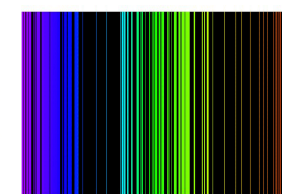
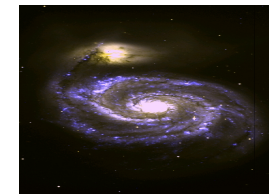
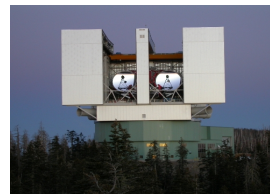




THE OHIO STATE UNIVERSITY



Supercomputer
Center



Research based online course:

**”Atomic and Molecular Astrophysics and Spectroscopy
with Computational workshops on R-matrix and
SUPERSTRUCTURE Codes I”**

**- PROF. SULTANA N. NAHAR,
PROF. ANIL K. PRADHAN**

Astronomy Department, Ohio State University, USA



THE OHIO STATE UNIVERSITY



A.P.J. Abdul Kalam STEM-ER Center
(Indo-US collaboration)

- Organized under the Indo-US STEM Education and Research Center of OSU-AMU, AMU, Aligarh, India, & OSU, Columbus, USA

May 4 -30, 2024

Support: OSU-AMU STEM ER Center, AMU, OSU, OSC

ATOMIC PROCESSES PRODUCING ASTROPHYSICAL SPECTRA *and* Relevant Atomic Parameters

RADIATIVE PROCESSES:

1. Photoexcitation & De-excitation (bound-bound transition):

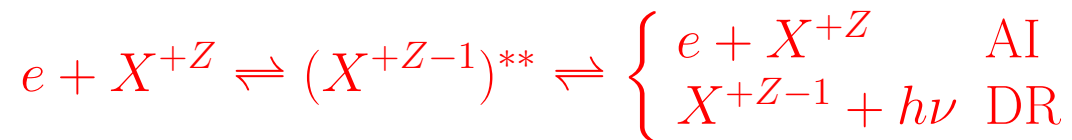


- Oscillator Strength (f), Radiative Decay Rate (A -value)
- Examples: Seen as lines in astrophysical spectra
- Determines opacities in astrophysical plasmas

2. Photoionization (PI) & Radiative Recombination (RR):



3. Autoionization (AI) & Dielectronic recombination (DR):



The doubly excited state - "autoionizing state" - introduces resonances

- 2 & 3. Photoionization Cross Sections (σ_{PI}), Recombination Cross Sections (σ_{RC}) and Rate Coefficients (α_{RC})

Examples:

- Photoionization resonances - seen in absorption spectra,
- Recombination resonances - seen in emission spectra

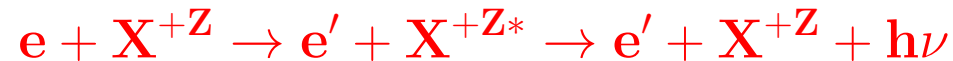
ATOMIC PROCESSES PRODUCING ASTROPHYSICAL SPECTRA

and Relevant Atomic Parameters

- Determine ionization fractions in astrophysical plasmas

COLLISIONAL PROCESSES:

4. Electron-impact excitation (EIE):



- Collision Strength (Ω)
- (i) Can go through an intermediate autoionizing state, (ii) gives out a photon as the ion de-excites. Ex. seen as forbidden lines in emission spectra

.5. Electron-impact Ionization:



- Ionization cross section and strength
- It does not involve any photon and hence can not be produce lines. However, it is needed for modeling to determine level populations, ionization fractions etc

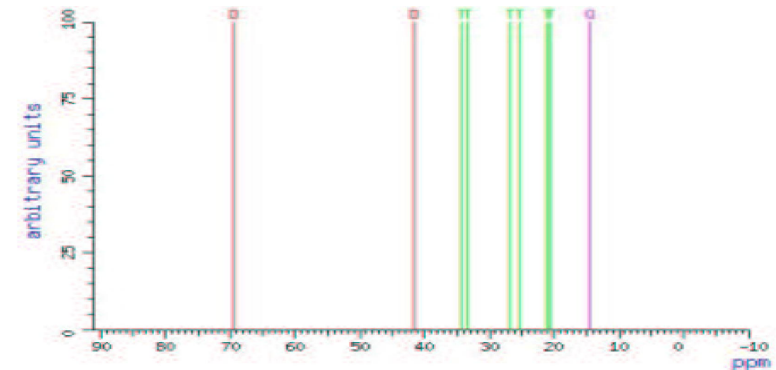
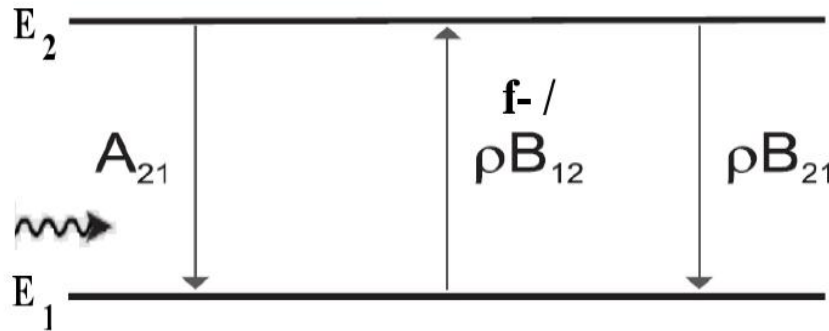
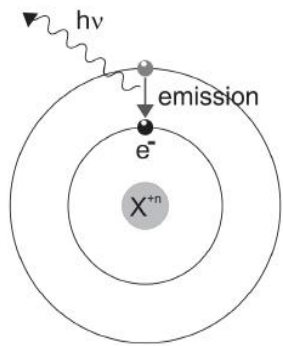
6. Hydrogen-impact excitation:



- Excitation rate coefficient and transition rate

1. "PHOTO-EXCITATION"

Photo-Excitation & De-excitation:



- Atomic quantities

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

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

B_{21} - Stimulated Decay with a radiation field

- P_{ij} , transition probability, $P_{ji} \sim | \langle j | H' | i \rangle |^2 \sim | \langle j | A.p | i \rangle |^2$

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

$$e^{ik \cdot r} = 1 + ik \cdot r + [ik \cdot r]^2 / 2! + \dots,$$

- Various terms in $e^{ik \cdot r} \rightarrow$ various transitions 1st term E1, 2nd term E2 and M1, ...
- The angular integrals determine the allowed and forbidden transitions - **selection rules**

TRANSITION MATRIX ELEMENTS WITH A PHOTON

- 1st term: **Dipole operator: $\mathbf{D} = \sum_i \mathbf{r}_i$:**
- Transition matrix for Photo-excitation & Deexcitation:

$$\langle \Psi_B || \mathbf{D} || \Psi_{B'} \rangle$$

Matrix element is reduced to generalized line strength (length form):

$$S = \left| \left\langle \Psi_f \left| \sum_{j=1}^{N+1} \mathbf{r}_j \right| \Psi_i \right\rangle \right|^2 \quad (2)$$

- There are also "Velocity" & "Acceleration" forms

Allowed electric dipole (E1) transitions

The oscillator strength (f_{ij}) and radiative decay rate (A_{ji}) for the bound-bound transition are

$$f_{ij} = \left[\frac{E_{ji}}{3g_i} \right] S, \quad \sigma_{PI}(\nu) = 8.064 \frac{E_{ij}}{3g_i} S^{E1} \text{ [Mb]}, \text{ , ,}$$

$$A_{ji}(\text{sec}^{-1}) = \left[0.8032 \times 10^{10} \frac{E_{ji}^3}{3g_j} \right] S$$

Selection Rules: Allowed & Forbidden Transitions

Angular momentum integrals introduce the selection rules

General rules: x =type of transition: For total J ,

• $\Delta J = J_2 - J_1 = 0, \pm 1, \dots, \pm x$; $J_1 + J_2 \geq x$, $\Delta M = 0, \pm 1, \dots, \pm x$

For the parity

$\Delta P = (-1)^x$ for E_x and $-(-1)^x$ for M_x transitions

Allowed: i) Electric Dipole (E1) transitions - a) same-spin (stronger) & intercombination (different spin, relatively weaker) transitions
($\Delta J = 0, \pm 1$, $\Delta L = 0, \pm 1, \pm 2$; parity changes)

Forbidden:

ii) Electric quadrupole (E2) transitions

($\Delta J = 0, \pm 1, \pm 2$, parity does not change)

iii) Magnetic dipole (M1) transitions

($\Delta J = 0, \pm 1$, parity does not change)

iv) Electric octupole (E3) transitions

($\Delta J = \pm 2, \pm 3$, parity changes)

v) Magnetic quadrupole (M2) transitions

($\Delta J = \pm 2$, parity changes)

Allowed transitions are much stronger than Forbidden transitions

FORBIDDEN TRANSITIONS

i) Electric quadrupole (E2) transitions ($\Delta J = 0, \pm 1, \pm 2$, π - same)

$$A_{ji}^{E2} = 2.6733 \times 10^3 \frac{E_{ij}^5}{g_j} S^{E2}(i, j) \text{ s}^{-1}, \quad (3)$$

ii) Magnetic dipole (M1) transitions ($\Delta J = 0, \pm 1$, π - same)

$$A_{ji}^{M1} = 3.5644 \times 10^4 \frac{E_{ij}^3}{g_j} S^{M1}(i, j) \text{ s}^{-1}, \quad (4)$$

iii) Electric octupole (E3) transitions ($\Delta J = \pm 2, \pm 3$, π changes)

$$A_{ji}^{E3} = 1.2050 \times 10^{-3} \frac{E_{ij}^7}{g_j} S^{E3}(i, j) \text{ s}^{-1}, \quad (5)$$

iv) Magnetic quadrupole (M2) transitions ($\Delta J = \pm 2$, π changes)

$$A_{ji}^{M2} = 2.3727 \times 10^{-2} \text{ s}^{-1} \frac{E_{ij}^5}{g_j} S^{M2}(i, j). \quad (6)$$

LIFETIME:

$$\tau_k(s) = \frac{1}{\sum_i A_{ki}(s^{-1})}.$$

Monochromatic Opacity (κ_ν): $\kappa_\nu(i \rightarrow j) = \frac{\pi e^2}{mc} N_i f_{ij} \phi_\nu$

Selection Rules: ALLOWED & FORBIDDEN TRANSITIONS

- E1 transitions are strong and are given the name allowed while E2, E3, ..., M1, M2, ... are much weaker and are referred to as forbidden. However, with higher charges, E2 which varies as z^6 and M1 as z^8 increases faster than E1 which varies as z^2 .
- E2 and M1 can become comparable to each other with highly charged ions, as seen in tungsten case.
- The forbidden transitions within the ground 3P state of highly charged Fe XIII was strong to be observed in solar flare by Edlen. He calculated and found that the flare temperature over million degrees compared to the assumed value of a few thousand degrees. Solar surface temperature is 5770 K.

He-LIKE ION: ALLOWED & FORBIDDEN TRANSITIONS

Diagnostic Lines of He-like Ions: w,x,y,z

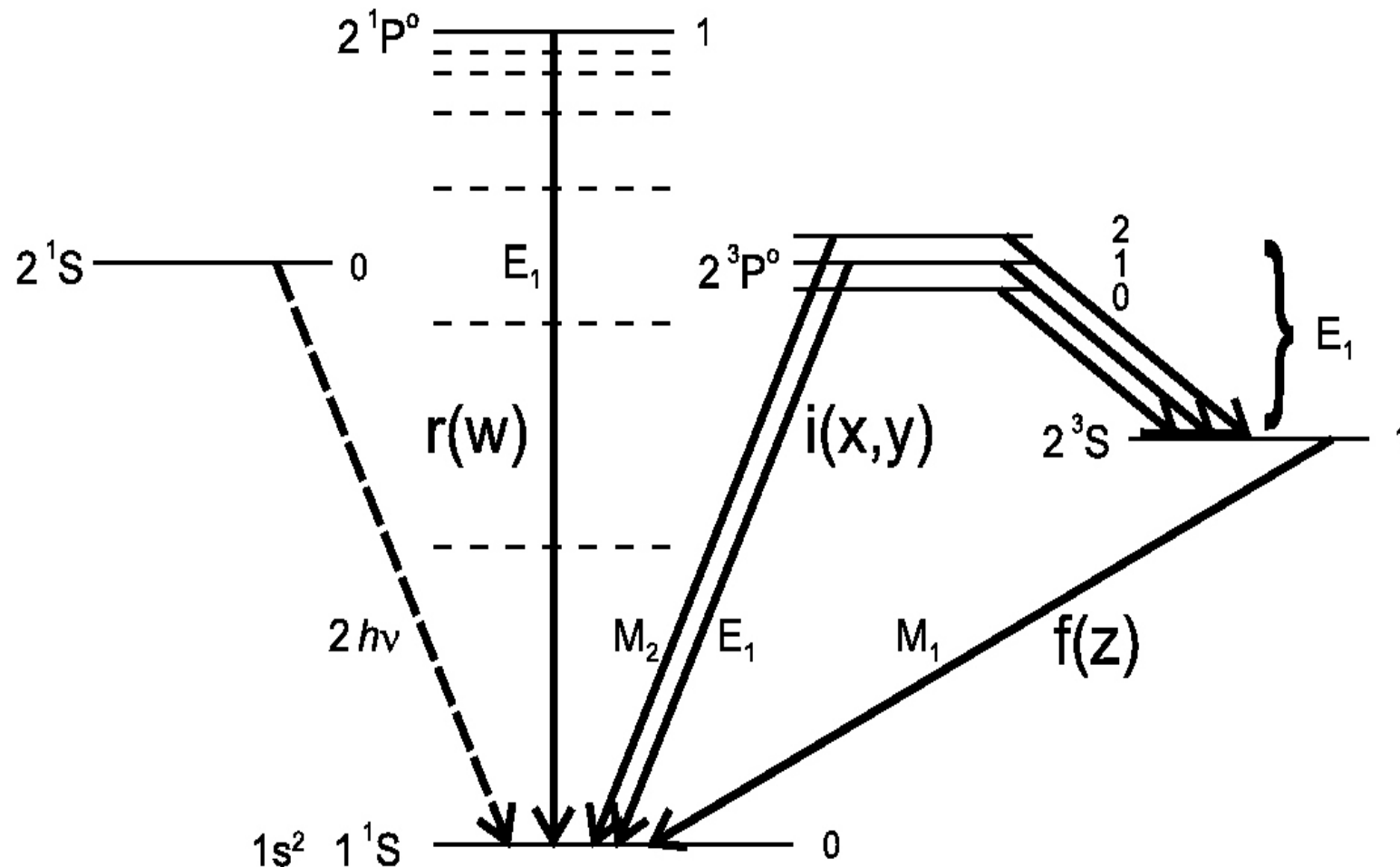
w(E1) : $1s2p(^1P_1^o) - 1s^2(^1S_0)$ (Allowed Resonant)

x(M2) : $1s2p(^3P_2^o) - 1s^2(^1S_0)$ (Forbidden)

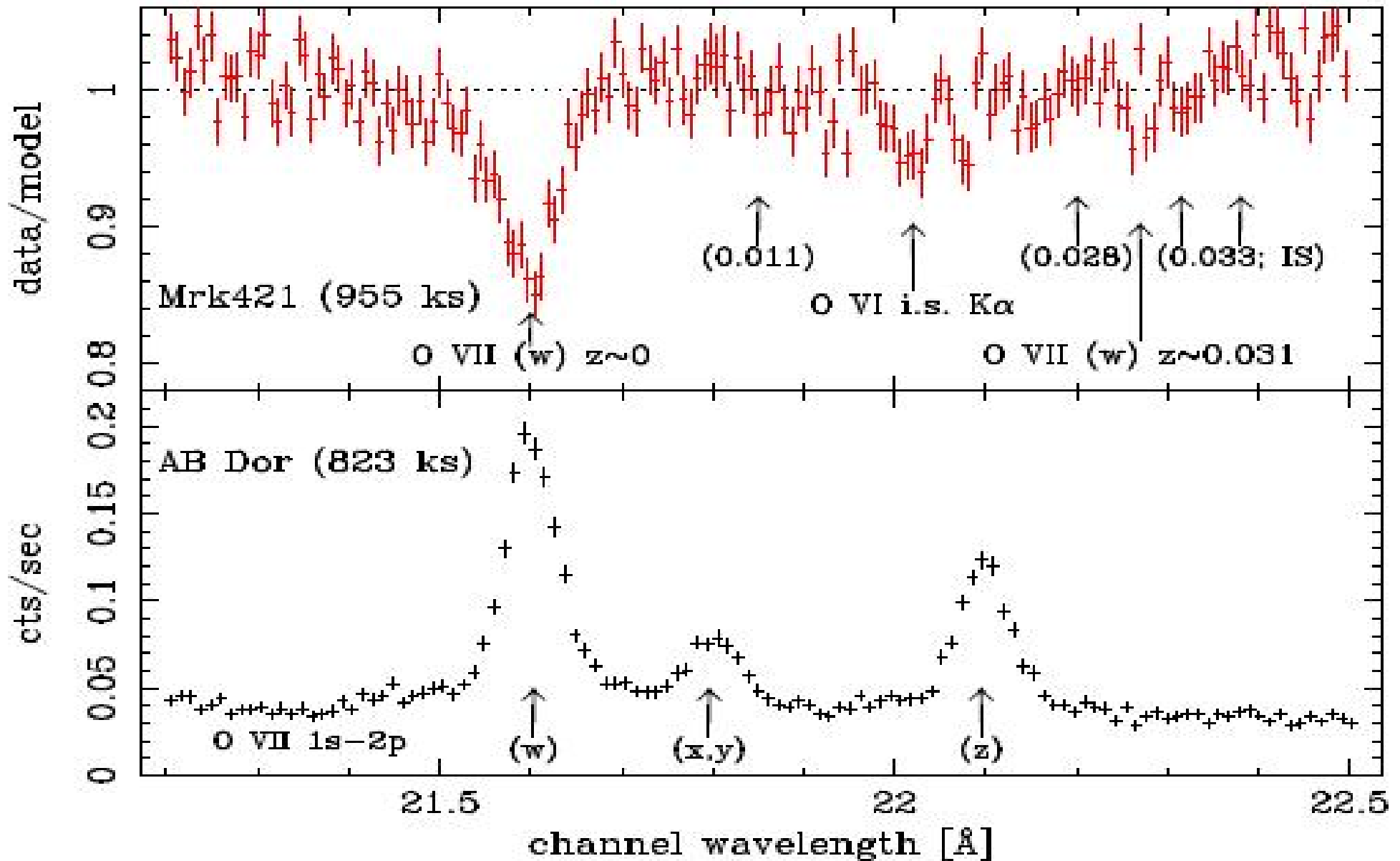
y(E1) : $1s2p(^3P_1^o) - 1s^2(^1S_0)$ (Intercombination)

z(M1) : $1s2s(^3S_1) - 1s^2(^1S_0)$ (Forbidden)

NOTE: 1s-2p are the K_α transitions



O VII w,x,y,z LINES IN ASTROPHYSICAL SPECTRA

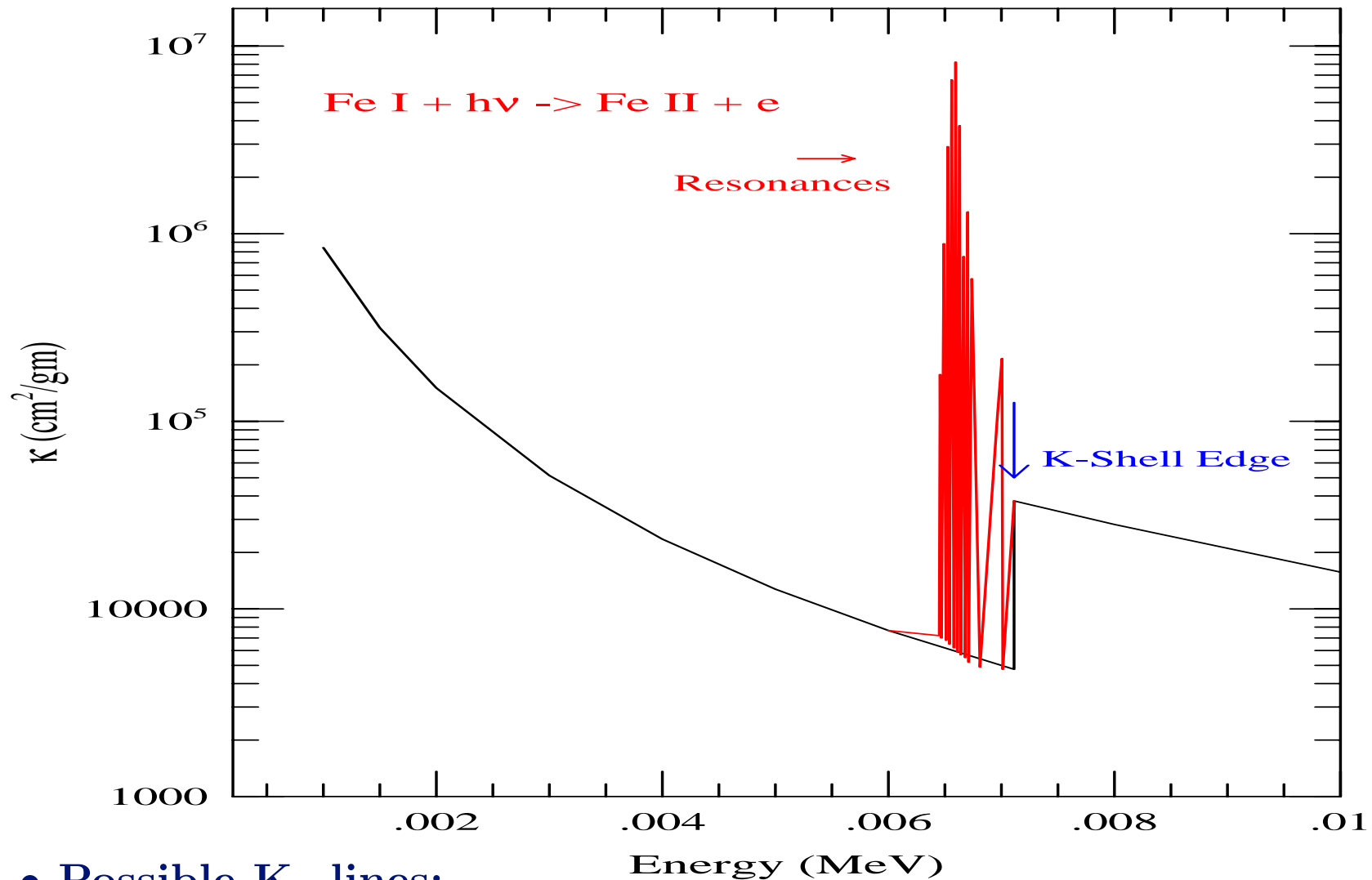


- These lines are detected in the X-ray spectra of AB DOR (AB Doradus is a quadruple star system in the constellation Dorado), and of Mrk 421 galaxy by XMM-Newton observatory (Rasmussen et al 2007)

K- α RESONANCES IN Fe PHOTOIONIZATION

(Pradhan, Nahar, Montenegro et al 2009)

Photo-Absorption Coefficient of Iron



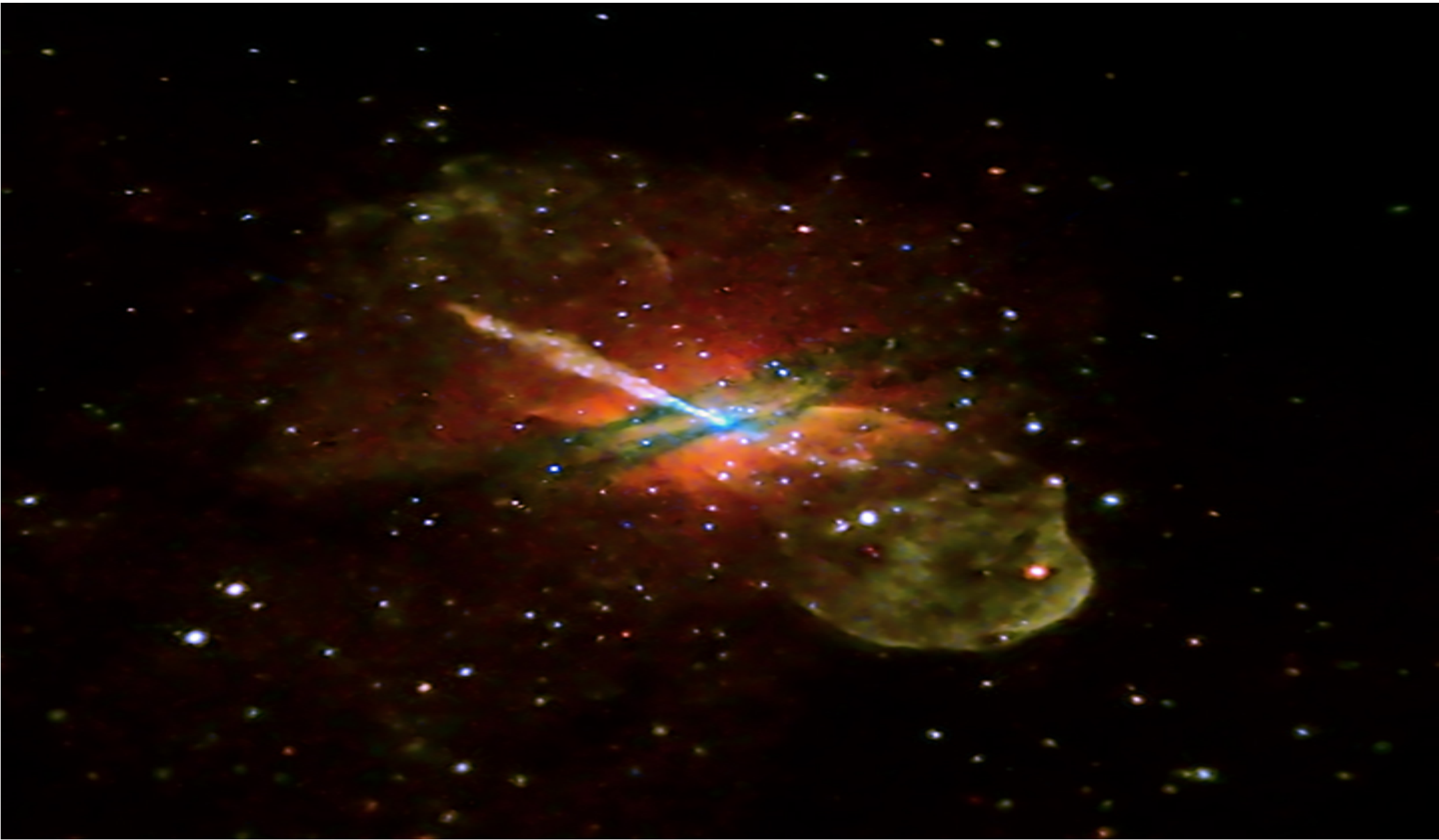
- Possible K $_{\alpha}$ lines:

$1s^2 \rightarrow 2p^5, 2p^4, 2p^3, 2p^2, 2p, 2p^-$

$1s \rightarrow 2p^5, 2p^4, 2p^3, 2p^2, 2p, 2p^-$

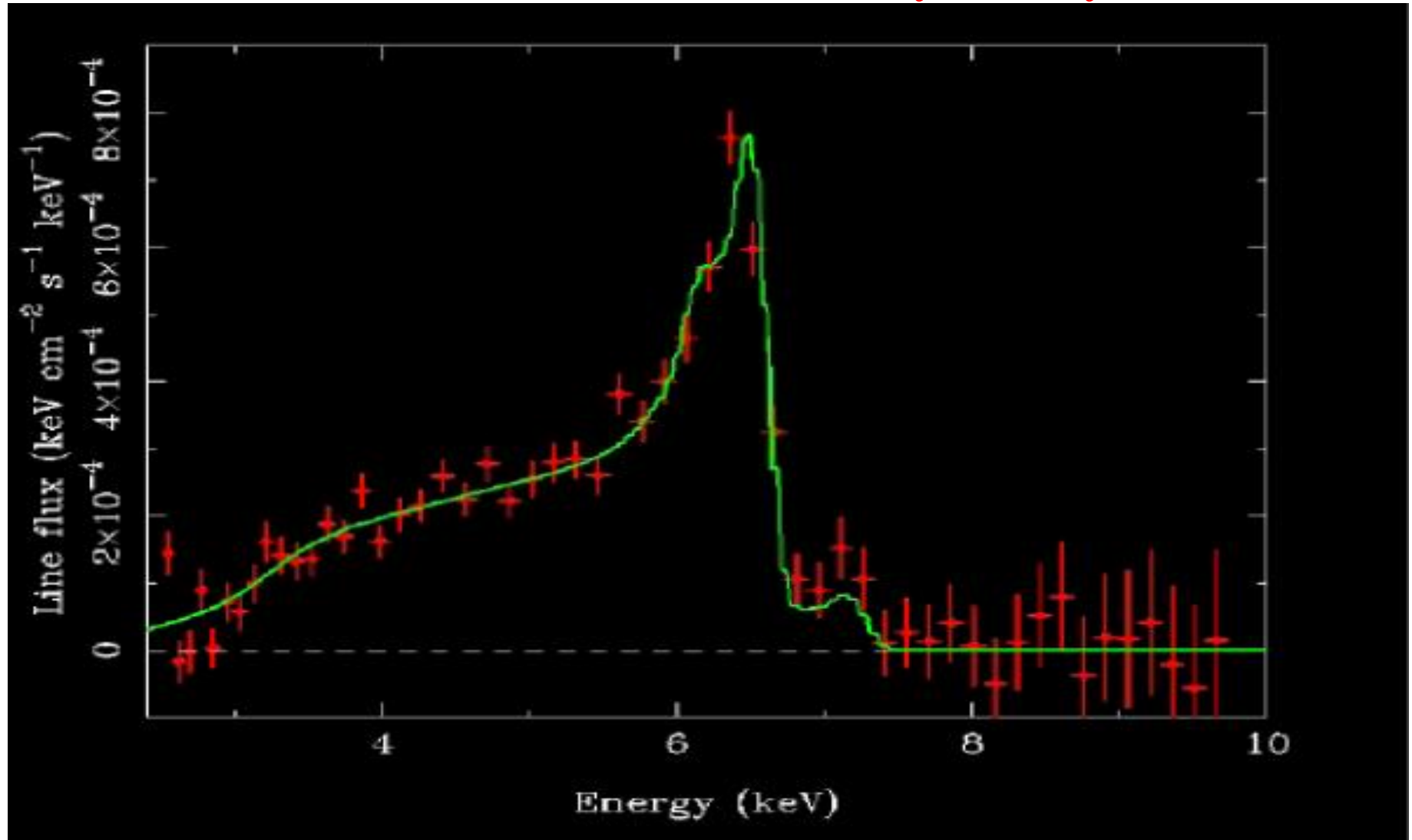
- There are 112 narrow resonances in the energy range of 6.457 - 7 keV formed due to 1s-2p (K $_{\alpha}$) transitions

X-RAYS FROM A BLACK HOLE - CENTAURUS A GALAXY (Chandra)



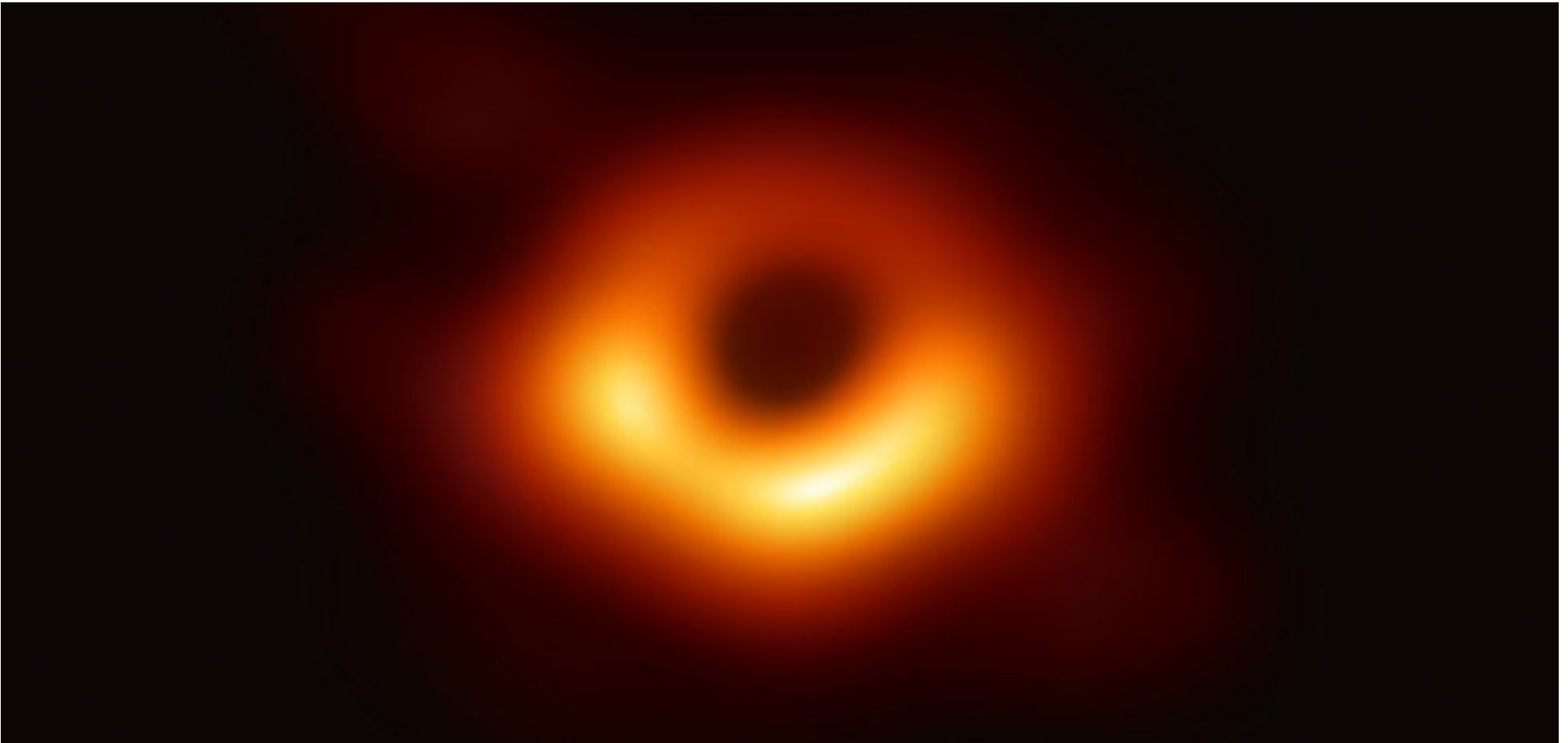
- Photometric image: red - low, green - intermediate, blue - high energy X-rays. Dark green & blue bands - dust lanes that absorb X-rays
- Blasting from the black hole a jet of a billion solar-masses extending to 13,000 light years

SIGNATURE OF A BLACK HOLE: SeyfertI Gy MCG-6-30-15 6



- The energy range for 1s-2p transitions in Fe = 6.4 - 7 keV. However, the large extension of the lines toward low energy, 3 - 7 keV, indicate that the escaped photons have lost energies in the gravitational force of the black hole. (Illustrated in AAS, Pradhan and Nahar 2011)

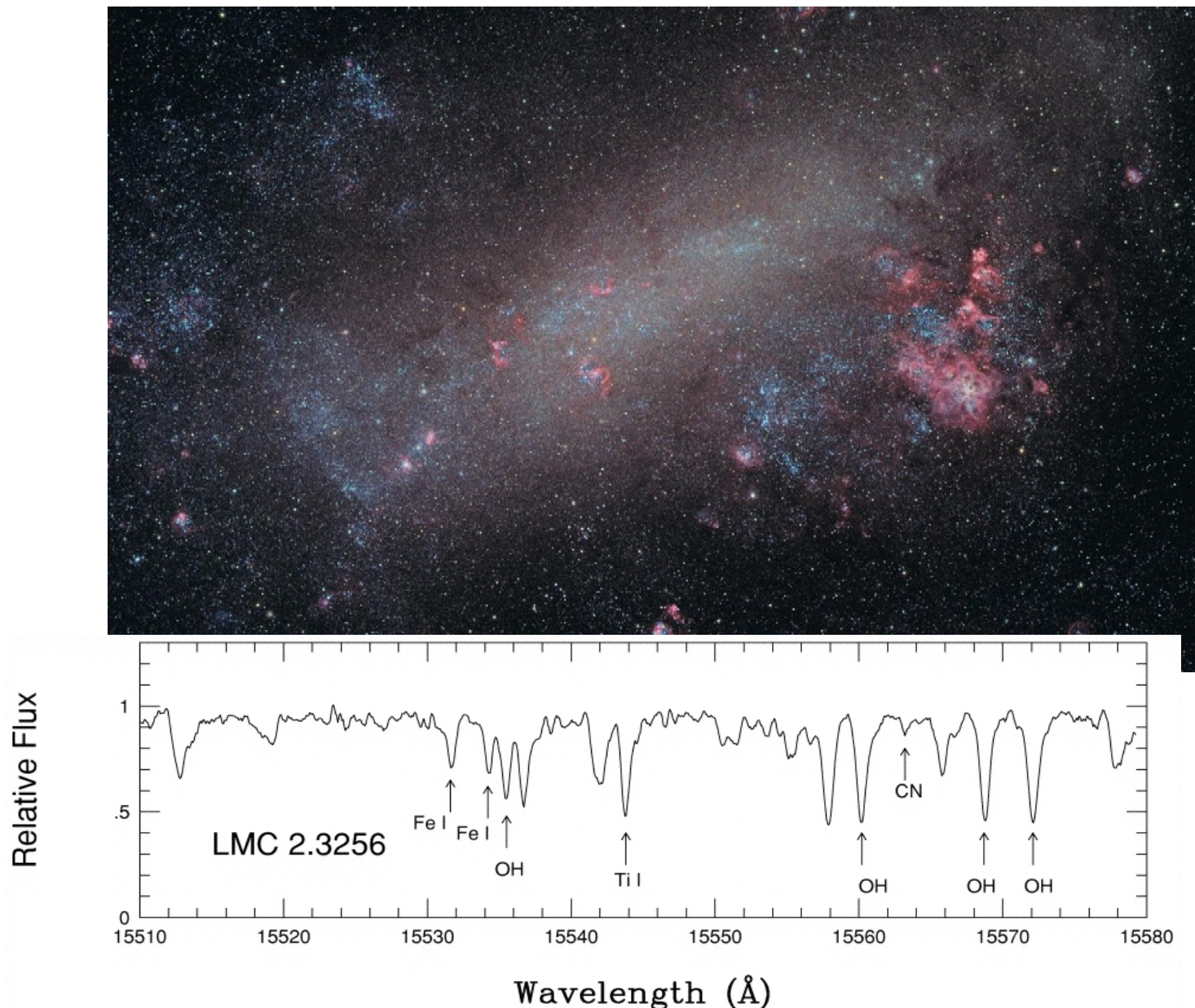
First ever black hole image released, Apr 10, 2019



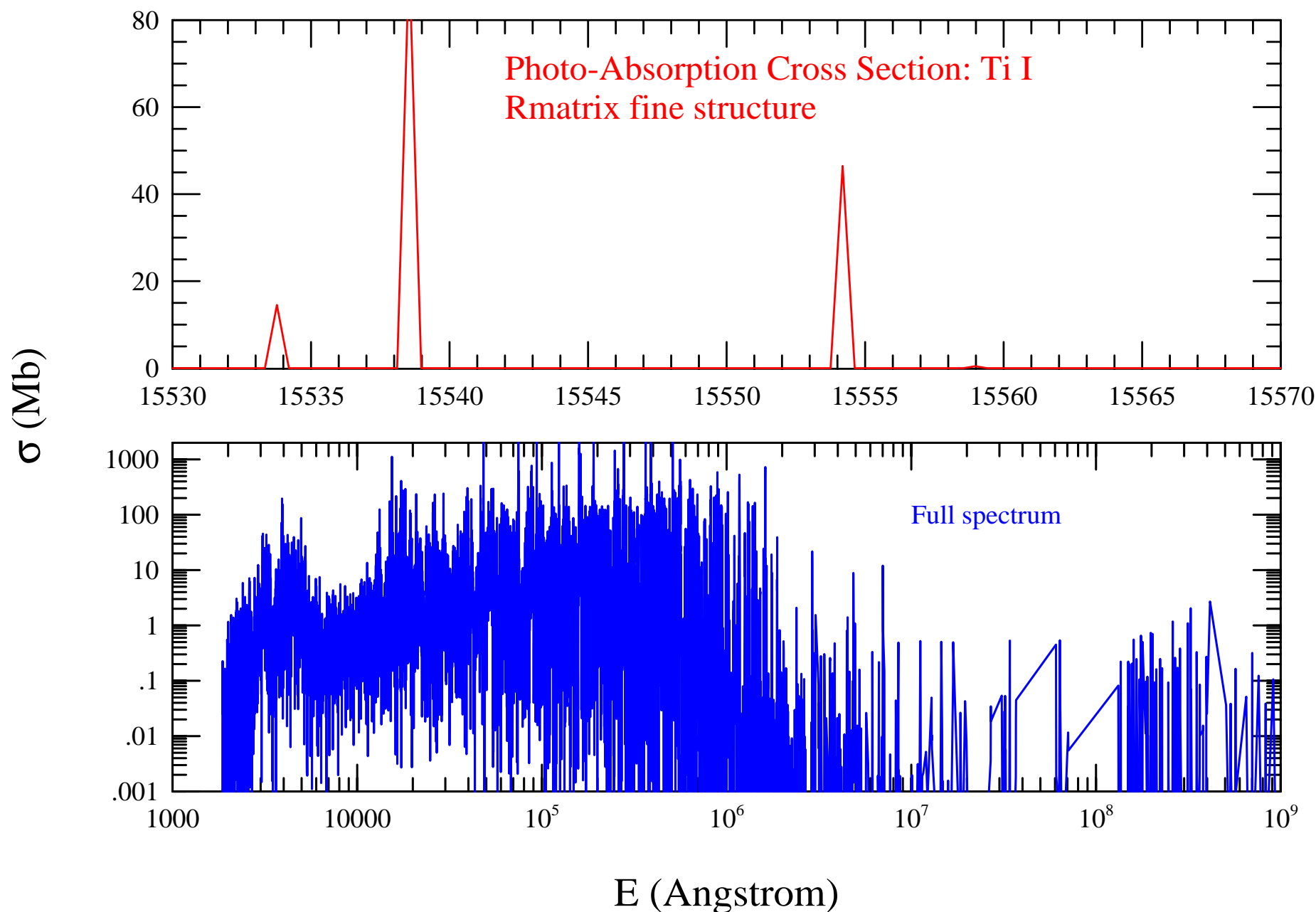
- The first ever image of a black hole, located in a distant galaxy, measures 40 Bkm across - 3M times the size of the Earth - and has been described as "a monster". It was composed from photographs by a network of eight "Event Horizon" telescopes across the world.
- The monster black hole in the center of our Milky Way galaxy: 4M time heavier than our Sun, tracked by the movement of 28 stars circling around it - Nobel prize in 2020

OBSERVATION OF Ti I LINES:

- LMC (Cloud around our Milky Way) 157 ly away, but is a prime target to probe the chemical evolution of stars.
- Ti I in LMC Spectra: PHOENIX, Gemini South.
- Ti line at 15544 Å.



PREDICTED SPECTRUM OF Ti I: IDENTIFY LINE



- TOP: lines in 15535 - 15560 indicating the observed line of LMC •
- Bottom: Total spectrum, number of lines / transitions = 270,423

SPECTROSCOPY OF LINES IN PLASMAS USING OSCILLATOR STRENGTHS

- For a plasma condition dependent spectrum, the theoretical spectrum can be run through the popularly used astrophysical **SME spectra program** (a python based program) with temperature and abundances of elements. (check website: <https://www.stsci.edu/valenti/sme.html> - valenti and piskunov)

- When two lines, 1 and 2. in **an LTE plasma (follow Boltzman-Saha equation)** are observed which are originating from the same level but going to different levels, temperature and density dependence for the lines are the same and hence do not enter in the diagnostics. Only ratio of A-values can be used to predict the observed ratio.

level 1 of energy E_1 (in eV) emits a photon of wavelength λ_1 with transition probability A_1 and decaying to the level with statistical weight factor g_1 , and level 2 has the similar parameters denoted by subscript 2. The line intensity I ratio of the two lines are given by

$$R = \frac{I_1}{I_2} = \frac{\lambda_2 A_1 g_1}{\lambda_1 A_2 g_2} \exp \left[-\frac{E_1 - E_2}{KT} \right] \quad (7)$$

where K is the Boltzmann constant, T is the plasma temperature is K, E is the transition energy in eV. The overall number of electron collisions must be high to achieve LTE.

SPECTROSCOPY OF LINES IN PLASMAS

The McWhirter criterion establishes the minimal or limiting value of electron density n_e in cm^{-3} for this purpose.

$$n_e \geq 1.6 \times 10^{12} \sqrt{T} (\Delta E)^3 \quad (8)$$

where T is plasma temperature in Kelvin, and $\Delta E = (E_1 - E_2)$ in eV. The other plasma parameters such as plasma frequency, skin depth and coupling parameter can be related with electron density as

$$n_e = 0.124 \times 10^{-9} \omega_e^2$$

$$n_e = 28.1961 \times 10^{10} \delta^{-2}$$

$$\Gamma = \frac{q_e^2}{4\pi\epsilon_0 k} \left[\frac{4\pi}{3} \right]^{1/3} \frac{n_e^{1/3}}{T_e}$$

In the above equations ω_e , δ , Γ are the plasma frequency, skin depth, and coupling parameter, respectively. Skin depth, δ , is defined as the depth where the current density is just $1/e$ (about 37%) of the value at the surface; it depends on the frequency of the current and the electrical and magnetic properties of the conductor.