

Infrared spectral signatures of light r-process elements in kilonovae

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ABSTRACT

A central question regarding neutron star mergers is whether they are able to produce all the r-process elements, from first to third peak. The high abundances of first-peak elements (atomic number $Z \sim 31 - 40$) in the solar composition means they may dominate the ejecta mass in kilonovae. We here study theoretical infrared signatures of such light elements with spectral synthesis modelling. By combining state-of-the-art NLTE physics with new radiative and collisional data for these elements, we identify several promising diagnostic lines from Ge, As, Se, Br, Kr and Zr. The models give self-consistent line luminosities and indicate specific features that probe emission volumes at early phases (~ 10 d), the product of ion mass and electron density in late phases ($\gtrsim 75$ d), and in some cases direct ionic masses at intermediate phases. Emission by [Se I] $5.03 \mu\text{m}$ + [Se III] $4.55 \mu\text{m}$ can produce satisfactory fits to the Spitzer photometry of AT2017gfo. However, the models show consistently that with a Kr/Te and Se/Te ratio following the solar r-process pattern, Kr + Se emission is dominant over Te for the blend at $2.1 \mu\text{m}$ observed in both AT2017gfo and AT2023vfi. The somewhat better line profile fit with [Te III] may suggest that both AT2017gfo and AT2023vfi had a strongly sub-solar production of the light r-process elements. An alternative scenario could be that Kr + Se in an asymmetric morphological distribution generates the feature. Further JWST spectral data, in particular covering the so far unobserved $> 5 \mu\text{m}$ region, holds promise to determine the light r-process production of kilonovae, and in particular whether the light elements are made in a slow disk wind or in a fast proto-NS outflow. We identify specific needs for further atomic data on recombination rates and collision strengths for $Z = 31 - 40$ elements.

Keywords: Neutron star, kilonova, spectra, radiative transfer, r-process, NLTE

1. INTRODUCTION

The James Webb Space Telescope (JWST) is currently revolutionising many branches of astronomy, opening up the near infrared (NIR) and mid infrared (MIR) regimes which can now be studied with excellent sensitivity and spectral resolution. For explosive transients, such as supernovae (SNe) and kilonovae (KNe),

the infrared contains rich signatures of atomic transitions that are often less affected by uncertain physical conditions than optical lines. While the Spitzer Space Telescope revealed much information about Type II SNe (Kotak et al. 2006, 2009), other SN types were not observed. The first kilonova, AT2017gfo, was photometrically detected in the Spitzer warm phase (Kasliwal et al. 2022). However, it is JWST, and in a few years the Extremely Large Telescope (ELT), that will give us detailed spectral information about these transients in the infrared.

The importance of the infrared regime for trans-iron elements has been established in studies of planetary nebulae (PNe). The first detection of neutron-capture elements in a PN, or any type of nebula, was the detection of optical Kr and Xe lines by [Pequignot & Baluteau \(1994\)](#). The near-infrared range subsequently yielded detections of [Kr III] 2.199 μm and [Se IV] 2.287 μm ([Dinerstein 2001](#)), [Zn IV] 3.625 μm ([Dinerstein & Geballe 2001](#)), [Rb IV] 1.5973 μm , [Cd IV] 1.7204 μm , [Ge VI] 2.1930 μm ([Sterling et al. 2016](#)), [Br V] 1.6429 μm , [Te III] 2.1019 μm ([Madonna et al. 2018](#)), and [Rb III] 1.356 μm ([Dinerstein et al. 2021](#)). These detections prompted work to develop the needed atomic data for these elements to carry out abundance analyses (e.g., [Sterling 2011](#); [Sterling & Witthoeft 2011](#); [Sterling et al. 2015](#); [McLaughlin & Babb 2019](#); [Macaluso et al. 2019](#)). The post-diffusion phase ($t \gtrsim 1$ week for kilonovae) gives unique information about explosive transients as the innermost layers, typically containing most of the ejecta mass, become visible as the nebula becomes more transparent. With radiative transfer playing a smaller role, and Doppler broadening being smaller for the inner layers, spectral signatures emerge more cleanly than in the diffusion phase. At the same time, modelling of the physical conditions becomes more challenging, as the necessary abandonment of Local Thermodynamic Equilibrium (LTE) for full non-LTE (NLTE) collisional radiative modelling brings about sensitivity to a large variety of collisional and radiative processes (e.g. [Jerkstrand 2025](#)), and requires a much more extensive computational machinery. For kilonova work, the only published NLTE modelling so far is by [Hotokezaka et al. \(2021, 2022, 2023](#), simplified NLTE in the optically thin limit) and by [Pognan et al. \(2022a,b, 2023, 2024\)](#); [Banerjee et al. \(2025](#), full NLTE with radiative transfer).

What is looked for in nebular analysis are signatures that, based on inspection of processes in the line formation mechanisms, can be established as diagnostics with good robustness (i.e., not too sensitive to conditions or uncertain physics). In this endeavor, the infrared is a particularly potent regime. Under typical nebular plasma conditions, IR lines often originate from forbidden transitions within the ground term of a given ion, and with the relatively small excitation energies ($T_{exc} \lesssim 2000 (\lambda/2 \mu\text{m})^{-1}$ K), the line luminosities can be in a quite temperature-insensitive regime (if $T \gtrsim T_{exc}$). Further, as transitions between fine structure states of a given term tend to have small A-values and large collision strengths, the critical densities for them are quite low and they can be close to LTE for quite long times, giving no or weak sensitivity to the electron density. Finally, line opacity generally declines

with wavelength, so there are no or weak radiative transfer effects. What results from these properties is that IR lines are excellent diagnostics of ionic masses (optically thin case) and/or emission volume (optically thick case) ([Jerkstrand et al. 2012](#)).

These benign properties of the infrared regime give expectations of strong scientific return with JWST for explosive transients. Extending the observable limit from up to 2.5 μm (accessible from the ground) to 30 μm , and with excellent sensitivity, JWST is expected to be able to reveal key spectral signatures of KNe and other transients. It has already shown its value by the observations of infrared emission of the presumed kilonova AT2023vfi at a distance of 292 Mpc ([Levan et al. 2024](#)).

With these prospects, it is imperative to improve our theoretical understanding of kilonova infrared emission, and to develop model predictions for a variety of merger types. This topic was opened up by [Hotokezaka et al. \(2021\)](#), who studied nebular spectral emission by neodymium, including in the IR. [Hotokezaka et al. \(2022\)](#) produced theoretical predictions of IR emission from solar composition ejecta with fixed parameterised physical conditions (temperature and ionization), in a limited NLTE approach. The strongest emission was obtained for [Se III] 5.74 μm , whereas the Spitzer 4.5 and 3.6 μm bands were found to be dominated by [Se III] 4.55 and Br + As lines, respectively.

From this exploratory modelling, the next step is modelling with calculation of physical conditions, with some consideration of the density structure of the ejecta. This is the main goal of this paper. We have presented the optical (and some near-infrared) properties of 1D full NLTE spectral models in [Pognan et al. \(2022a, 2023\)](#) - here the focus is on the near- and mid-infrared emission of models with a similar setup. With the strong sensitivity to accurate atomic physics, we have adopted an approach to initially limit the focus to the infrared emission from light r-process elements only, $Z \leq 40$ (with one exception, Te ($Z = 52$)), carrying out an extensive atomic data compilation and calibration effort for these elements.

2. MODELLING SETUP

Our goal is to establish an orientation of the nebular near and mid-infrared signatures of light r-process elements in KN ejecta, being aided by self-consistent physical NLTE modelling with the SUMO code ([Jerkstrand et al. 2011, 2012](#)). We adopt a 1D approach where our base-line model is similar to the models in [Pognan et al. \(2023\)](#). Because the light r-process elements ($Z \leq 40$) make up about 80% of the solar r-process composition by mass (and 87% by number, Fig. 1), it is plausible

that the ejecta of many KNe are dominated by these elements. The ejecta mass of AT2017gfo has been estimated to be about $0.05 M_{\odot}$ (e.g. Smartt et al. 2017; Villar et al. 2017; Tanaka et al. 2017; Wollaeger et al. 2018; Vieira et al. 2025), which is the value we use for the ejecta model here.

Light r-process elements are made in significant amounts in regions where the electron fraction Y_e (number of protons relative to number of nucleons) is raised to $\gtrsim 0.3$ due to positron capture and neutrino irradiation. In current simulations, dynamic, secular (disk wind), and hypermassive neutron star (HMNS) polar wind components can all have parts with such conditions (e.g. Wanajo et al. 2014; Goriely et al. 2015; Fujibayashi et al. 2020; Just et al. 2023; Curtis et al. 2023). However, only the disk wind component reaches, in current simulations, the kind of masses inferred for AT2017gfo (and one may also note that ejecta mass was likely yet larger in AT2023vfi). It is therefore reasonable to associate the baseline model with such ejecta. The disk wind can achieve this high Y_e due to either neutrino irradiation by a hypermassive neutron star (Metzger & Fernández 2014), or by self-irradiation (Just et al. 2023).

The density profiles of various high- Y_e components can vary, both between simulations and within a simulation with position angle. The analytic limit for a disk wind is a -2 power law, whereas other components can be steeper, -3 or -4 power laws (e.g. Kawaguchi et al. 2021; Just et al. 2022; Fernández et al. 2024). We use a -3 power law throughout as a value that lies relatively close to all scenarios.

The mean velocity of a disk wind outflow is significantly lower than for dynamic ejecta or HMNS outflows, although with magnetohydrodynamic effects the difference is somewhat reduced (Kiuchi et al. 2023). We choose an inner boundary velocity $v_{in} = 0.02c$ to obtain mean velocities ($\langle \beta \rangle = 0.078$ for a -3 power law) roughly consistent with disk wind simulations (e.g., $\langle \beta \rangle \sim 0.05$ in the simulations of Just et al. 2023), but a higher value $v_{in} = 0.08c$ (giving $\langle \beta \rangle = 0.13$ for a -3 power law) in an alternative model which would correspond closer to the other components (e.g., $\beta = 0.1 - 0.2$ for the PNS wind in the simulations of Just et al. 2023). The ejecta are terminated at $v_{out} = 0.2c$, with material faster than this playing a subdominant role at nebular phases.

The abundances are set to the solar r-process pattern for $Z = 31 - 40$ and $Z = 52$, as estimated by Prantzos et al. (2020), plus 1% abundance each (by mass) of Fe, Ni and Zn. Although the study is focused on the $Z \leq 40$ elements, Te ($Z = 52$) was added due to its possible identification in both AT2017gfo (Hotokezaka et al.

2023) and AT2023vfi (Levan et al. 2024). Inspection of the detailed abundance patterns in the simulations of Kawaguchi et al. (2021); Just et al. (2023); Fujibayashi et al. (2023); Fernández et al. (2024), shows that the $Z = 34 - 40$ pattern is relatively close to the solar one for most simulations. For $Z = 31 - 33$, there is, however, more variation and simulations tend to produce lower abundances than solar. Goriely (1999) assesses the solar r-process abundances of $Z = 31$ (Ga) as very uncertain, with potentially a value much lower than the standard one.

All the simulations mentioned above give abundances of $Z = 26, 28, 30$ being the highest in the $Z = 20 - 30$ range, and of order 1% of the $Z = 31 - 40$ total abundance, which we adopt. By using the solar r-process abundance distribution we make our model as generic as possible, but still in broad agreement with KN simulations, although not tied to any particular one.

The zoning is done with logarithmic 10% steps in velocity, resulting in of order 20 zones (depending on v_{in} and v_{out}). This is an increase compared to the 5 zones used in Pognan et al. (2023), which improves the radiative transfer accuracy and better spatially resolves the physical conditions.

Radioactive powering varies significantly with composition (e.g. Wanajo et al. 2014) and also with uncertain nuclear physics for fixed Y_e (Barnes et al. 2021). Kilonovae have multiple ejecta components, with different Y_e and different morphologies. For this reason, we allow a certain freedom for the power deposition. The baseline powering, "low power", has the decay power of a $Y_e = 0.35$ composition (Wanajo et al. 2014), whereas "high power" multiplies this by a factor f . This scenario could represent e.g. a $Z = 30 - 40$ ejecta component exposed to radioactive decay particles from another more neutron-rich composition in the ejecta. We choose an approach where we boost the power in the high-velocity model with a factor $f = 3$. This allows us to probe the likely span of ionization states, with the low-velocity, low-power model giving a quite neutral ejecta, whereas the high-velocity, high-power one gives high ionization (both low density and high power work to increase ionization). In this way we can bracket the range of possible lines from the studied elements. Thermalization is computed in the same way as in previous papers, with time-delay accounted for using the analytic methods of Kasen & Barnes (2019) and Waxman et al. (2019), but specific flows into heating and ionization channels (non-thermal excitation is ignored) using the Spencer-Fano routine of SUMO.

The baseline atomic data is the FAC calculation set presented in Pognan et al. (2023). However, we have

here also carried out extensive calibrations of energy levels, wavelengths, and A-values relevant for IR lines, and also added in new recombination and collision rates, with details outlined in Appendix A. Of particular importance are the new dielectronic recombination rates for light r-process elements computed in Banerjee et al. (2025). For collision strengths, computed values are used for several ions. When the values are unknown, we make a separate treatment between forbidden fine-structure lines (most important for this study) and others, because the fine-structure transitions often have significantly larger collision strengths than higher-energy ones. For the first group, we fitted the formula $\Upsilon = \text{const} \times g_u g_l$ (Axelrod 1980), where g_u and g_l are the statistical weights of upper and lower levels, to all the calculated fine-structure data for the included elements (see appendix), obtaining a best-fit coefficient of $\text{const} = 0.41$. For the others, we used the Axelrod value derived for iron ($\text{const} = 0.004$) boosted by a factor 10 to bring better agreement with recent calculations for trans-iron elements (Bromley et al. 2023; Mulholland et al. 2024a, 2025; Dougan et al. 2025; McCann et al. 2025).

We study two models, A-low and B-high, with properties summarized in Table 1. We compute the models at 10d, 40d and 80d, in the steady-state approximation (see Pognan et al. 2022a, for an in-depth study of this approximation), at wavelengths from 400 Å to 30 μm .

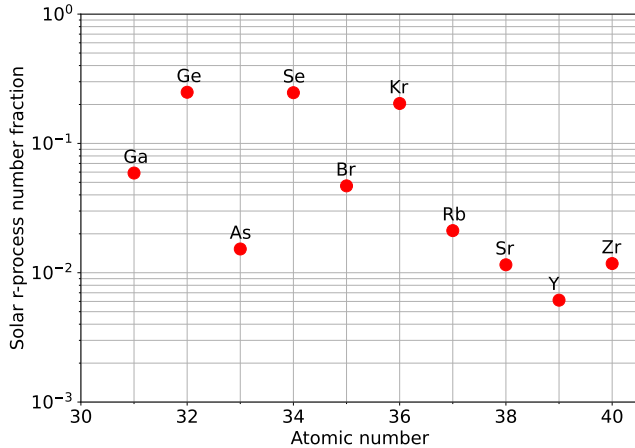


Figure 1. The solar r-process number abundances in the $Z = 31 - 40$ range, according to the Prantzos et al. (2020) estimation. The value for Te ($Z = 52$, not plotted) is 2.3%.

3. DATA

We will make comparisons of the computed models to observations of AT2017gfo and AT2023vfi.

We will make use of the +10.4d spectrum of AT2017gfo presented in Pian et al. (2017). We use

the reduced version of the ENGRAVE data release¹. The spectrum has been corrected for redshift with $z = 0.009843$ (luminosity distance $D_L = 40$ Mpc) and extinction with $E(B - V) = 0.11$ mag.

Kasliwal et al. (2022) reported on the detection of AT2017gfo in the Spitzer 4.5 μm band at +43d and at +74d (see also Villar et al. 2018, for an alternative data reduction). The Spitzer observations also gave upper limits in the 3.6 μm band. The reported 4.5 μm band flux at +43d is $F_\nu = 6.43 \times 10^{-29} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Hz}^{-1}$, which corresponds to

$$F_\lambda = F_\nu \frac{c}{\lambda^2} = 9.5 \times 10^{-12} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ cm}^{-1} \\ = 9.5 \times 10^{-20} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Å}^{-1}. \quad (1)$$

This is equivalent to $F_\lambda \times \lambda_{\mu\text{m}} = 4.3 \times 10^{-19} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Å}^{-1}$ ($\lambda_{\mu\text{m}} = 4.5$). We control our conversion by taking

$$L_{\text{band}} = F_\lambda \times \Delta\lambda_{\text{band}} \times 4\pi d^2 \\ \approx 9.5 \times 10^{-20} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Å}^{-1} \times 10^4 \text{ Å} \times 4\pi \times \\ (40 \times 10^6 \times 3.08 \times 10^{18} \text{ cm})^2 = 1.8 \times 10^{38} \text{ erg s}^{-1}, \quad (2)$$

similar to the value $2 \times 10^{38} \text{ erg s}^{-1}$ reported in Hotokezaka et al. (2022).

The 3.6 μm -band upper limit magnitude at +43d of 23.21 corresponds to a flux limit of $F_\nu = 1.9 \times 10^{-29} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Hz}^{-1}$ ², or equivalently $F_\lambda \lambda_{\mu\text{m}} = 1.6 \times 10^{-19} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Å}^{-1}$. For the +74d data, the corresponding values in the 4.5 μm band are $F_\nu = 1.04 \times 10^{-29} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Hz}^{-1}$, corresponding to $F_\lambda \lambda_{\mu\text{m}} = 6.9 \times 10^{-20} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Å}^{-1}$. The 3.6 μm band upper limit of 23.05 corresponds to $F_\lambda \lambda_{\mu\text{m}} = 1.8 \times 10^{-19} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Å}^{-1}$.

We use the JWST spectra of GRB 230307A/AT2023vfi, taken at +29d and +61d (Levan et al. 2024), utilizing the reduction of Gillanders & Smartt (2025). The reduced spectra were downloaded from <https://ora.ox.ac.uk/objects/uuid:5032f338-aff0-4089-9700-03dc5c965113>. They were corrected for redshift with $z = 0.0646$ (luminosity distance 292 Mpc).

4. ANALYTIC LIMITS OF IR LINE FORMATION

Before we proceed to study the model spectra, we review the various analytic limits of nebular line formation (see also Jerkstrand 2017).

¹ <http://www.engrave-eso.org//AT2017gfo-Data-Release>

² <https://lweb.cfa.harvard.edu/~dfabricant/huchra/ay145/mags.html>

Name	Composition	Deposition	v_{in}
A-low	Solar for $Z = 31 - 40, 52 + 26, 28, 30$ at 1%	Low ($f = 1$)	0.02
B-high	Same as A-low	High ($f = 3$)	0.08

Table 1. Summary of the models studied. Both models have $v_{out} = 0.2c$ and -3 power law density profiles.

4.1. Optically thick, LTE limit

In this limit, the line luminosity is

$$L = V \times n_u A \beta h \nu = V \frac{n_u A h \nu}{n_l A \lambda^3 \frac{1}{8\pi} \frac{g_u}{g_l} t \left(1 - \frac{g_l}{g_u} \frac{n_u}{n_l}\right)}$$

$$= V \frac{8\pi h \nu}{\lambda^3} t^{-1} \frac{e^{-h\nu/kT}}{(1 - e^{-h\nu/kT})} = \frac{4\pi V}{ct} \lambda B_\lambda(T), \quad (3)$$

where V is the volume, n_u and n_l are the number densities of the upper and lower states, A is the Einstein coefficient for spontaneous emission, β is the Sobolev escape probability, g_u and g_l are the statistical weights of the upper and lower levels, t is time, and the other symbols have their usual meaning. If $h\nu \ll kT$, then $e^{-h\nu/kT} \approx 1 - h\nu/kT$, giving

$$L \approx \frac{8\pi k}{\lambda^3 t} VT. \quad (4)$$

4.2. Strong NLTE limit

Assuming that collisional excitation from n_l dominates the inflow to n_u , but the electron density n_e is low enough that deexcitation is always radiative, we have

$$n_u A \beta \approx n_l n_e \frac{8.6 \times 10^{-6}}{\sqrt{T}} \frac{1}{g_l} \Upsilon e^{-h\nu/kT}, \quad (5)$$

where Υ is the effective collision strength. Then

$$L = V \frac{hc}{\lambda} n_l n_e \frac{8.6 \times 10^{-6}}{\sqrt{T}} \frac{1}{g_l} \Upsilon e^{-h\nu/kT}. \quad (6)$$

Taking $n_l \approx n_{ion}$, and $M_{ion} = V n_{ion} \mu m_p$, where μ is the atomic weight of the ion, this becomes

$$L \approx \frac{8.6 \times 10^{-6} hc}{\lambda g_l \mu m_p} T^{-1/2} e^{-h\nu/kT} M_{ion} n_e \Upsilon. \quad (7)$$

If $h\nu \ll kT$, then the exponential factor approaches unity. Because Υ -factors have weak T -dependencies, the temperature dependency is then approximately $\propto T^{-1/2}$.

4.3. Optically thin, LTE limit

This limit yields

$$L = V n_l \frac{g_u}{g_l} e^{-h\nu/kT} A h \nu = \frac{hc}{\lambda \mu m_p} \frac{g_u}{g_l} e^{-h\nu/kT} M_{ion} A. \quad (8)$$

If $h\nu \ll kT$, then the exponential factor approaches unity, so there is no temperature-dependency.

4.4. Summary

Thus, line formation can occur in three different regimes. For $T \gg T_{exc}$ (often fulfilled for MIR lines), the optically thick LTE regimes probes $V \times T$ (Eq. 4), the strong NLTE regime probes $M_{ion} \times n_e / \sqrt{T}$ (Eq. 7), and the optically thin LTE regime probes M_{ion} (Eq. 8). Even if luminosity is generated over a region with varying physical conditions, the total luminosity may still robustly reveal information on masses or volumes. For example, if formation is in the third regime, it does not matter how T and n_e vary over the region. If formation is in the first regime, the emission volume can be inferred no matter what the n_e distribution is (and if a good average temperature can be assessed).

Note that while lines with $\lambda < hc/kT$ are more sensitive to temperature than the Eq. 4, 7, 8 limits, ratios of such lines with similar excitation energies can still give abundances ratios to good accuracy.

Figure 2 plots the position in the departure coefficient (level population relative to its value for the case of an atom in LTE) - optical depth plane for the [Kr II] 1.86 μm and [Ge I] 17.94 μm lines, in model A-low at 10d, as examples. For each epoch, the values in the innermost 10 zones are plotted, which are the ones with the most energy deposition, and therefore will be dominant for line formation. Dividing lines between the different line formation limits discussed above are also drawn.

[Kr II] 1.86 μm is at 10d mostly in the upper right corner, which means its luminosity probes volume but not mass. At 40d and 80d, on the other hand, it has moved to the left side domain, which means its luminosity probes the product of Kr II mass and electron number density. Thus, by the time the Kr II mass can be diagnosed, the regime is already where there is dependency on n_e - the line never (cleanly) passes through the $M_{ion} A$ regime (bottom right).

[Ge I] 17.94 μm (bottom panel) behaves differently. It straddles the upper right and bottom right regimes at 10d, indicating hybrid formation that needs detailed modelling for interpretation. Then, at 40d and 80d the line is fully in the bottom right corner, which means direct probing of M_{ion} . As the departure coefficients are close to unity (LTE), the line is far away from any n_e sensitivity which gives good robustness for mass inferences.

By studying the spatial and temporal variation of these formation regimes, it is possible to identify which

lines give what diagnostic information at which epochs - valuable for developing high-return observation strategies.

5. RESULTS

5.1. Model A-low, evolution of physical conditions

Over the modelled time span (10-80d), model A-low has a radioactive powering (after thermalization) ranging from $4.6 \times 10^{39} \text{ erg s}^{-1}$ at 10d to $9.1 \times 10^{38} \text{ erg s}^{-1}$ at 80d, which is a factor 5.1 decline. This is a significantly smaller power decline than a canonical $t^{-1.3}$ decay (and declining thermalization efficiency would steepen further) which would give a factor $\gtrsim 15$. The reason is that at this Y_e a few isotopes dominate the power output rather than a large ensemble. The power for $Y_e \sim 0.35$ is lower than for low- Y_e compositions at 10d (by a factor 3-4), but higher at 80d (by a factor ~ 2) (Wanajo et al. 2014).

Figure 3 (top) shows the cumulative radioactive deposition versus velocity in model A-low. Some $\gtrsim 80\%$ of the deposition occurs in the layers inside $0.07c$, corresponding to the inner ~ 10 shells of the total 25. The central region dominance can be seen to increase with time, as thermalization inefficiency increasingly sets in for the outer layers. This effect will lead to a narrowing of emission lines with time, and hence cleaner, less blended spectra at late nebular epochs.

Figure 3 (middle) shows the temperature versus velocity at the three epochs. At 10d the ejecta are close to isothermal at around 2300 K in the line-forming region ($v/c \lesssim 0.07$). With time there is then a general trend of increasing temperatures, as radioactive powering decreases more slowly than the collisional cooling efficiency (Hotokezaka et al. 2021; Pognan et al. 2022a), although the innermost few zones break this trend and become somewhat cooler between 10d and 40d. In contrast to at 10d, there is at later epochs a quite steep temperature gradient ($\sim 2000 - 5000 \text{ K}$ over $v/c = 0.02 - 0.07$ at 40d and $\sim 2500 - 8000 \text{ K}$ at 80d). The general temperature scale in the line-forming region indicates that emission lines with $\lambda \gtrsim hc/(k \times 2500 \text{ K}) \gtrsim 6 \mu\text{m}$ will be quite insensitive to the detailed temperature (proportional to T^α , where $\alpha = -1/2, 0, 1$, depending on regime, as opposed to exponential dependency if $\lambda < hc/kT$), making mid-infrared lines uniquely powerful probes.

Figure 3 (bottom) shows the ionization (electron fraction x_e) versus velocity. In the line forming region ($\lesssim 0.07c$) the characteristic value is $x_e \sim 0.7$ at 10d (neutrals and singly ionized species dominate), increasing to $x_e \sim 1.5$ at 40d (singly and doubly ionized species dominate) and $x_e \sim 1.8$ at 80d (doubly ionized species dominate). While x_e does increase with velocity coordinate,

this effect only slightly dampens the electron density profile from the model density profile ($n_{nuclei} \propto v^{-3}$), roughly to a $n_e \propto v^{-2}$ form in the inner layers. As such, the electron density varies by about an order of magnitude over the line-forming region ($\sim 0.02 - 0.07c$).

Figure 4 shows the escape probability for a photon emitted at the centre of the nebula versus wavelength. At 10d, the optical range is completely opaque, and much of the NIR as well, although certain escape windows exist there, where the line opacity is sufficiently low. The MIR range is optically thin for the most part at 10d although some lines remain optically thick, causing absorption ranges. By 40d the NIR range has largely opened up, and at 80d conditions are mostly optically thin down to $\sim 5000 \text{ \AA}$, although a few lines remain optically thick in the innermost zones, e.g. Rb I 7802, 7949 $\text{\AA}$. The variation of T and n_e is important information for assessing single-zone approaches.

5.2. Spectrum of model A-low, 10d

Figure 5 shows the model spectrum at 10d. Line emission is dominated by [Br I] 2.71, [Br II] 3.19 μm , [Se I] 5.03 μm , [Ge II] 5.66 μm , [Ge I] 11.72 μm , [Ge I] 17.94 μm and [Se I] 18.35 μm . There is also some emission in the allowed Sr I transitions between $5s4d(^3D)$ to $5s5p(^3P^o)$ at 2.60-3.01 μm . Significantly weaker, but still relatively clean lines, are seen for [Ni III] 7.35 μm , [As II] 9.40 μm , [Zr III] 14.67 μm (some blending with [Br II] 14.26 μm), [Fe III] 22.9 μm , [Fe I] 24.0 μm , and [Fe II] 26.0 μm .

Figure 6 (upper left) shows the zone-averaged formation regimes of the main lines at 10d. We can see that LTE is a quite good approximation, with all departure coefficients $\gtrsim 0.7$. We can also see that many of the lines are still optically thick. In those cases the specific ion masses are not important; each line samples a blackbody (at characteristic inner region temperature of $\sim 2300 \text{ K}$) and only emission volume and temperature matters (Eq. 3).

At 2300 K, a blackbody peaks at $hc/(3.82kT) = 1.6 \mu\text{m}$. The closest optically thick line to this is [Kr II] 1.86 μm , which therefore becomes the strongest line in the spectrum. Other optically thick lines then follow on the black-body curve with peak luminosities in rough agreement with the theoretical limit (optically thick LTE case). Radiative transfer effects still operate for $\lambda \lesssim 2 \mu\text{m}$ (Fig. 4) which there complicates this simple picture.

Comparison to AT2017gfo at +10.4d shows that AT2017gfo was brighter by a factor several in the NIR compared to the model. As described above, the $Y_e \approx 0.35$ composition has significantly less decay power than

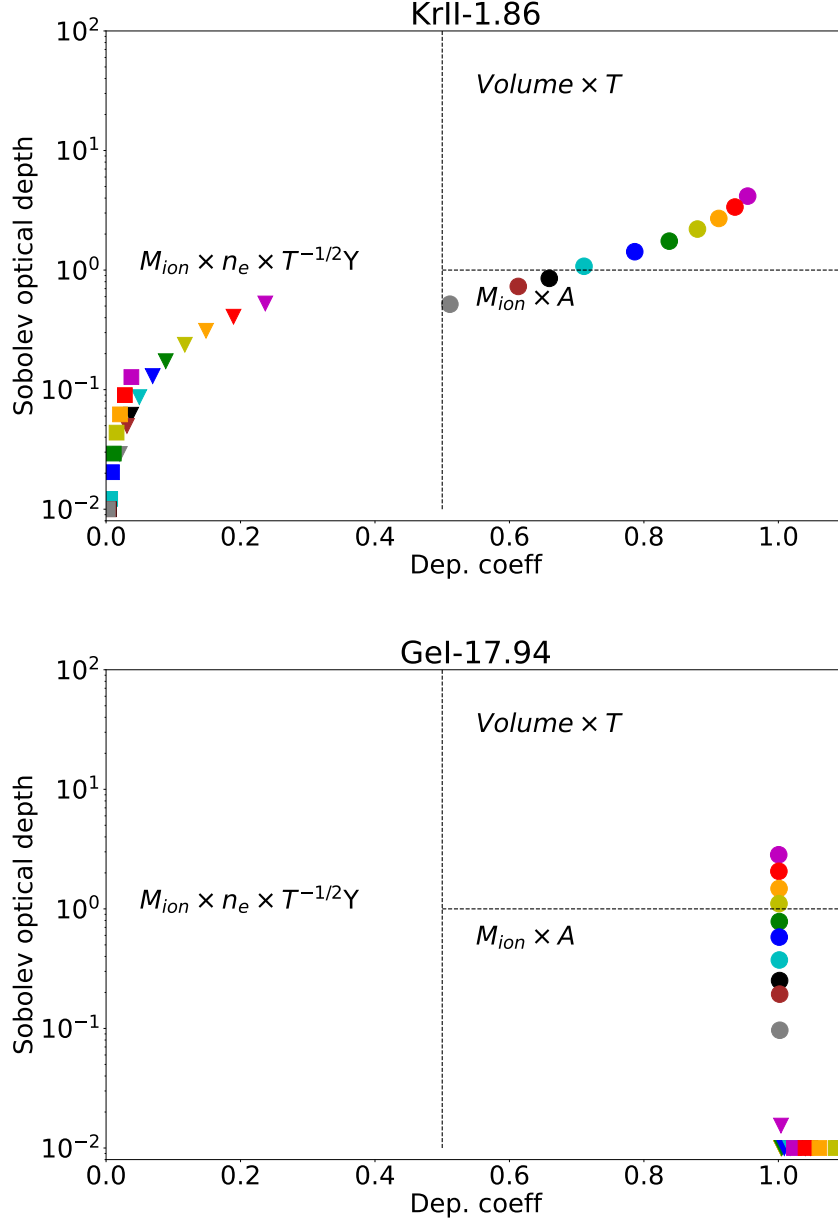


Figure 2. Formation regimes for [Kr II] 1.86 μm (top) and [Ge I] 17.94 μm (bottom), in model A-low at 10d (circles), 40d (triangles) and 80d (squares). Each color corresponds to a zone, with purple the innermost zone. Zone 1 has $v \sim 0.02c$, zone 10 has $v \sim 0.06c$. The stated temperature-dependencies are for the limit $T \gg T_{exc}$.

lower- Y_e compositions at this epoch, and the discrepancy is possibly explained by the presence of such low- Y_e material.

Looking at spectral details, the model gives distinct emission lines in the NIR from Zr I 1.37 μm (this may be [Rb III] 1.36 μm scattering in Zr I), and [Kr II] 1.86 μm . These lines unfortunately lie in regions of strong atmospheric absorption, and hence the reconstructed flux of Pian et al. (2017) is highly uncertain at these wavelengths. If one takes the reconstructed fluxes at

face value, the lack of these features in the observations around 10d might be due to several reasons. One is opacity provided by heavier elements ($Z > 40$ elements are not included in the model, except Te); Fig. 4 shows that even this light composition is largely optically thick in the NIR at 10d, and heavier elements would further enhance the opacity. Another is cooling by heavier elements (this would require these elements to be co-spatial). Another is that AT2017gfo has significantly less $Z = 30 - 40$ elements than in this model

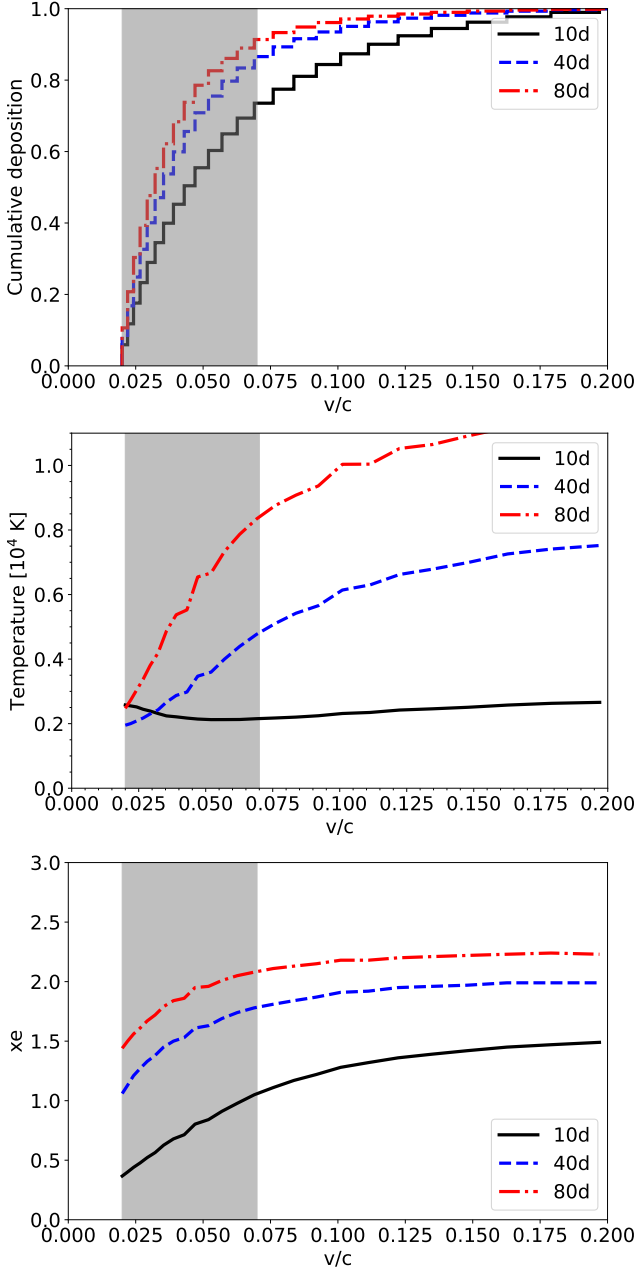


Figure 3. Physical conditions in model A-low; radioactive deposition (top), temperature (middle), electron fraction (bottom), at 10d (black, solid), 40d (blue, dashed) and 80d (red, dash-dotted). The $\gtrsim 80\%$ deposition region is marked gray.

(solar). A final possibility is that the velocity distribution in this model is unrepresentative. However, definitive conclusions cannot be drawn from the ground-based spectra of AT2017gfo. JWST observations of KNe, such as those for AT2023vfi (Levan et al. 2024), are needed to accurately measure the strengths of these Zr I/[Rb III], and [Kr II] features.

Irrespective of which, or combination of which factors, one valuable conclusion is that none of these $Z = 30 - 40$ elements provide a compelling candidate line to explain the strong observed $2.1 \mu\text{m}$ feature. [Kr III] $2.20 \mu\text{m}$ would be the line closest in wavelength, but it is relatively weak in the model, with most Kr being in the I and II states. There is also a Zr I line at $2.24 \mu\text{m}$ ($0.02c$ separation) that is optically thick out to $\sim 0.05c$, absorbing some of the [Kr III] $2.20 \mu\text{m}$ emission. The tellurium feature is a blend of [Te I] $2.10 \mu\text{m}$ and [Te III] $2.10 \mu\text{m}$ in this model. Its luminosity is substantially below the observed value. The Te I lines becomes stronger than the Te III line when ionization is low/moderate, and can give signatures also in CCSNe (Ricigliano et al. 2025).

Kr discussion.—[Kr III] $2.20 \mu\text{m}$ is one of only three lines (the others being [Te III] $2.10 \mu\text{m}$ and [Br II] $3.19 \mu\text{m}$) that directly probe ion mass at this epoch (Fig. 6). It is however quite weak, as only about 1% of the Kr in the model is in the III state. Dividing Eq. 8 with Eq. 3, and using $A = 2.0 \text{ s}^{-1}$, $M_{\text{Kr III}} = 10^{-4} M_{\odot}$, $v = 0.05c$, gives $L_{\text{LTE,thin}}/L_{\text{LTE,thick}} \sim 0.1$.

Let us consider ways to bring the [Kr III] line up towards observed levels for the $2.1 \mu\text{m}$ feature. If the ionization would increase the Kr III abundance by a factor 10, the line would move into the optically thick regime, for the same overall density, and line luminosity would go up by a factor ~ 10 , all else remaining similar, according to the above ratio. Changing the volume would not easily achieve this, as a smaller volume would reduce the LTE, optically thick regime luminosity, and a larger volume would not achieve optical thickness (and would also move the regime towards NLTE). Increasing power would be more promising. It would lead to more Kr III, and a higher temperature. But, as long as a significant Kr II abundance exists, [Kr II] $1.86 \mu\text{m}$ would also strengthen. It would seem difficult to achieve a strong [Kr III] line but a weak [Kr II] line (with the caveat that most of the [Kr II] line lies in the atmospheric band), unless the doubly ionized state becomes dominant to the singly ionized state; in the model the opposite relation holds, and calculated recombination rates for the Kr ions are in use (even though DR calculations for the quite low temperatures here carry uncertainties, e.g. Ferland 2003; Sterling et al. 2015).

5.3. Spectrum of model A-low, 40d

The spectrum at 40d is shown in Fig. 7. The neutral germanium lines have now significantly weakened. The iron-group elements give relatively strong emission between $10 - 13 \mu\text{m}$, and also by [Ni II] $7.35 \mu\text{m}$, whereas Br II and Zr III create a blend at around $14 \mu\text{m}$. Clear

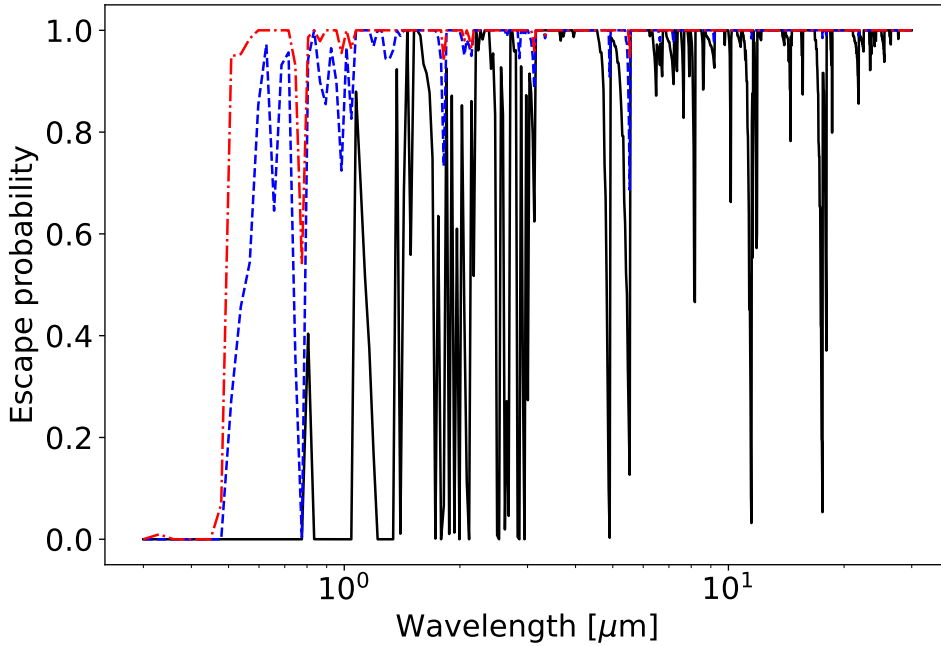


Figure 4. Escape probability for a photon emitted at the centre of the nebula at the modelled epochs (10d; black, solid, 40d; blue, dashed, 80d; red, dash-dotted) for model A-low.

detection potential is predicted for Ni, As, Br, Kr, Se, and Ge.

All strong lines are now optically thin (Fig. 6). The long-wavelength lines are still close to LTE, whereas the shorter-wavelength ones are now in the NLTE regime - it is however still the same lines that dominate as at 10d. The somewhat higher ionization leads to the [Kr III]/[Kr II], [Br II]/[Br I], and [Ge II]/[Ge I] line ratios now being higher.

The model predicts the best targets for direct ion mass determinations (optically thin, close to LTE, and weak T sensitivity) to be [Ge I] 17.94 μm , [Ge I] 11.72 μm , [Ge II] 5.66 μm , and [Se I] 5.03 μm . Neutral Ge makes up 1-10% of the Ge in the line-forming region, and singly ionized Ge $\gtrsim 60\%$. Therefore joint observations of the Ge I and Ge II emission lines holds promise to get a good constraint on the total Ge mass. Selenium has a substantial Se II abundance ($\gtrsim 50\%$), which means observations of the I and III lines (Se II gives no strong lines) still need a significant correction factor to estimate the total Se mass.

The strongest line in the model is, as at 10d, [Kr II] 1.86 μm . There is no sign of this line in the +29d JWST spectrum of AT2023vfi. At this epoch, there is also no possibility to shift model flux over to the [Kr III] 2.20 μm line (by a higher ionization state); it is already too strong by a factor several in the model compared to observations. While at 10d radiative transfer effects at

these wavelengths are still present to some degree, at 40d they are minor (at least from the elements included here, and models including also heavier elements show little absorption by these, Pognan et al. 2025, in prep.); the model predicts none that could absorb [Kr II] 1.86 μm or [Kr III] 2.20 μm emission.

It would seem difficult to resolve this "Kr issue" with either an ionization effect (only small fractions reside in I and IV states) or a radiative transfer effect (epoch is too late). Apart from the option of there being very little Kr in the ejecta, the remaining option is a lower temperature. If the temperature were 1500 K instead of the roughly 3000 K in the model, the [Kr II] 1.86 μm luminosity would go down a factor 13. This might happen if there are many other cooling lines from heavier elements, not included in the model, as observations of AT2023vfi may suggest with its smooth spectrum. A counterpoint to this is that the power in model A-low is quite low, clearly lower than what is needed for AT2017gfo at +10d (by a factor ~ 5) and for AT2023vfi at +29d (factor ~ 2) - but heavier elements will bring in higher power, acting to raise the temperature.

The Te emission is at this epoch almost exclusively due to [Te III] 2.10 μm . The luminosity is, as at 10d, similar to the [Kr II] + [Kr III] emission. The observed feature in AT2023vfi has a peak close to 2 μm , not in clean agreement with any line.

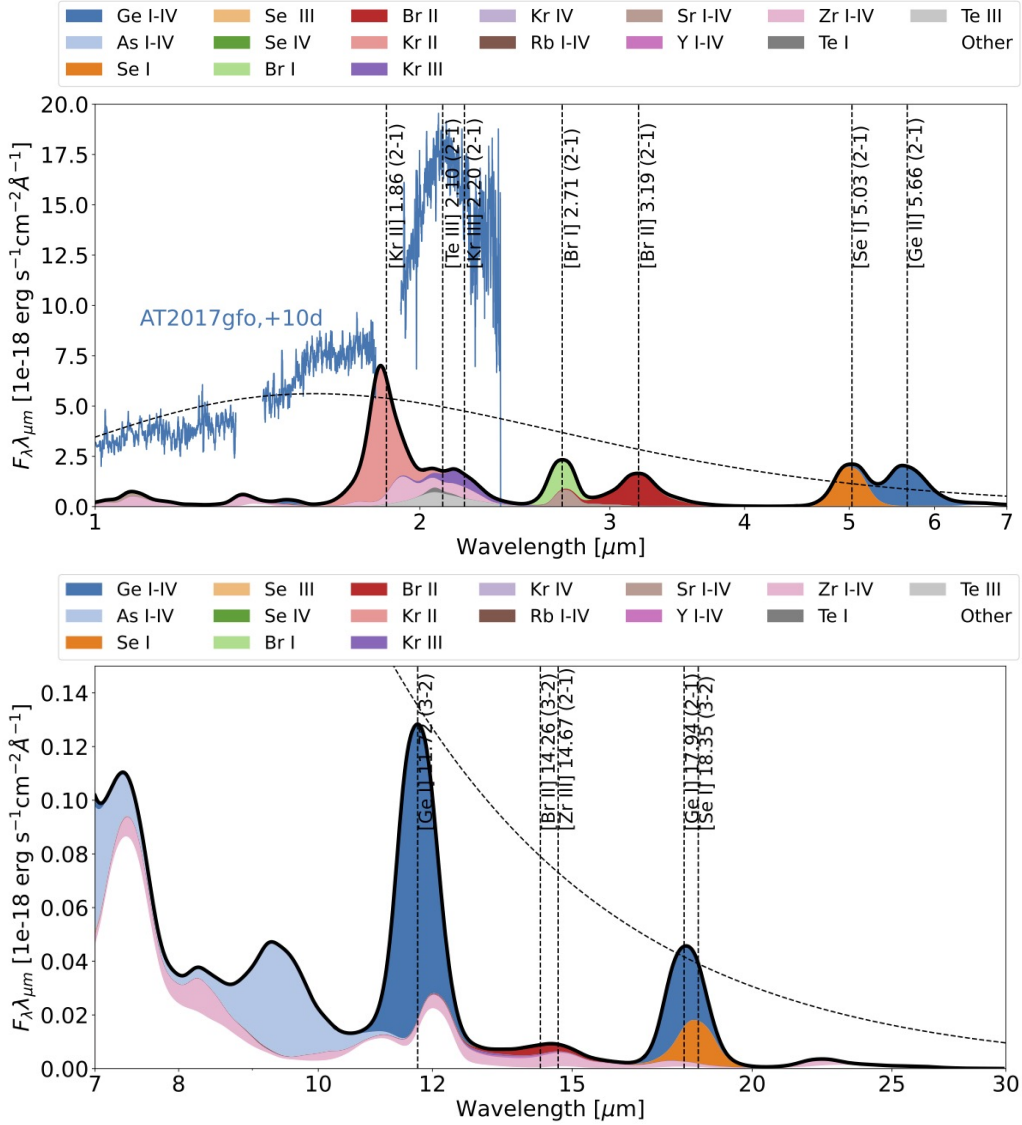


Figure 5. Spectrum of model A-low at 10d. The observed (ground-based) spectrum of AT2017gfo at +10.4d (Pian et al. 2017) is plotted in blue. Overplotted is also a 2400 K blackbody (black, dashed) - lines forming in the optically thick LTE regime have peak fluxes at or close to this curve.

5.4. Spectrum of model A-low, 80d

The spectrum at 80d is shown in Fig. 8. The ejecta are now somewhat hotter (characteristic temperature in the line-forming region of ~ 5000 K) and more ionized (characteristic x_e of ~ 1.8), than at 40d. The $1 - 10 \mu\text{m}$ region is qualitatively similar as at +40d, although the line luminosities are down by a factor ~ 2 . The most notable change is that the neutral lines have now mostly disappeared. In the $10 - 30 \mu\text{m}$ range some bigger changes are seen. The Ge I lines have disappeared, while some of the other features remain at similar luminosities as at 40d. The iron-group cluster at $10 - 13 \mu\text{m}$ has strengthened further, and it blends into a complex of lines from Ge I, Zr III, Kr III, and Br II extending up to $15 \mu\text{m}$.

The +74d Spitzer $4.5 \mu\text{m}$ observation of AT2017gfo is matched well by the combination of [Se I] $5.03 \mu\text{m}$ and [Se III] $4.55 \mu\text{m}$ emission in the model. As at 40d, the $3.6 \mu\text{m}$ upper limit is at or somewhat below the model prediction - with [Br II] $3.19 \mu\text{m}$ tending to give a bit too much luminosity.

For AT2023vfi, the predicted [Br II] $3.19 \mu\text{m}$ line is not, as at 40d, observed, and the issue with [Kr II] $1.86 \mu\text{m}$ is also still there. The observed bump seen close to $2.1 \mu\text{m}$ is somewhat more towards the red at +61d, and would match with a relatively flat-topped [Kr III] $2.20 \mu\text{m}$ line - in model A-low the line is however too narrow. Both the [Kr III] $2.20 \mu\text{m}$ and [Te III] $2.10 \mu\text{m}$ model lines are stronger than in AT2023vfi.

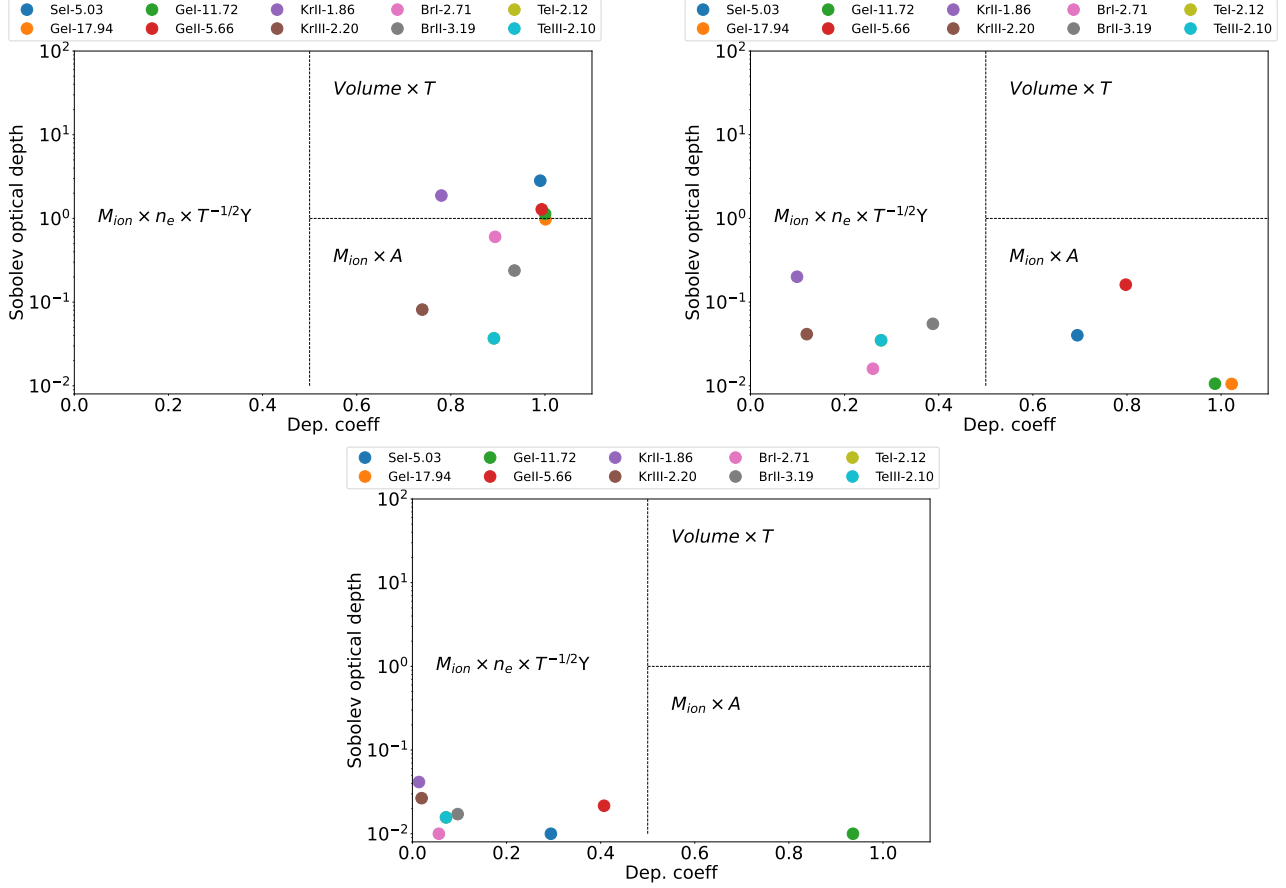


Figure 6. Formation regimes in model A-low at 10d (upper left), 40d (upper right) and 80d (bottom). Each point represents the zone-averaged value over the innermost 8 shells. Optical depths below 10^{-2} are plotted at this floor value. The stated temperature dependencies are for the limit $T \gg T_{exc}$.

5.5. Model B-high - evolution of physical conditions

The physical conditions in model B-high are plotted in Fig. 9. Model B-high reaches 80% deposition at $v/c \sim 0.15$, thus emission lines are expected to emerge a factor 2-3 broader than in model A-low. In terms of power levels, the factor ~ 3 decay boost combines with lower thermalization efficiencies (due to the lower densities) to give deposition ratios (relative to model A-low) of 2.2, 1.3 and 0.9 at 10d, 40d and 80d, respectively.

The higher deposition (except for at 80d) and the lower densities lead to higher temperatures, especially at 40d and 80d when model B-high reaches characteristic temperatures of 10,000 and 25,000 K, much higher than model A-low (~ 3000 and ~ 6000 K, respectively). This means that more IR lines now come into the regime $T_{exc} \ll T$. Ionization is also higher, with x_e values up by factors ~ 1.5 .

5.6. Spectrum of model B-high - 10d

The spectrum of model B-high at 10d is shown in Figure 10. [Kr II] $1.86 \mu\text{m}$ is, as in model A-low, the strongest line. [Kr III] $2.20 \mu\text{m}$ is significantly stronger

than in model A-low, which together with the [Te III] $2.10 \mu\text{m}$ contribution moves the blend towards the red, giving a peak at $\sim 2 \mu\text{m}$. The Kr lines are now formally consistent with the AT2017gfo spectrum, but the shape of the triple-blend feature is also not in particularly good agreement with the observed feature, which is quite well described by a Gaussian centred at $2.1 \mu\text{m}$ (which would correspond to a Gaussian emissivity distribution if by a single line, Jerkstrand 2017). Considering the 7.4d-10.4d evolution, Gillanders et al. (2024) favor a fit consisting of two Gaussians centred at $2.05 \mu\text{m}$ and $2.14 \mu\text{m}$, respectively, with $v_{FWHM} = 0.1c$. It is of interest that these wavelengths would match [Te III] $2.10 \mu\text{m}$ and [Kr III] $2.20 \mu\text{m}$ if both have a blueshift of $\sim 0.05/2.1 = 0.024c$. Such a blueshift could arise either due to an intrinsic ejecta asymmetry, or due to radiative transfer effects (Jerkstrand et al. 2015).

At longer wavelengths, [Br II] $3.19 \mu\text{m}$ and [Ge II] $5.66 \mu\text{m}$ are distinct, as in model A-low. The neutral lines, [Br I] $2.71 \mu\text{m}$ and [Se I] $5.03 \mu\text{m}$ are now however mostly gone, as is the quasi-continuum created by zir-

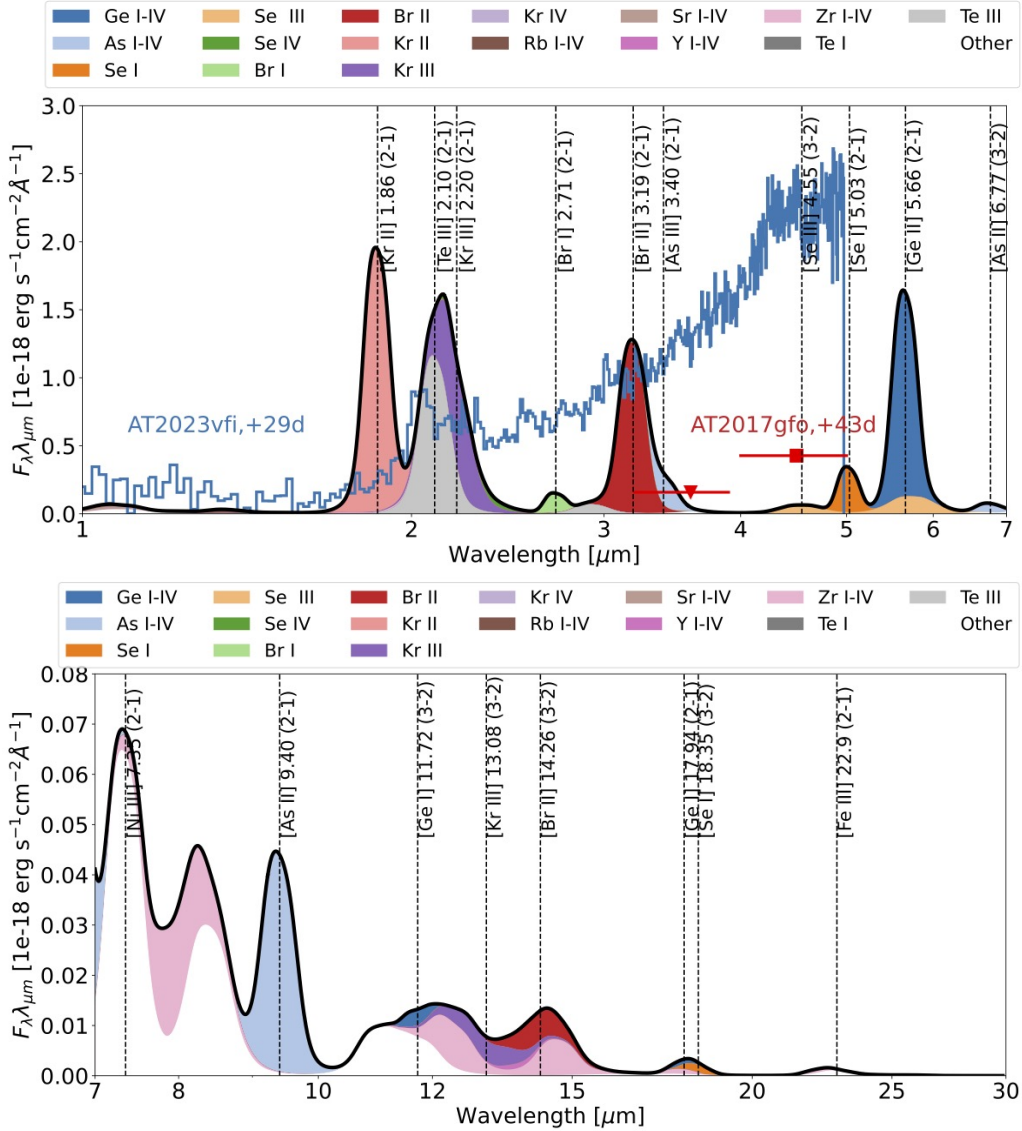


Figure 7. Spectrum of model A-low at 40d. Observed photometry of AT2017gfo at +43d and observed spectra of AT2023vfi at +29d are also shown. The model and AT2023vfi spectra have been scaled to a distance of 40 Mpc (distance of AT2017gfo).

conium (much of it is Zr I in model A-low, and neutral abundances are generally lower in model B-high).

Beyond 10 μm , the neutral Ge lines in model A-low are gone, and instead [Kr III] 13.08 μm and [Br II] 14.26 μm are prominent - the flux levels are however low and there is severe blending throughout. This model predicts observations between 1-7 μm to be most rewarding, and Br II and Ge II appear promising for detection at $\sim 10\text{d}$ irrespective of the velocity of the light r-process component (strong lines predicted by both models A-low and B-high). Inspection of the line formation regimes (Fig. 11) shows that Br II and Ge II form in the optically thin LTE regime, thus with this type of ejecta ionic masses are possible to directly probe at 10d. The fractions of Br and Ge in the singly ionized states are quite high in the

model, so these ionic masses are in turn useful tracers of the total element masses.

5.7. Spectrum of model B-high - 40d

The spectrum of model B-high at 40d is shown in Figure 12. The strong narrow [Kr II] 1.86 μm line in model A-low has here morphed into a more discrete, broader feature. It is now subdominant to [Kr III] 2.20 μm and in addition [Se IV] 2.29 μm has emerged, with about equal strength to the [Kr III] line. Together with a relatively modest [Te III] 2.10 μm contribution, the 2.1 feature is therefore now a four-way blend. The model feature is in reasonably good agreement with the observed feature in AT2023vfi, both in terms of luminosity and (roughly) line profile - although the detailed interpreta-

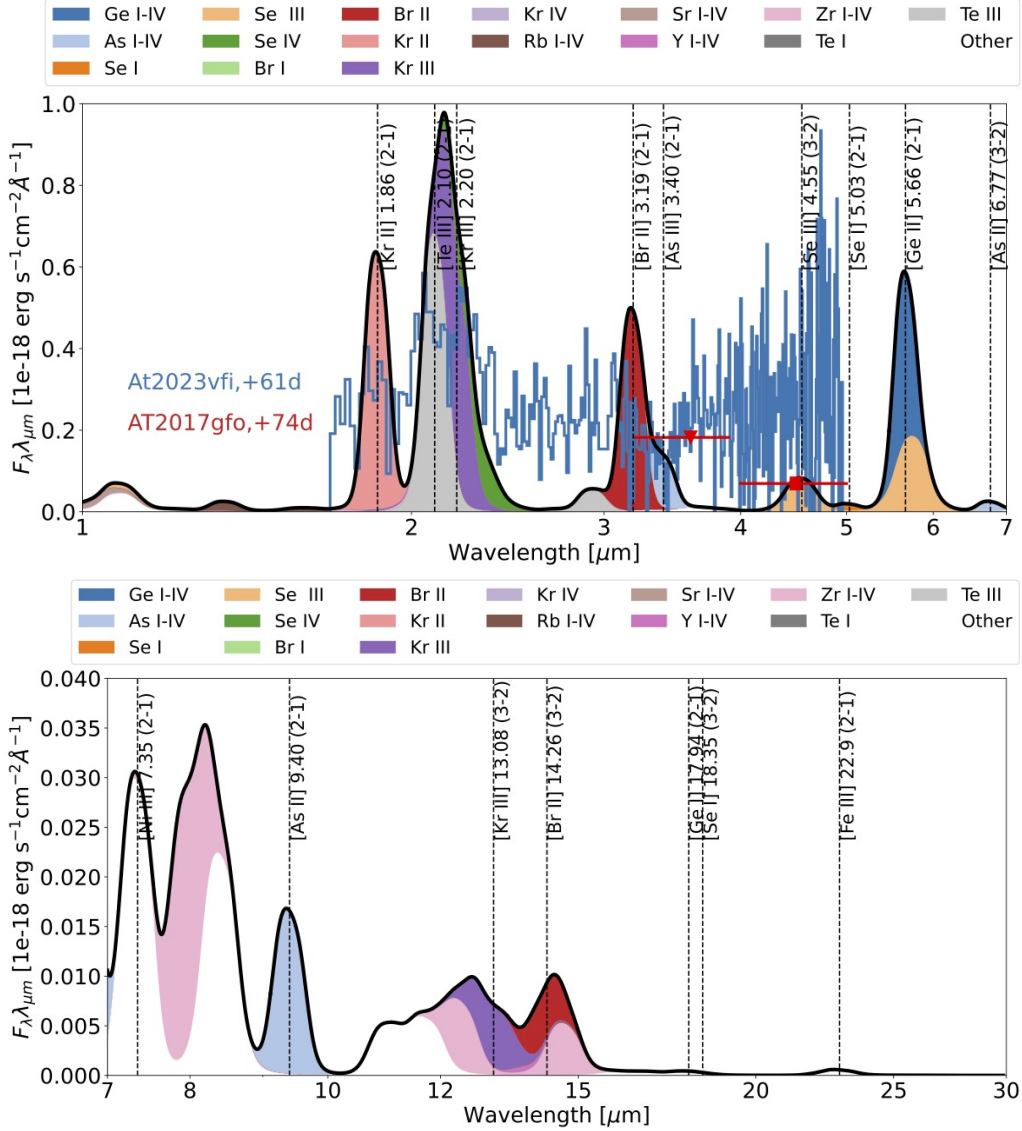


Figure 8. Spectrum of model A-low at 80d. Observed photometry of AT2017gfo at +74d and observed spectra of AT2023vfi at +61d are also shown. The model and AT2023vfi spectra have been scaled to a distance of 40 Mpc (distance of AT2017gfo).

tion depends on what one assumes about the underlying (quasi)-continuum.

Neutral Br and Ge lines are weak, while [Br II] 3.19 μm is distinct. Both [Se I] 5.03 μm and [Ge II] 5.66 μm have disappeared and given way to [Se III] 4.55 μm and [Se III] 5.74 μm . What one may note is that in both a low and high velocity model, it is always selenium that would produce the type of flux observed with Spitzer for AT2017gfo - neutral selenium in the first case and doubly ionized selenium in the second case. At longer wavelengths, [Zr IV] 8.00 μm and [Kr III] 13.08 μm are the dominant lines.

All lines are now well into the low density limit in the line formation plane (Fig. 11) - thus A-values play no role for the line luminosities, which instead are directly

proportional to collision strengths. In addition, as temperature is $\gtrsim 10,000$ K, relative IR line luminosities are temperature insensitive and differ mainly by the combination of ionic masses and collision strengths. As such it is important to remember that the models make use of detailed collision strengths for the Kr II, Kr III, Se III, Se IV, Te III and Zr IV lines but not for the Br II lines.

5.8. Spectrum of model B-high - 80d

The spectrum of model B-high at 80d is shown in Figure 13. Changes to +40d are quantitative but not qualitative. [Se IV] 2.29 μm has now taken over as the dominant line in the 2.1 μm blend, with [Kr III] 2.20 μm second strongest. As at 40d, a solar ratio between Te

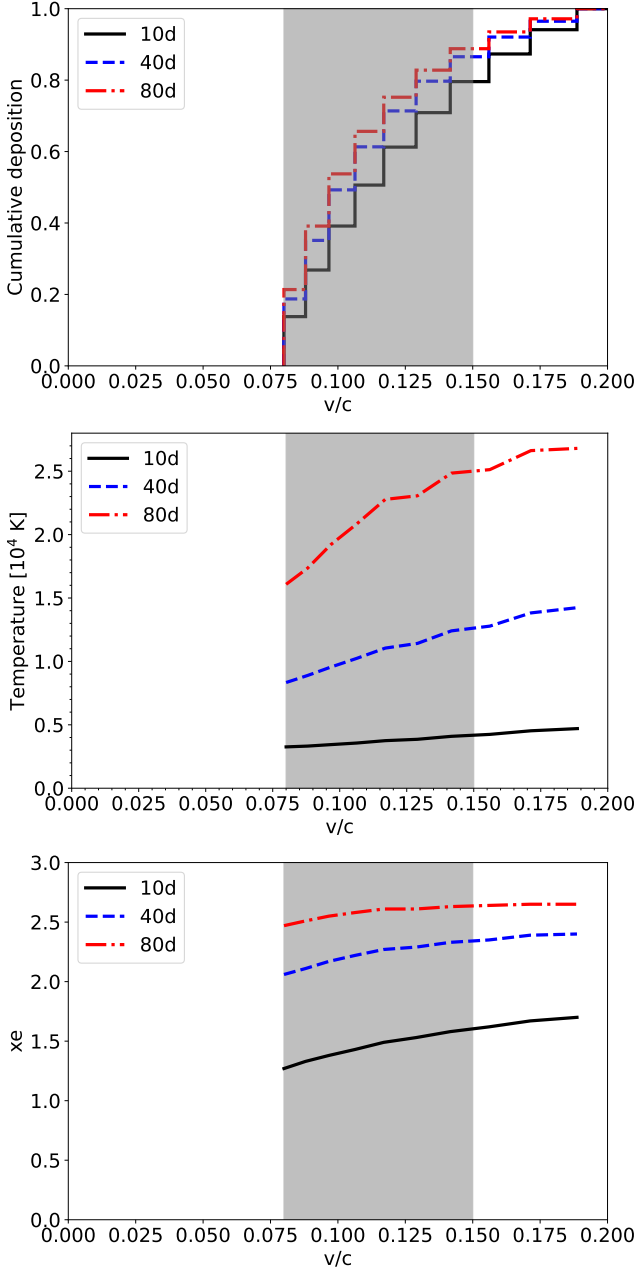


Figure 9. Physical conditions in model B-high; radioactive deposition (top), temperature (middle), electron fraction (bottom), at 10d (black, solid), 40d (blue, dashed) and 80d (red, dash-dotted). The $\gtrsim 80\%$ deposition region is marked gray.

and the lighter elements would mean Te does not dominate the feature. The [Se III] $4.55 \mu\text{m}$ line remains in good agreement with the Spitzer observations - spectral observations with JWST of the $5\text{--}7 \mu\text{m}$ region hold potential to confirm or reject Se III based on the $5.74 \mu\text{m}$ line.

Ion	Line	Detectable in
Ge I	11.72	A10
	17.94	A10
Ge II	5.66	A10-80, B10
As II	6.77	A40-80,
	9.40	A10-80, (B10)
As III	3.40	A40-80, (B40-B80)
Se I	5.03	A10-80
Se III	4.55	A40-80, B40-80
	5.74	(A40-80), B40-80
Se IV	2.29	(B40), B80
Br I	2.71	A10-40
Br II	3.19	A10-80, B10-40
	14.26	(A10-80), (B10-40)
Br IV	3.34	(B40-80)
	3.81	(B40-80)
Kr II	1.86	A10-80, B10-80
Kr III	2.20	(A10-80), (B10-80)
Zr I	14.91	(A40-80),
Zr II	22.28	A10
Zr III	12.42	(A10-80), (B10)
Zr IV	8.00	(B40-80)

Table 2. Summary of predicted IR lines. Lines that suffer significant blending are marked in parenthesis.

Evolution beyond $10 \mu\text{m}$ is minor - the same lines are seen as at 40d and they are formed in the same regime, the model therefore predicts limited additional value of observing at the long wavelengths again if data at $\sim 40\text{d}$ already exists.

5.9. Summary of predicted signatures

Table 2 summarizes predicted signatures from the $Z = 31 - 40$ elements in the two models. Six of these ten elements have predicted detectable lines; Ge, As, Se, Br, Kr and Zr. The other four elements - Ga, Rb, Sr, Y - give no strong lines in the models, at any epoch.

This table can be used to design a JWST observation strategy depending on target element. For example, detection of Ge is predicted to require one MIRI spectrum at around 10d - (unblended) Ge I lines should emerge if ejecta conditions are similar to model A, and Ge II lines if they are similar to conditions in model B. Analogously, a NIRSpect spectrum at 10-40d holds potential to reveal Br I and Br II for model A conditions and Br II (and perhaps Br IV) for model B conditions.

6. DISCUSSION

From the considered model set, krypton stands out as an element giving strong predicted lines that are not clearly seen in observations. We therefore look in some

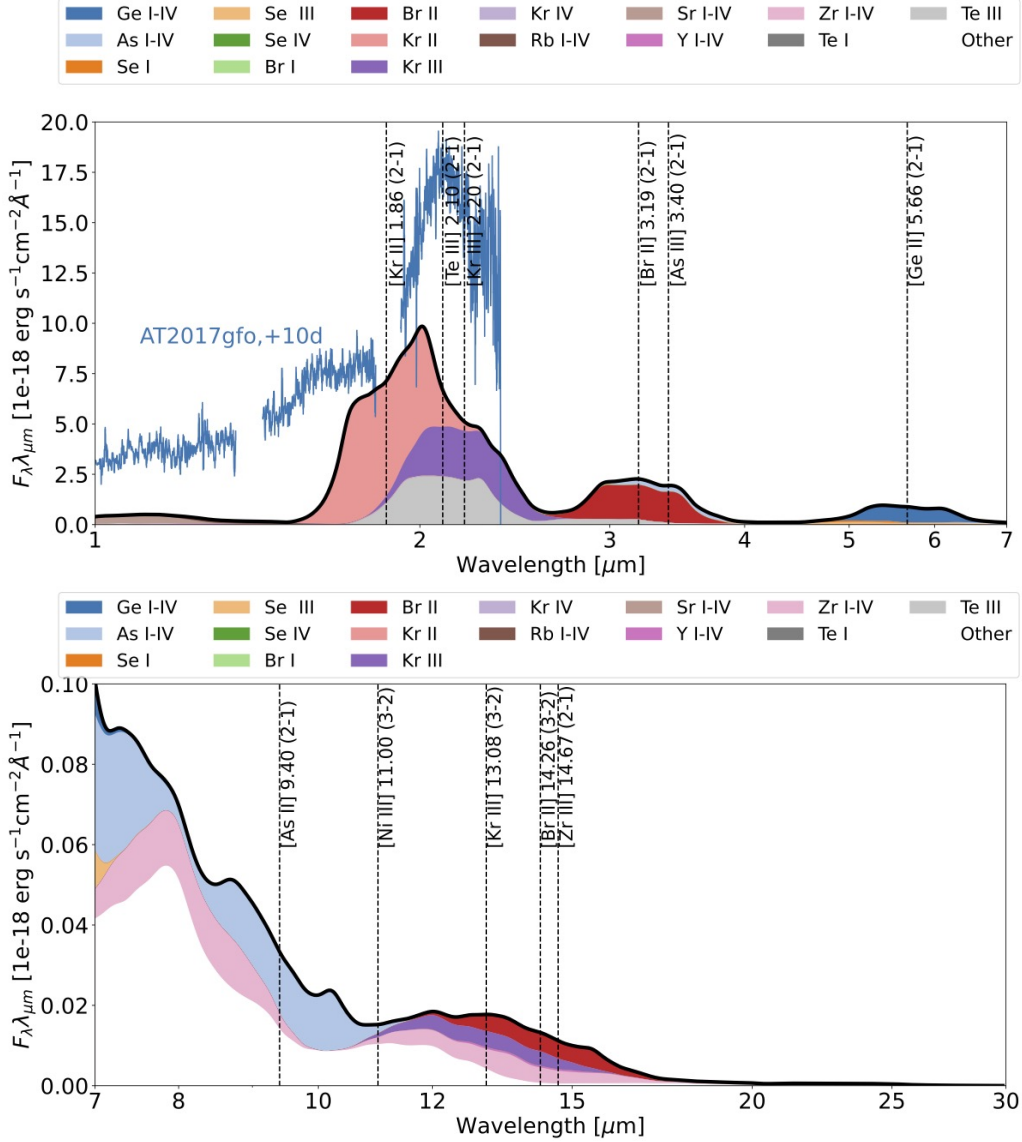


Figure 10. Spectrum of model B-high at 10d, compared to the same data as in Fig. 5.

detail into the formation of these lines, and what constraints may be put on krypton abundances.

In the optically thin LTE phase, the line ratio of [Kr III] 2.20 μm and [Te III] 2.10 is given by

$$\frac{L(\text{Kr III})}{L(\text{Te III})} = \frac{x_{36} y_{36,3} g_{u,\text{Kr III}}/Z_{\text{Kr III}} A_{\text{Kr III}} e^{\frac{302K}{T}}}{x_{52} y_{52,3} g_{u,\text{Te III}}/Z_{\text{Te III}} A_{\text{Te III}}} \approx 2.9 \frac{y_{36,3}}{y_{52,3}}. \quad (9)$$

where x_Z denotes the number fraction of species with atomic number Z and $y_{Z,n}$ denotes the fraction of that species in ionization state n , with $n = 1$ representing the neutral atom. The last equation uses the solar value of $x_{36}/x_{52} = 8.7$ (Lodders 2003), and, because the temperature is much higher than 302 K, the last term has been put to unity.

Past some time ($\gtrsim 40\text{d}$ in model B-high), the lines both form in the low-density NLTE regime. Their luminosity ratio is then

$$\frac{L(\text{Kr III})}{L(\text{Te III})} = \frac{x_{36} y_{36,3} \Upsilon_{\text{Kr III}}/g_{u,\text{Kr III}} e^{\frac{302K}{T}}}{x_{52} y_{52,3} \Upsilon_{\text{Te III}}/g_{u,\text{Te III}}}, \quad (10)$$

Inserting the known values of the collision strengths (Schöning 1997; Madonna et al. 2018), and again putting the temperature factor to unity, this becomes

$$\frac{L(\text{Kr III})}{L(\text{Te III})} \approx 5.1 \frac{y_{36,3}}{y_{52,3}}. \quad (11)$$

Thus, for a solar Kr/Te ratio the Te III line can dominate the Kr III one only if the fraction of Te in the doubly ionized state is at least a factor 5 larger than the fraction of Kr in the doubly ionized state.

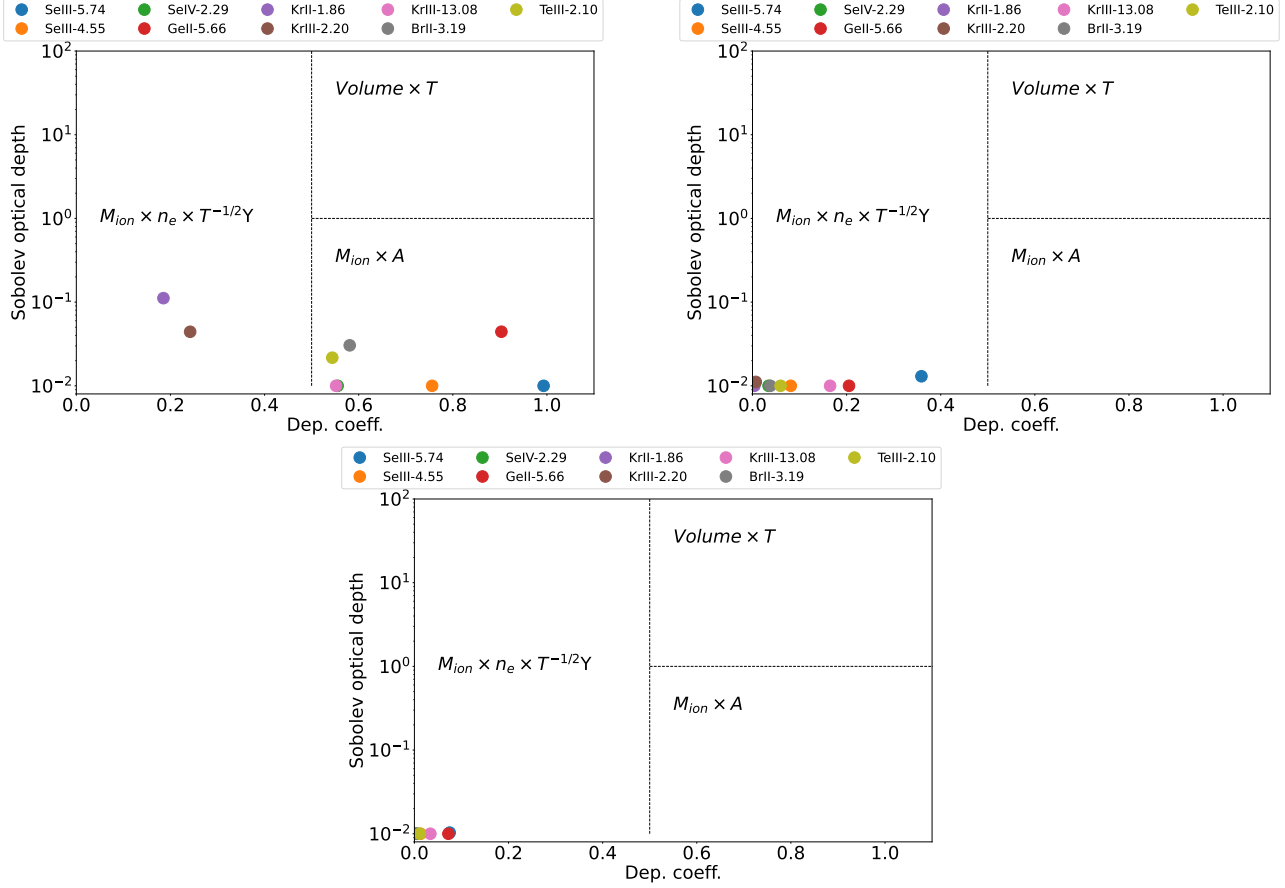


Figure 11. Formation regimes in model B-high at 10d (top), 40d (middle) and 80d (bottom). Each point represents the zone-averaged values over the innermost 8 shells. Optical depths below 10^{-2} are plotted at this floor value. The stated temperature dependencies are for the limit $T \gg T_{exc}$.

Kr I and Kr II have higher ionization potentials (14.0 and 24.4 eV, respectively) than Te I and Te II (9.0 and 18.6 eV, respectively). All else equal, this would imply that more Kr stays in neutral and singly ionized states compared to Te. However, recombination rates also affect this. For Kr we use dedicated calculations (Sterling 2011), so there is limited uncertainty from this direction (although DR calculations are challenging due to uncertain positions of doubly excited states). While for Te only the Te III to Te II recombination stage has published rates (Singh et al. 2025), this does not directly affect the question of how to achieve a lower $y_{36,3}/y_{52,3}$ ratio (to allow Te III to explain the 2.1 line at solar Kr/Te values), as in the models here $y_{52,3}$ is already large, $\gtrsim 0.3$.

In model A-low, the characteristic $y_{36,3}$ value in the line-forming region is $\sim 1\%$ at 10d, growing to $\sim 10\%$ at 40d and $\sim 30\%$ at 80d (Figs. 14-16). The corresponding $y_{52,3}$ values are $\sim 5\%$, 50% , and 70% . Thus, at 40d and 80d, the $y_{52,3}$ value is close to its maximum (unity), and to make a significantly weaker [Kr III] line would mean reducing $y_{36,3}$. But $y_{36,2}$ is already high, and would, for

a movement toward a less ionized solution, become yet higher, further overproducing the [Kr II] 1.86 μm line.

In model B-high, both $y_{36,3}$ and $y_{52,3}$ are high at all epochs, $\gtrsim 40\%$ (Figs 17-19). At 40d and 80d, the neutral and singly ionized states are subdominant and Kr and Te are mainly in the doubly and triply ionized states. But again, because the Kr IV to III recombination rate is known, it is not straightforward to reduce the $y_{36,3}$ value.

An analogous analysis of [Kr II] 1.86 μm gives, in the optically thin LTE phase

$$\frac{L(\text{Kr II})}{L(\text{Te III})} \approx 3.4 \frac{y_{36,2}}{y_{52,3}} e^{\frac{-884K}{T}}, \quad (12)$$

and in the low-density limit

$$\frac{L(\text{Kr II})}{L(\text{Te III})} \approx 0.72 \frac{y_{36,2}}{y_{52,3}} e^{\frac{-884K}{T}}. \quad (13)$$

Both model A-low and B-high give $\frac{y_{36,2}}{y_{52,3}} \gtrsim 1$ (an exception is model B-high at 80d where the ratio is lower). Thus, a solar Kr/Te ratio yields a [Kr II] 1.86 μm line

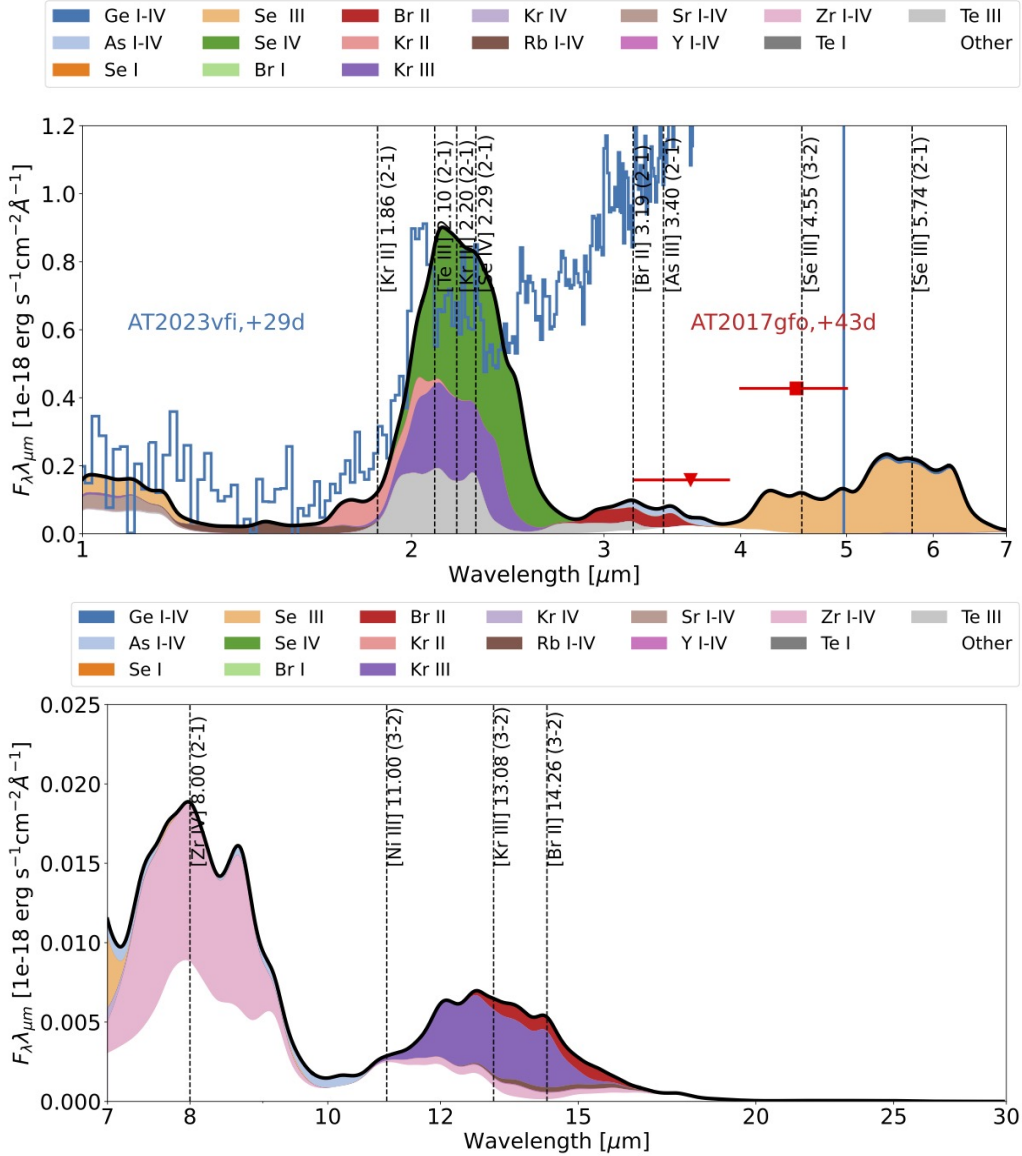


Figure 12. Spectrum of model B-high at 40d, compared to the same data as in Fig. 7.

comparable in strength to [Te III] 2.20 μm , as $T \gg 884$ K.

From these considerations, identification of the observed feature at ~ 2.1 μm in AT2017gfo and AT2023vfi with [Te III] 2.10 μm would rather robustly implicate a Kr/Te ratio significantly below the solar r-process pattern one (at least in the ejecta component giving rise to the [Te III] 2.10 μm line). Krypton gives uniquely constraining information because both Kr II and Kr III have strong 2-1 lines in this spectral region - but the general picture of a subsolar production of light r-process elements is also reinforced by the fact that quite strong predicted [Br II] 3.19 μm is not observed in AT2023vfi. The most straightforward interpretation is that Kr and

Br abundances are both significantly subsolar compared to Te.

What if Kr and Te exist in different regions, with different physical conditions? The excitation temperatures are between 6500-7700 K for these three lines. At face value, this means that also relatively small zone temperature differences could drive big differences in relative luminosities. But - if the ejecta mass is $\sim 0.05 M_{\odot}$ and the 31-40 elements are produced in solar ratios, there must be strong Kr lines produced - as we show here equal or stronger to observed features and/or non-detections in AT2017gfo and AT2023vfi. Thus - one could boost Te by postulating that it exists in another, hotter and/or more ionized zone - but such a model would not fit the

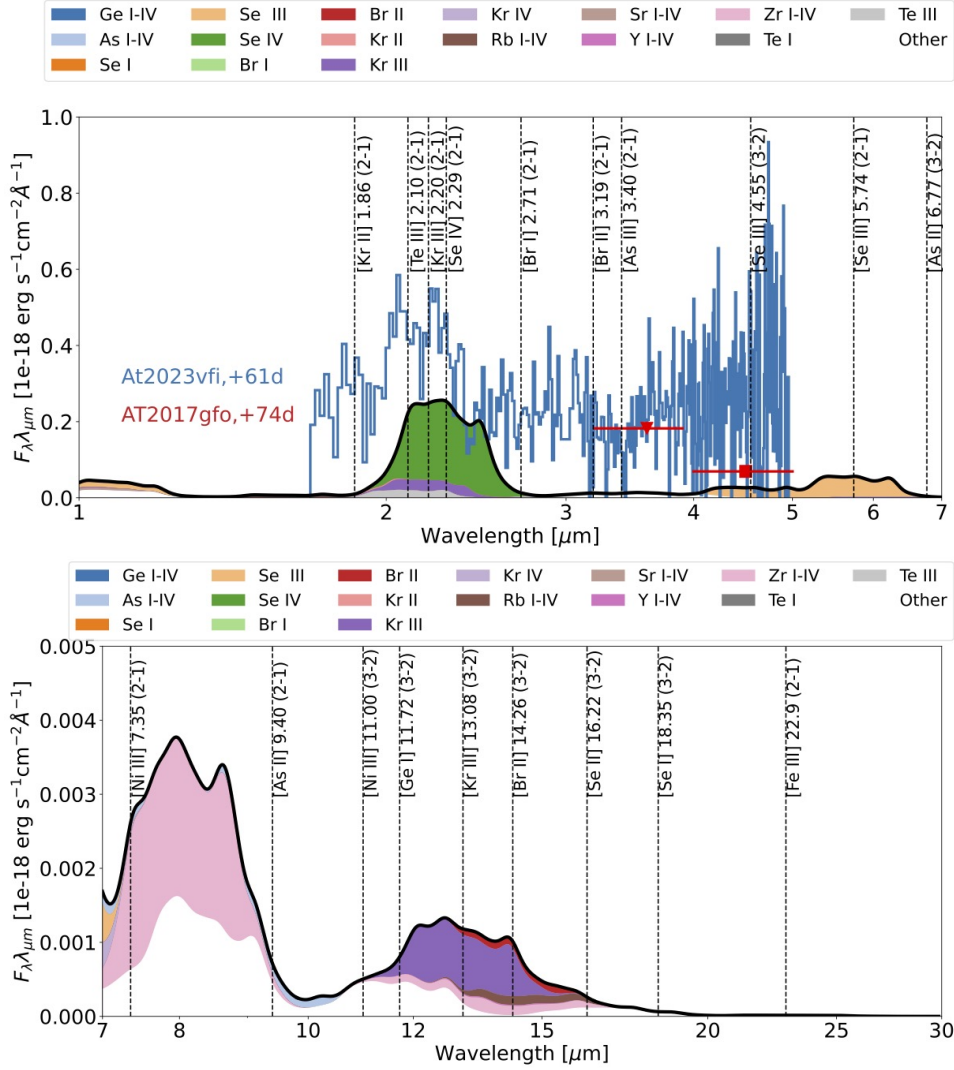


Figure 13. Spectrum of model B-high at 80d, compared to the same data as in Fig. 8.

data as the Kr + Te + Se complex would be much too strong.

If this is the case in the first two observed KNe, important consequences follow for the question of the origin of the light r-process elements. Alternative sources for r-process nucleosynthesis - neutrino-driven winds in CCSNe, collapsar disks, and jets and magnetorotational SNe, in many studies appear promising for light r-process production (e.g. Travaglio et al. 2004; Cowan et al. 2021; Arcones & Thielemann 2023).

At low metallicity, the weak s-process is not yet effective in massive stars, and therefore can their heavy element ejection be ascribed to explosive nucleosynthesis. Germanium shows no correlation with europium (Eu) in low-metallicity stars (Cowan et al. 2005), suggesting two different sources. At the same time, Ge correlates well with Fe, which suggests a coproduction. But already Se and Sr show close to solar r-process abundances

with respect to heavier elements in several metal-poor stars (Roederer & Lawler 2012; Roederer et al. 2022). These results suggest the main r-process (presumably from kilonovae with perhaps a contribution by collapsars) may be capable to make the solar r-process pattern from $Z = 34$.

These results appear to be in good agreement with several current KN nucleosynthesis models, which achieve patterns close to solar from $Z = 34$, but sub-solar for $Z = 31 - 33$. There is however some tension with nucleosynthesis yield models for CCSNe (Sukhbold et al. 2016; Wanajo et al. 2018), which tend to give close to solar production all the way up to $Z \sim 38$.

Two interesting hypothesis tests, with consideration of what the models in this paper show, now present themselves. One is that the Ge r-process component (estimated as 36% by Prantzos et al. (2020)) comes mainly from CCSNe. This is already a quite convincing scenario

from CCSN theory, NSM theory, and low-metallicity star observations - but detections or constraining upper limits on Ge emission directly from r-process sources are needed to fully test this. The models here show that the hypothesis is testable with MIR observations of KNe, e.g. of the [Ge II] 5.66 μm line.

The other hypothesis is that the r-process components of Se and Kr (both estimated at 61% by Prantzos et al. (2020)) come mainly from KNe. There is tension here between CCSN theory, NSM theory, and metal-poor r-process enriched stars - and there is also a certain degree of tension within the KN analysis presented here. Selenium, at solar abundance, is able to explain the Spitzer photometry of AT2017gfo. On the other hand, the lack of observed Kr lines suggest significantly subsolar Kr production. Further JWST data, and yet more accurate models, hold clear promise to settle this question. There is also a close relation to the question of strontium production by KNe (Watson et al. 2019; Domoto et al. 2021; Perego et al. 2022; Tarumi et al. 2023), as well as possible identifications of Y (Sneppen & Watson 2023) and/or Rb (Pognan et al. 2023).

With the complex ejecta structures and physical formation processes, the interpretation of kilonova spectra is still in its infancy. Significant work has been done in the past few years to identify possible signatures, in particular in the infrared where radiative transfer effects and line blending tend to be less severe. Hotokezaka et al. (2023) used a single-zone emissivity model where the composition is the solar one, but starting at $Z = 38$. The physical conditions were fixed to ionization structure I – II – III – IV = 0.25, 0.4, 0.25, 0.1 for all elements, and temperature to $T = 2000$ K. The model has ejecta mass $0.05 M_{\odot}$ and uniform density with $v_{\text{max}} = 0.07c$ (as such the characteristic line widths are somewhere between models A-low and B-high here).

The luminosity of a line can vary significantly with density, composition, and energy deposition, which determine the temperature and ionization. As an example, the [Te III] 2.10 μm luminosity in model A-low here at 10d is significantly below the one of Hotokezaka et al. (2023). There are two main reasons for this. First, the Te mass fraction in the models here is 3.8% (the solar value), whereas in the Hotokezaka et al. (2023) model it is 11%; with the same total ejecta mass of $0.05 M_{\odot}$ this means a factor ~ 3 lower Te mass in our case. Second, our lower value for $y_{52,3}$ of ~ 0.05 in model A-low, compared to the assumed 0.25 in Hotokezaka et al. (2023), combines with the 3 times lower Te mass to give a Te III mass ratio of ~ 15 . Both in model A-low here, and in the model of Hotokezaka et al. (2023), electron densities are larger than $n_{e,\text{crit}}$, so the line is formed close to

LTE and only ion mass and temperature matter. The typical temperature in model A-low is around 2400 K, and while this seems close to the assumed 2000 K in Hotokezaka et al. (2023), it leads to a factor 1.5 higher emissivity through the Boltzmann factor (entering both in LTE and NLTE limits), lowering the difference to a factor ~ 10 .

When the line does not form in LTE, the situation is even more complex. In model B-high, the much larger volume of the line-forming region leads to lower electron densities (factor ~ 30), and the [Te III] 2.10 μm line forms in the transition regime between LTE and NLTE at 10d (Fig. 11). The luminosity ratio of NLTE vs LTE emission is $L(\text{NLTE})/L(\text{LTE}) = g_l/g_u (n_e/n_{e,\text{crit}})$, so the emission per Te III ion is lower in NLTE (as then $n_e < n_{e,\text{crit}}$), all else similar. However, a higher temperature (~ 4000 K) significantly brings up the Boltzmann factor (factor 3.1 from 2400 K and factor 5.1 from 2000 K), and now $y_{52,3}$ has increased to $\gtrsim 0.5$, together giving a factor 35 increase for LTE emission compared to model A-low, and a factor 10 increase compared to Hotokezaka et al. (2023). But going into NLTE damps this to factors of ~ 3.5 and ~ 1 . Finally, our lower Te mass gives a luminosity of $\sim 1/2$ of the one of Hotokezaka et al. (2023).

The above analysis illustrates how the luminosity of a line can vary quite dramatically with density, composition, and energy deposition, which determine the temperature and ionization, in a model. In model A-low, the density to energy deposition ratio is too high to allow for sufficient Te in the doubly ionized state. In model B-high, it is too low, but with a lesser discrepancy.

6.1. Complementary information from Pognan et al. (2024)

In Pognan et al. (2025), a SUMO model grid is constructed where ejecta mass and composition (held fixed here) is varied. This grid gives complementary information about how lines can change over ejecta parameter space. One result is that for the case of no dynamic ejecta component ($f_{\text{dyn}} = 0$, the composition most similar to the one used here), the spectrum is not strongly sensitive to ejecta mass, in the sense that Se I + Se III, Br I, Br II, Ni III lines are dominant for all cases at 10d. The Ni III lines are stronger than here because the abundance is higher (about 7% compared to 1% here). Some more sensitivity is seen around the 2 μm region. The [Kr II] 1.86 μm line is strong, as in the models here, but [Te III] 2.10 μm becomes increasingly important with lower ejecta mass. The [Kr III] 2.20 μm line is always also much weaker than in the model here. While the Pognan et al. (2025) model grid does not use as de-

tailed recombination rates and collision strengths for the $Z = 30 - 40$ elements as this paper (but instead includes more elements), this nevertheless indicates that a full understanding of the formation of the $2.1 \mu\text{m}$ bump in AT2017gfo and AT2023vfi is challenging. There are several ways such a broad bump could be generated - from a single feature dominating (for which one can directly infer the velocity of the emitting region) to blends of two or more features (where such extractions are more difficult). The grid also demonstrates that as long as mixing with heavier matter is limited (e.g., a full solar composition would have $f_{\text{dyn}} \lesssim 0.1$), the light r-process elements still fully dominate the IR spectra - thus removing a major source of uncertainty regarding how generic results from this paper (using models with only light elements) may be taken.

7. CONCLUSIONS AND FUTURE WORK

We have studied the infrared spectral signatures of light r-process elements ($Z \leq 40$, plus tellurium, $Z = 52$) in kilonovae, over the epochs 10-80d using 1D NLTE models. We conclude the following.

- From the $Z = 31 - 40$ range, distinct signatures in the MIR are predicted for [Ge I] $11.72 \mu\text{m}$, [Ge I] $17.94 \mu\text{m}$, [Ge II] $5.66 \mu\text{m}$, [As II] $6.77 \mu\text{m}$, [As II] $9.40 \mu\text{m}$, [As III] $3.40 \mu\text{m}$, [Se I] $5.03 \mu\text{m}$, [Se I] $18.35 \mu\text{m}$, [Se III] $4.55 \mu\text{m}$, [Se III] $5.74 \mu\text{m}$, [Se IV] $2.29 \mu\text{m}$, [Br I] $2.71 \mu\text{m}$, [Br II] $3.19 \mu\text{m}$, [Br II] $14.26 \mu\text{m}$, [Kr II] $1.86 \mu\text{m}$, [Kr III] $2.20 \mu\text{m}$, [Kr III] $13.08 \mu\text{m}$, and [Zr IV] $8.00 \mu\text{m}$. Low-velocity ejecta (associated e.g. with a disk wind) generate lines mainly from neutral, singly and doubly ionized species, whereas high-velocity ejecta (associated e.g. with a PNS component) generate lines mainly from singly, doubly, and triply ionized species.
- Lines evolve over time from an initially optically thick LTE regime (probing emission volume) to an optically thin NLTE regime (probing the product of ionic mass and electron density). Some lines pass through an optically thin LTE regime (directly probing ionic mass). Longer wavelength lines are less sensitive to temperature and can therefore more robustly be used to infer emission volumes and/or ionic masses.
- Comparison to AT2017gfo Spitzer photometry, from $Z \leq 40$ candidates only [Se I] $5.03 \mu\text{m}$ and [Se III] $4.55 \mu\text{m}$ produce significant luminosity in the $4.5 \mu\text{m}$ band, and model predictions are in rough agreement with the observed band fluxes.

Following the proposal of [Se III] $4.55 \mu\text{m}$ using models with parameterized physical conditions (Hotokezaka et al. 2022), these are the first self-consistent models successfully explaining this data (using a Se mass of $0.014 M_{\odot}$). In the $3.6 \mu\text{m}$ band, [Br II] $3.19 \mu\text{m}$ and [As III] $3.40 \mu\text{m}$ are the dominant contributors, with fluxes at or below the upper limits.

- Comparison to AT2023vfi JWST spectra, a light composition-only component cannot produce the smooth observed spectrum, instead giving discrete emission lines with gaps between with low flux. This may suggest that heavier elements are present that either do much of the cooling, and/or reprocess the light element emission.
- For a low-velocity, light-composition ejecta, [Kr II] $1.86 \mu\text{m}$ and [Kr III] $2.20 \mu\text{m}$ produce narrow, well-separated lines, inconsistent with observations of both AT2017gfo and AT2023vfi. In a higher velocity model these features partially overlap giving a bright feature centred close to $2.1 \mu\text{m}$, as observed in both AT2017gfo and AT2023vfi. While the detailed line profile in AT2017gfo still fits better with a single line centred at $2.1 \mu\text{m}$ (with Te III $2.10 \mu\text{m}$ the leading candidate, Hotokezaka et al. 2023), the situation is less clear for AT2023vfi. A solar Br/Te ratio leads to predicted strong lines from [Br I] $2.71 \mu\text{m}$ and [Br II] $3.19 \mu\text{m}$, which are not observed in AT2023vfi. The summary picture suggests that both AT2017gfo and AT2023vfi ejected significantly less light r-process material than a solar composition. This is of interest in the context of various challenges with KNe being the main source of first r-process peak elements.

The results in this paper provide indications of sub-solar production of light r-process elements in KNe. However, to more firmly establish this, progress is needed along at least three fronts.

The first is more atomic data for NLTE modelling. While the atomic data situation has significantly improved for the $Z = 30 - 40$ range in the last years, now enabling nebular emission modelling for both planetary nebulae and kilonovae with quite good accuracy, certain important data is still missing. This includes collision strengths for Ge I and II, As II and III, Se I and II, Br I, II and III, as well as recombination rates for Ge and As ions. For heavier elements, this kind of data is still mostly missing.

The second is improved NLTE spectral models taking into consideration deviations from spherical symme-

try (being done already for the LTE phase, e.g. [Collins et al. 2023](#)), the multi-component nature of KNe, and doing thermalization and other microphysics to higher level of detail. While MIR lines are quite insensitive to temperature, NIR lines are more so, and there is always a direct sensitivity to ionization state. We put significant focus here on ratios of nearby lines of similar ions,

but individual line luminosities are sensitive to physical conditions.

The third is observations of more KNe in the infrared - we establish here the unique diagnostic possibilities of this range, but the data so far is very limited. Progress requires JWST observations with unique r-process signatures predicted all along the 1-30 micron range.

APPENDIX

A. ATOMIC DATA UPDATES

The dielectronic recombination rates calculated for Se, Rb, Sr, Y, and Zr by [Banerjee et al. \(2025\)](#) and Kr ([Sterling 2011](#)) were used. The dielectronic and radiative recombination rates for Br and the radiative recombination rates for Rb, from Kerlin et al. (in prep.), were also incorporated.

As outlined in more detail below, some energy levels were corrected to experimental values or, lacking that, to more accurate theoretical ones. In such calibrations, lines connecting to the level had A-values rescaled by a factor $(\lambda_{old}/\lambda_{new})^3$ ([Hotokezaka et al. 2021](#)). The numbering of levels in the descriptions below refer to the energy-ordering in the FAC model atoms (using a spectroscopic configuration-interaction (SCI) method, [Pognan et al. 2023](#)).

A.1. Ga I

The energy of level 2 was corrected to NIST ([Shirai et al. 2007](#)). The Ga I isoelectronic sequence (Ga I, Ge II, As III, Se IV,...) has a single p-shell valence electron, giving a doublet ground term 2P with $J = 3/2$ or $J = 1/2$ depending on the spin of the electron. A potential IR line is therefore $^2P_{3/2}^o - ^2P_{1/2}^o$ (2-1, 12.10 μm , $A = 4.6 \times 10^{-3} \text{ s}^{-1}$).

A.2. Ga II

The first excited state in Ga II lies high at 47,367 cm^{-1} , no calibrations were made. The Ga II isoelectronic sequence (Zn I, Ga II, Ge III, As IV, ...) has a $4s^2$ ground configuration with no fine structure splitting.

A.3. Ga III

The first excited state in Ga III lies high at 65,169 cm^{-1} , no calibrations were made. The Ga III isoelectronic sequence (Cu I, Zn II, Ga III, Ge IV, ...) has a single-electron ($4s$) ground configuration.

A.4. Ga IV

The first excited state in Ga IV lies high at 149,512 cm^{-1} , no calibrations were made. The Ga IV isoelectronic sequence (Cu II, Zn III, Ga IV,...³) has a $3d^{10}(^1S)$ ground configuration with no splitting.

A.5. Ge I

The energies for levels 2-5 were corrected to NIST values ([Sugar & Musgrove 1993](#)). Theoretical A-values for transitions between these first 5 levels are provided by [Biémont & Hansen \(1986a\)](#), Hartree-plus-statistical-exchange and Hartree-Fock with relativistic corrections). The Ge I isoelectronic sequence (Ge I, As II, Se III, Br IV, ..) has 2 p-shell electrons. In the ground term the spins are aligned (so $2S + 1 = 3$); and splitting occurs by three allowed values for the orbital magnetic number giving $J = 2, 1, 0$. Transitions with $\Delta J = 1$ have significantly higher A-values than $\Delta J = 2$, giving two main lines from the ground term. Potential IR lines are $^3P_1 - ^3P_0$ (2-1, 17.94 μm , $A = 3.3 \times 10^{-3} \text{ s}^{-1}$), $^3P_2 - ^3P_1$ (3-2, 11.72 μm , $A = 8.0 \times 10^{-3} \text{ s}^{-1}$), and (trans-term) $^1D_2 - ^3P_0$ (4-3, 1.75 μm , $A = 0.098 \text{ s}^{-1}$).

A.6. Ge II

The energy of level 2 was corrected to NIST ([Sugar & Musgrove 1993](#)). A potential IR line is $^2P_{3/2}^o - ^2P_{1/2}^o$ (2-1, 5.66 μm , $A = 0.050 \text{ s}^{-1}$).

³ Ni I breaks pattern with a different ground term

A.7. *Ge III*

The first excited state in Ge III lies high at 61,733 cm⁻¹, no calibrations were made.

A.8. *Ge IV*

The first excited state in Ge IV lies high at 81,311 cm⁻¹, no calibrations were made.

A.9. *As I*

The energies of levels 2-5 were corrected to NIST values (Moore 1971). Theoretical A-values for transitions between the first 5 levels are provided by Biémont & Hansen (1986a, their table 6). The As I isoelectronic sequence (As I, Se II, Br III, Kr IV, ..) has a 4p³(⁴S) ground configuration with no splitting. IR lines can only be generated from the second term, 4p³(²D°). For As I the ²D_{5/2}^o–²D_{3/2}^o transition is however beyond JWST range at 31 μm, and with a low A-value.

A.10. *As II*

The energies of levels 2-5 were corrected to NIST values (Moore 1971). Theoretical A-values for transitions between the first 5 levels are provided by Biémont & Hansen (1986a). Potential IR lines include ³P₁–³P₀ (2-1, 9.40 μm, A = 0.022 s⁻¹) and ³P₂–³P₁ (3-2, 6.77 μm, A = 0.043 s⁻¹).

A.11. *As III*

The energy of level 2 was corrected to the NIST value (Moore 1971). A potential IR line is ²P_{3/2}⁰–²P_{1/2}⁰ (2-1, 3.40 μm, A = 0.23 s⁻¹).

A.12. *As IV*

The first excited state in As IV lies high at 75,812 cm⁻¹, no calibrations were made.

A.13. *Se I*

The energies of levels 2-5 were corrected to NIST values (Moore 1971). Theoretical A-values for transitions between the first 5 levels are provided by Biémont & Hansen (1986b, Hartree-Fock with relativistic corrections, their Table 8). The Se I isoelectronic sequence (Se I, Br II, Kr III, Rb IV,..) has a 4p⁴(³P) ground term with J = 2, 1, 0. Potential IR lines include ³P₁–³P₂ (2-1, 5.03 μm, A = 0.17 s⁻¹), ³P₀–³P₁ (3-2, 18.35 μm, A = 0.010 s⁻¹), and ¹D₂–³P₂ (4-1, 1.04 μm, A = 0.63 s⁻¹).

A.14. *Se II*

The energies of levels 2-5 were corrected to NIST values (Moore 1971). Theoretical A-values for transitions between the first 5 levels are provided by Biémont & Hansen (1986a, their Table 6). The ²D_{5/2}⁰–²D_{3/2}⁰ transition (within the second term) is at 16.22 μm, with A = 2.9 × 10⁻³ s⁻¹.

A.15. *Se III*

The energies of levels 2-5 were corrected to NIST values (Moore 1971). Theoretical A-values for transitions between the first 5 levels are provided by Biémont & Hansen (1986a) and Sterling et al. (2017), we use the latter source as it also reports R-matrix calculations of collision strengths for these transitions. Potentially important IR lines include ³P₂–³P₁ (3-2, 4.55 μm, A = 0.16 s⁻¹), and ³P₁–³P₀ (2-1, 5.74 μm, A = 0.082 s⁻¹).

A.16. *Se IV*

Level 2 was corrected to the NIST value (Moore 1971). Collision strengths for this transition were implemented (K. Butler, priv. comm.). A potential IR line is ²P_{3/2}⁰–²P_{1/2}⁰ (2-1, 2.29 μm, A = 0.75 s⁻¹).

A.17. *Br I*

Level 2 was corrected to the NIST value (Tech 1963). The Br I isoelectronic sequence (Br I, Kr II, Rb III, Sr IV, ..) has a 4p⁵(²P) ground term with J = 3/2, 1/2. A potential IR line is ²P_{1/2}–²P_{3/2} (2-1, 2.71 μm, A = 0.90 s⁻¹).

A.18. *Br II*

The energies of levels 2-5 were corrected to NIST values (Moore 1971). Theoretical A-values for transitions between the first 5 levels are provided by Biémont & Hansen (1986b, their Table 8). Potential IR lines include $^3P_1-^3P_0$ (2-1, 3.19 μm , $A = 0.67 \text{ s}^{-1}$) and $^3P_0-^3P_1$ (3-2, 14.26 μm , $A = 0.022 \text{ s}^{-1}$).

A.19. *Br III*

The energies of levels 2-5 were corrected to NIST values (Moore 1971). A potential IR line is (second-term) $^2D_{5/2}^0-^2D_{3/2}^0$ (3-2, 7.94 μm , $A = 2.0 \times 10^{-2} \text{ s}^{-1}$).

A.20. *Br IV*

The energies of levels 2-4 were corrected to NIST values (Joshi & Budhiraja 1971). Theoretical A-values for transitions between the first 5 levels are provided by Biémont & Hansen (1986a). Potential IR lines include $^3P_1-^3P_0$ (2-1, 3.81 μm , $A = 0.32 \text{ s}^{-1}$) and $^3P_2-^3P_1$ (3-2, 3.34 μm , $A = 0.33 \text{ s}^{-1}$).

A.21. *Kr I*

The first excited state of Kr I lies high at 79,971 cm^{-1} , no calibrations were made. The Kr I isoelectronic sequence (Kr I, Rb II, Sr III, Y IV,...) has a $4p^6(^1S)$ ground term with no splitting.

A.22. *Kr II*

The energy of level 2 was corrected to the NIST value (Saloman 2007). The third state lies high at 109,000 cm^{-1} . Collision strengths were implemented for the 2-1 transition (K. Butler, priv. comm.) A potential IR line is $^2P_{1/2}-^2P_{3/2}$ (2-1, 1.86 μm , $A = 2.78 \text{ s}^{-1}$).

A.23. *Kr III*

The energies of levels 2-5 were corrected to the NIST values (Saloman 2007). Theoretical A-values for transitions between the first 5 levels are provided by Biémont & Hansen (1986b, their Table 8). Schöning (1997) provide R-matrix calculations of collision strengths. Potential IR lines include $^3P_1-^3P_2$ (2-1, 2.20 μm , $A = 2.0 \text{ s}^{-1}$) and $^3P_0-^3P_1$ (3-2, 13.08 μm , $A = 0.029 \text{ s}^{-1}$).

A.24. *Kr IV*

The energies of levels 2-5 were corrected to NIST values (Saloman 2007). Schöning (1997) provide R-matrix calculations of collision strengths. A potential IR line is (second-term) $^2D_{5/2}^0-^2D_{3/2}^0$ (3-2, 6.01 μm , $A = 0.046 \text{ s}^{-1}$).

A.25. *Rb I*

The energies of levels 2-6 were corrected to NIST values (Sansonetti 2006), which included a reordering of levels 4-6. Rb I has no expected strong IR lines. Rb I has a single-electron $5s(^2S)$ ground state.

A.26. *Rb II*

The first excited state of Rb II lies high at 133,341 cm^{-1} , no calibrations were made.

A.27. *Rb III*

The energy of level 2 was corrected to the NIST value (Sansonetti 2006). The third level lies high at 130,032 cm^{-1} . A potential IR line is $^2P_{1/2}-^2P_{3/2}$ (2-1, 1.36 μm , $A = 7.21 \text{ s}^{-1}$).

A.28. *Rb IV*

The energies of levels 2-5 were corrected to NIST values (Sansonetti 2006). Theoretical A-values for transitions between the first 5 levels are provided by Biémont & Hansen (1986b, their Table 8). We use collision strengths for the first 5 levels from Sterling et al. (2016)⁴. Potential IR lines include $^3P_1-^3P_2$ (2-1, 1.60 μm , $A = 4.65 \text{ s}^{-1}$) and $^3P_0-^3P_1$ (3-2, 14.54 μm , $A = 2.3 \times 10^{-2} \text{ s}^{-1}$).

⁴ Sterling et al. (2016) also compute A-values, but list zero for several transitions that have non-zero entries in Biémont & Hansen (1986b). In their discussion they also use the Biémont & Hansen (1986b) values as benchmark.

A.29. *Sr I*

The energies of levels 2-9 were corrected to NIST values (Sansonetti & Nave 2010), which involved some reorderings. Sr I has a $5s^2(^1S)$ ground term with no splitting.

A.30. *Sr II*

The energies of levels 2-17 were corrected to NIST values (Moore 1971). Collision strengths from Mulholland et al. (2024a) were used.

A.31. *Sr III*

The first excited state of Sr III lies high at $176,434 \text{ cm}^{-1}$, no calibrations were made.

A.32. *Sr IV*

The energy of level 2 was corrected to the NIST value (Persson 1978). A potential IR line is $^2P_{1/2}-^2P_{3/2}$ (2-1, $1.028 \mu\text{m}$, $A = 15.8 \text{ s}^{-1}$).

A.33. *Y I*

The energies of levels 2-8 were corrected to NIST values (Palmer 1977), which involved some reorderings. Because the FAC energy structure is significantly different to the NIST one for higher levels, the model atom was limited to these 8 states. Y I has a $4d5s^2(^2D)$ ground configuration with splitting into $J = 3/2, 5/2$ (Zr II, Nb III, etc. have other ground configurations so the isoelectronic sequencing here breaks down). A potential IR line is $^2D_{5/2}-^2D_{3/2}$ (2-1, $18.85 \mu\text{m}$, $A = 5.5 \times 10^{-4} \text{ s}^{-1}$).

A.34. *Y II*

The energies of levels 2-12 were corrected to NIST values (Nilsson et al. 1991). We implemented collision strengths for transitions between the first 12 levels from Mulholland et al. (2024a). Y II has a rich level structure and many lines, difficult to assess beforehand if IR lines may become strong. Y II has a $5s^2(^1S)$ ground term with no splitting.

A.35. *Y III*

The energies of levels 2-17 were in Pognan et al. (2023) calibrated to NIST values. Here, we also add A-values for transitions between the first three states from Sahoo et al. (2008). Y III has a $4p^6(^2D)$ ground term with $J = 3/2, 5/2$ splitting. Potential IR lines include $^2D_{5/2}-^2D_{3/2}$ (2-1, $13.81 \mu\text{m}$, $A = 4.1 \times 10^{-3} \text{ s}^{-1}$), $5s^2S-4d^2D_{3/2}$ (3-1, $1.34 \mu\text{m}$, $A = 9.4 \times 10^{-2} \text{ s}^{-1}$), and $5s^2S-4d^2D_{5/2}$ (3-2, $1.48 \mu\text{m}$, $A = 4.5 \times 10^{-2} \text{ s}^{-1}$).

A.36. *Y IV*

The first excited state in Y IV lies high at $209,651 \text{ cm}^{-1}$, no calibrations were made.

A.37. *Zr I*

The energies of levels 2-12 were corrected to NIST values (Moore 1971). Potential IR lines include $^3F_3-^3F_2$ (2-1, $17.53 \mu\text{m}$, $A = 3.2 \times 10^{-3} \text{ s}^{-1}$), $^3F_4-^3F_3$ (3-2, $14.91 \mu\text{m}$, $A = 4.7 \times 10^{-3} \text{ s}^{-1}$), and a blend of lines between $2 - 2.5 \mu\text{m}$.

A.38. *Zr II*

The energies of levels 2-4 were corrected to NIST values (Moore 1971). Potential MIR lines include $^4F_{9/2}-^4F_{7/2}$ (4-3, $17.87 \mu\text{m}$, $A = 2.7 \times 10^{-3} \text{ s}^{-1}$) and $^4F_{7/2}-^4F_{5/2}$ (3-2, $22.28 \mu\text{m}$, $A = 2.1 \times 10^{-3} \text{ s}^{-1}$).

A.39. *Zr III*

The energies of levels 2-13 were corrected to NIST values (Reader & Acquista 1997). We also replaced the FAC A-values for transitions between these states with those of Rynkun et al. (2020, Multi-Configuration Dirac-Hartree-Fock (MCDHF) and relativistic configuration interaction (RCI) calculations using GRASP2018). Potential IR lines include $^3F_3-^3F_2$ (2-1, $14.67 \mu\text{m}$, $A = 7.5 \times 10^{-3} \text{ s}^{-1}$) and $^3F_4-^3F_3$ (3-2, $12.42 \mu\text{m}$, $A = 1.0 \times 10^{-2} \text{ s}^{-1}$).

A.40. *Zr IV*

The energies of levels 2-5 were corrected to NIST values (Reader & Acquista 1997). Level 6 lies high at $137,413 \text{ cm}^{-1}$. Collision strengths for transitions between these first 5 levels were implemented (Dinerstein et al. 2006, K. Butler, priv. comm.). A potential IR line is $^2D_{5/2}-^2D_{3/2}$ (2-1, $8.00 \mu\text{m}$, $A = 0.012 \text{ s}^{-1}$).

A.41. *Te I*

The energies of levels 2-10 were calibrated to NIST values (Morillon & Vergès 1975). Because higher levels showed discrepancy between the FAC model and NIST, the model atom was capped at 10 levels - the eleventh level lies quite high at $54,683 \text{ cm}^{-1}$. We use collision strengths from Mulholland et al. (2024b). A potential IR line is $^3\text{P}_1 - ^3\text{P}_2$ (3-1, $2.10 \text{ }\mu\text{m}$, $A = 2.27 \text{ s}^{-1}$).

A.42. *Te II*

The energies of levels 2-8 were calibrated to NIST values (Eriksson 1974). Because higher levels showed discrepancy between the FAC model and NIST, the model atom was capped at 8 levels - the ninth level lies high at $78,448 \text{ cm}^{-1}$. A potential IR line is $^2\text{D}_6^\circ - ^2\text{D}_4^\circ$ (3-2, $4.55 \text{ }\mu\text{m}$, $A = 0.098 \text{ s}^{-1}$).

A.43. *Te III*

The energies of levels 2-4 were calibrated to NIST values (Moore 1971). Because higher levels showed discrepancy between the FAC model and NIST, the model atom was capped at 4 levels - the fifth level lies high at $82,885 \text{ cm}^{-1}$. A-values and collision strengths from Madonna et al. (2018) were used. Potential IR lines include $^3\text{P}_1 - ^3\text{P}_0$ (2-1, $2.10 \text{ }\mu\text{m}$, $A = 1.19 \text{ s}^{-1}$) and $^3\text{P}_2 - ^3\text{P}_1$ (3-2, $2.92 \text{ }\mu\text{m}$, $A = 0.52 \text{ s}^{-1}$).

A.44. *Te IV*

The energy of level 2 was calibrated to NIST values (Moore 1971). Because higher levels showed discrepancy between the FAC model and NIST, the model atom was capped at 2 levels - the third level lies high at $92,772 \text{ cm}^{-1}$. A potential IR line is $^2\text{P}_{3/2}^\circ - ^2\text{P}_{1/2}^\circ$ (2-1, $1.084 \text{ }\mu\text{m}$, $A = 7.1 \text{ s}^{-1}$).

B. IONIZATION PROFILES

Figures 14-19 show the detailed ionization structures in the line-forming regions in the models, for elements with distinct lines.

C. FULL SPECTRAL RANGE PLOTS

Figures 20-21 show the evolution of model A-low and B-high (with some rescaling factors stated in the legend) covering 0.3-30 microns on the x-axis.

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DATA AVAILABILITY

All computed model spectra are available upon email request to the author, and will also be made available at the Zenodo archive.

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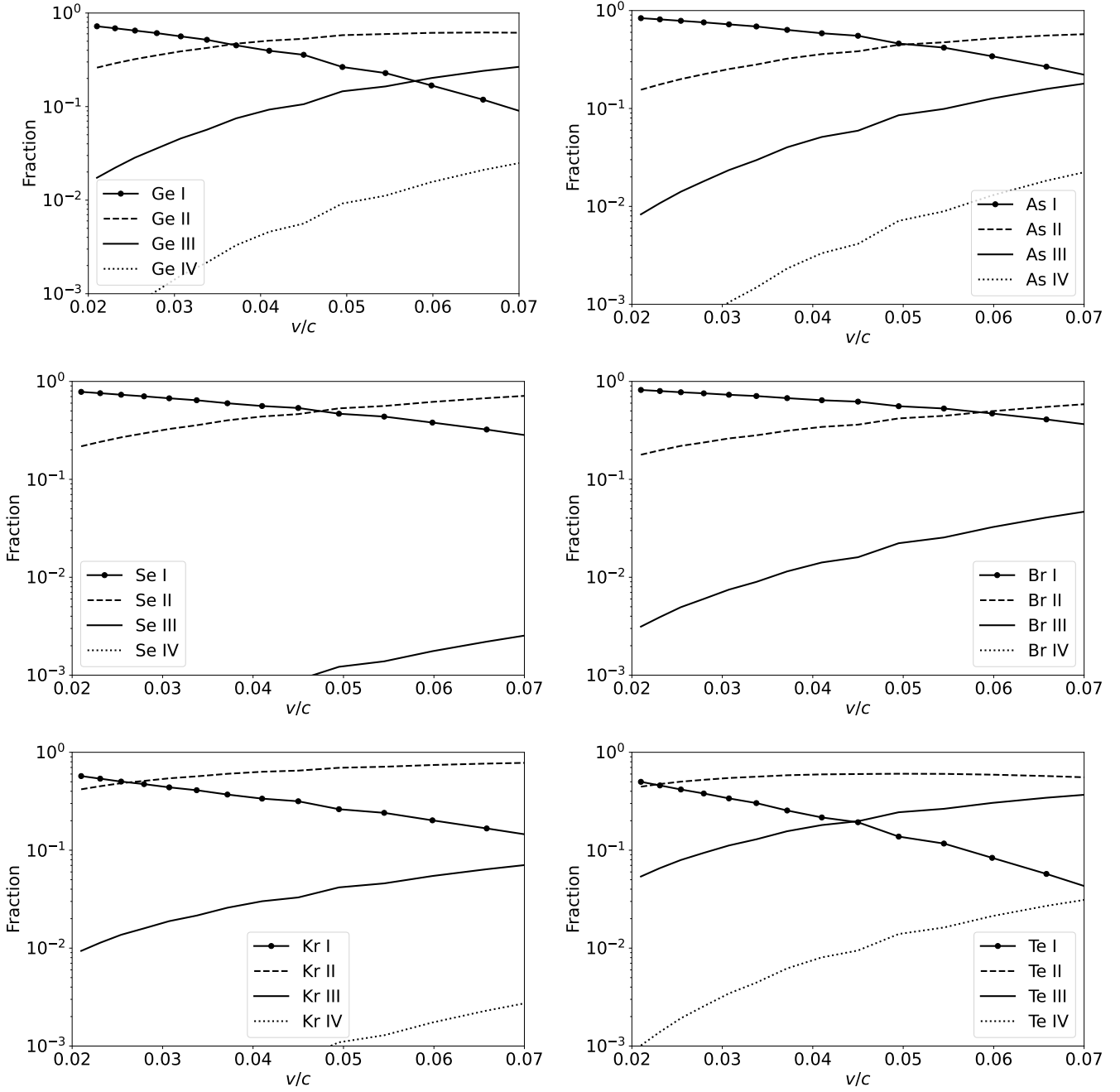


Figure 14. Ionization profiles of selected important elements in model A-low, at 10d, zoomed in on the region $v/c \leq 0.07$ (which has $\gtrsim 80\%$ of the radioactive energy deposition). Neutral abundances are plotted with solid lines with dots, singly ionized with dashed lines, doubly ionized with solid lines, and triply ionized with dotted lines.

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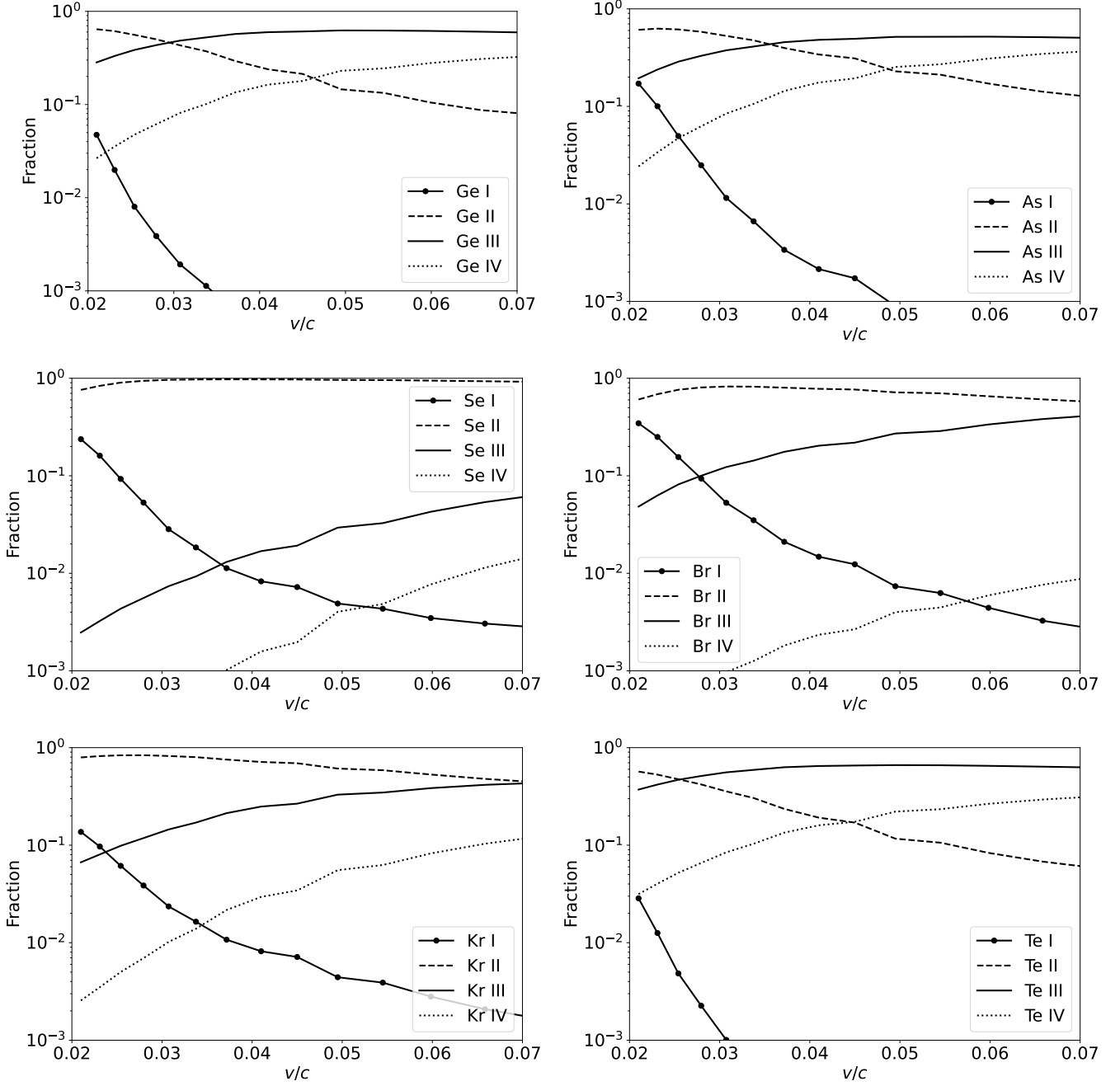


Figure 15. Same as Fig. 14, at 40d.

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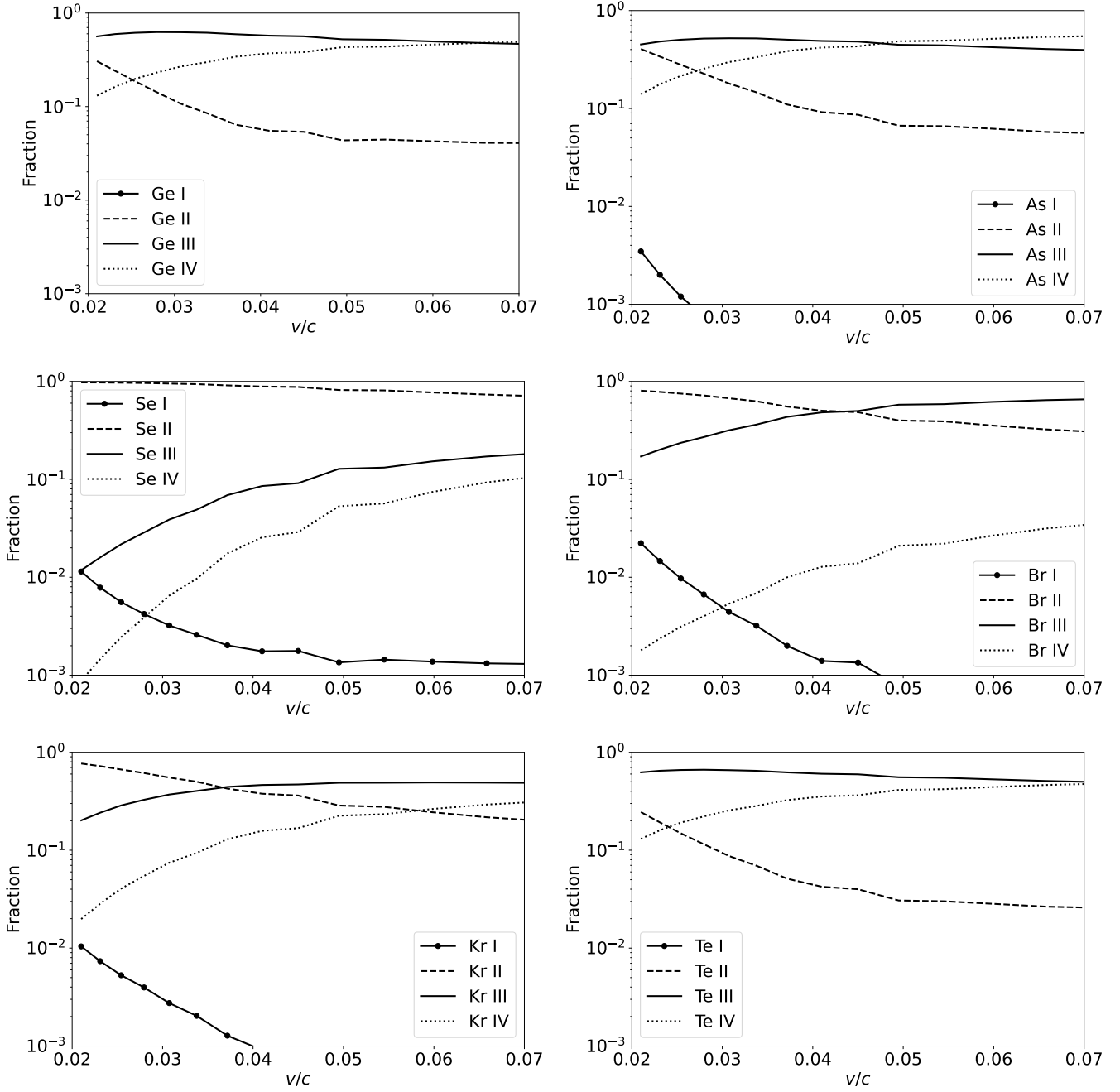


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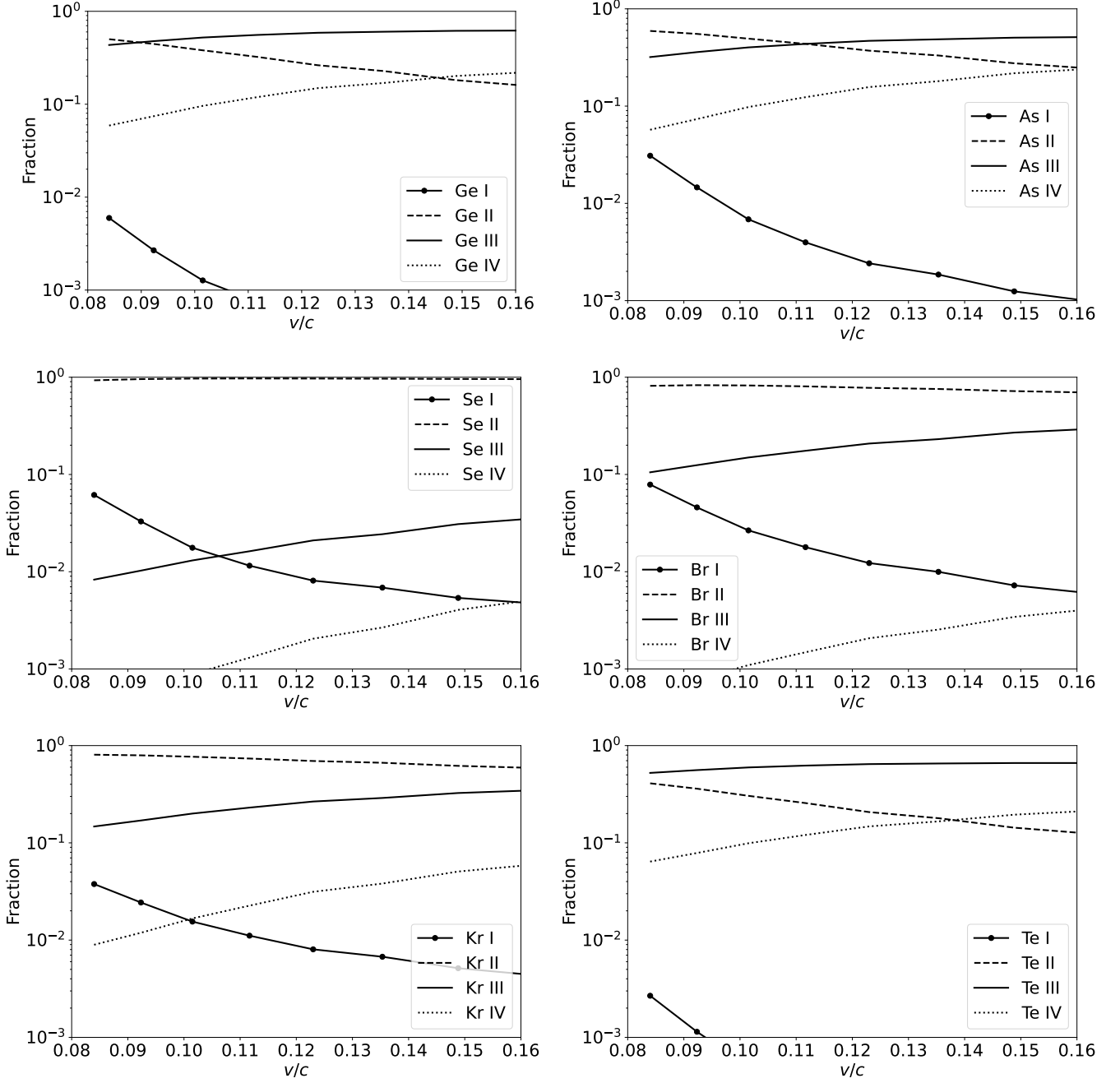


Figure 17. Same as Fig. 14, but model B-high at 10d. The inner boundary is here at $v/c = 0.08$ and the $\gtrsim 80\%$ radioactive deposition limit at $v/c = 0.16$.

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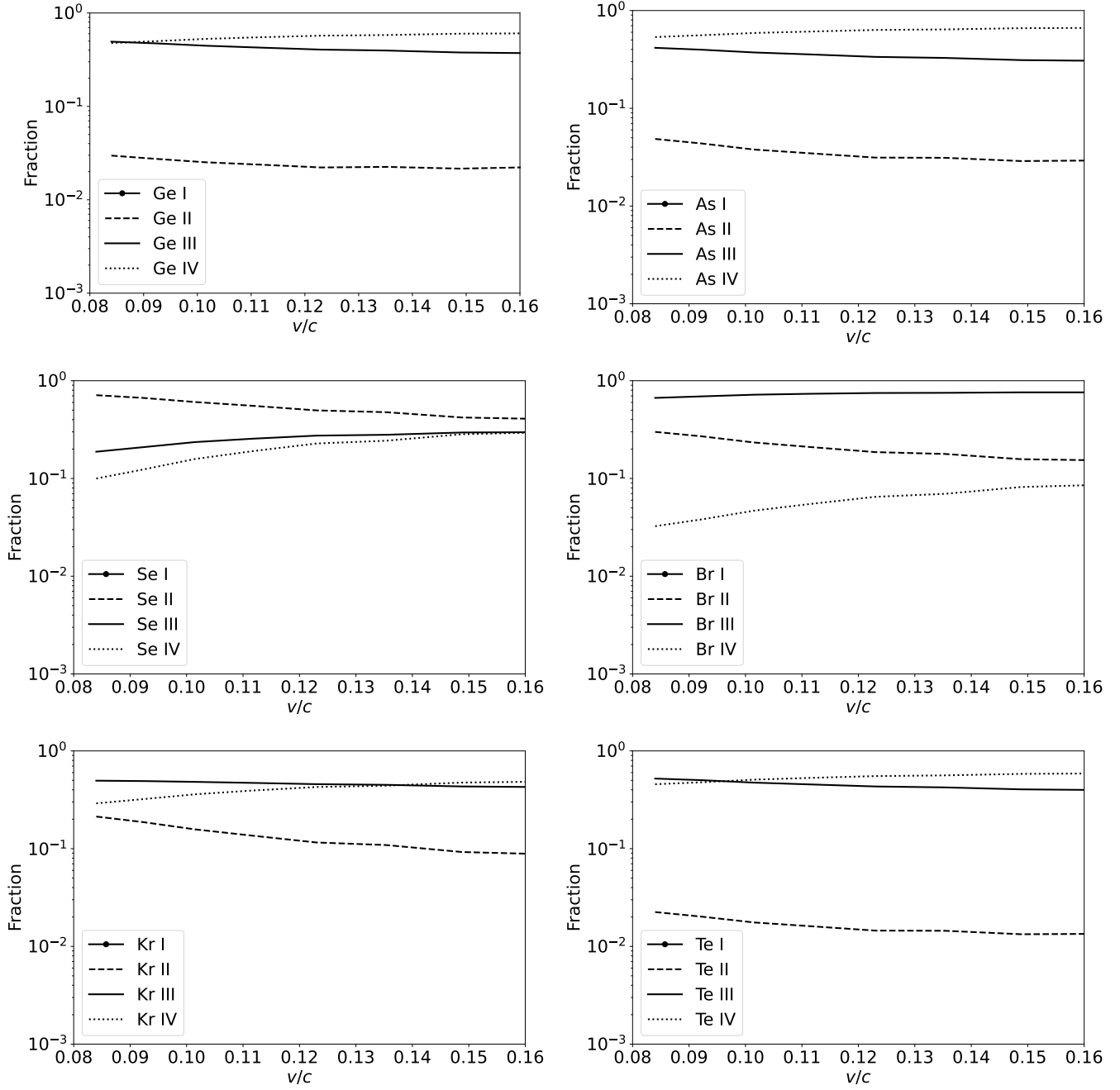


Figure 18. Same as Fig. 17, at 40d.

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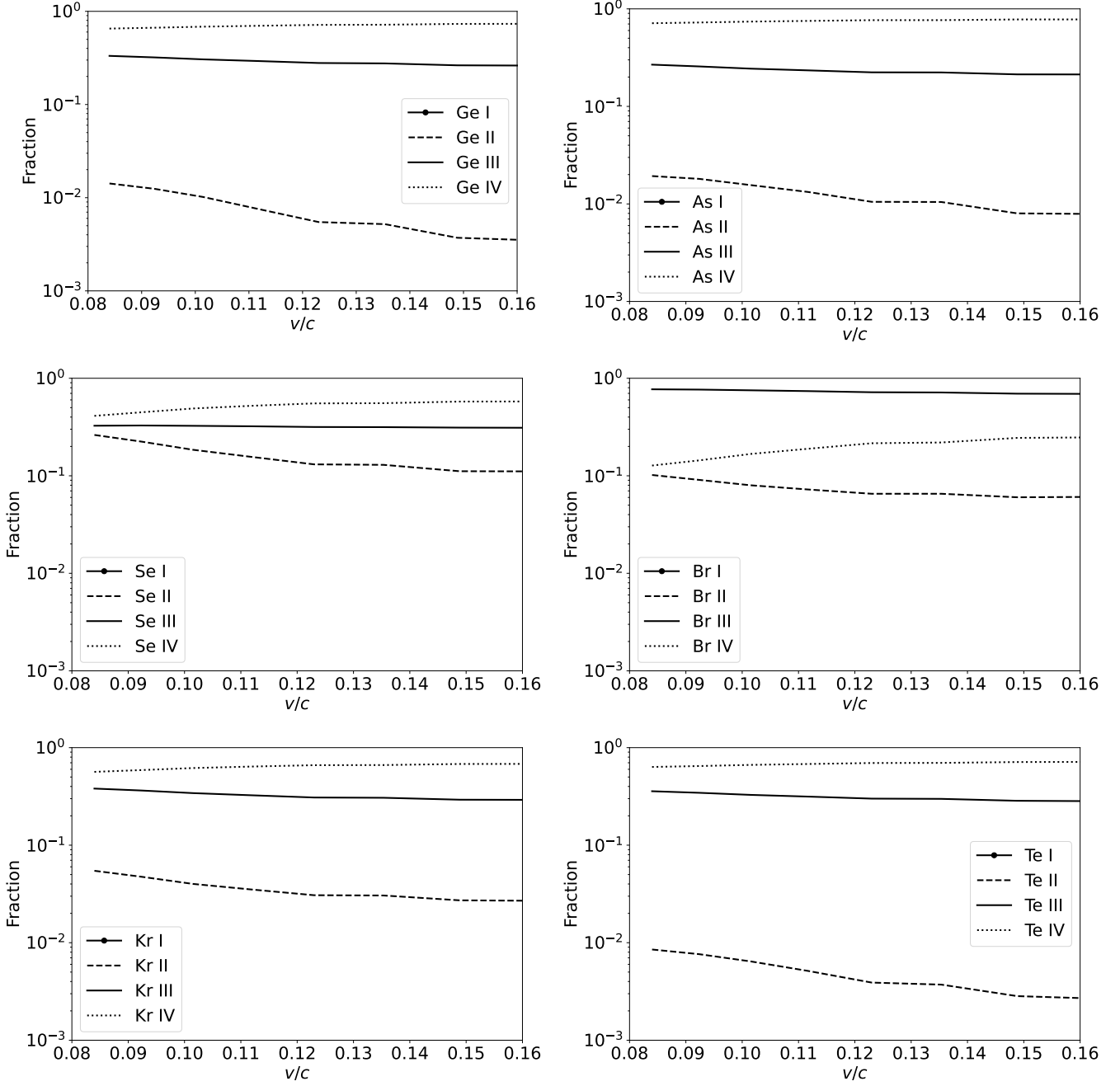


Figure 19. Same as Fig. 17, at 80d.

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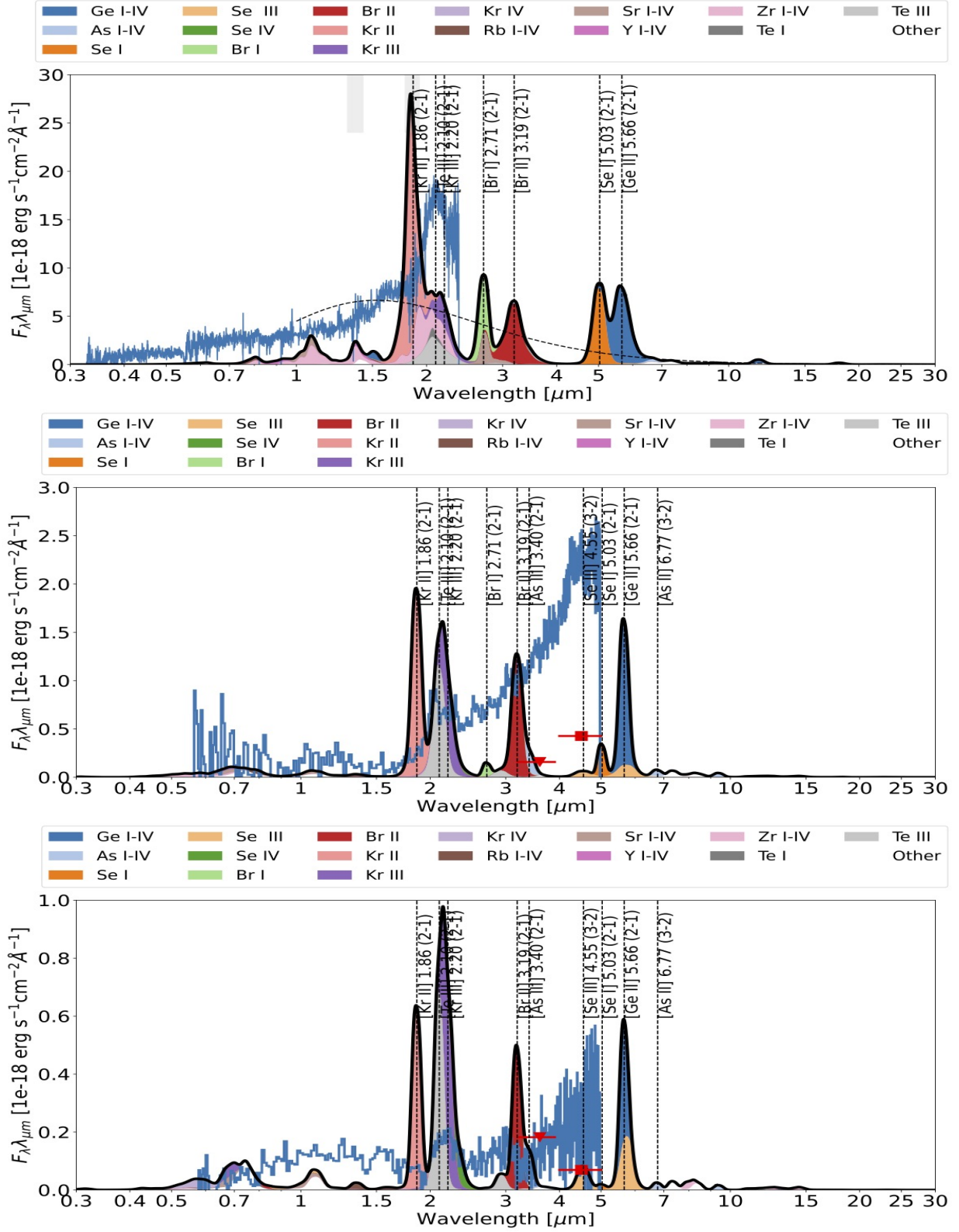


Figure 20. Evolution of model A-low from 10-80d over the 0.3-30 μm range, and comparison to data (top panel: spectrum of AT2017gfo at 10.4d, middle panel AT2023vfi at +43d (blue) and photometry of AT2017gfo (red points)), bottom panel AT2023vfi at +61d (blue) and photometry of AT2017gfo (red points). The model at 10d has been rescaled with a factor of 3 for better flux matching.

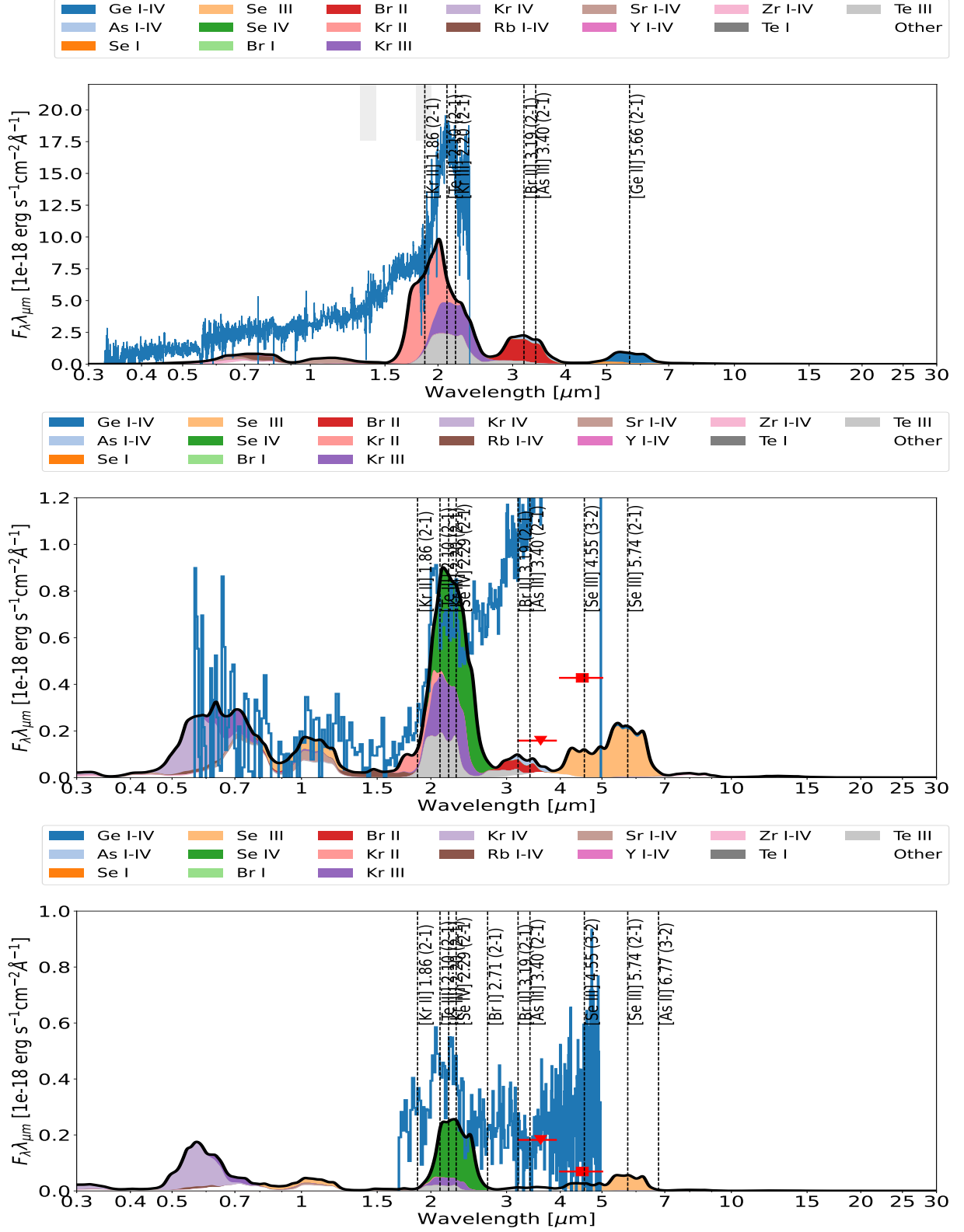


Figure 21. Evolution of model B-high from 10-80d over the 0.3-30 μm range, and comparison to data.

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