Spectral modelling of supernovae and kilonovae, and the role of atomic data for inferring their element production

Anders Jerkstrand

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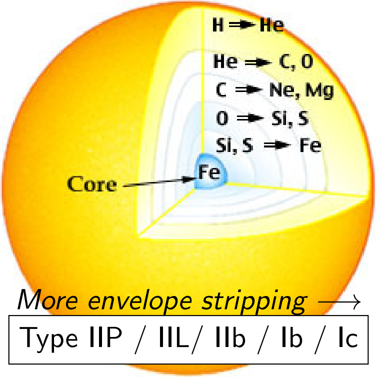
Supernovae - the death of stars

$\boxed{1}$ Core-collapse of a **massive star** ($M_{ZAMS} \gtrsim 8\ M_\odot$) as it runs out of fuel at the end of its life.

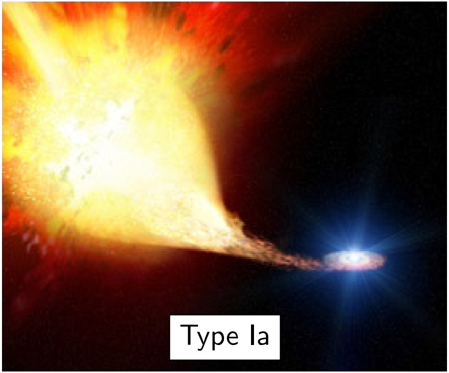


More envelope stripping ⟶

Type IIP / IIL/ IIb / Ib / Ic

www.phys.olemiss.edu

$\boxed{2}$ Thermonuclear explosion of a **white dwarf** exceeding the Chandrasekhar limit (1.4 $M_\odot$).

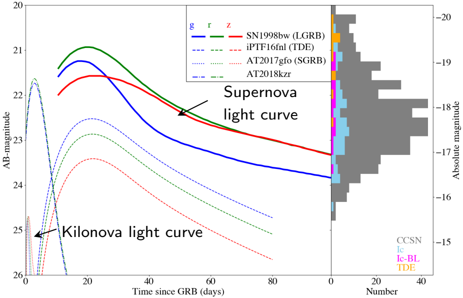


Type Ia

hetdex.org

Kilonovae - the death of dead stars

Merger of two **neutron stars**, with ejection of $0.01 - 0.1\ M_{\odot}$ of r-processed material.



Supernova light curve

Kilonova light curve

Courtesy: A Levan.

A first prediction for the ages!

Monthly Notices of the ROYAL ASTRONOMICAL SOCIETY

Mon. Not. R. Astron. Soc. **406,** 2650–2662 (2010) doi:10.1111/j.1365-29

Electromagnetic counterparts of compact object mergers powered the radioactive decay of *r*-process nuclei

B. D. Metzger,[1★†] G. Martínez-Pinedo,[2] S. Darbha,[3] E. Quataert,[3] A. Arcones, D. Kasen,[5‡] R. Thomas,[6] P. Nugent,[6] I. V. Panov[7,8,9] and N. T. Zinner[10]

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[4] *Institut für Kernphysik, TU Darmstadt, Schlossgartenstr. 9, D-64289 Darmstadt, Germany*
[5] *University of California, Santa Cruz, CA 95064, USA*
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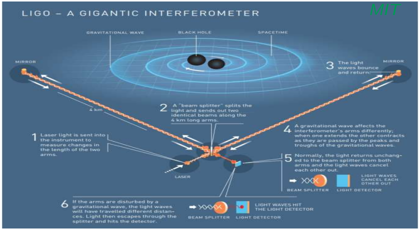
[9] *Russian Research Centre Kurchatov Institute, pl. Kurchatova 1, 123182 Moscow, Russia*
[10] *Department of Physics, Harvard University, Cambridge, MA 02138, USA*



1 Laser light is sent into the instrument to measure changes in the length of the two arms.

2 A "beam splitter" splits the light and sends out two identical beams along the 4 km long arms.

3 The light waves bounce and return.

4 A gravitational wave affects the interferometer's arms differently; when one extends the other contracts as they are passed by the peaks and troughs of the gravitational waves.

5 Normally, the light returns unchanged to the beam splitter from both arms and the light waves cancel each other out.

6 If the arms are disturbed by a gravitational wave, the light waves will have travelled different distances. Light then escapes through the splitter and hits the detector.

MIT

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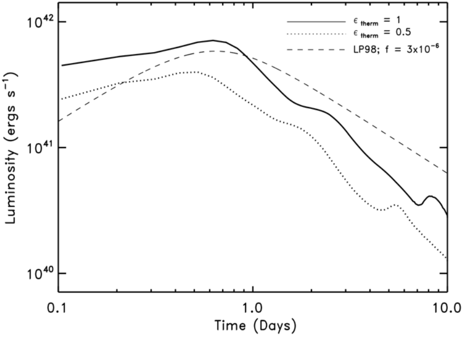

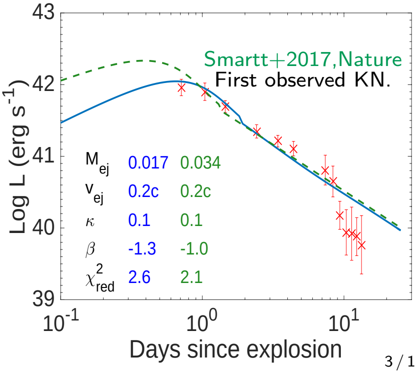

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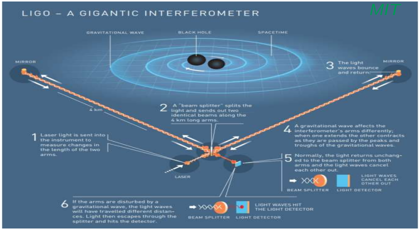

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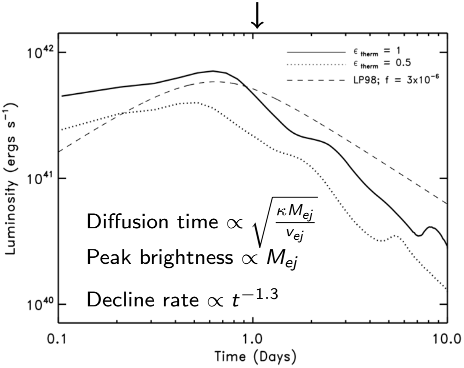
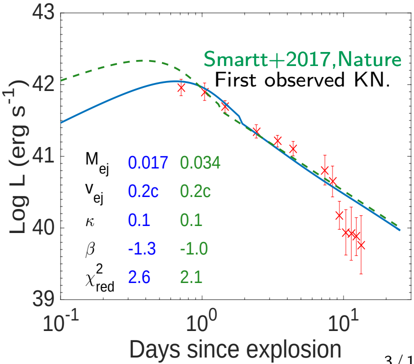


Diffusion time $\propto \sqrt{\frac{\kappa M_{ej}}{v_{ej}}}$

Peak brightness $\propto M_{ej}$

Decline rate $\propto t^{-1.3}$



Smartt+2017,Nature

First observed KN.

M_{ej}	0.017	0.034
v_{ej}	0.2c	0.2c
κ	0.1	0.1
β	-1.3	-1.0
$\chi^2_{\rm red}$	2.6	2.1

The origin of the elements

CCSN : Core-collapse supernova. TNSN: Thermonuclear supernova

Ab.	El.	Main source	Nebular lines seen in SNe
1	H	Big Bang	Many
2	He	Big Bang	He I 5016, 7065, 1.08 μm, 2.06 μm
3	O	CCSN	[O I] 5577, [O I] 6300, 6364, O I 7774, O I 9263 + ..
4	C	AGB stars+CCSN	[C I] 8727, 9824+9850, 1.44 μm, CO lines
5	Fe	CCSN+TNSN	[Fe II] 7155, 1.26 μm, 1.64 μm, 18 μm, 26 μm
6	Ne	CCSN	[Ne II] 12.8 μm
7	Si	CCSN+TNSN	[Si I] 1.10 μm, 1.20 μm, 1.60/1.64 μm, SiO lines
8	N	AGB stars	[N II] 6548, 6583
9	Mg	CCSN	Mg I] 4571, 1.50 μm
10	S	CCSN	[S I] 1.082 μm, 1.13 μm
11	Ar	CCSN	[Ar II] 6.99 μm
12	Ni	CCSN+TNSN	[Ni II] 7378, 1.93 μm, 6.6 μm, 10.7 μm, [Ni I] 3.1 μm
13	Ca	CCSN	[Ca II] 7291,7323 NIR triplet, Ca I 4200
14	Al	CCSN	-
15	Na	CCSN	Na I 5890, 5896, 1.14 μm

- Most distinct lines typically low-lying forbidden lines of neutral or singly ionized atoms, excited by thermal electron collisions.

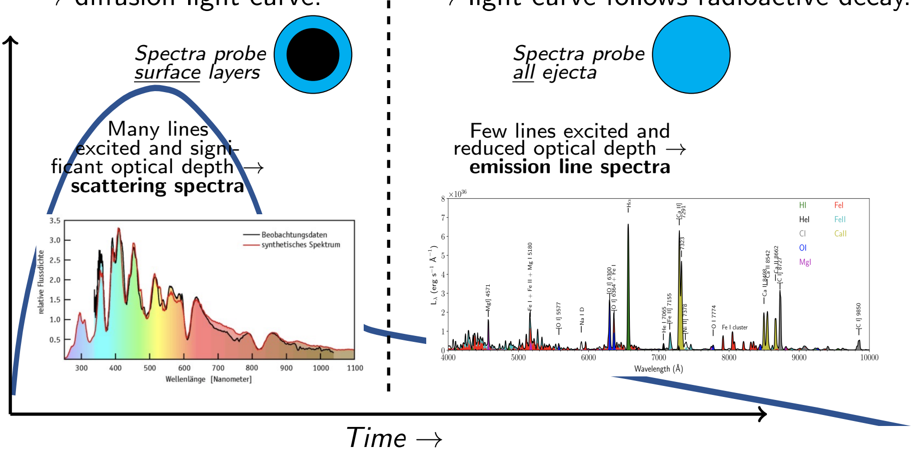
Two main phases in transient evolution

Photospheric phase

Long escape time for radiation
→ diffusion light curve.

Nebular phase

Short escape time for radiation
→ light curve follows radioactive decay.



Spectra probe
<u>surface</u> layers

Many lines
excited and significant optical depth →
scattering spectra

Spectra probe
<u>all</u> ejecta

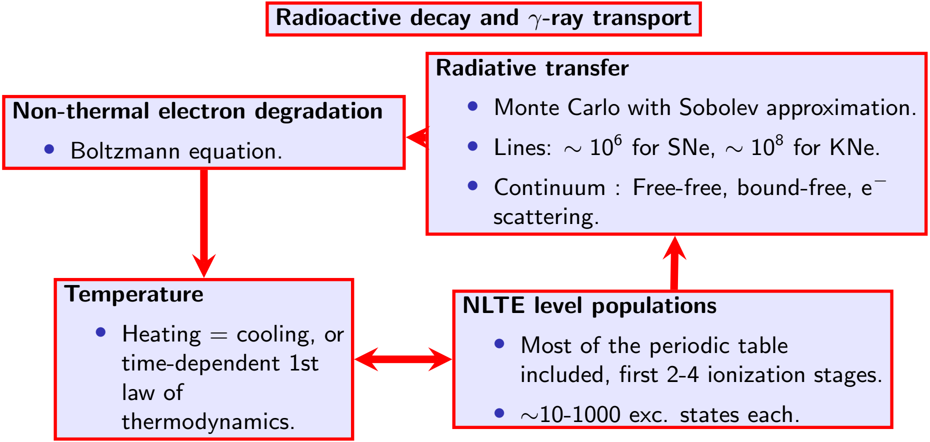
Few lines excited and
reduced optical depth →
emission line spectra

Simple microphysics (LTE)

Complex michrophysics (NLTE)

The SUMO code : a tool when NLTE needed

Jerkstrand 2011, PhD thesis, Jerkstrand, Fransson & Kozma 2011, Jerkstrand+2012
Adaptation to KNe : Q. Pognan (PhD thesis, ongoing)



Radioactive decay and γ-ray transport

Radiative transfer

- Monte Carlo with Sobolev approximation.
- Lines: $\sim 10^6$ for SNe, $\sim 10^8$ for KNe.
- Continuum : Free-free, bound-free, e^- scattering.

Non-thermal electron degradation

- Boltzmann equation.

Temperature

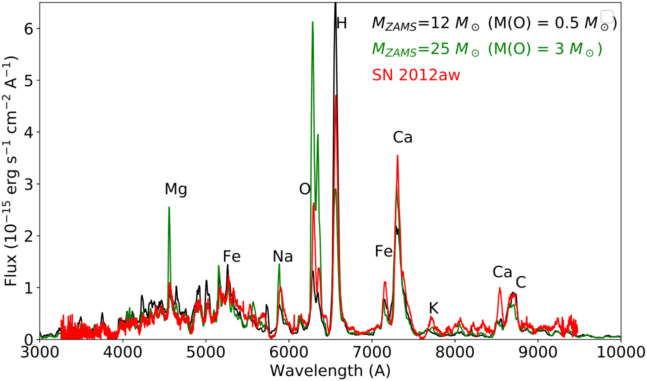
- Heating = cooling, or time-dependent 1st law of thermodynamics.

NLTE level populations

- Most of the periodic table included, first 2-4 ionization stages.
- ∼10-1000 exc. states each.

- Code is 1D but allows for (3D-informed) artificial mixing by a **virtual grid** method.
- A 3D version of SUMO ("ExtraSS") now coming into place (Jerkstrand+2020,van Baal+2023).

Spectral modelling example : Type II SNe



Jerkstrand+2014,2017

- Over the last decade, the first spectral models in reasonable agreement with observed spectra emerged.
- Can now test stellar evolution and explosion models in detail, and determine nucleosynthesis yields (e.g. oxygen) to within factor ∼2 (if atomic data ok).
- Temperatures $10^3 - 10^4$ K, mostly neutral and singly ionized species emit.

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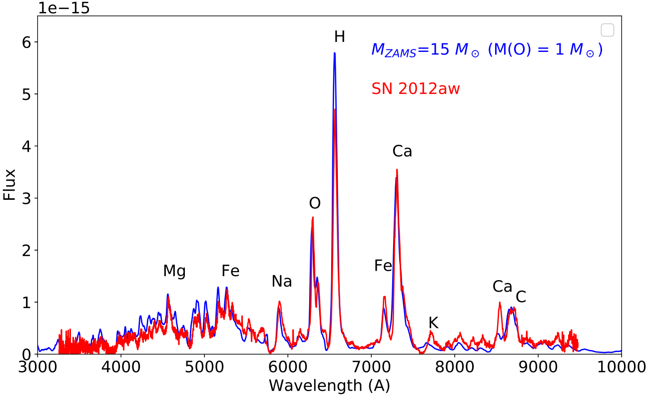

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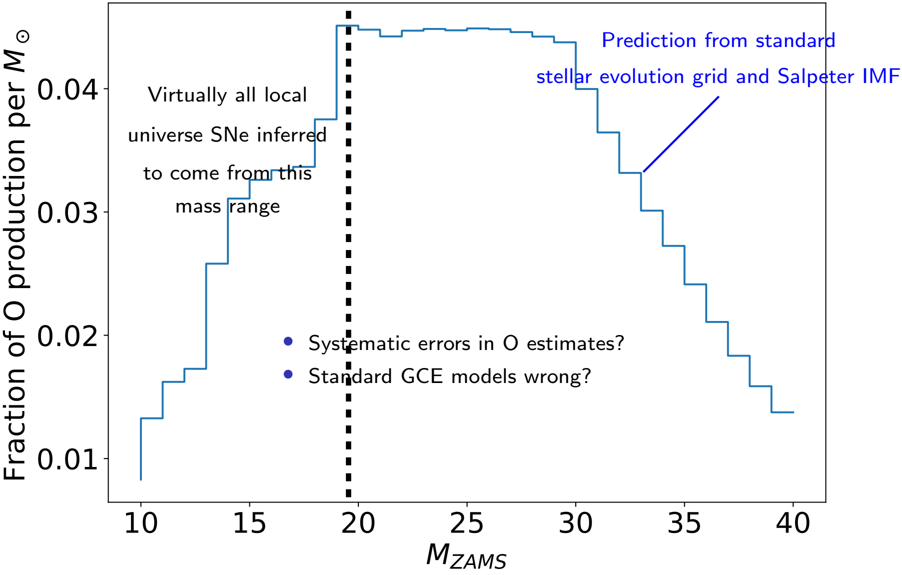
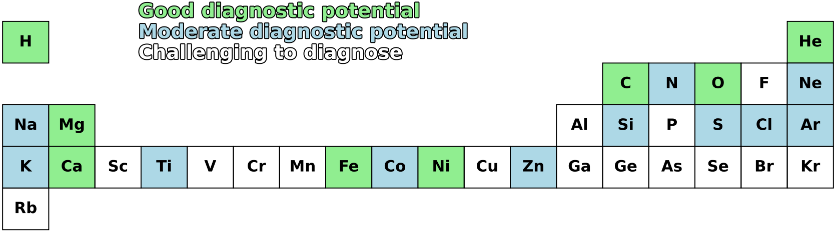
Which stars actually make most of our oxygen?



- Systematic errors in O estimates?
- Standard GCE models wrong?

Elements we can diagnose from supernova nebular-phase spectra


Good diagnostic potential
Moderate diagnostic potential
Challenging to diagnose

See Jerkstrand 2017, Handbook of SNe, for a review.

Current atomic data situation for nebular SN modelling

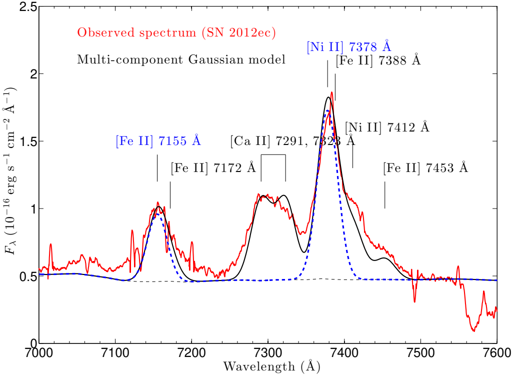
For $Z \leq 28$, SUMO treats 70 atoms/ions in NLTE, $\sim$ 150 levels each. About $\sim$300,000 transitions with specific atomic data. Around$\sim$10,000 level solutions in each zone.

- **Energy levels** : Good. Main source : NIST, Kurucz CD 23.
- **A-values** : Good. NIST, Kurucz CD 23.
- **Thermal collision strengths** : Medium. Probably cover most important (low-lying) transitions. Pradhan.
- **Non-thermal collision cross sections** : Poor/Medium. Arnaud & Rothenflug 1985, plus Bethe approximation.
- **Photoionization cross sections** : Medium. GS ok (Verner+1996), meta-stable some (TOPBASE).
- **Recombination rates** : Medium. Nahar.
- **Charge transfer rates** : Poor. 150 rates, lack for many important metal-metal reactions.

Current reference library maintained at https://ttt.astro.su.se/ anje1871/atomicdata

Diagnosing explosive nucleosynthesis : example of nickel

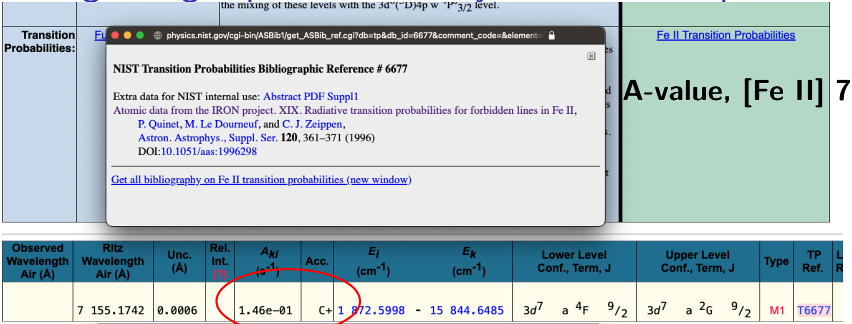
- Main diagnostic line: **[Ni II] 7378**



Jerkstrand+2015,MNRAS

- Use forward model to identify which lines present in spectral region (result: 7) and in which regime they form.
- Make 4-component fit (atomic data constraints remove 4 DOF) for $L_{\mathrm{Ni\ II\ 7378}}$, $L_{\mathrm{Fe\ II\ 7155}}$, $L_{\mathrm{Ca\ II\ 7300}}$, ΔV
- Obtain Ni/Fe ratio analytically.

Diagnosing explosive nucleosynthesis : example of nickel



the mixing of these levels with the 3d^{6}(^{5}D)4p w ^{4}P$^{o}_{3/2}$ level.

Transition Probabilities:

physics.nist.gov/cgi-bin/ASBib1/get_ASBib_ref.cgi?db=tp&db_id=6677&comment_code=&element=

NIST Transition Probabilities Bibliographic Reference # 6677

Extra data for NIST internal use: Abstract PDF Suppl1

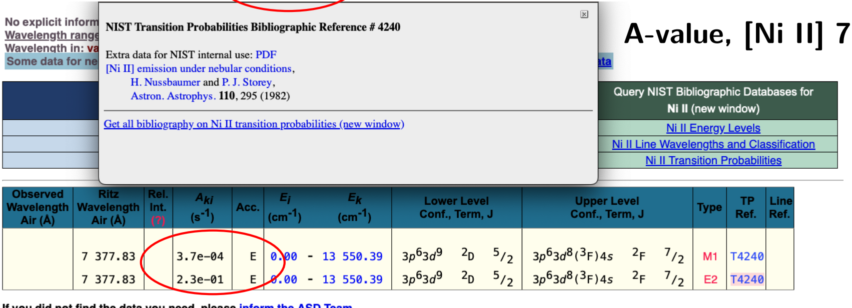
Atomic data from the IRON project. XIX. Radiative transition probabilities for forbidden lines in Fe II,
P. Quinet, M. Le Dourneuf, and C. J. Zeippen,
Astron. Astrophys., Suppl. Ser. **120**, 361–371 (1996)
DOI:10.1051/aas:1996298

Get all bibliography on Fe II transition probabilities (new window)

Fe II Transition Probabilities

A-value, [Fe II] 7155

Observed Wavelength Air (Å)	Ritz Wavelength Air (Å)	Unc. (Å)	Rel. Int. (?)	A_{ki} (s^{-1})	Acc.	E_i (cm^{-1})		E_k (cm^{-1})	Lower Level Conf., Term, J			Upper Level Conf., Term, J			Type	TP Ref.	L R
	7 155.1742	0.0006		1.46e-01	C+	1 872.5998	-	15 844.6485	3d^7	a ^{4}F	$^9/_2$	3d^7	a ^{2}G	$^9/_2$	M1	T6677	



No explicit inform
Wavelength range
Wavelength in: va
Some data for ne

NIST Transition Probabilities Bibliographic Reference # 4240

Extra data for NIST internal use: PDF

[Ni II] emission under nebular conditions,
H. Nussbaumer and P. J. Storey,
Astron. Astrophys. **110**, 295 (1982)

Get all bibliography on Ni II transition probabilities (new window)

A-value, [Ni II] 7378

ata

Query NIST Bibliographic Databases for
Ni II (new window)

Ni II Energy Levels
Ni II Line Wavelengths and Classification
Ni II Transition Probabilities

Observed Wavelength Air (Å)	Ritz Wavelength Air (Å)	Rel. Int. (?)	A_{ki} (s^{-1})	Acc.	E_i (cm^{-1})		E_k (cm^{-1})	Lower Level Conf., Term, J			Upper Level Conf., Term, J			Type	TP Ref.	Line Ref.
	7 377.83		3.7e-04	E	0.00	-	13 550.39	3p^{6}3d^9	^{2}D	$^5/_2$	3p^{6}3d^8(^{3}F)4s	^{2}F	$^7/_2$	M1	T4240	
	7 377.83		2.3e-01	E	0.00	-	13 550.39	3p^{6}3d^9	^{2}D	$^5/_2$	3p^{6}3d^8(^{3}F)4s	^{2}F	$^7/_2$	E2	T4240	

If you did not find the data you need, please inform the ASD Team

Diagnosing explosive nucleosynthesis : example of nickel

Collision strengths:

Fe **II** : Zhang & Pradhan 1995

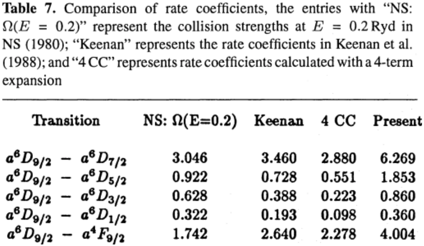


Table 7. Comparison of rate coefficients, the entries with "NS: $\Omega(E = 0.2)$" represent the collision strengths at $E = 0.2$ Ryd in NS (1980); "Keenan" represents the rate coefficients in Keenan et al. (1988); and "4 CC" represents rate coefficients calculated with a 4-term expansion

Transition	NS: Ω(E=0.2)	Keenan	4 CC	Present
$a^6D_{9/2} - a^6D_{7/2}$	3.046	3.460	2.880	6.269
$a^6D_{9/2} - a^6D_{5/2}$	0.922	0.728	0.551	1.853
$a^6D_{9/2} - a^6D_{3/2}$	0.628	0.388	0.223	0.860
$a^6D_{9/2} - a^6D_{1/2}$	0.322	0.193	0.098	0.360
$a^6D_{9/2} - a^4F_{9/2}$	1.742	2.640	2.278	4.004

Ni **II** : Cassidy, Ramsbottom & Scott +2010

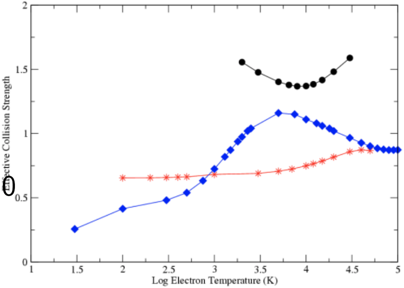


Fig. 7. Effective collision strength as a function of log electron temperature in Kelvin for the $3d^9\ ^2D^e_{5/2} - 3d^8 4s\ ^2F^e_{7/2}$ fine-structure transition: diamonds – present 295 level calculation, circles – 77 level calculation of Bautista (2004), stars – 17 level calculation of Bautista & Pradhan

The significance of collision strengths

New thermal collision strengths from Barklem+2017 applied to a Type Ib SN model:

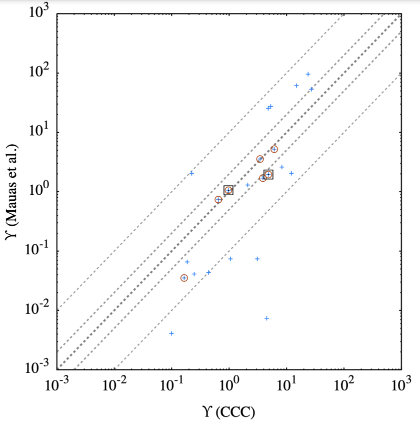
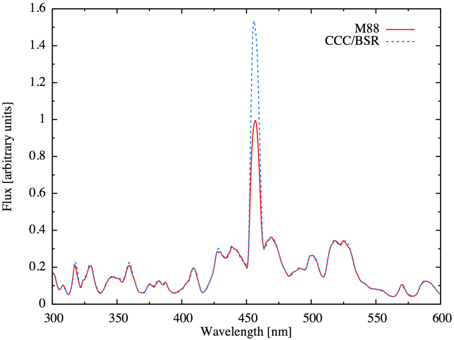


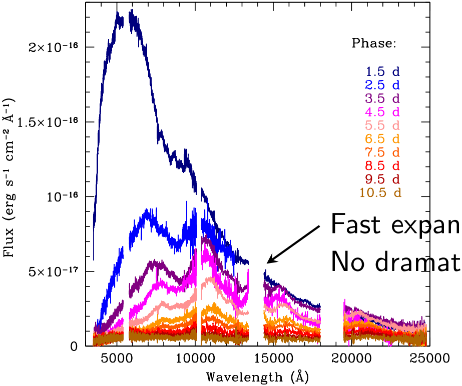
Fig. 5. Comparison of the effective collision strengths Υ_{ij} from Mauas et al. (1988), with those from the CCC calculations, at 5000 K. The lines and points follow the description in Fig. 4.



Supernovae vs kilonovae

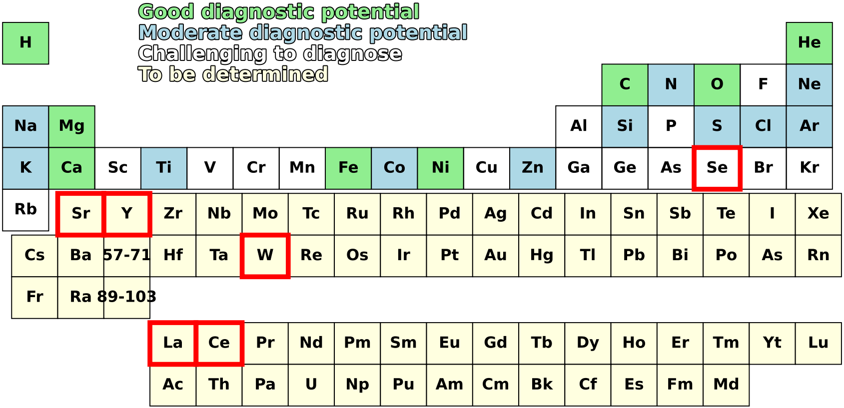
	SN	**KN**
M	5 $M_\odot$	0.05 $M_\odot$
V	0.01c	0.1c
t_{peak}	20d	2d
ρ_{peak}	10^{-11}	10^{-13}

- Everything about KNe make them more challenging to analyse than SNe - except that all ejecta is now radioactive.
- In particular, significantly lower densities for a given evolutionary phase → expect NLTE more important.



Fast expansion (0.1-0.2c) → severe line blending.
No dramatic spectral change as tail phase begins.

Elements we can diagnose from SN/KN spectra



Good diagnostic potential
Moderate diagnostic potential
Challenging to diagnose
To be determined

H																	He
													C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	57-71	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	As	Rn
Fr	Ra	89-103															
			La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yt	Lu
			Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md		

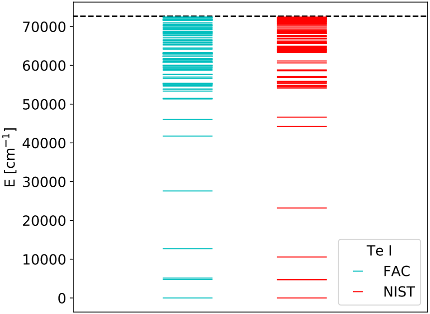
Claimed (possible) detection in 2017gfo, or potential for detection

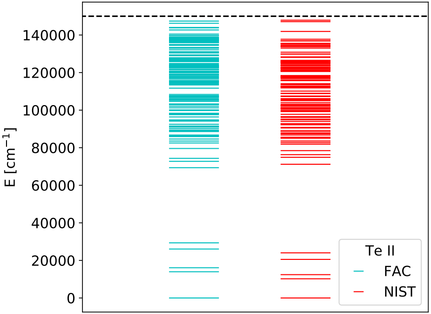
Watson+2019,Domoto+2021,2022,Hotokezaka+2022,Sneppen+2023

r-process energy levels and A-values

Calculated by J. Grumer with the **Flexible Atomic Code** (Gu 2008,open-s.)

- Overall term structure captured but moderate accuracy for energies → wavelengths 10-20% uncertainty.
- Models should be able to predict SED reasonably well, but not exact line features.

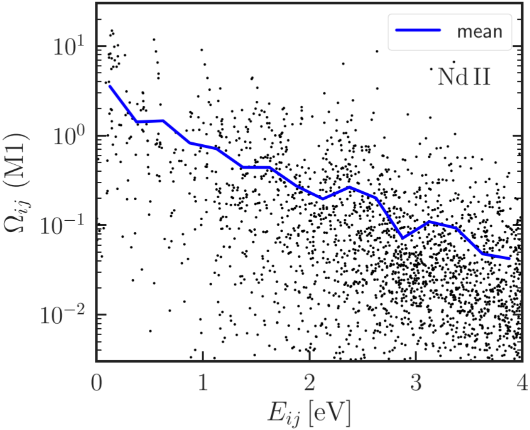




Pognan, Jerkstrand & Grumer, MNRAS 2022a

r-process collision strengths

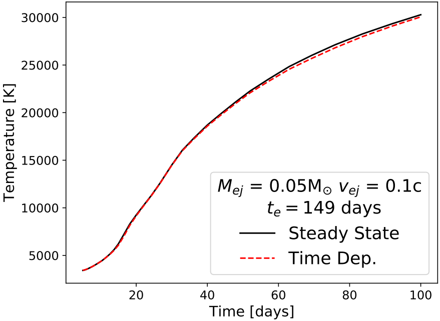
- SUMO: van Regemorter for allowed, $\Upsilon = 0.004 g_l g_u$ (Axelrod 1980, fit to iron) for forbidden.
- Other treatments in literature : HULLAC calculations (Nd only so far), $\Upsilon = 1$ others (Hotokezaka 2021)



Hotokezaka+2021

The temperature evolution of kilonovae

Heating: $H \propto t^{-1.3} \cdot f_{therm}(t)$
Cooling: $C \propto t^{-3} \cdot x_e(t) \cdot \Lambda(T)$



Typically $\Lambda(T) \propto T^{2\alpha}$, with $\alpha \gtrsim 1$.

For fixed x_e, Υ, equating $H = C \rightarrow$:

Early ($f_{therm}(t) \approx 1$) :
$\Lambda(T) \propto t^{1.7} \rightarrow \boldsymbol{T \propto t^{0.85/\alpha}}$

Late ($f_{therm}(t) \propto t^{-1.5}$):
$\Lambda(T) \propto t^{0.2} \rightarrow \boldsymbol{T \propto t^{0.1/\alpha}}$

Radiation trapping may raise T beyond radioactivity balance. We see however no strong effect of this : all models are getting hotter from ~3-5d.
Ionization: Neutrals to triply ionized.

Current atomic data situation for SUMO KN modelling

For $Z \geq 30$, SUMO treats 30 atoms/ions in NLTE, $\sim 10^3$ levels each. About $\sim$X transitions with specific atomic data. Around$\sim$X level solutions in each zone.

- **Energy levels** : Medium. Main source : FAC.
- **A-values** : Medium. FAC.
- **Thermal collision strengths** : Poor. van Regemorter + Axelrod approximations.
- **Non-thermal collision cross sections** : Poor/Medium. Lotz 1967, plus Bethe approximation.
- **Photoionization cross sections** : Poor. Hydrogenic.
- **Recombination rates** : Poor. Constant.
- **Charge transfer rates** : Poor. None.