ion stages under consideration. Our goal was to accurately determine the lowest 25–40 levels of each ion stage, from a much larger configuration set. Although the National Institute of Standards and Technology Atomic Spectra Database (NIST ASD; Kramida et al. 2020) provides a more comprehensive list of energy levels for the neutral ion stages of platinum and gold, the higher ion stages have sparse, incomplete energy state listings. Furthermore, we appreciate that the Einstein A-coefficients for the lowest levels of each ion stage involve non-dipole transitions that scale α E5, and therefore we have utilized the option with GRASP to adopt spectroscopically accurate energy separations before the calculation of transition matrix elements, where available. The typical differences in the calculated wavelengths and those adopted after scaling to experimentally measured energies are 1–13 per cent for the strongest permitted transitions, and ≤ 4 per cent for the strongest forbidden transitions. The typical differences between the calculated A-values and those adopted after scaling are 3–31 per cent for the strongest permitted transitions, and 1–14 per cent for the strongest forbidden transitions. For example, the 10761 Å transition (A = 20.1 s−1) of Pt I had a calculated wavelength of 10454 Å (and A = 21.9 s−1) in GRASP.

For Pt I, the first 32 energy levels were calibrated to the energies given in the NIST ASD (Kramida et al. 2020). For Pt II, the first 40 levels were calibrated. For Au I, the first 37 levels were calibrated, excluding levels 21, 28, 31, and 34, which did not have identifiable counterparts. The first 21 levels of Au II were calibrated. The NIST ASD has no atomic data for either Pt III or Au III, aside from the ground level. Therefore, all energy levels in these structures are taken as calibrated in GRASP. The configurations that contain calibrated energy levels in neutral and singly ionized platinum and gold are shown in Table 1. GRASP has also been further modified to interface with TARDIS to provide easier future integration of new atomic data sets.

Although these atomic structure calculations provide the foundation of any plasma modelling under LTE conditions, a companion paper (McCann et al., in preparation) will provide greater detail on the atomic structure calculations, as well as the electron-impact excitation of neutral gold. This excitation calculation shall be benchmarked against the spectra of ongoing gold experiments (Bromley et al. 2020) and provide insight into populating mechanisms, when the observed spectra drop out of LTE into the collisional radiative regime. This will also address the incompleteness of data for the more highly charged systems, where observed and synthetic spectra may be compared to determine the identification of higher excited states. It will also provide the mechanisms by which excited states are populated, and hopefully provide temperature and density line ratios. For an in-depth discussion of the atomic data generation, see McCann et al. (in preparation). Finally, we note that all wavelengths presented throughout this paper are quoted as in vacuum.

4 MOTIVATION OF PARAMETERS

To determine what ejecta mass to use in our calculations, we considered both observational and theoretical estimates. We also performed our own calculation, to estimate Pt and Au production in KNe.

Observationally, the ejecta mass can be estimated from the light-curve modelling of AT2017gfo. The bolometric light curve and filter band light curves have been fit with ejecta masses between 0.01 and 0.05 M⊙ (Cowperthwaite et al. 2017; Smartt et al. 2017; Tanvir et al. 2017; Coughlin et al. 2018; Waxman et al. 2018). The expected mass of dynamical ejecta in BNS merger simulations is in the region 10−4 < Mdyn < 10−2 M⊙ (Bauswein et al. 2013;
Hotokezaka et al. 2013; Sekiguchi et al. 2016; Ciolfi et al. 2017; Radice et al. 2018), with a large fraction of neutron-rich material ($Y_e < 0.2$), which would favour Pt and Au production. However, disc wind ejecta can potentially be more massive ($10^{-2} < M_{\text{dw}} < 10^{-1} M_\odot$), slower moving ($v \approx 0.1c$; Wu et al. 2016; Siegel & Metzger 2017), and may be composed of either low or high $Y_e$ material. Nuclear trajectories for low $Y_e$ regimes (Bauswein et al. 2013; Goriely et al. 2013, 2015) indicate that Pt and Au compositions could be as high as 5–15 per cent, by mass, which would potentially mean ejecta masses of either element of $\sim 5 \times 10^{-4}$–$1.5 \times 10^{-2} M_\odot$, in low $Y_e$ ejecta.

A simple calculation to determine Pt and Au production in KNe, assuming they are the sole source of these elements in the Milky Way, also provides approximate Pt and Au masses per event. The currently accepted LIGO–Virgo rate for BNS mergers in our local Universe is $R_{\text{BNS}} = 320^{+330}_{-220}$ Gpc$^{-3}$ yr$^{-1}$ (The LIGO Scientific Collaboration 2020). From Abadie et al. (2010), the density of Milky Way equivalent galaxies (MWEG) is $\sim 1.16 \times 10^{-2}$ Mpc$^{-3}$. From these values, we calculated a rate of BNS mergers of in low model to evaluate the presence of Pt and Au signatures. In the paper, we model the spectra of AT2017gfo using a one-component model to evaluate the presence of Pt and Au signatures.

The focus of this photospheric phase modelling is not to fully reproduce, or ‘fit’ the observed spectra of AT2017gfo; rather, it is to place constraints on what features the ions of Pt and Au would produce if such elements were present in the ejecta. Therefore, we calculated model compositions that were composed entirely of either Pt or Au. While these compositions are not physical, they demonstrate which features of these heavy elements are potentially detectable, and illustrate what one can do with reliable atomic data.

This lack of realism is somewhat necessary since the absence of extensive atomic data for the third r-process peak elements prevents a calculation encompassing all expected heavy ions. For example, nucleosynthesis calculations of r-process element production in KNe events produce significant mass fractions of Os and Pb, in addition to Pt and Au (Bauswein et al. 2013; Goriely et al. 2013, 2015). The existing data for the first few ionization states of both Os and Pb is sparse. The NIST ASD has only 135, 97, and 41 lines for Pb I, II, and III, respectively. For Os I–III, there are 534, 38, and 1061 lines respectively, although all lines for Os III lie in the UV, with wavelengths <2100 Å. The lack of a complete atomic data set, spanning the optical and NIR, prevents us from making quantitative predictions for observable features for either of these elements. A fully consistent analysis for realistic compositions can only be achieved when atomic data sets for other elements have been calculated.

5 PHOTOSPERHIC PHASE

The spectra of AT2017gfo have been interpreted in different ways, with many authors invoking two components. A low opacity, blue component, and a red contribution from high opacity ejecta are physically motivated from numerical simulations of neutron star mergers. In particular, the models of Kasen et al. (2017) have been widely used to argue for two components to explain the SED of the spectra (see also e.g. Chornock et al. 2017; Coughlin et al. 2018). However, the existence of two components is by no means settled, with some work arguing that the evolution of the SED and the bolometric luminosity is dominated by one component with low to moderate opacity (Smartt et al. 2017; Waxman et al. 2018). In this paper, we model the spectra of AT2017gfo using a one-component model to evaluate the presence of Pt and Au signatures.

To determine if any photospheric phase spectral features could be produced by Pt or Au, we generated synthetic spectra using TARDIS (Kerzendorf & Sim 2014; Kerzendorf et al. 2019), a 1D Monte Carlo radiative transfer code capable of rapidly generating spectral features for explosive transients. TARDIS has been used previously to produce KN spectra (Smartt et al. 2017; Watson et al. 2019; Perego et al. 2020). We note that these previous works did not make use of the full relativistic treatment recently implemented for TARDIS (as outlined by Vogl et al. 2019), whereas we have incorporated this feature into our modelling here. The TARDIS code uses a photospheric approximation, where it assumes that the properties of the transient’s ejecta beneath some optically thick boundary can be approximated to a blackbody with a certain temperature, either selected by the user, or determined from the code based on some requested output luminosity for the model.

First, we used the new data to generate an atomic data set capable of being read by TARDIS. For this, we used the CARSUS package, which extracted the level energies and statistical weights, and also the Einstein $A$-values for all transitions from the GRASPY output. This was then parsed into an atomic data file for use in our TARDIS models. The atomic data set we produced for our modelling efforts is publicly available – see Data Availability.

5.1 Method

To determine if any photospheric phase spectral features could be produced by Pt or Au, we generated synthetic spectra using TARDIS (Kerzendorf & Sim 2014; Kerzendorf et al. 2019), a 1D Monte Carlo radiative transfer code capable of rapidly generating spectral features for explosive transients. TARDIS has been used previously to produce KN spectra (Smartt et al. 2017; Watson et al. 2019; Perego et al. 2020). We note that these previous works did not make use of the full relativistic treatment recently implemented for TARDIS (as outlined by Vogl et al. 2019), whereas we have incorporated this feature into our modelling here. The TARDIS code uses a photospheric approximation, where it assumes that the properties of the transient’s ejecta beneath some optically thick boundary can be approximated to a blackbody with a certain temperature, either selected by the user, or determined from the code based on some requested output luminosity for the model.

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all of our models, which had the general form:

\[
\rho(v,v_{\text{exp}}) = \rho_0 \left( \frac{v}{v_{\text{exp}}} \right)^3 \left( \frac{v}{v_0} \right)^{-\Gamma}
\]

for \( v_{\text{min}} < v < v_{\text{max}} \), where \( \rho_0, v_0, v_{\text{exp}}, \Gamma, \) and \( v_{\text{max}} \) are constants. The values for these constants were chosen empirically to reproduce the general shape of the early SED of AT2017gfo, assuming it is dominated by a single blackbody component. Table 2 lists these values. The choice of photospheric ejecta velocity \( (v_{\text{min}}) \) is in line with previous works that model the early spectra of AT2017gfo \((\sim 0.2 \pm 0.1 \text{ km s}^{-1})\) (Smartt et al. 2017; Watson et al. 2019). The time since explosion \( (t_{\text{exp}}) \) is well constrained based on the GW detection (Abbott et al. 2017b). A value of \( \Gamma = 3 \) was chosen as it typically agrees with hydrodynamical calculations (Hotokezaka et al. 2013; Tanaka & Hotokezaka 2013), and has been adopted by other modelling efforts for AT2017gfo (Watson et al. 2019). The values for \( \rho_0 \) were chosen either to correspond to models with a fixed ejecta mass, or such that the models had pronounced and observable features. The photospheric temperatures \( (T_{\text{ph}}) \) chosen for the models closely resemble the blackbody temperatures of the early spectra of AT2017gfo, but we allowed some variation to improve the match to the observed spectra. The photospheric luminosity \( (L_{\text{ph}}) \) for the models is then derived using:

\[
L_{\text{ph}} = 4\pi \left( \frac{v_{\text{min}}}{v_{\text{exp}}} \right)^2 \sigma T_{\text{ph}}^4.
\]

where \( \sigma \) is the Stefan–Boltzmann constant. We use the TARDIS LTE treatment for ionization, and dilute-LTE for excitation.

We present two sets of photospheric calculations in this paper, which differ primarily in ejecta mass. The term ‘ejecta mass’ in treatment for ionization, and dilute-LTE for excitation.

\[
t_{\text{exp}} \text{ (d)}
\]

5.2 Pt and Au realistic mass models

Our first set of TARDIS model spectra are presented in Fig. 1. These models have ejecta masses consistent with what is expected for the Pt and Au composition in KNe. As discussed in Section 4, we chose \( M_{\text{ej}} = 10^{-3} M_\odot \). These models are insensitive to any material beneath the photosphere, and so they overestimate the contribution that \( 10^{-3} M_\odot \) of Pt or Au would have on early KN spectra, since we have placed \( 10^{-3} M_\odot \) of Pt or Au above the photosphere. This neglects the fact that some of this material is likely travelling at slower velocities, and so is hidden beneath the optically thick boundary in our model. The models cover a range of temperature, which correlates strongly with \( t_{\text{exp}} \). These models illustrate the effect that a modest amount of Pt and Au can have on the evolution of early KN spectra.

Table 2. Input parameters used to generate the various TARDIS models presented in this work.

| Model | Pt | Au |
|-------|----|----|
| 0     | 1  | 1  |
| 1     | 2  | 2  |
| 2     | 3  | 3  |

\[
T (\text{K})
\]

5.2.1 Results

At wavelengths redwards of \( \sim 8000 \text{ Å} \), where we might hope to be able to detect features due to particular transitions, we find no strong, observable spectral features. For Pt, there is strong, line-blended, UV absorption \((500–4000 \text{ Å})\) at each temperature (with the absorption extending into the optical for the 6000 K model). This absorption is almost exclusively PtIII absorption for the 10 000 K and hotter models, a blend of PtII and PtIII absorption at 8000 K, almost exclusively PtII absorption for the 6000 K model, and almost exclusively PtI for the 4000 K model. The 16 000 K model exhibits little absorption, but this is a result of our atomic data only containing transitions up to doubly ionized Pt. At this temperature, most of the Pt present in the ejecta is at least triply ionized, as PtIV. The feature at \( \sim 7500 \text{ Å} \) in the 6000 K model is the same feature as in the \( +1.4 \text{ d} \text{ high ejecta mass Pt model, presented in Fig. 2.} \) This feature is produced by the 9863.8, 10026 Å Pt II transitions. Although there is visible absorption here, we require a significantly higher mass of Pt to produce a feature comparable in strength to the observed absorption feature.

The Au models exhibit similar behaviour to the Pt ones. The UV absorption is almost exclusively AuIII absorption for the 10 000 K and hotter models, a blend of AuII and AuIII absorption at 8000 K, almost exclusively AuII absorption for the 6000 K model, and almost exclusively AuI for the 4000 K model. Similarly, the 16 000 K model exhibits little absorption, for the same reason as discussed for the Pt case. The feature at \( \sim 5800 \text{ Å} \) in the 6000 K model is a result of the AuII 7796.0 Å transition (same feature as in the \( +1.4 \text{ d} \text{ high ejecta mass Au model in Fig. 2.} \) The feature at \( \sim 4500 \text{ Å} \) in the 4000 K model is the same feature as in the \( +2.4 \text{ d} \text{ high ejecta mass Au model in Fig. 2.} \) produced predominantly by the AuII 6279.9 Å transition.

5.2.2 Interpretation

The strong UV line blanketing exhibited in these models illustrates the effect Pt and Au have on the opacity of the ejecta material, and the continuum in the UV. However, this UV absorption is not likely
to be uniquely attributed to either Pt or Au in a KN spectrum, as UV line blanketing will be produced by many other heavy elements, either with d- or f-shell valence electrons. In addition, observing this region would require time-resolved spectra from a space-based telescope within the first 24 h, which could only be facilitated by a rapid response of the Hubble Space Telescope. We conclude that a mass of $\sim 10^{-3} M_\odot$ of either Pt or Au is unlikely to produce a detectable, uniquely identifiable feature in the photospheric phase spectra of a kilonova, with the exception of the few shallow features in the optical, as discussed. These features are not well pronounced, and would require more Pt or Au mass for them to be prominent enough to be detectable.

5.3 Pt and Au high mass models

Our second set of models, presented in Fig. 2, have unreasonably high masses compared to expectations for KN ejecta. The total ejecta mass for a BNS merger is likely to lie in the region $10^{-3} \lesssim M_{ej} \lesssim 10^{-1} M_\odot$, which will be a mixture of r-process elements (see Section 4). Our models have been constructed to determine the spectral regions showing the strongest features of Pt and Au ions that could exist in early phase KN spectra, and we find that such high mass models are necessary to illustrate these features. The masses enclosed in these TARDIS models ($M_{ej}$) are listed in Table 2. Since we only consider pure Pt and Au models, we are neglecting the free electron contribution from other species. To quantify this effect, we generated a test TARDIS model with equivalent Pt mass, but more total mass, such that Pt only made up 15 per cent of the total ejecta. This showed that the Pt to free electron ratio only marginally affects the resultant spectrum, and does not alter our conclusions. As discussed in Section 5.1, TARDIS uses a photospheric approximation, which models optically thick material beneath some inner boundary as a blackbody with a certain temperature. As a validation of our models presented here, the Planck-mean optical depths for our models (calculated within TARDIS from the sum of the Thomson scattering and line opacity, which is obtained using an expansion opacity formulation; Blinnikov et al. 1998) were computed, and were confirmed to be of the order of unity at this inner boundary, as expected.

Table 3 contains the properties of a subset of the strongest permitted lines that appear in our spectra for Pt I, II, III, and Au I, II, III, that we have selected from our atomic data. Also included in Table 3 are the $A$-values of the transitions as quoted in the NIST ASD, where available. Some lines are completely absent from the data base, and some of those that are present do not have known $A$-values, hence the sparse data. From the few values that are available, there is reasonable agreement between the values predicted by GRASP, and those in the NIST ASD (mostly agree within a factor $\lesssim 2$, with the only exception being the Pt I 7115.7 Å transition, which varies by a factor $\lesssim 5$). While Table 3 contains only the transitions that are highlighted in Fig. 2, we provide complete lists of all...
Figure 2. Comparison of our high ejecta mass TARDIS models for pure Pt and Au compositions to early spectra of AT2017gfo. Left-hand panels: Model spectra for our pure Pt KN models compared to observed spectra of AT2017gfo at the corresponding epochs (+0.5, +1.4, and +2.4 d, for the top, middle, and bottom panels, respectively). Right-hand panels: As left, but for pure Au KN models. The regions of the spectra that deviate strongly from a blackbody continuum, as a result of interaction with one (or many) strong transitions, are shaded and labelled. The shaded regions labelled with ‘Blend’ signify that the feature is produced as a result of many different transitions, all with comparable strength. The regions where the feature was produced predominantly by a few strong transitions are labelled in descending order of contribution.

permitted transitions in our models with a Sobolev optical depth (calculated by TARDIS), $\tau_s > 0.01$, and $\lambda > 3000\,\text{Å}$. The full atomic data information for the lower levels of the transitions (electronic configuration, term, $J$, parity and energy) are provided in Tables A1–A6.

Fig. 2 shows the high ejecta mass model spectra generated with TARDIS, compared with three of the earliest spectra of AT2017gfo, when the photospheric regime is most likely to be applicable. The overall SED of the models approximately match the observed spectra of AT2017gfo at the same epochs, indicating that the temperatures and photospheric radii of the models are appropriate.

5.3.1 Pt models
In the pure Pt model at +0.5 d post-merger (Pt model 0, with parameters as in Table 2), there is a shallow absorption feature,
Table 3. Subset of the strongest lines in our TARDIS models. The lines are ranked by their Sobolev optical depth ($\tau_s$) in the models. Only lines that are highlighted in Fig. 2 are included here. All lines with $\tau_s > 0.01$ and $\lambda > 3000$ Å are included in the supplementary tables. The full atomic data information for each of the lower level indices indicated here can be found in Tables A1–A6.

| Species | GRASP$^0$ lower level index | GRASP$^0$ upper level index | Sobolev optical depth, $\tau_s$ | Transition wavelength, $\lambda_{\text{peak}}$ (Å) | GRASP$^0$ A-value (s$^{-1}$) | NIST ASD A-value (s$^{-1}$) |
|---------|-----------------------------|-----------------------------|---------------------------------|---------------------------------|----------------------------|-----------------------------|
| Pt III  | 45$^a$                      | 64$^a$                      | 0.72                            | 6228.1                          | $3.85 \times 10^5$         | N/A                         |
|         |                             |                             | Pt model 0                      | Au model 0                      |                           |                             |
| Au III  | 13$^a$                      | 19$^a$                      | 3.81                            | 3849.9                          | 2.42 $\times 10^5$        | N/A                         |
|         |                             |                             | Pt model 1                      | Au model 1                      |                           |                             |
| Pt II   | 16                          | 22                          | 12.8                            | 4515.4                          | $5.63 \times 10^5$        | $5.0 \times 10^5$           |
|         |                             |                             | Pt model 2                      | Au model 2                      |                           |                             |
| Pt II   | 19                          | 22                          | 3.61                            | 5966.2                          | $3.24 \times 10^5$        | N/A                         |
|         |                             |                             | Pt model 3                      | Au model 3                      |                           |                             |
| Au I    | 3                           | 4                           | 2.76                            | 6279.9                          | $1.70 \times 10^6$        | $3.4 \times 10^6$           |
|         |                             |                             | Pt model 4                      | Au model 4                      |                           |                             |
| Au II   | 7                           | 16                          | 1.44                            | 4053.9                          | $2.08 \times 10^6$        | N/A                         |
|         |                             |                             | Pt model 5                      | Au model 5                      |                           |                             |
| Au II   | 7                           | 17                          | 1.26                            | 3805.1                          | $1.57 \times 10^6$        | N/A                         |
|         |                             |                             | Pt model 6                      | Au model 6                      |                           |                             |
| Au II   | 7                           | 14                          | 0.94                            | 4017.2                          | $2.31 \times 10^6$        | N/A                         |
|         |                             |                             | Pt model 7                      | Au model 7                      |                           |                             |
| Au II   | 8                           | 10                          | 0.51                            | 7796.0                          | $2.15 \times 10^5$        | N/A                         |
|         |                             |                             | Pt model 8                      | Au model 8                      |                           |                             |
| Au I    | 5                           | 10                          | 0.33                            | 7512.8                          | $8.29 \times 10^7$        | $4.24 \times 10^7$          |
|         |                             |                             | Pt model 9                      | Au model 9                      |                           |                             |
| Pt I    | 9                           | 15                          | 32.1                            | 5841.7                          | $4.13 \times 10^5$        | $8.0 \times 10^5$           |
|         |                             |                             | Pt model 10                     | Au model 10                     |                           |                             |
| Pt I    | 11                          | 15                          | 8.66                            | 7115.7                          | $2.03 \times 10^5$        | $9.4 \times 10^5$           |
|         |                             |                             | Pt model 11                     | Au model 11                     |                           |                             |
| Pt I    | 12                          | 24                          | 3.22                            | 6328.3                          | $2.87 \times 10^5$        | N/A                         |
|         |                             |                             | Pt model 12                     | Au model 12                     |                           |                             |
| Pt I    | 12                          | 18                          | 2.95                            | 8227.0                          | $1.20 \times 10^5$        | N/A                         |
|         |                             |                             | Pt model 13                     | Au model 13                     |                           |                             |
| Pt I    | 13                          | 18                          | 0.26                            | 13363                          | N/A                       | N/A                         |
|         |                             |                             | Pt model 14                     | Au model 14                     |                           |                             |
| Au I    | 3                           | 4                           | 27.7                            | 6279.9                          | $1.70 \times 10^6$        | $3.4 \times 10^6$           |
|         |                             |                             | Pt model 15                     | Au model 15                     |                           |                             |
| Au I    | 3                           | 5                           | 5.62                            | 5066.0                          | $3.27 \times 10^5$        | $5.2 \times 10^5$           |
|         |                             |                             | Pt model 16                     | Au model 16                     |                           |                             |
| Au I    | 5                           | 10                          | 0.43                            | 7512.8                          | $8.29 \times 10^7$        | $4.24 \times 10^7$          |

Note. $^a$These levels were not scaled to any experimental data. All others levels were scaled to experimentally calculated levels (Kramida et al. 2020).

5.3.2 Au models

In the pure Au model at $+0.5$ d post-merger (Au model 0), there is strong absorption and emission due to Au II and Au III, bluewards of 3200 Å. The features are a result of a myriad of Au II and Au III transitions, all with comparable strength. The transition with the strongest contribution in this region is the Au III 3849.9 Å transition. No distinct transitions redwards of 3000 Å are clearly visible at this temperature.

The second pure Au model (Au model 1), at $+1.4$ d, has a shallow absorption feature centred at 6100 Å, which is produced by a blend of the Au I 5066.0 Å line, and the Au II 7796.0 Å line. Centred at 5000 Å, there is another, much more pronounced absorption feature, which is dominated by the Au I 6279.9 Å line. There is also another feature at $\approx 3000$ Å, which is produced by the Au II 3805.1, 4017.2, 4053.9 Å lines.

The third spectrum, Pt Model 2, calculated $+2.4$ d after merger, displays a photosphere that has cooled sufficiently such that the Pt II lines present in the previous model have disappeared, and all observed features are now produced by Pt I. The NIR transition at 31363 Å is visible as a shallow absorption at 11000 Å. There are two additional absorption features, centred at 5500 and 6700 Å, and these are produced by the Pt I 5841.7, 6328.3, 7115.7, and 8227.0 Å transitions. Table 3 contains the details of these strong optical and NIR lines that produce the distinct features in the TARDIS models.
The overall SED of the models approximately reproduce the observed spectra of AT2017gfo, as expected, since the velocities and temperatures in our TARDIS models were chosen to produce a match to the luminosity of the transient. Although the models are simply pure Pt or Au, they do serve a purpose for determining if any absorption-like features in the photospheric spectra of AT2017gfo could be identified as Pt or Au, and for making predictions for future events.

We find no plausible transition of any of the three ionization states of Pt or Au can be uniquely matched with the features in AT2017gfo. There is strong absorption between ∼7000–10 000 Å in the observed spectra at +1.4 and +2.4 d, which is not replicated well by contributions from Pt or Au models. Additionally, the model spectra exhibit strong absorption in regions where the observed spectra do not (e.g. Au model 1 at ∼5000 Å). From these model spectra, it is clear that the early phase spectra of AT2017gfo are not dominated by Pt or Au features. This is not to say that there is none of these elements present in the ejecta of AT2017gfo, but it does mean that, if present, their contribution to the spectra are not prominent. It is possible that the Pt II blend of the 9863.8, 10026 Å transitions contribute to the broad absorption observed at 8000 Å, at +1.4 d. However, this feature has been attributed to Sr II by Watson et al. (2019), and only a very large mass of Pt would produce a significant contribution.

The masses of Pt and Au in the high ejecta mass models presented here represent rough estimates for upper limits of these species in the ejecta of AT2017gfo. From these, we can conclude that there is less than ∼1 M⊙ of Pt in the ejecta. If indeed there was ∼0.1 M⊙ of Pt present, then, based on our calculation of the relative ratios of Pt and Au synthesis presented in Section 4, we would expect ∼0.02 M⊙ of Au to also be present, which we can accommodate in the early phase spectra of AT2017gfo. It should be noted however, that these masses are comparable to, or larger than, the total ejecta mass expected from a BNS merger (10^-3 ≤ Mej ≤ 10^-1 M⊙). Therefore, our upper limits are not constraining for the amounts of Pt and Au produced by AT2017gfo.

The spectra of AT2017gfo exhibit rapid evolution, the rate of which is unprecedented, compared to other optical and NIR extragalactic transients. By ∼1 week after explosion, broad features appear in the spectra that could be interpreted as being emission lines arising in a quasi-nebular plasma. Here, we make some physically motivated estimates for the different properties of a KN (temperature, density, ejecta velocity), and then make predictions for which lines we would expect to dominate the nebular phases of these transients, assuming there is some component of the ejecta made up of Pt or Au. From these model spectra, it is clear that the early phase spectra of AT2017gfo are not dominated by Pt or Au features. This is not to say that there is none of these elements present in the ejecta of AT2017gfo, but it does mean that, if present, their contribution to the spectra are not prominent.

6 NEBULAR PHASE

The spectra of AT2017gfo exhibit rapid evolution, the rate of which is unprecedented, compared to other optical and NIR extragalactic transients. By ∼1 week after explosion, broad features appear in the spectra that could be interpreted as being emission lines arising in a quasi-nebular plasma. Here, we make some physically motivated estimates for the different properties of a KN (temperature, density, ejecta velocity), and then make predictions for which lines we would expect to dominate the nebular phases of these transients, assuming there is some component of the ejecta made up of Pt or Au. This information is then used to generate simple, synthetic emission spectra, under the assumption of LTE level populations. Due to the simplicity of our models, we treat ionization as a free parameter in our models, and treat the individual ions of each species independently. While such calculations are not as physically realistic as those in radiative transfer codes such as CMFGEN (Hillier & Miller 1998; Dessart & Hillier 2005), ARTIS (Kromer & Sim 2009; Shingles et al. 2020), SUMO (Jerkstrand, Fransson & Kozma 2011), and JEKYLL (Ergon et al. 2018), they serve the purpose of identifying the strongest predicted transitions of these two elements.

We provide a qualitative comparison with the observed spectra of AT2017gfo, in the phases where the continuum weakens and line features become prominent. For AT2017gfo, the high ejecta velocity and low mass (v\text{ej} ∼ 0.2 c and M\text{ej} ∼ 0.03 M⊙; Smartt et al. 2017) imply the electron density drops to n_e ≤ 10^9 cm^{-3} after ≥3 d, assuming singly ionized ejecta and a filling factor of 0.1, and assuming a uniform expanding sphere (Jerkstrand 2017). To favour radiative de-excitation, we require transitions with Einstein A-values < 100 s^{-1} (Jerkstrand 2017). Such transitions would potentially give rise to nebular emission lines in the spectra of AT2017gfo, taken after ∼ a few days.

The spectra taken from +7.4 to +10.4 d show broad, emission-like features at 0.79, 1.08, 1.23, 1.40, 1.58, and 2.07 μm. In a companion paper (Gillanders et al., in preparation), we propose that these are consistent with being emission features of width 35 600 ± 6600 km s^{-1}, and could be arising from optically thin, nebular-phase emission. We use this hypothesis to compare the forbidden (electric quadrupole and magnetic dipole) transitions of Pt and Au to the positions of these features. Further discussion on the nature of these late-time spectra will be provided by Gillanders et al. (in preparation).

6.1 Method

To identify candidate transitions that may appear in emission in the late-time KN spectra, we first exclude any that originate from an upper level with energy greater than the ionization energy of the species under consideration (acquired from the NIST ASD; Kramida et al. 2020). Such levels would be expected to have very small populations, and therefore the corresponding transitions would have negligible contributions to our synthetic spectra.

We further excluded all transitions that originate from an upper level that was not metastable, on the grounds that the upper levels of such transitions can be expected to be strongly depopulated (relative to LTE) under nebular conditions. We calculated the radiative lifetimes of all levels using:

\[ \tau_{\text{rad}} = \left( \sum_{L > 0} A_{L} \right)^{-1}, \]  

(3)

where \( \tau_{\text{rad}} \) is the mean radiative lifetime of the level, and \( A_{L} \) is the Einstein A-coefficient for spontaneous decay, from upper state \( U \) to lower state \( L \). In this work, we consider any levels with a mean radiative lifetime, \( \tau_{\text{rad}} \geq 10^{-5} \) s, to be metastable (based on the discussion above). Therefore, all transitions originating from non-metastable levels (i.e. \( \tau_{\text{rad}} < 10^{-5} \) s) were discarded, as the rate of emission in these transitions at late times is likely to be much lower than in LTE (which we adopt to estimate the level populations – see below). For more on nebular phase spectra, see Jerkstrand (2017).

Although this leaves a large number of plausible lines (96, 593, and 1510 for Pt I, II, and III respectively, and 10, 87, and 339 for the same three ionization stages of Au), the vast majority of these transitions come from relatively highly excited levels, which will be heavily disfavoured in our subsequent analysis, as discussed below.

To determine the approximate strengths of emission lines arising from our selected transitions, we assume LTE excitation, and estimate the population of atoms and ions in different excited states, using the Boltzmann equation:

\[ N_{i} = N_{\text{e}} \left( \frac{g_{i}}{Z} \right) e^{-\frac{E_{i}}{kT}}, \]  

(4)

where \( N_{i} \) is the number of atoms or ions in the excited state, \( N_{\text{e}} \) is the total number of atoms or ions, \( g_{i} \) is the statistical weight of the upper level, \( Z \) is the LTE partition function, \( E_{i} \) is the energy of the upper level, \( k_{\text{B}} \) is the Boltzmann constant, and \( T \) is the temperature.
With the estimates for $N_0$, and the Einstein $A$-values from the atomic data, we are able to calculate the total line luminosity arising from each transition, for temperatures $T \in [2000, 3500, 5000] \, \text{K}$, assuming optically thin emission:

$$L_{\text{em}} = A_{13} N_0 \left( \frac{hc}{\lambda_{\text{vac}}} \right). \quad (5)$$

In order to test the accuracy of our LTE assumption on the level populations, we obtained collision strength information for the lowest 5 levels of Au I (see the upcoming companion paper, McCann et al., in preparation). With this, we were able to calculate level populations, and compare them to our simple LTE estimates. We found that there was reasonable agreement (within a factor $\lesssim 3$), for electron densities on the order of $\sim 5 \times 10^8 \, \text{cm}^{-3}$.

The strongest transitions of Pt I, II, III, and Au I, II, III in the framework of the simple LTE approximation (at a temperature of 3500 K) are listed in Tables 4 and 5. These tables only contain the strongest transitions from our analysis; i.e. only transitions that have $L_{\text{em}} > 1$ per cent of the strongest line luminosity in our analysis are included. As expected, electric dipole transitions do not appear in either table, as these have been desected due to the radiative lifetime cut, leaving only forbidden lines. As in Table 3, the corresponding $A$-values for the transitions from the NIST ASD are included, where available. Again, there is good agreement between these values, and the theoretically obtained values from GRASP, with values agreeing to within a factor $\lesssim 2$. The full atomic data information for the lower and upper levels of the transitions (electronic configuration, term, $J$, parity and energy) are provided in Tables A1–A6. We note that $\tau_{\text{sub}} < 1$ for all our calculated transitions, indicating that we are in an optically thin regime, as expected.

To produce a simple visualization of how nebular emission lines may appear, we generated Gaussian emission features for all transitions. These were centred on the rest-wavelength of the lines, may appear, we generated Gaussian emission features for all transitions. Then, these Gaussians were all co-added to form one composite emission spectrum. This spectrum illustrates the relative strengths of all the transitions that we predict should be prominent in an observed nebular spectrum, which contains the species under consideration. These composite spectra are plotted in Fig. 3.

### 6.2 Model results

Before we analyse the individual features in our models, it is worth noting that, for the Einstein $A$-values of the strongest Pt lines, at a temperature, $T = 3500 \, \text{K}$, with total ion masses, $M_\text{ion} = 10^{-3} \, \text{M}_\odot$ (which is comfortably within the range of expected Pt and Au masses discussed in Section 4), we calculate line luminosities on the order $L_\text{em} \sim 10^{38} \, \text{erg s}^{-1}$. These luminosities are similar in strength to the observed features in the late-time spectra of AT2017gfo, if indeed these features are a result of emission. This motivates the study of individual features of Pt, and by extension, Au, and other third $r$-process peak elements that are expected to be produced in KNe, as we have determined that they may be capable of producing features similar in strength to those observed in AT2017gfo.

In Fig. 3, we present the LTE synthetic emission spectra for Pt I, II, III, and Au I, II, III, at three example temperatures (2000, 3500, and 5000 K). In each case, the ion masses are $M_\text{ion} = 10^{-3} \, \text{M}_\odot$, motivated by the discussion in Section 4. The intensity of the lines scales linearly with mass, or $N_0$, as shown in equations (4) and (5). We predict these lines to be the strongest features, when the ejecta has reached the optically thin regime. As discussed in Section 6.1, low mass and high velocity ejecta can reach this regime in a few days. While high velocities and a multitude of heavy elements will likely make line blending common place in the spectra of KNe (Kasen et al. 2017; Tanaka et al. 2020), the optical and NIR wavelength range covered in Fig. 3 appears to be the optimal place to observe signatures of these two elements. Tables 4 and 5 indicate that these lines are all at wavelengths observable from the ground (0.33 – 2.52 $\mu$m), apart from the [Au II] line at 3.8446 $\mu$m.

We compare the line positions and approximate intensities to the late-time spectra of AT2017gfo in Fig. 4. The strongest features that could be emission lines have peaks at 0.79, 1.08, 1.23, 1.40, 1.58, and 2.07 $\mu$m (Gillanders et al., in preparation). The strong 1.08 $\mu$m feature weakens significantly between +7.4 d and + 8.4 d. It is possible that this is the evolution of the emission component of the P-Cygni line of Sr II, identified by Watson et al. (2019), causing the 8000 $\AA$ absorption dip in the +1.4 d spectrum, but it could also be unrelated emission developing, coincidentally, at the same wavelength.

#### 6.2.1 Pt models

There is an interesting coincidence between this observed emission feature, and our predicted strongest [Pt I] 10761 $\AA$ and [Pt II] 10917 $\AA$ lines. If there was a significant contribution of [Pt I] 10761 $\AA$ to this feature, then the next strongest transitions of [Pt II] would be at 7409.5 $\AA$ and 15227 $\AA$. These do not align with the peaks of the 7900 $\AA$ and 15800 $\AA$ observed features, but both of those features show asymmetric profiles, with a significant excess in the blue wing. Hence, it is possible that the 5 strongest [Pt I] transitions in our models are contributing emission in the +7.4 d spectrum of AT2017gfo. Fig. 5 illustrates how different ion masses for Pt I, II, and III could contribute to the observed features of AT2017gfo at $+7.4 \, \text{d}$. If two (or more) of these ions were to co-exist in the ejecta at this epoch, then the spectra could be co-added to produce a composite Pt emission spectrum, which may reproduce some of the observed features.

There is only one strong line of [Pt III], at 10917 $\AA$, which lies at a similar wavelength to the strong [Pt I] line, at 10761 $\AA$, and no further statement can be made as to the presence of this ion. The three strongest [Pt II] lines at 7512.5, 11877 and 21883 $\AA$ do not correspond to any of the most pronounced peaks in the +7.4 to +10.4 d spectra of AT2017gfo, but the 7512.5 and 11877 $\AA$ lines do lie on the asymmetric wings of observed features. We predict a [Pt II] line at 21883 $\AA$, but this is much redder than the observed peak of the feature at 20700 $\AA$. As the AT2017gfo spectra evolve from $+7.4$ to $+10.4$ d, the emission peaks between 0.8 and 1.6 $\mu$m weaken, and no other strong features emerge. Therefore, no further conclusive evidence for the presence of neutral or low ion stages of Pt emerge. The possible coincidences we highlight are interesting but not conclusive, and even if some Pt I or Pt II is contributing at a low or moderate level, the spectrum is dominated by other species.

From the model comparisons in Figs 4 and 5, we can estimate approximate upper limits for the individual ions of Pt. Clearly,
Table 4. Strongest [Pt I], [Pt II], and [Pt III] transitions, at a temperature of 3500 K. The full atomic data information for each of the level indices indicated here can be found in Tables A1–A3.

| Species | GRASP0 lower level index | GRASP0 upper level index | Transition wavelength, $\lambda_{\text{vac}}$ (Å) | GRASP0 A-value (s$^{-1}$) | NIST ASD A-value (s$^{-1}$) | Transition type | Relative intensity |
|---------|--------------------------|--------------------------|-----------------------------------------------|---------------------------|----------------------------|------------------|-------------------|
| Pt I    | 2                        | 6                        | 10761                                         | 20.1                      | 24.0                       | M1               | 1.0               |
| Pt I    | 1                        | 5                        | 15227                                         | 4.21                      | 2.6                        | M1               | 0.45              |
| Pt I    | 3                        | 7                        | 10688                                         | 9.28                      | 13.3                       | M1               | 0.20              |
| Pt I    | 1                        | 8                        | 7409.5                                        | 7.68                      | 15.6                       | M1               | 0.10              |
| Pt I    | 3                        | 9                        | 6790.7                                        | 7.33                      | N/A                        | M1               | 0.049             |
| Pt I    | 5                        | 9                        | 11193                                         | 3.97                      | N/A                        | M1               | 0.015             |
| Pt I    | 2                        | 12                       | 4729.6                                        | 10.8                      | N/A                        | M1               | 0.012             |
| Pt I    | 3                        | 8                        | 7861.4                                        | 0.905                     | N/A                        | M1               | 0.011             |
| Pt I    | 3                        | 5                        | 17266                                         | 0.111                     | N/A                        | M1               | 0.011             |
| Pt II   | 1                        | 3                        | 11877                                         | 9.05                      | 8.75                       | M1               | 1.0               |
| Pt II   | 2                        | 4                        | 21883                                         | 2.54                      | 1.38                       | M1               | 0.21              |
| Pt II   | 2                        | 8                        | 7512.5                                        | 15.2                      | 21.1                       | M1               | 0.10              |
| Pt II   | 1                        | 6                        | 6332.6                                        | 3.61                      | N/A                        | M1               | 0.036             |
| Pt II   | 4                        | 7                        | 13397                                         | 6.46                      | 13.3                       | M1               | 0.030             |
| Pt II   | 4                        | 5                        | 25170                                         | 1.96                      | N/A                        | M1               | 0.020             |
| Pt II   | 1                        | 4                        | 10688                                         | 0.0970                    | N/A                        | M1               | 0.016             |
| Pt II   | 1                        | 8                        | 5525.5                                        | 1.42                      | N/A                        | E2               | 0.013             |

Note. *These levels were not scaled to any experimental data. All others levels were scaled to experimentally calculated levels (sourced from Kramida et al. 2020).

Table 5. Strongest [Au I], [Au II], and [Au III] transitions, at a temperature of 3500 K. The full atomic data information for each of the level indices indicated here can be found in Tables A4–A6. Note the [Au II] 38446 Å transition, which does not appear in Fig. 3. We predict this to be one of the strongest [Au II] features in our nebular phase model spectra.

| Species | GRASP0 lower level index | GRASP0 upper level index | Transition wavelength, $\lambda_{\text{vac}}$ (Å) | GRASP0 A-value (s$^{-1}$) | NIST ASD A-value (s$^{-1}$) | Transition type | Relative intensity |
|---------|--------------------------|--------------------------|-----------------------------------------------|---------------------------|----------------------------|------------------|-------------------|
| Au I    | 2                        | 3                        | 8147.3                                        | 29.8                      | N/A                        | M1               | 1.0               |
| Au I    | 1                        | 2                        | 10916                                         | 0.0229                    | N/A                        | E2               | 0.13              |
| Au I    | 1                        | 3                        | 4665.2                                        | 1.20                      | N/A                        | E2               | 0.071             |
| Au II   | 1                        | 3                        | 5668.7                                        | 0.405                     | N/A                        | E2               | 1.0               |
| Au II   | 2                        | 5                        | 6857.9                                        | 27.1                      | N/A                        | M1               | 0.36              |
| Au II   | 3                        | 4                        | 9876.4                                        | 27.2                      | N/A                        | M1               | 0.20              |
| Au II   | 1                        | 5                        | 3376.0                                        | 8.27                      | N/A                        | E2               | 0.25              |
| Au II   | 2                        | 3                        | 38446                                         | 0.287                     | N/A                        | M1               | 0.10              |
| Au II   | 3                        | 5                        | 8346.8                                        | 1.74                      | N/A                        | M1               | 0.021             |
| Au III  | 1                        | 2a                       | 8382.3                                        | 27.4                      | N/A                        | M1               | 1.0               |

Note. *These levels were not scaled to any experimental data. All others levels were scaled to experimentally calculated levels (sourced from Kramida et al. 2020).

\[ \sim 5 \times 10^{-4} - \sim 1 \times 10^{-3} \, M_\odot \] produces features comparable in strength to those observed in the late-time spectra of AT2017gfo, and so we place an upper limit of \[ \sim a \times 0^{-3} \, M_\odot \] on the total abundance of Pt in these spectra.

6.2.2 Au models

In the case of Au, the two strongest transitions are close in wavelength and would be blended if they co-existed: [Au I] 8147.3 Å, and [Au III] 8382.3 Å. One may dominate over the other depending on temperature and ionization. There is no obvious signature of an emission line or excess flux in any of the spectra of AT2017gfo at \( \lambda \sim 8250 \, \text{Å} \), and any other lines of these ions would likely be weaker. The strongest [Au I] lines are at 5668.7 Å and 6857.9 Å, but again, no obvious feature is distinguishable above the noise in the AT2017gfo spectra, although this is a region where many lines may blend together in a pseudo-continuum (Gillanders et al., in preparation). Fig. 5 illustrates how different ion masses for Au I, II, and III may produce features comparable in strength to those observed in the +8.4 d spectrum of AT2017gfo. It is clear that the combination of two (or more) of these ionization stages are unable to be co-added to reproduce any of the strong observed features of AT2017gfo.

From Figs 4 and 5, we constrain the amount of Au III present at late times to \[ \sim 5 \times 10^{-4} \, M_\odot \]. The [Au I] and [Au II] features are much weaker and so our models can accommodate much more of these ions (\[ \sim 5 \times 10^{-3} \, M_\odot \] of each). From this, we place a tentative upper limit of \[ \sim 10^{-2} \, M_\odot \] on the mass of Au present at late times, although we note that this is heavily dependent on the ionization state of Au. From our calculations in Section 4, we predict \( \sim 5 \times 10^{-3} \, M_\odot \) to the AT2017gfo spectra.
be synthesized than Au. If the upper limit of Pt (∼ a few $10^{-3} M_\odot$) were to be present in the ejecta, then we could easily accommodate 5 times less Au in the spectra, assuming that Pt and Au are similarly ionized.

We further note that one of the strongest [Au II] transitions lies beyond the observed range of the X-shooter data for AT2017gfo. The 3.8446 μm transition would be of particular interest in the future, as the mid-infrared regime opens up with the capability of the James Webb Space Telescope (JWST), and the expectation that the 3 – 4 μm region may suffer from less line-blending effects. In summary, we find no obvious coincidence with the predictions for the strongest [Au] lines and features in the spectra of AT2017gfo, at any epoch.

7 CONCLUSIONS

The main aim of this work was to highlight the usefulness of good quality atomic data for the exploration of r-process element synthesis. Here we have presented our new atomic data for neutral, singly, and doubly ionized Pt and Au, and we have also presented some models we generated with these data. We specifically investigated the mergers of binary neutron star systems as a source of r-process...
material in this work, and performed some spectral analysis of the kilonova AT2017gfo.

First, we used TARDIS to produce model spectra with properties similar to those expected for KNe at early times, while still in the photospheric phase (see Figs 1 and 2). We were able to demonstrate that, for realistic masses of Pt and Au, we see broad-line blended absorption in the UV. This property is not unique to Pt and Au, and is expected for many heavy elements. We also found that we required unrealistically large amounts of material (up to 0.5 $M_\odot$ in cases, see Table 2) to produce observable individual features of any ion of Pt or Au.

We generated simple emission spectra for the individual species under investigation here (Pt I, II, III and Au I, II, III), using a simple LTE excitation approximation. These models are presented in Figs 3, 4, and 5. With these models, we make strong predictions for forbidden emission lines that could be detectable in the late-time, nebular-phase spectra of a KN, which has ejecta rich in these species. Many of our features lie at wavelengths $>8000$ Å, demonstrating that the best method of identifying these species is through obtaining NIR spectra of future objects. X-shooter is capable of observing $\lesssim 2.5 \mu m$, which would capture all but one of our strongest predicted lines; the [Au II] 3.8446 $\mu m$ transition would only be detectable through JWST observations.

We compared our model photospheric and nebular-phase spectra to the observed spectra of AT2017gfo. The TARDIS model spectra were computed at the epochs of the early spectral observations of AT2017gfo (+0.5, +1.4, and +2.4 d). We find that the strong observed feature at $\sim 7000-10000$ Å in the +1.4 d spectrum may be reproducible by Pt, but the model requires a very large amount of material to do so. We identify no evidence of Au features in the early observations. We conclude that it is unlikely there are prominent Pt or Au features in the early spectra of AT2017gfo.

Comparisons of our late-time model spectra with those of AT2017gfo were presented in Section 6. At the beginning of this section, we demonstrated that, for the temperatures and masses that we have estimated for our models, the strongest forbidden transitions in our analysis have line luminosities on the order of $\sim 10^{38}$ erg s$^{-1}$. This demonstrates that we can expect features from these elements to be bright enough to be observed.

We identify some coincidence with the [Pt I] 10761 Å and the [Pt III] 10917 Å transitions, and a strong emission-like feature in the +7.4 d spectrum of AT2017gfo. If there is Pt present in the ejecta, then strong features from Pt should be detectable at wavelengths of 7409.5 Å, and 15227 Å. There are features near these wavelengths ($\sim 7900$ Å and $\sim 15800$ Å), with asymmetric profiles, displaying excess blue-wing flux. This flux could be a result of these [Pt I] features, and so we conclude it is plausible that there is [Pt I] emission in the observed late-time spectra of AT2017gfo. A definitive statement, however, will depend on future work with atomic data for many more elements, as needed to synthesize a full spectrum.

It is harder to motivate the presence of Pt III in the ejecta, as we only predict one prominent strong [Pt III] line (at 10917 Å), preventing
Pt and Au constraints on kilonova spectra

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Figure 5. Comparison of the synthetic emission spectra for [Pt] and [Au] transitions, with the +7.4 and +8.4 d AT2017gfo spectra. Upper panel: Pt I, II, and III M1 and E2 synthetic emission spectra plotted with the +7.4 d AT2017gfo spectrum. We have scaled the relative ion masses arbitrarily to qualitatively match the emission features in the observed spectrum of AT2017gfo. The ion masses used for Pt I, II, III are $M_{\text{ion}} = 10^{-3}$, $10^{-3}$ and $5 \times 10^{-4} \, M_\odot$, respectively. Lower panel: Au I, II and III M1 and E2 synthetic emission spectra plotted with the +8.4 d AT2017gfo spectrum. Similar to the Pt synthetic emission spectra above, we have arbitrarily scaled the ion masses: $M_{\text{ion}} = 5 \times 10^{-3}$, $5 \times 10^{-3}$, and $5 \times 10^{-4} \, M_\odot$ for the Au I, II, III spectra, respectively. The synthetic emission spectra are shifted to qualitatively match the continua of the observed spectra, for clarity.

us from drawing further conclusions on its presence. We predict three strong [Pt II] features, none of which correspond exactly to the observed emission features, but they do lie on asymmetric wings. We conclude that it is possible that there is some contribution from Pt in the late-time spectra of AT2017gfo, but it is likely that the spectra are dominated by other species.

Similar comparisons with the late-time AT2017gfo spectra and our model Au spectra do not yield such informative results. We predict a handful of strong [Au I], [Au II], and [Au III] lines, none of which correspond to observed emission features. We conclude that there is no evidence for the presence of Au in the late-time spectra of AT2017gfo.

From our early, photospheric phase analysis, we were unable to meaningfully constrain the mass of Pt and Au present in the ejecta of AT2017gfo. However, our nebular phase analysis proved to be more constraining. From that, we place tentative upper limits on the Pt and Au masses of $\lesssim 10^{-3} \, M_\odot$ and $\lesssim 10^{-2} \, M_\odot$, respectively. Spectroscopic follow-up for as long as possible after any future event should be a top priority, as it is this data that we think will be the most useful for helping identify individual lines for specific elements and species in future KN events.

Pt and Au are expected to be co-produced in KN ejecta. Therefore, if we observe spectral signatures for one, it is reasonable to expect to see signatures of the other. However, in Section 4, we highlighted the ratio of Pt and Au production; specifically, Pt is expected to be $\sim$ a few times more abundant than Au. Hence, it is reasonable for us to speculate that Pt may be contributing towards features in the spectra of AT2017gfo, without also detecting any Au features.

Despite the fact we cannot definitively prove the presence of Pt or Au in the spectra of AT2017gfo, we have demonstrated the usefulness of having access to complete atomic data, and have also demonstrated the study that can be performed with such data. This work supports the idea that having complete atomic data for the heavy elements is useful, and we hope that these data become available in the near future. A complete set of atomic data could then be used for quantitative modelling works, where many elements are included, and more physical KN ejecta compositions are explored in detail.

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**DATA AVAILABILITY**

The atomic data file used for the TARDIS modelling, and extended versions of the tables presented in this work are available, and can be accessed [here](#).

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**APPENDIX A: LEVEL CONFIGURATION TABLES**

Here we present tables containing information for the relevant levels that are of interest in our work, for Pt I, II, III, and Au I, II, III. The tables include the level configuration and term, as well as J, parity, and energy. We have flagged any levels that were not calibrated to experimental measurements. While these tables only contain information for the most important transitions highlighted in our work, we have included online versions, which contain all levels related to transitions presented anywhere in this work. Additionally,
Table A1. Pt I energy levels. Only levels that are relevant to the transitions discussed in the main text have been included.

| GRASP0 level index | Configuration | Term | J | Parity | Energy (cm\(^{-1}\)) |
|-------------------|---------------|------|---|--------|---------------------|
| 1                 | 5d\(^6\)6s | \(^3\)D | 3 | even | 0.00 |
| 2                 | 5d\(^6\)6s\(^2\) | \(^3\)F | 4 | even | 823.66 |
| 3                 | 5d\(^6\)6s | \(^1\)D | 2 | even | 775.88 |
| 4                 | 5d\(^4\)6s | \(^1\)D | 0 | even | 6140.17 |
| 5                 | 5d\(^6\)6s | \(^3\)D | 2 | even | 6567.45 |
| 6                 | 5d\(^6\)6s\(^2\) | \(^3\)F | 3 | even | 10116.72 |
| 7                 | 5d\(^6\)6s | \(^3\)D | 1 | even | 10131.87 |
| 8                 | 5d\(^6\)6s | \(^1\)D | 2 | even | 13496.26 |
| 9                 | 5d\(^6\)6s\(^2\) | \(^3\)F | 2 | even | 15501.83 |
| 10                | 5d\(^6\)6s\(^2\) | \(^3\)P | 0 | even | 16983.44 |
| 11                | 5d\(^6\)6s\(^2\) | \(^3\)P | 1 | even | 18566.54 |
| 12                | 5d\(^6\)6s\(^2\) | \(^1\)G | 4 | even | 21967.10 |
| 13                | 5d\(^6\)6s\(^2\) | \(^1\)D | 2 | even | 26638.58 |

Figure A1. Pt I energy level diagram. Only transitions that are specified in Table 4 are shown.

we have included energy level diagrams, to visualize the strongest forbidden emission transitions.

Table A2. Same as Table A1 but for Pt II energy levels.

| GRASP0 level index | Configuration | Term | J | Parity | Energy (cm\(^{-1}\)) |
|-------------------|---------------|------|---|--------|---------------------|
| 1                 | 5d\(^6\) | \(^2\)D | \(\frac{1}{2}\) | even | 0.00 |
| 2                 | 5d\(^6\)6s | \(^4\)F | \(\frac{1}{2}\) | even | 4786.65 |
| 3                 | 5d\(^6\) | \(^2\)D | \(\frac{1}{2}\) | even | 8419.84 |
| 4                 | 5d\(^6\)6s | \(^4\)F | \(\frac{1}{2}\) | even | 9356.32 |
| 5                 | 5d\(^6\)6s | \(^4\)P | \(\frac{1}{2}\) | even | 13329.28 |
| 6                 | 5d\(^6\) | \(^2\)D | \(\frac{1}{2}\) | even | 15791.31 |
| 7                 | 5d\(^6\)6s | \(^4\)F | \(\frac{1}{2}\) | even | 16820.93 |
| 8                 | 5d\(^6\)6s | \(^4\)F | \(\frac{1}{2}\) | even | 18097.76 |
| 9                 | 5d\(^6\)6s | \(^2\)F | \(\frac{1}{2}\) | even | 29262.01 |
| 10                | 5d\(^6\)6s\(^2\) | \(^4\)F | \(\frac{1}{2}\) | even | 34647.27 |
| 11                | 5d\(^6\)6s\(^2\) | \(^4\)P | \(\frac{1}{2}\) | even | 41434.12 |
| 12                | 5d\(^6\)6s\(^2\) | \(^2\)G | \(\frac{1}{2}\) | even | 43737.43 |

Figure A2. Pt II energy level diagram. Only transitions that are specified in Table 4 are shown.

Table A3. Same as Table A1 but for Pt III energy levels.

| GRASP0 level index | Configuration | Term | J | Parity | Energy (cm\(^{-1}\)) |
|-------------------|---------------|------|---|--------|---------------------|
| 1                 | 5d\(^8\) | \(^3\)F | 4 | even | 0.00 |
| 2\(^a\)           | 5d\(^8\) | \(^1\)D | 2 | even | 6776.39 |
| 3\(^a\)           | 5d\(^8\) | \(^3\)F | 3 | even | 9159.88 |
| 4\(^a\)           | 5d\(^8\) | \(^3\)F | 2 | even | 14798.78 |
| 45\(^a\)          | 5d\(^7\)6s\(^2\) | \(^3\)D | 4 | even | 79582.08 |

Note. \(^a\)These levels were not scaled to any experimental data. All others levels were scaled to experimentally calculated levels (sourced from Kramida et al. 2020).
Table A4. Same as Table A1 but for Au I energy levels.

| GRASP0 level index | Configuration | Term | J   | Parity | Energy (cm$^{-1}$) |
|--------------------|---------------|------|-----|--------|-------------------|
| 1                  | 5d$^{10}$s   | 2S   | ½   | even   | 0.00              |
| 2                  | 5d$^{8}$s$^2$| 2D   | ½   | even   | 9161.18           |
| 3                  | 5d$^{8}$s$^2$| 2D   | ½   | even   | 21435.19          |
| 4                  | 5d$^{10}$p   | 2P   | ½   | odd    | 37358.99          |
| 5                  | 5d$^{10}$p   | 2P   | ½   | odd    | 41174.61          |

Note. These levels were not scaled to any experimental data. All others levels were scaled to experimentally calculated levels (sourced from Kramida et al. 2020).

Table A5. Same as Table A1 but for Au II energy levels.

| GRASP0 level index | Configuration | Term | J   | Parity | Energy (cm$^{-1}$) |
|--------------------|---------------|------|-----|--------|-------------------|
| 1                  | 5d$^{10}$     | 1S   | 0   | even   | 0.00              |
| 2                  | 5d$^{8}$s     | 3D   | 3   | even   | 15039.57          |
| 3                  | 5d$^{8}$s     | 3D   | 2   | even   | 17640.62          |
| 4                  | 5d$^{8}$s     | 1D   | 2   | even   | 27765.76          |
| 5                  | 5d$^{8}$s$^2$| 3F   | 4   | even   | 40478.75          |
| 6                  | 5d$^{8}$s$^2$| 1D   | 2   | even   | 48510.89          |
| 7                  | 5d$^{8}$s$^2$| 3F   | 3   | even   | 52176.51          |

Figure A5. Au II energy level diagram. Only transitions that are specified in Table 5 are shown.

Table A6. Same as Table A1 but for Au III energy levels.

| GRASP0 level index | Configuration | Term | J   | Parity | Energy (cm$^{-1}$) |
|--------------------|---------------|------|-----|--------|-------------------|
| 1                  | 5d$^{9}$      | 2D   | ½   | even   | 0.00              |
| 2$^a$              | 5d$^{9}$      | 2D   | ½   | even   | 11929.84          |
| 13$^a$             | 5d$^{8}$s$^2$| 2G   | ½   | even   | 59286.41          |

Note. $^a$These levels were not scaled to any experimental data. All others levels were scaled to experimentally calculated levels (sourced from Kramida et al. 2020).
**Figure A6.** Au III energy level diagram. Only transitions that are specified in Table 5 are shown.

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