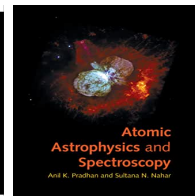
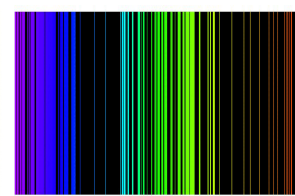
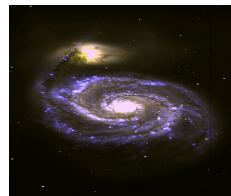
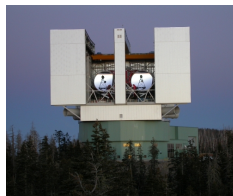




THE OHIO STATE UNIVERSITY



"PREDICTING DIAGNOSTIC LINES FOR GALACTIC EVOLUTION FROM SPECTROSCOPY OF Mn III"

SULTANA N. NAHAR¹

Collaborators: Zher Samak², Anil K. Pradhan¹

¹The Ohio State U, USA; Al-Aqsa U, Palestine



The VIII International
Conference on Molecular
Modeling and Spectroscopy

03 - 05 October 2026

The 8th International Conference on Molecular Modeling and
Spectroscopy (ICMMS8)

Organizer: NRC and Ain Shams University, Egypt

Platform: Online, October 3-5, 2026

SUPPORT:



Supercomputer
Center

Mn: ITS ABUNDANCE AND IMPORTANCE DAILY AND ASTROPHYSICALLY

- Manganese (Mn, Z=25) is known to us as vitamin and use in steels, industries.
- Elements are created by Stars, Supernova Explosions, Neutron Star Mergers, and through processes of i) nuclear fusion and ii) neutron captures. Mn is formed mainly through white dwarf supernova explosion and is poorly abundant,

Group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H	He																
2	Li	Be																
3	Na	Mg																
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo

Frequently used fundamental physical constants
For the most accurate values of these and other constants, visit physics.nist.gov/constants
1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ^{133}Cs
Speed of light in vacuum $c = 299\,792\,458\text{ m s}^{-1}$ (exact)
Planck constant $h = 6.626\,07 \times 10^{-34}\text{ J s}$ ($h = N h/2\pi$)
Elementary charge $e = 1.602\,177 \times 10^{-19}\text{ C}$
Electron mass $m_e = 9.109\,383 \times 10^{-31}\text{ kg}$
Proton mass $m_p = 1.672\,622 \times 10^{-27}\text{ kg}$
Fine-structure constant $\alpha = 1/137.035\,999$
Rydberg constant $R_\infty = 10\,973\,731.569\text{ m}^{-1}$
Boltzmann constant $k_B = 1.380\,658 \times 10^{-23}\text{ J K}^{-1}$

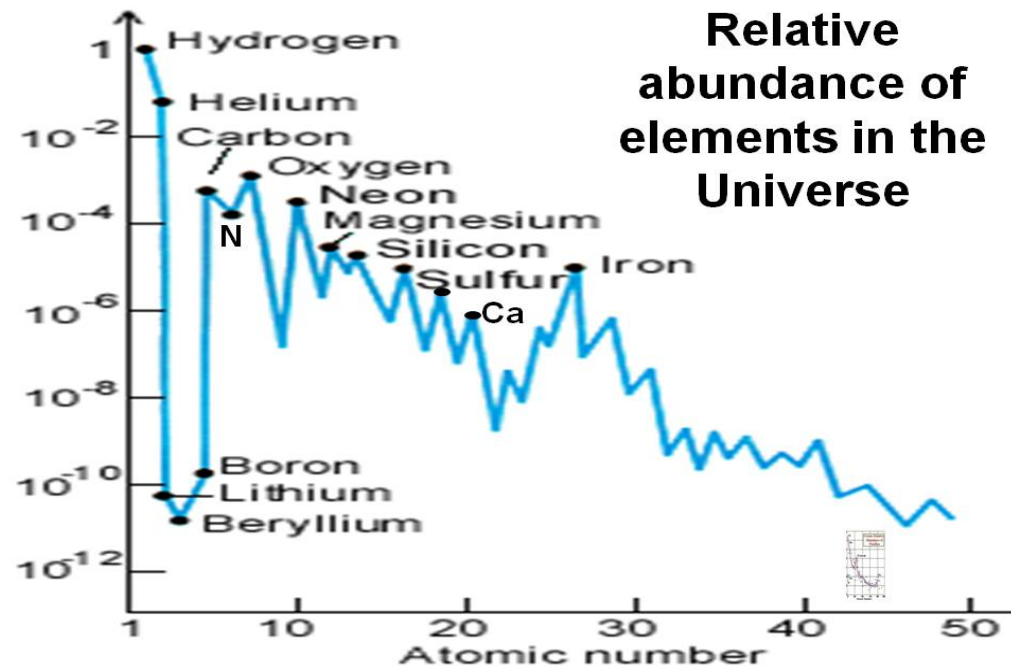
Physical Measurement Laboratory
www.nist.gov/pml

Standard Reference Data
www.nist.gov/srd

Legend:
Solids (white)
Liquids (light blue)
Gases (light green)
Artificially Prepared (pink)

Atomic Properties:
Atomic Number (Z)
Standard Atomic Weight (A_r)
Ground-state Ionization Energy (eV)

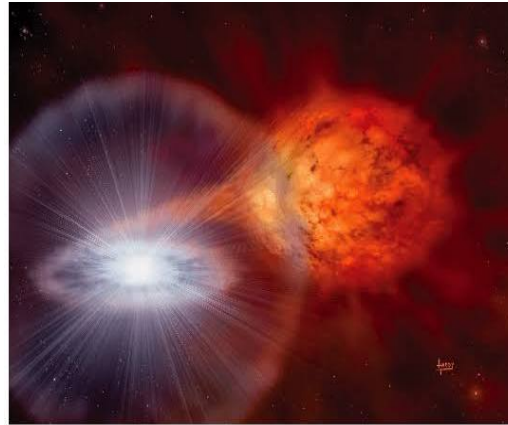
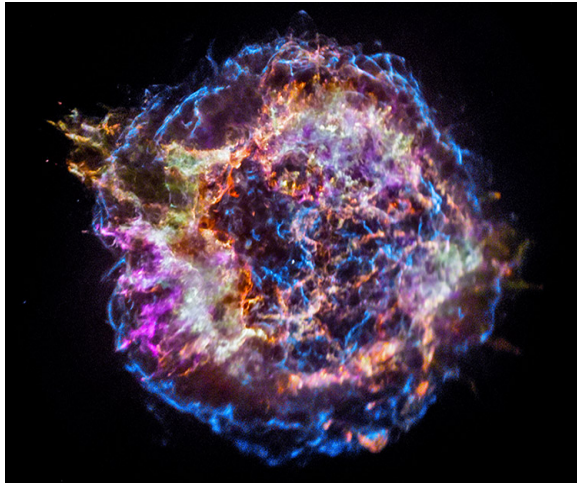
Footnote:
*Based upon ^{12}C . (i) indicates the mass number of the longest-lived isotope.
†IUPAC conventional atomic weights; standard atomic weights for these elements are expressed in intervals; see spacing for an explanation and values.
For a description of the data, visit physics.nist.gov/data
NIST SP 966 (September 2014)



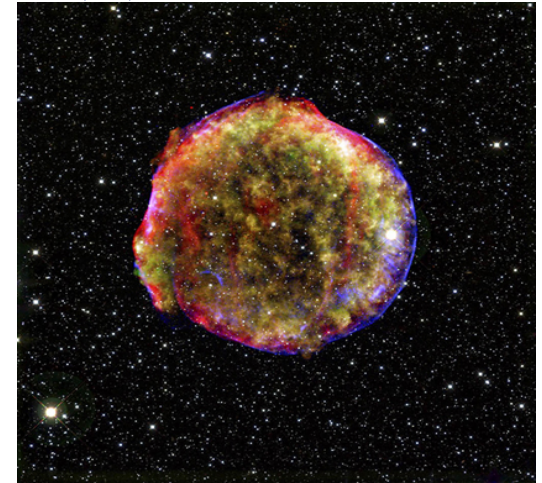
- Mn is important astrophysically, particularly ratio: Mn/Fe - Cosmic Clock: Its changing abundance relative to iron allows researchers to gauge a galaxy's age and evolutionary phase.
- poor Mn/Fe ratio - Ancient galaxy or star
- rich Mn/Fe ratio - newer galaxy or star, e.g, the Sun

Mn ABUNDANCE & ASTROPHYSICAL IMPORTANCE

- A supernova explosion can happen through i) nucleosynthesis of Core Collapse at the end of a star's life (**Supernova II**, e.g. Cassiopeia A, left fig), ii) thermonuclear reaction in a white dwarf binary system after the star has accumulated heavily matter from the companion (middle Fig) and explode (**Supernova Ia**, e.g. Tycho Brahe. It was concluded from Mn abundance in Tycho Brahe atmosphere)).



Artist's rendition of a white dwarf accumulating mass from a nearby companion star. This type of progenitor system would be considered singly-degenerate.



- Both SN produces Fe and Mn. But SN II produces Mn poorly, but richly by SN 1a. Fe abundance is a stable number since SN II happens more frequently (in Million years), but Mn abundance increases with SN 1a (in giga years). Hence abundance ratio Mn/Fe for a galaxy provides age and chemical evolution history - both are very important quantity.
- How do we detect Mn in a Supernova explosion - through SPECTROSCOPY OF LINES emitted by the ion

Project: PREDICT Mn DIAGNOSTIC LINES DETECTABLE BY JWST, and HENCE HELP ANALYZE GALACTIC CHEMICAL EVOLUTION

”Emissivity line ratios for [Mn iii] and spectral diagnostics of H ii regions”, Samak, Nahar, Pradhan MNRASL (2026)

- Received media attention after publication of Mn III diagnostic lines

New chemical clues shine a light on galactic evolution

 news.osu.edu/new-chemical-clues-shine-a-light-on-galactic-evolution
The Ohio State University

August 31, 2026



- The interest grow because of the possibility of detection by JWST.
- Photons from very large distance are stretched (z redshift- a measure of the past) with time due to accelerated expansion of the universe as

$$\lambda_{obs} = (z + 1)\lambda_{org}$$

Hence even shorter wavelengths, like ultraviolet, optical can stretch to infra-red photons that JWST can catch and analyze.

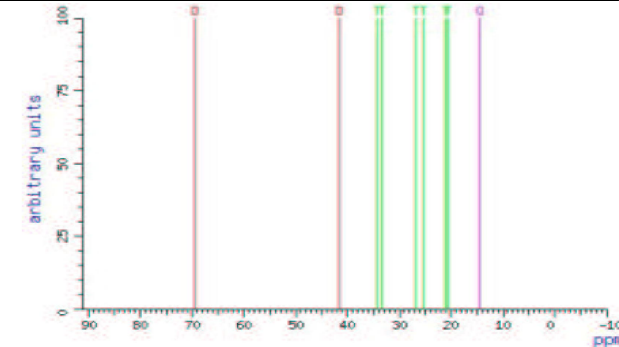
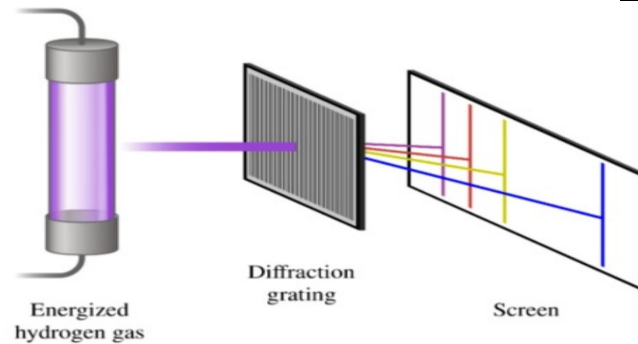
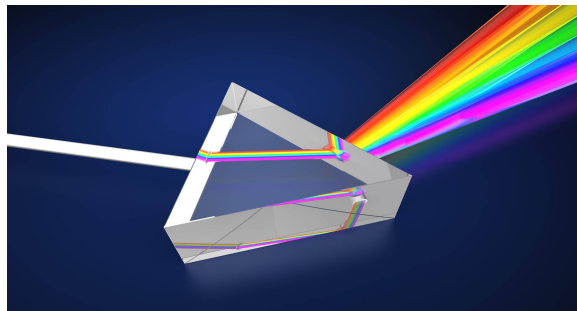
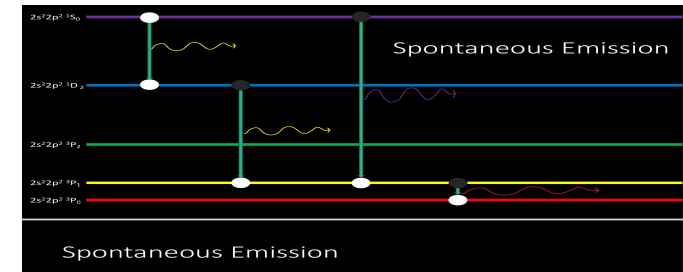
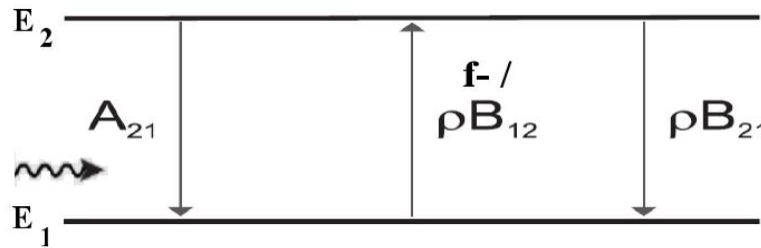
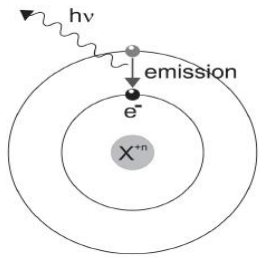
- Underlying science is the spectroscopy of lines emitted by Mn -the presentation objective

SPECTRAL LINE FORMATION: "PHOTO-EXCITATION"

Photo-Excitation & De-excitation:



- Most common method for infinite number of spectral line formation



- Physical atomic quantities describing the process

B_{12} - Photo-excitation, Oscillator Strength (f)

A_{21} - Spontaneous Decay, - Radiative Decay Rate (A -value)

The transition probability is given by $P_{ji} \sim | \langle j | H' | i \rangle |^2 \sim | \langle j | A \cdot p | i \rangle |^2$

$$P_{ij} = 2\pi \frac{c^2}{h^2 \nu_{ji}^2} | \langle j | \frac{e}{mc} \hat{e} \cdot p e^{ik \cdot r} | i \rangle |^2 \rho(\nu_{ji}). \quad (1)$$

- Strength of a line depends on the type of transitions, allowed for strong lines and forbidden for weaker lines

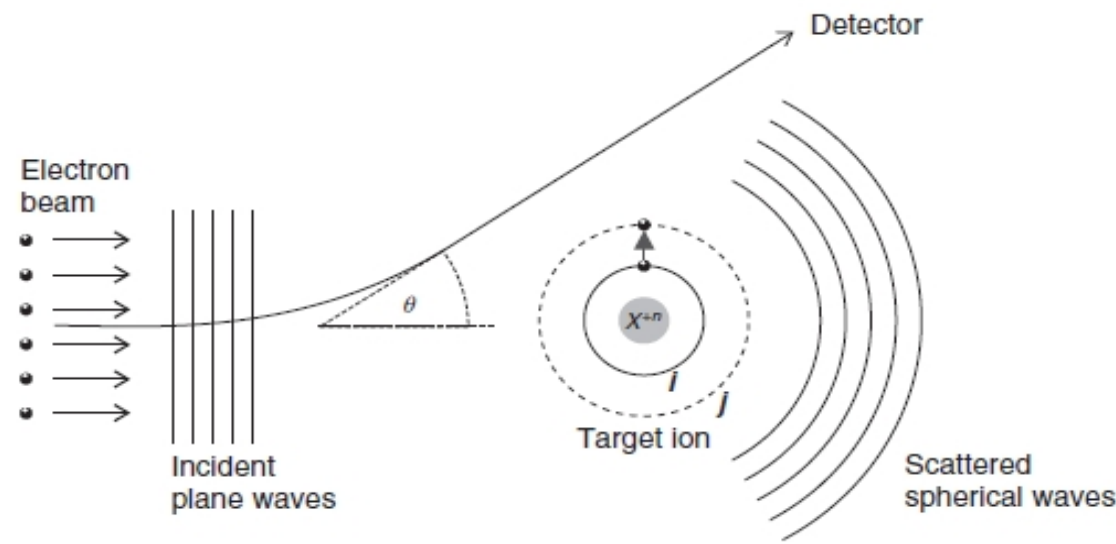
ELECTRON-IMPACT EXCITATION (EIE)

Most common process in cold, thin plasma, e.g., planetary nebulae, ISM, - mostly diagnostic forbidden lines



- Light is emitted as the excitation decays
- Scattered electron shows features with energy & can have autoionizing resonances
- Atomic quantity: i) Collision Strength (Ω)
ii) Effective collision strength $\Upsilon(T)$
iii) Excitation rate coefficient $q_{ij}(T)$

Line ratio: I_{ji}/I_{ik} depends on ratio of q_{ij}/q_{ik} , and hence used for determination of plasma diagnostics, ρ and T

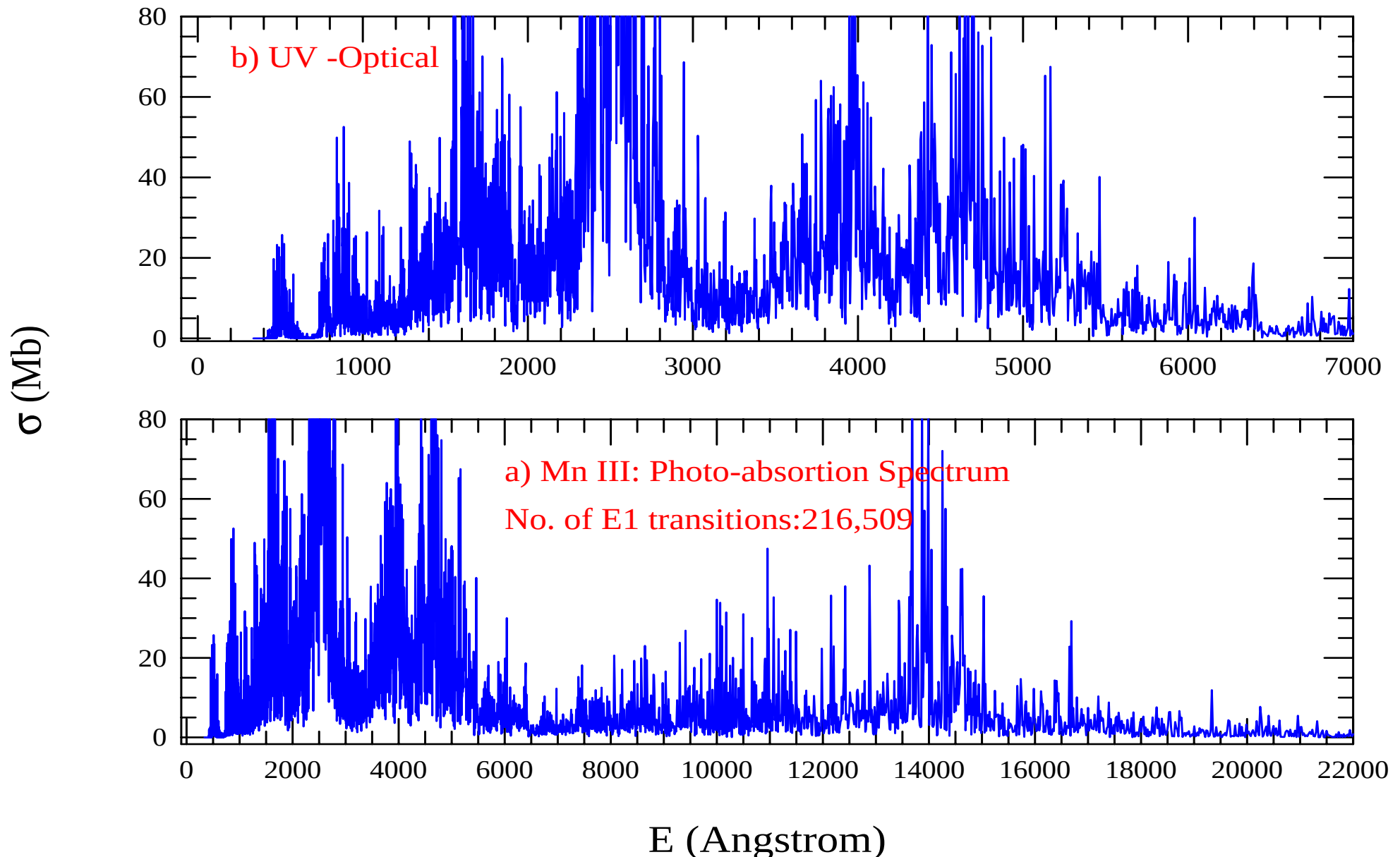


• **Mn III Energies:** We carried out relativistic Breit-Pauli atomic structure calculations for photo-excitation of Mn III. Used program SUPERSTRUCTURE (SS) (Eissner et 1974, Nahar et al. 2003). We obtained an optimization set of configurations of Mn III, $3d^5$, $3d^44s$, $3d^44p$, $3d^44d$, $3d^44f$, $3d^45s$, $3d^45p$, $3d^45d$, $3d^45d$ with closed orbitals $1s^2$, $2s^2$, $2p^6$, $3s^2$, and $3p^6$ for the transitions. Calculated energies are compared with those at NIST table.

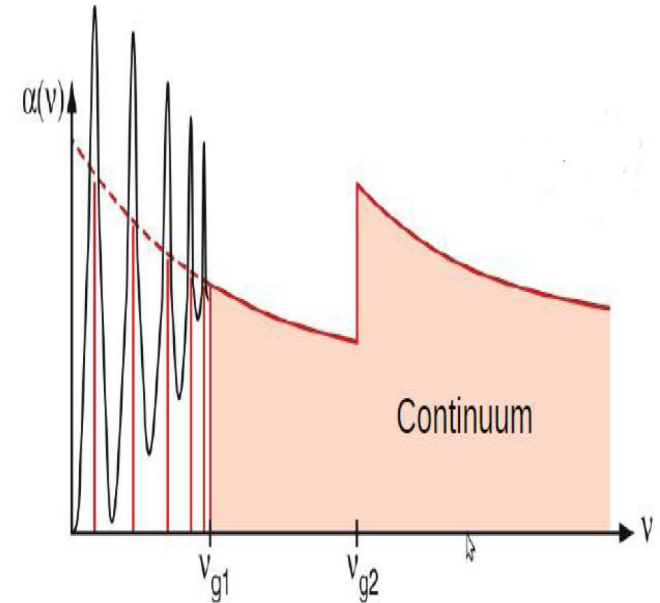
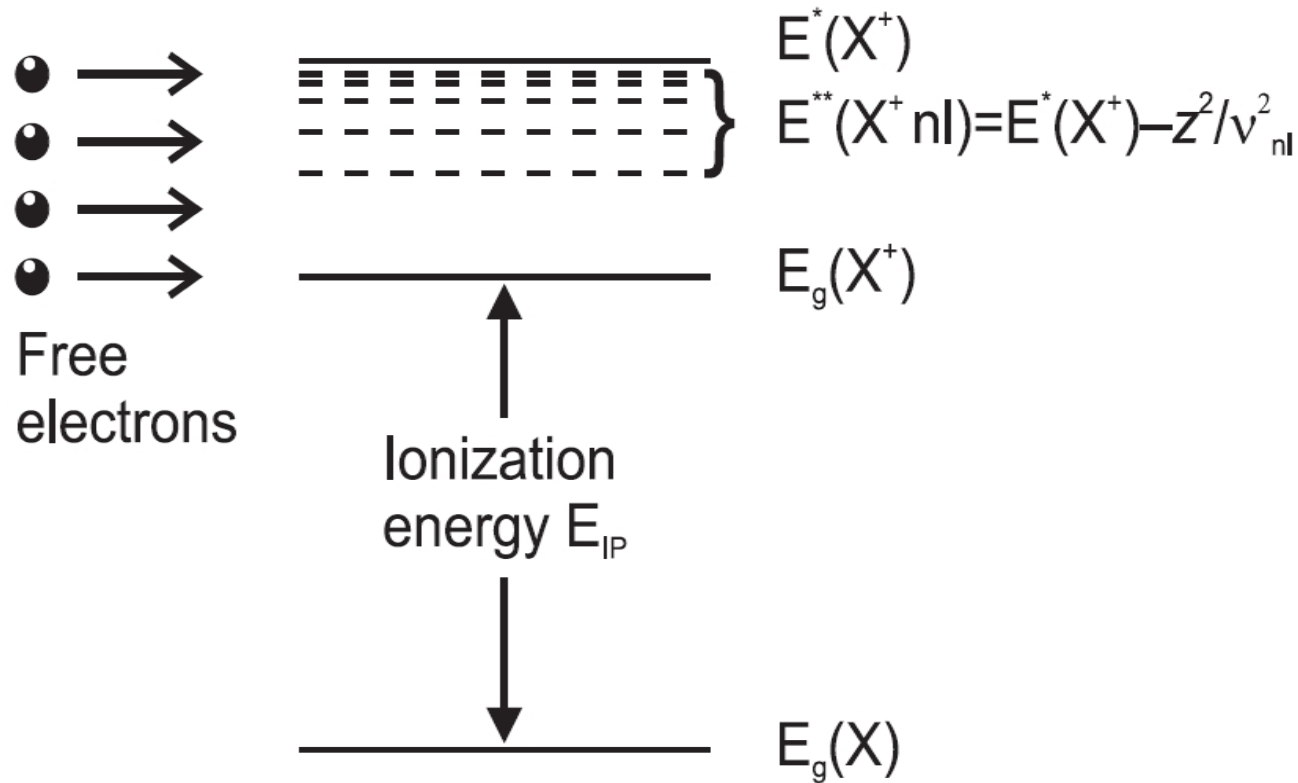
K	Configuration Term	E_{SS} (Ry)	E_{NIST} (Ry)	K	Configuration Term	E_{SS} (Ry)	E_{NIST} (Ry)
1	$3d^5(^6S_{5/2})$	0	0	20	$3d^5(^4F_{7/2})$	0.39707	0.41713
2	$3s^5(^4G_{11/2})$	0.248202	0.24444	21	$3d^5(^4F_{5/2})$	0.397335	0.41729
3	$3s^5(^4G_{9/2})$	0.244685	0.24819	22	$3d^5(^4F_{3/2})$	0.397940	0.417457
4	$3s^5(^4G_{5/2})$	0.244746	0.24802	23	$3d^5(^2H_{11/2})$	0.397940	0.417457
5	$3s^5(^4G_{7/2})$	0.244765	0.24812	24	$3d^5(^2H_{9/2})$	0.425295	0.437430
6	$3s^5(^4P_{5/2})$	0.244765	0.28297	25	$3d^5(^2G_{7/2})$	0.435968	0.444860
7	$3s^5(^4P_{3/2})$	0.265796	0.28315	26	$3d^5(^2G_{9/2})$	0.437456	0.446042
8	$3s^5(^4P_{1/2})$	0.266157	0.28339	27	$3d^5(^2F_{5/2})$	0.464771	0.477299
9	$3s^5(^4D_{7/2})$	0.266467	0.30367	28	$3d^5(^2F_{7/2})$	0.465290	0.476864
10	$3s^5(^4D_{5/2})$	0.294406	0.30412	29	$3d^5(^2S_{1/2})$	0.507373	0.523485
11	$3s^5(^4D_{3/2})$	0.294967	0.30401	30	$3d^5(^2D_{3/2})$	0.561160	0.587047
12	$3s^5(^4D_{1/2})$	0.295102	0.30378	31	$3d^5(^2D_{5/2})$	0.507373	0.587074
13	$3s^5(^2I_{13/2})$	0.295111	0.35738	32	$3d^44s(^6D_{1/2})$	0.569150	0.611694
14	$3s^5(^2I_{11/2})$	0.357003	0.35717	33	$3d^44s(^6D_{3/2})$	0.570162	0.612304
15	$3s^5(^2F_{5/2})$	0.356983	0.39410	34	$3d^44s(^6D_{5/2})$	0.571797	0.613311
16	$3s^5(^2D_{3/2})$	0.375789	0.39591	35	$3d^44s(^6D_{7/2})$	0.573997	0.614696
17	$3s^5(^2F_{7/2})$	0.378812	0.40675	36	$3d^44s(^6D_{9/2})$	0.576699	0.616441
18	$3s^5(^2D_{5/2})$	0.388259	0.40851	37	$3d^5(^2G_{7/2})$	0.627790	0.649227

SIMULATED SPECTRUM OF Mn III

- Total transitions (allowed + forbidden) = 958,499.
- Strong transitions are in the UV (1500 - 5500 Å) and in the infrared (14000 Å) regions. Some lines with higher z are expected to be detected by JWST (0.6 - 28.5 μm)



Lines from Rydberg Series of Autoionizing States



- Rydberg series of autoionizing states $(LS)_c \nu l$ lie above the ionization threshold & below an excited core state $(LS)_c$
- Energy of the state is given by the Rydberg formula

$$E^{**}(X^+ \nu l) = E_{Res} = E_c - z^2 / \nu^2$$

$E_c = E^*(X^+) =$ an excited threshold of the residual ion X^+

- ν = effective quantum number, $\Delta \nu \sim 1$ for each series
- Resonances can appear as lines in the spectra. However, they are typically weaker than bound-bound lines, often are dissolved by the high ρ and T of the plasma, and enhance the spectrum background.

Close-Coupling (CC) Wave Function & R-matrix Method

- CC approximation generates resonances naturally
- CC Wave Function expansion includes excited states of the residual ion which generate resonant states:

$$\Psi_E(\mathbf{e} + \mathbf{ion}) = A \sum_i^N \chi_i(\mathbf{ion}) \theta_i + \sum_j c_j \Phi_j(\mathbf{e} + \mathbf{ion})$$

$\chi_i \rightarrow$ Core ion wavefunction, $\Phi_j \rightarrow$ correlation functions $\theta_i \rightarrow$ interacting electron wavefunction (continuum or bound)

- Substitution of $\Psi_E(\mathbf{e} + \mathbf{ion})$ in Schrodinger equation results in a set of coupled equations which are solved using the R-matrix method

$$\mathbf{H}\Psi_E = E\Psi_E$$

The Breit-Pauli Hamiltonian is

$$\mathbf{H}_{N+1}^{\text{BP}} = \mathbf{H}_{\text{NR}} + \mathbf{H}_{\text{mass}} + \mathbf{H}_{\text{Dar}} + \mathbf{H}_{\text{so}} + \frac{1}{2} \sum_{i \neq j}^N [\mathbf{g}_{ij}(\text{so} + \text{so}') + \mathbf{g}_{ij}(\text{ss}') + \mathbf{g}_{ij}(\text{css}') + \mathbf{g}_{ij}(\mathbf{d}) + \mathbf{g}_{ij}(\mathbf{oo}')]. \quad (2)$$

- $E < 0 \rightarrow$ Bound (e+ion) states Ψ_B
- $E \geq 0 \rightarrow$ Continuum states Ψ_F
- Ψ_B & Ψ_F are used for parameters of the atomic processes

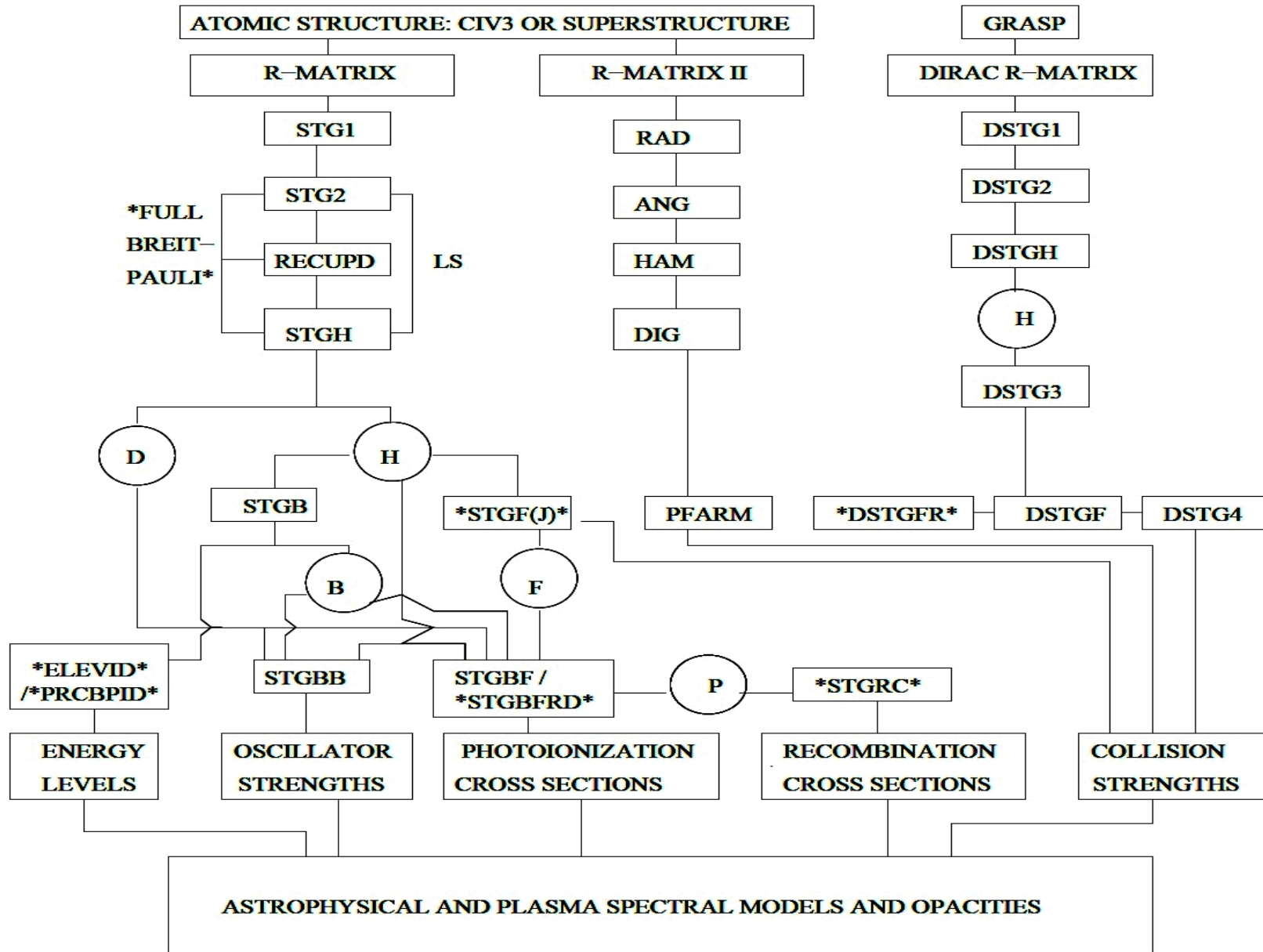
R-MATRIX CODES (for Close Coupling approximation)

- Large-Scale Atomic Calculations at OSC

- Various Computational Stages

• R-matrix calculations • Results - 1) Energy Levels, 2) Oscillator Strengths, 3) Photoionization Cross sections, 4) Recombination Rate Coefficients, 5) Collision Strengths; - Astrophysical Models

THE R-MATRIX CODES AT OSU



ELECTRON IMPACT EXCITATION (EIE)

- EIE Scattering matrix $S_{SL\pi}(i, j)$ is obtained from the wave function phase shift. The EIE collision strength is

$$\Omega(S_i L_i - S_j L_j) = \frac{1}{2} \sum_{SL\pi} \sum_{l_i l_j} (2S + 1)(2L + 1) |S_{SL\pi}(S_i L_i l_i - S_j L_j l_j)|^2$$

Ω is a dimensionless quantity, introduced by Seaton. It does not diverge like the cross section, σ_{EIE} at origin,

$$\sigma_{\text{EIE}} = \pi / (g_i k^2) \Omega a_o^2,$$

- The quantity used in models is **effective collision strength** $\Upsilon(T)$, the Maxwellian averaged collision strength:

$$\Upsilon(T) = \int_0^\infty \Omega_{ij}(\epsilon_j) e^{-\epsilon_j/kT} d(\epsilon_j/kT)$$

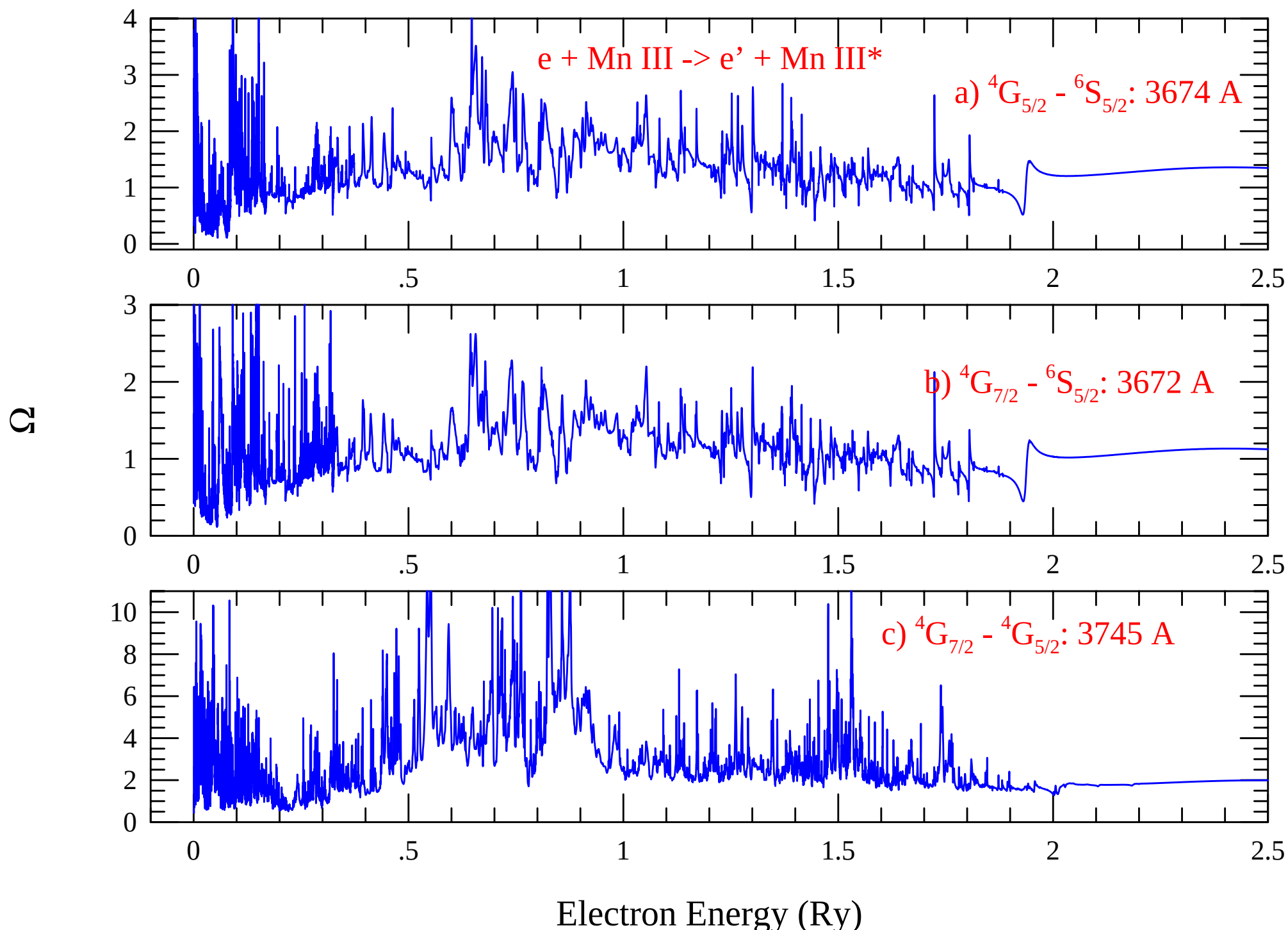
- The **excitation rate coefficient** $q_{ij}(T)$ is given by

$$q_{ij}(T) = \frac{8.63 \times 10^{-6}}{g_i T^{1/2}} e^{-E_{ij}/kT} \Upsilon(T) \text{ cm}^3 \text{ s}^{-1}$$

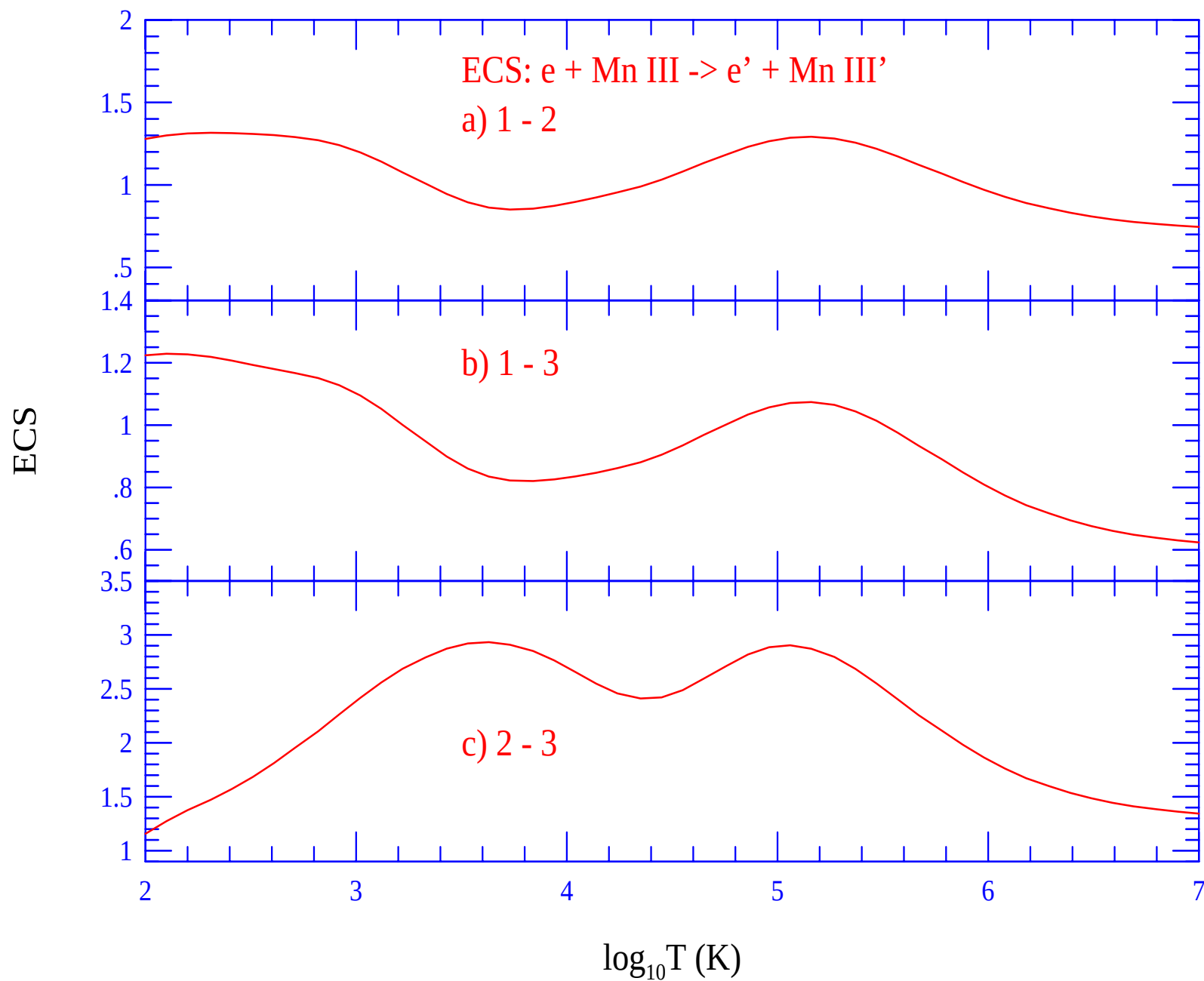
$E_{ij} = E_j - E_i$ in Ry, T in K, $(1/kT = 157885/T)$

Ω EIE SPECTRUM OF Mn III (in preparation)

Collision strength: $e + \text{Mn III} \rightarrow e' + \text{Mn III}'$ (Lowest 3 excitation)



EIE: EFFECTIVE COLLISION STRENGTHS OF Mn III



ASTROPHYSICAL APPLICATIONS: Elemental Abundances, Plasma Diagnostics

i) DETERMINATION OF ELEMENTAL ABUNDANCES

From the intensity of a line

$$I_{ba}(X^+, \lambda_{ba}) = \frac{h\nu}{4\pi} n_e n_{ion} Q_{ba}$$

population of a level b can be written as

$$N(b) = n_{ion} Q_{ba}$$

Abundance of element X w.r.t. H , $n(X)/n(H)$, can be obtained from

$$I(X^+, \lambda_{ba}) = \frac{h\nu}{4\pi} A_{ba} \frac{N(b)}{\sum_j N_j(X^+)} \frac{n(X^+)}{n(X)} \left[\frac{n(X)}{n(H)} \right] n(H)$$

A_{ba} = radiative decay rate, $\sum_j N_j$ = total populations of all excited levels, $N(b)/\sum_j N_j(X^+) =$ population fraction, $\frac{n(X^+)}{n(X)}$ - ionization fraction (from photoionization model)

ii) PLASMA DIAGNOSTICS

- The ratio of intensities (emissivity ratio), of two different lines arising from the same level can be used for T & ρ diagnostics.

$$\frac{I_{ji}(\lambda_{ji})}{I_{lk}(\lambda_{lk})} = \frac{\nu_{ji} n'_{ion} Q_{ji}}{\nu_{lk} n''_{ion} Q_{lk}}$$

The density or T are varied for the line ratios to carry out the diagnostics of plasma

”FOUR DIAGNOSTIC LINE RATIOS FOR JWST” (MNRASL 2026)

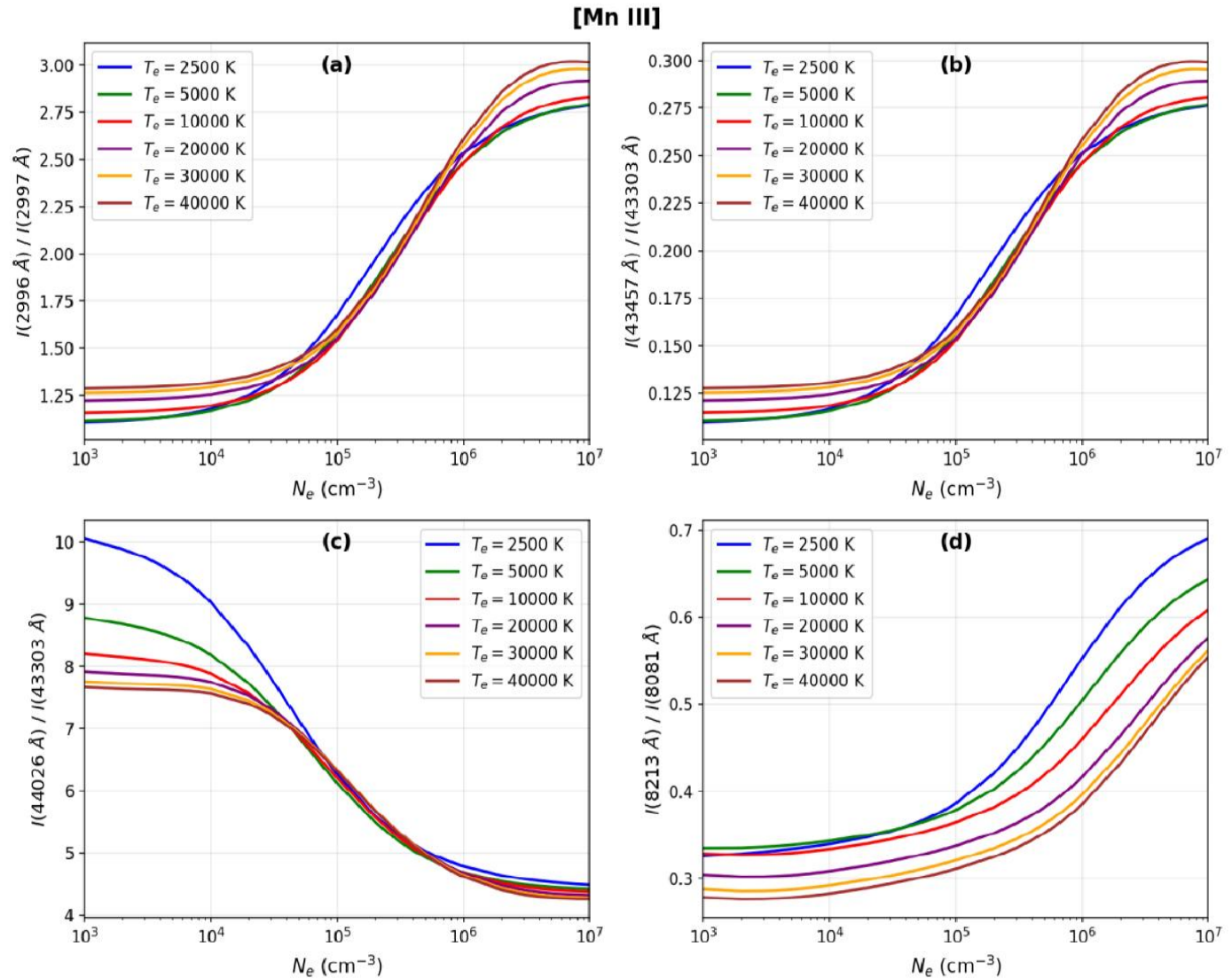
RESULTS

Four New Diagnostic Line Ratios

PURE DENSITY

R_1, R_2

Nearly independent of T_e across 2500–40,000 K
— clean N_e probes for $3 \lesssim \log_{10} N_e \lesssim 7 \text{ cm}^{-3}$.

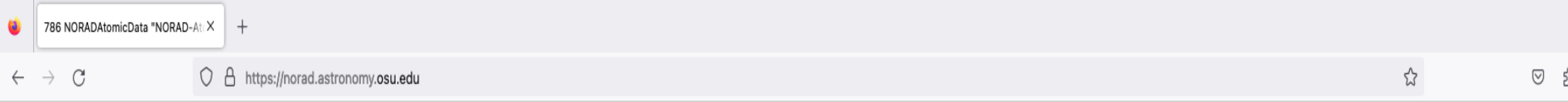


T_e & N_e COMBINED

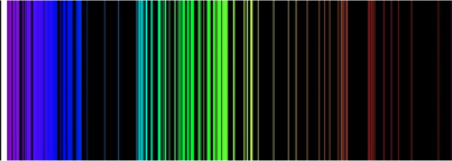
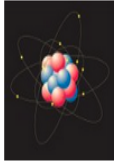
R_3, R_4

Sensitive to both parameters
used together with R_1/R_2 to
break the T_e – N_e degeneracy.

• ONLINE DATABASE: NORAD-Atomic-Data - 5 types of data



Sultana N. Nahar



"NORAD-Atomic-Data (NORAD: Nahar-OSU-Radiative-Atomic-Data)"

Introduction	Accuracy & Benchmarking	Atomic Radiative Data 1 (Z upto 28)	Atomic Radiative Data 2 (Z > 28)	EIE Collision Data 3
Measured Lines & Energies Data 5	Measured Photoionization Data 6	Program Codes	PUBLICATIONS, NEWS	Line Ratios



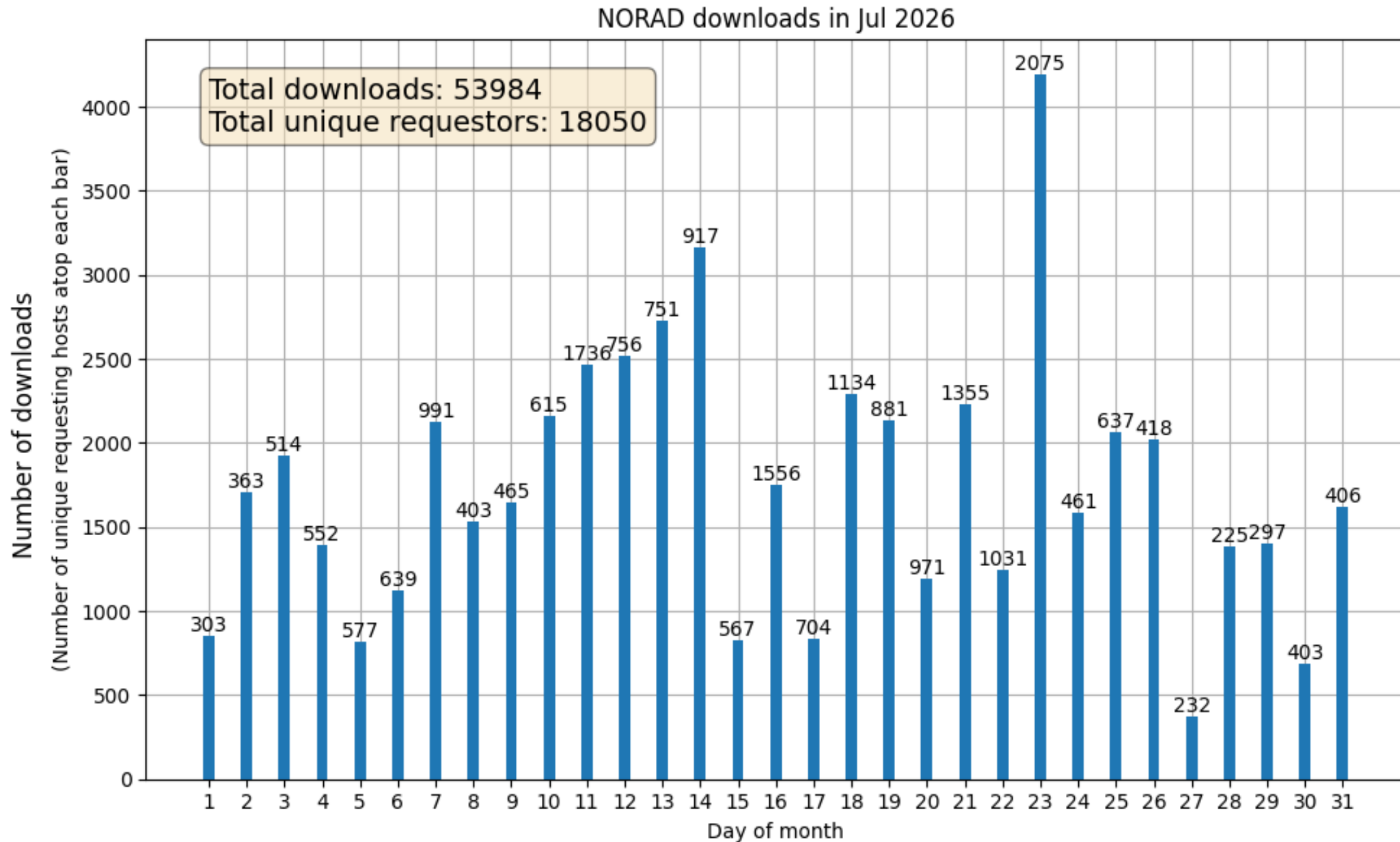
[- NORAD-Atomic-Data Access metric charts](#)

Introduction:

- **Brief Description of NORAD-Atomic-Data database:**
- The on-line [NORAD-Atomic-Data](#) based at the Ohio State University contains large amount calculated atomic data relevant to various radiative and collisional atomic processes, such as, excitation of energies, photoionization, electron-ion recombination, radiative transitions, lifetimes, etc relevant to astrophysical and laboratory plasmas. They are obtained mainly from large scale R-MATRIX calculations and some from atomic structure program SUPERSTRUCTURE carried at the Ohio Supercomputer Center (OSC) by Nahar et al
- [Atomic Data files](#) contents:
 - i) Energies,
 - ii) Oscillator Strengths, transition probabilities for allowed and forbidden transitions,
 - iii) Photoionization cross sections,
 - iv) Electron-Ion Recombination cross sections and rate coefficients,
 - v) Lifetimes,

Following additional data are in process to be added

- NORAD-Atomic-Data was created in 2007. Most users: Astronomers. Physicists, Engineers, Chemists, atmospheric modelers etc.
- The amount of accessible is expected to considerably
- Following figure shows the metric of monthly usage: July 2026, total data downloads= 782,818 (Dec 2023 - Aug 2026)



CONCLUSIONS

- Study of Mn II spectra formation and line ratio are presented
- The study focuses on the underlying science of atomic processes forming lines, their features and impacts
- All published data are available at the Ohio State University database:
NORAD-Atomic-Data (<https://norad.astronomy.osu.edu>)