

Elements in and Spectroscopy of Astrophysical Plasmas, and Elemental Identification of the Black Hole X-rays of GRO J1655–40

High School Research Thesis

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Abstract

Taking a spectroscopic signature of any astronomical event or object gives insight into many important characteristics of the subject, such as composition, temperature, motion, etc. This project looks at the spectroscopic signature of elements coming from the GRO binary star system, which consists of the F3 IV–F6 IV star along with a black hole. This black hole emits radiation in the soft X-ray band. Using the atomic structure program SUPERSTRUCTURE, the wavelength and atomic probability emitted by various ions, identified by Miller et al., found in the accretion disk of the black hole were calculated and recorded. These theoretical calculations were then compared with those experimentally found by NIST.

Dedication

Dedication to my parents for their constant love and support for my passions. And to my brother for pursuing his passions and being a role model which I can follow.

Acknowledgments

I would like to first thank God. I would also like to thank my family for their endless support. Thank you to Dr. Nahar for providing me guidance and mentorship throughout the project, and to the Indo-US APJ Abdul Kalam STEM Center of The Ohio State University and Aligarh Muslim University along with their Research Promotion Program for providing the research scope, financial support, and opportunity for my research project.

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1. Introduction

Spectroscopy uses the science of electron transitions and the quantum mechanics of atoms to study astronomic objects and their physical features. Spectrums produced by atoms within the object can tell us about composition, temperature, and processes of faraway environments. Spectroscopy is especially useful in far environments like black holes, where information normally can't be obtained due to the black hole's strong gravity. Using spectroscopy, the radiation from accretion disk of the black hole can be analyzed to learn about the black hole itself. The binary star system GRO J1655-40, containing a black hole and a star, is an example of this where the black hole's accretion disk can be analyzed using spectroscopy. In this paper, the spectrum of the disk is analyzed and found to include the ions Mg XII, Si XIII, Si XIV, Al XIII, Fe XXIV, and Ni XXVI. Using the atomic structure program SUPERSTRUCTURE, I calculated the energy levels and characteristics of different properties, and compared them with data from the National Institute of Standards and Technology (NIST) atomic database. This paper demonstrates the application of atomic structure and spectroscopy to astrophysical systems.

2. Theoretical background

2.1. Creation of Elements

The elements which make up the world around us weren't always present in their current state.

2.1.1. Nuclear Mechanisms

Elements were "created" through two separate processes or mechanisms.

1. Nuclear Fusion is the combination or fusion of two atoms into one. The act of chemically forming something new, in this case the creation of an element, causes energy to be released as a byproduct. The resulting element, with atomic number n , occurs according to the sum of the protons, a and b , in the atoms fused where $n = a + b$.
2. Neutron Capture occurs when free-floating neutrons are attracted to a nearby atom as a result of the nuclear force. These new neutrons upset the proton-neutron balance in the atom, causing neutrons to undergo beta decay and become a proton while emitting an electron and an antineutrino. This process can occur relatively quickly (the r -process) or slowly (s -process). In neutron-dense environments, the r -process is more common and causes multiple neutron captures before a single beta decay.

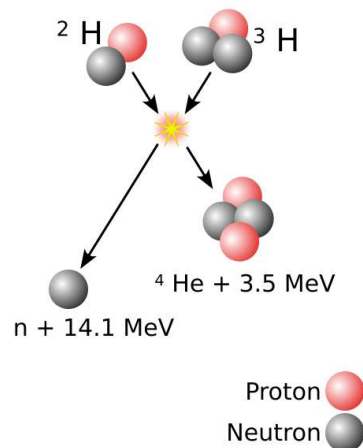


Figure 1: Nuclear Fusion: Fusion of deuterium (Hydrogen-2) and tritium (Hydrogen-3) to create Helium-4; This releases 17.59 MeV of energy

2.1.2. Astrophysical Systems

The universe holds a vast collection of differing environments. Based on the present environment and available reactants, elements might be created in different ways. Different environments cause different mechanisms to occur, and as a result different elements.

At the beginning of the universe, around the Big Bang, neutrons and electrons interconverted but there was no change in the universe's overall composition. Due to the explosive nature of the Big Bang, the early universe was too hot to sustain anything other than fundamental particles. Nucleosynthesis began once temperatures cooled to less than 1 Mega-Electron Volt (MeV). At this time, protons and electrons began to make up hydrogen atoms, allowing nuclear fusion to create elements from Helium-4 up to Lithium.

Since the beginning of the universe, nuclear fusion has continued to occur as the source of energy in stars. Inside of stars, hydrogen fusion and other catalytic cycles like the CNO-I cycle (using C, N, and O as intermediaries to cycle between elements producing energy) maintain the needed energy of stars. Stars finally die when these processes end due to the depletion of Hydrogen within the star and fusion hitting a “roadblock” at iron.

A star's death can also be an environment ripe for the creation of elements. When a relatively “small” star dies, it causes a nova explosion to occur. This explosion causes the elements remaining in the old star to get shuffled within a region, allowing for nuclear fusion to occur.

A supernova is the result of the death of a particularly massive star or white dwarf. This explosion causes explosive nucleosynthesis, neutron capture, and nuclear fusion to all occur due to the rich resulting environment. Explosive nucleosynthesis refers to the synthesis

of elements from Oxygen (O) to the Iron (Fe) group. This mechanism is what powers the brightness of the explosion. Due to the resulting high temperatures, neutron capture occurs almost immediately, and creates gold, platinum, uranium, and other rare earth elements. Lastly, nuclear fusion occurs in the outer layer of the explosion and creates ^{92}Mo and ^{144}Sm . Such an explosion is especially important for our current understanding of the universe because its violent nature causes its products to spread out and enrich the surrounding areas.

One of the most consequential events is known as a neutron star merger. Neutron stars are extremely neutron-dense bodies formed from the collapsed core of a massive giant star. The merger of two of these neutron stars creates an extremely chaotic and explosive environment full of free neutrons. The resulting kilonova and neutron-dense region allows neutron capture to repeatedly occur in a relatively short period of time. This “rapid” version of neutron capture is known as r -process neutron capture. Neutron star mergers create around half of the possible isotopes past iron.

2.2. Plasma

Plasma, also known as the fourth state of matter, is a result of gas undergoing ionization. Plasma consists largely of charged particles. It makes up 99.9% of the Universe, including stars and dominates regions like intracluster and intergalactic mediums. Plasma can be described by the abundance of certain elements within it; the abundance (percent) of Hydrogen within the material is denoted as X , the abundance of Helium is denoted as Y , and the abundance of all other elements, known as metals, is denoted as Z . The last of these (metal abundance), despite making up a low percent of the material, is the main cause of

the material's spectral features.



Figure 2: Dark strands of plasma hovering above the Sun's surface engaging in a "tug of war".

Conducting research involving charged materials can be difficult due to the great distance between us and them and the inability to manipulate the subject as we please. To address this, various instruments are used in laboratories to replicate plasma. These include Electron Beam Ion Traps (EBIT), plasma trapped in rings interacting with electron beams, and Advanced Light Sources (ALS), photons mounted on accelerators targeting "stored" ions.

2.3. Spectroscopy & Quantum Mechanics

Spectroscopy is the study of interactions between matter and electromagnetic radiation, and is crucial to the study of astronomical systems and objects. It is built upon the work of many

prominent scientists, and spans several topics from the radiation of the sun to the behavior of fermions and bosons.

2.3.1. A brief history

Spectroscopy dates back to Sir Isaac Newton. Around the 17th century, he conducted experiments with sunlight and prisms to learn about color. His experiments led to many discoveries, like the identification of the visible band of light and that white light is a combination of all colors.

While Newton’s initial experiments would lay the foundations of spectroscopy, the beginning of spectroscopy used for astronomical purposes was in 1802 and 1815, when Wollaston and Fraunhofer independently discovered “dark lines”—an absorption spectrum—of the sun.

One of the most important physicists, Johannes Rydberg, helped propel spectroscopy even further. Rydberg’s most important contributions were his efforts to analyze spectral lines, the creation of the Rydberg formula along with the accompanying constant, the Rydberg.

All of this work by past physicists would benefit greatly throughout the 20th century, when various innovations would also be made in the world of quantum mechanics. This includes the discovery of Schrödinger’s equation by Erwin Schrödinger, the Pauli Exclusion Principle by Wolfgang Pauli, and many others by the likes of Heisenberg and Einstein.

Another important contribution is Russell & Saunders’ utilization of quantum mechanics to find algebraic rules for S (total spin) and L (angular momenta) of electrons in an atom. This led to the creation of Russell-Saunders coupling (aka LS coupling), which lays

the basis for the spectral ID of states of an atom.

2.3.2. Spectroscopy

When an electron changes states (locations), this means there is an electron transition within the atom. These electron transitions can cause photons, particles of light, to be emitted or absorbed. The wavelength of this radiation is proportional to the difference in energies between the final and initial state of the electron. This is one of the central ideas of spectroscopy.

Spectroscopy analyzes radiation detected from a subject in the universe, and organizes it into a high resolution spectrum based on wavelengths. Variables describing the subject such as motion, temperature, and composition can be found using this spectrum.

2.3.3. The Physics behind Spectroscopy

Each electron within an atom inhabits a different area, called a subshell. This “area” is actually a probabilistic region that the electron is most likely to be in. These areas/regions are denoted as the s, p, d, and f sub-level with each being a different shape: a sphere, “dumbbell”, clover, and complex shape respectively. However, these are not the only four areas that electrons can inhabit. Each of the regions within an atom can have a different size corresponding to the energy of that region; the larger the area, the higher the energy. These regions are determined by the wavefunction, a fundamental equation in Quantum Mechanics.

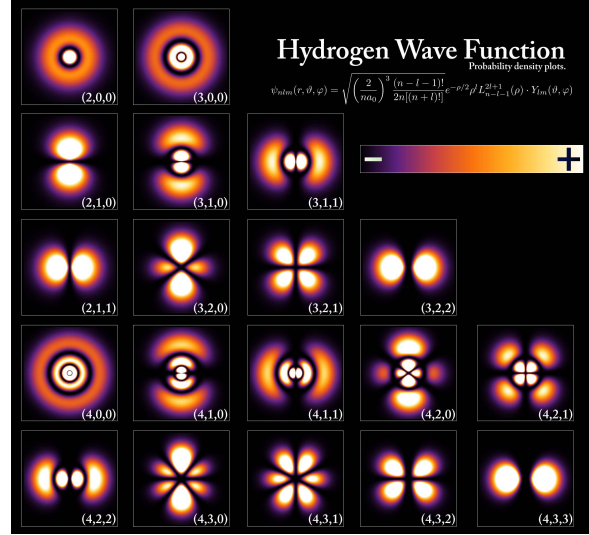


Figure 3: A visualization of the subshells of Hydrogen as calculated by the wavefunction. The probability of finding the electron is given by the color, as shown in the key in the top right.

The radiation detected from an atom is due to a change in state of an electron within the atom. This change in state can be one of two kinds: an absorption or an emission. An absorption is caused when a particle of light, or a photon, is absorbed by an electron. This sudden burst in energy allows the electron to move past its initial “ground state” into a higher, excited state. The energy of the absorbed photon is equal to the difference in energies between the two states.

However, an electron in an excited state is unstable. Due to this instability, the electron eventually must jump back down to its original ground state. When it jumps, the electron emits a photon equal to the difference in energies of its excited and ground states.

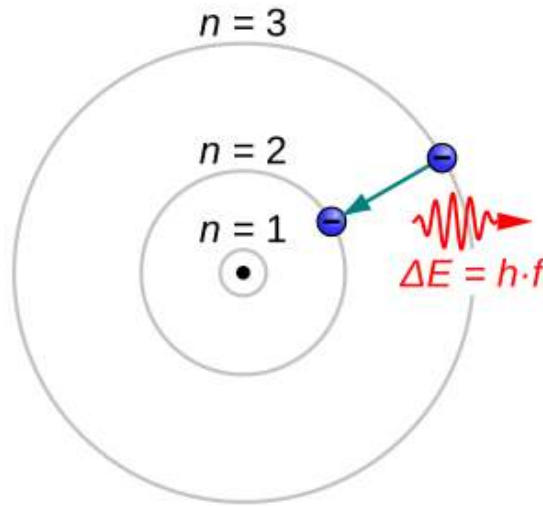


Figure 4: An electron jumping from $n = 3$ to $n = 2$, from its excited state to its ground state, and emitting a photon **Source:** <https://commons.wikimedia.org/wiki/File:Bohr-atom-electron-to-jump.svg>.

2.3.4. Spectroscopy Applications

As previously mentioned, Johannes Rydberg was a pioneer in the world of spectroscopy. The Rydberg Equation

$$\frac{1}{\lambda} = R_H \left[\frac{1}{n^2} - \frac{1}{n'^2} \right]$$

$$\Delta E_{n,n'} = \frac{hc}{\lambda}$$

was discovered by Rydberg and allows us to find the energy of a photon emitted or absorbed by an atom using the initial and final state of the electron that interacted with it. However, this equation, similar to some others dealing with atoms, has only fully been solved for the single-electron system of the Hydrogen atom.

For other single-electron systems, the equation remains mostly unchanged aside from the coefficient, which goes from R_H to RZ^2 :

$$\frac{1}{\lambda} = RZ^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Series transitions are another useful application of spectroscopic data. By itself, these series only aim to group electron transitions, but when used for other things their helpfulness is highlighted. Series transitions describe transitions from $n_1 = k$ to any higher level $n_2 = j$ as being part of the same transition series. These series represent solutions to the Rydberg equation for a chosen lower energy level. These series transitions are labeled according to the physicists who discovered them: $n_1 = 1$ is the Lyman Series, $n_1 = 2$ is the Balmer Series, and the rest being the Paschen Series, Brackett Series, etc. for increasing n_1 . Within each series, transitions can be specified further using Greek letters. For any series, a step to the immediate next level (n_1 to $n_1 + 1$) is denoted as α ; a jump two levels up is β ; a jump three levels up is γ ; etc. Series transitions can also be used to find the region a specific transition lies on the electromagnetic spectrum. By using the Rydberg Equation, and setting the final energy level (n') to infinity, the wavelength a series converges to can be found and plotted on the spectrum.

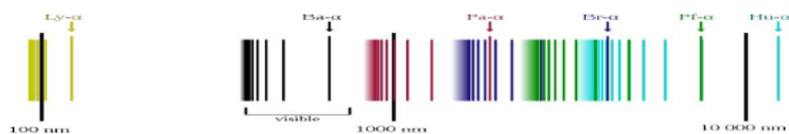


Figure 5: All the transition series' plotted on the electromagnetic spectrum **Source:** <https://wikimedia.org>.

Quantum Mechanics

Spectroscopy and everything dealing in the quantum world is built on the laws of Quantum Mechanics.

The wave function is one of the foundation concepts in Quantum Mechanics. This function describes the quantum state of an isolated system, and provides probabilistic solutions such as the position of an electron. This equation can only be applied to the Hydrogen Atom, for which it can be split into a function for each coordinate: $R(r)$ for the radial function and Y_l^m as the spherical harmonic.

Quantum Numbers

An electron can be described by four quantum numbers. These four quantum numbers are n , the principal quantum number; l , the azimuthal or angular momentum quantum number; m_l , the magnetic quantum number; and m_s , the spin quantum number.

The principal quantum number communicates the main energy level the electron resides in. This corresponds to the size of the electron's orbit and its radial distance from the nucleus. n can only be a positive number.

The azimuthal quantum number specifies the specific subshell of the electron. This number can be any non-negative integer up to $n - 1$, but is most commonly 0, 1, 2, or 3 (matching the s, p, d, and f subshells respectively).

The magnetic quantum number tells us the spatial orientation of the orbital. This number can be integers from $-l$ to l where l is the azimuthal quantum number.

Lastly, the spin quantum number tells us the spin of the electron. It can be either $-1/2$ or $1/2$.

Quantum Rules

There are certain rules which govern the behavior of electrons. A fundamental rule is that no two electrons in a single atom can share the same four quantum numbers. Every electron has its own identifiers, making each one unique.

The most important of these rules is the Pauli exclusion principle, which dictates that no two electrons can inhabit the same orbital. Orbitals are one level of specificity deeper than the subshell. These orbitals can only contain two electrons at most. Within each subshell type, there is a corresponding number of orbitals.

Other rules include:

- Hund's Rule of Maximum Multiplicity which states that all the orbitals in a subshell should house a single electron before any orbital gains a second.
- The Aufbau principle says orbitals and subshells should be filled in order of increasing energy. A subshell with energy $n = 1$ should be filled before one with energy $n = 2$.
- Madelung's Rule specifies the exact formula, $n + l$, to use when ordering subshells and orbitals for the Aufbau principle.

Types of particles

All particles of a given kind (ex. electrons, protons, photons, etc.) are physically indistinguishable from other particles of the same kind due to the "principle of indistinguishability." However, not all elementary particles share identical properties. All particles can be divided into two groups based upon their spin. These groupings depict their interaction with the wavefunction and probabilities derived from it.

Bosons are particles with a zero or integral spin. These particles can share the same state due to their characteristics causing symmetric (indistinguishable) solutions to the wavefunction. Examples of these include photons, which carry/transmit the electromagnetic force; gluons, which carry/transmit the strong nuclear force; and atomic nuclei with an even mass number (sum of neutrons and protons is even).

Fermions can be thought of as the opposite of bosons. Fermions have a half-integral spin because they have asymmetrical solutions to the wavefunction. This means fermions cannot share the same state. Examples of fermions include electrons (this is why they obey the Pauli exclusion principle); quarks, fundamental particles which make up large particles; protons, positive particles in atomic nuclei; and atomic nuclei with an odd mass number.

2.4. The X-ray Spectrum of a Black Hole

Black holes are some of the densest things in the universe. The most distinguishable characteristic of black holes is their extreme gravity, which prevents even light from escaping.

Black holes have several defining features:

- The center of a black hole is the singularity, where curvature of spacetime is infinite.
- The event horizon is a boundary some length r_1 from the singularity that marks the point of no return for light. From this point inwards, gravity is so strong it pulls even light in.
- The innermost stable circular orbit is a boundary some length r_2 from the singularity that describes the closest an object can be to have a stable orbit around the black hole.
- When a black hole has other bodies of matter near it, an accretion disk can form.

This is a circular disk surrounding the black hole formed from matter that the black hole has attracted towards it. The matter in this accretion disk slowly spirals into the singularity as it feels the pull of the black hole’s gravity.

For our purposes, the most important feature of a black hole is the accretion disk. The unique characteristic of this disk is the presence of matter in close proximity to the singularity. Due to many different possible factors like friction, gravity, or magnetic fields, accretion disks often emit radiation in the form of soft or hard X-rays (lower and higher energy X-rays). This radiation can be studied to learn about the black hole itself and also the system around it.

3. Methodologies and Description of the work

The target system and the basis of this research mirror the work done in “The magnetic nature of disk accretion onto black holes” by Miller et al.

3.1. The Miller Paper

The paper “The magnetic nature of disk accretion onto black holes” by Miller et al. focuses on the target system GRO J1655–40. This system is a binary star system, consisting of a star named F3 IV–F6 IV and a black hole. This star is about $2.3\times$ the mass of our sun, and has a 2.6 day orbit. The black hole has a mass $7\times$ that of our sun and accretes (takes) matter from its accompanying star. These two bodies are a distance of 3.2 kiloparsec (about 9.874×10^{16} kilometers) from each other. Along with these astronomical bodies, highly ionized winds caused by the accretion disk of the black hole are present.

Through a study of the spectral signature of the accretion disk, the reason for these

disk winds is hoped to be uncovered. This spectrum consists of X-rays in the soft X-ray band, and was observed through the Chandra X-ray telescope.

The resulting spectrum showcased 90 absorption lines significant at the 5σ level of confidence or higher. Using this spectrum, 76 lines with resonance can be confidently identified from over 32 charge states. Additionally, this spectrum is consistent with absorption in a geometric model of the accretion disk (constant-density slab).

Using this data, Miller et al. were able to determine that the disk winds were magnetically driven because all other plausible causes could be ruled out:

1. The disk winds were too highly ionized to be driven by radiation pressure; absorption was mainly from He-like and H-like species, causing little UV opacity in the wind.
2. The ionization parameters indicate any UV emission lines couldn't add any force.
3. Wind could be driven by magnetic **and** centrifugal force, but no data is available on tangential velocities.

3.2. Calculations and Simulations

Using the ions in the accretion disk, identified by Miller et al. through Chandra, I was able to conduct my own calculations using the SUPERSTRUCTURE program along with corroboration by the NIST database.

3.2.1. SUPERSTRUCTURE

SUPERSTRUCTURE is an atomic structure program created and optimized by Eissner et al. (1974) and Nahar et al. (2003). It utilizes a Fortran network for organization, and modified wavefunctions to calculate characteristics of ions, their configurations, and corresponding

transitions.

3.2.2. Utilization of NIST

The National Institute of Standards and Technology (NIST), a federal agency of the US government, houses an in-depth public database of data on atomic spectra. This data was obtained by various experiments over the years and includes information on transition lines, configuration energies, and more.

Using this database, I was able to compare the calculated values obtained using SUPERSTRUCTURE with experimental values in NIST. The values had agreement with percent differences around 1% or lower.

4. Results and Discussions

4.1. Results

4.1.1. Energy Comparison Tables

Tables 1–6, six in total, show a comparison between the calculated (SS) and measured (NIST) energies for each ion (Mg XII, Si XIII, Si XIV, Fe XXIV, Ni XXVI, and Al XIII) up to the transitional levels observed in their spectrum.

There was good agreement between the calculated and measured values, with the percent difference being consistently below 1%.

These energies were then compared with the observed spectrum, and had good agreement for all but one.

Table 1: Comparison between calculated (SS) and measured (NIST) energies of Al XIII

K	Configuration Term	E _{SS} (Ry)	E _{NIST} (Ry)	% Diff	K	Configuration Term	E _{SS} (Ry)	E _{NIST} (Ry)	% Diff
1	1s ($^2S_{1/2}$)	0	0	0	9	3d ($^2D_{5/2}$)	150.598	150.569	0.02
2	2p ($^2P^{\circ}_{1/2}$)	127.012	126.983	0.02	10	4p ($^2P^{\circ}_{1/2}$)	158.799	158.770	0.02
3	2p ($^2P^{\circ}_{3/2}$)	127.107	127.078	0.02	11	4p ($^2P^{\circ}_{3/2}$)	158.811	158.781	0.02
4	2s ($^2S_{1/2}$)	127.012	126.986	0.02	12	4s ($^2S_{1/2}$)	158.799	158.770	0.02
5	3p ($^2P^{\circ}_{1/2}$)	150.561	150.531	0.02	13	4d ($^2D_{3/2}$)	158.811	158.781	0.02
6	3p ($^2P^{\circ}_{3/2}$)	150.589	150.560	0.02	14	4d ($^2D_{5/2}$)	158.815	158.785	0.02
7	3s ($^2S_{1/2}$)	150.561	150.532	0.02	15	4f ($^2F^{\circ}_{5/2}$)	158.815	158.785	0.02
8	3d ($^2D_{3/2}$)	150.589	150.560	0.02	16	4f ($^2F^{\circ}_{7/2}$)	158.817	158.787	0.02

Table 2: Comparison between calculated (SS) and measured (NIST) energies of Mg XII

K	Configuration Term	E _{SS} (Ry)	E _{NIST} (Ry)	% Diff	K	Configuration Term	E _{SS} (Ry)	E _{NIST} (Ry)	% Diff
1	1s ($^2S_{1/2}$)	0	0	0	9	3d ($^2D_{5/2}$)	128.273	128.250	0.02
2	2p ($^2P^{\circ}_{1/2}$)	108.190	108.167	0.02	10	4p ($^2P^{\circ}_{1/2}$)	135.263	135.239	0.02
3	2p ($^2P^{\circ}_{3/2}$)	108.259	108.237	0.02	11	4p ($^2P^{\circ}_{3/2}$)	135.272	135.248	0.02
4	2s ($^2S_{1/2}$)	108.190	108.170	0.02	12	4s ($^2S_{1/2}$)	135.263	135.240	0.02
5	3p ($^2P^{\circ}_{1/2}$)	128.246	128.223	0.02	13	4d ($^2D_{3/2}$)	135.271	135.248	0.02
6	3p ($^2P^{\circ}_{3/2}$)	128.266	128.243	0.02	14	4d ($^2D_{5/2}$)	135.274	135.251	0.02
7	3s ($^2S_{1/2}$)	128.246	128.224	0.02	15	5p ($^2P^{\circ}_{1/2}$)	138.509	138.486	0.02
8	3d ($^2D_{3/2}$)	128.266	128.243	0.02	16	5p ($^2P^{\circ}_{3/2}$)	138.513	138.490	0.02

K	Configuration Term	E _{SS} (Ry)	E _{NIST} (Ry)	% Diff	K	Configuration Term	E _{SS} (Ry)	E _{NIST} (Ry)	% Diff
17	5s ($^2S_{1/2}$)	138.509	138.486	0.02	20	6s ($^2S_{1/2}$)	140.272	140.249	0.02
18	6p ($^2P^{\circ}_{1/2}$)	140.272	140.249	0.02	21	7p ($^2P^{\circ}_{1/2}$)	141.335	141.312	0.02
19	6p ($^2P^{\circ}_{3/2}$)	140.275	140.251	0.02	22	7p ($^2P^{\circ}_{3/2}$)	141.336	141.313	0.02

Table 3: Comparison between calculated (SS) and measured (NIST) energies of Si XIII

K	Configuration Term	E _{SS} (Ry)	E _{NIST} (Ry)	% Diff	K	Configuration Term	E _{SS} (Ry)	E _{NIST} (Ry)	% Diff
1	1s ² (¹ S ₀)	0	0	0	9	1s 3p (³ P ^o ₀)	160.251	160.185	0.04
2	1s 2s (³ S ₁)	135.281	135.197	0.06	10	1s 3p (³ P ^o ₁)	160.260	160.190	0.04
3	1s 2p (³ P ^o ₀)	136.272	136.234	0.03	11	1s 3p (³ P ^o ₂)	160.281	160.209	0.05
4	1s 2p (³ P ^o ₁)	136.305	136.250	0.04	12	1s 3s (¹ S ₀)	160.254	160.195	0.04
5	1s 2p (³ P ^o ₂)	136.380	136.316	0.05	13	1s 3d (³ D ₁)	160.438	160.367	0.04
6	1s 2s (¹ S ₀)	136.358	136.316	0.03	14	1s 3d (³ D ₂)	160.440	160.367	0.05
7	1s 2p (¹ P ^o ₁)	137.162	137.075	0.06	15	1s 3d (³ D ₃)	160.448	160.474	0.02
8	1s 3s (³ S ₁)	159.972	159.900	0.05	16	1s 3d (¹ D ₂)	160.455	160.382	0.05

Table 4: Comparison between calculated (SS) and measured (NIST) energies of Si XIV

K	Configuration Term	E _{SS} (Ry)	E _{NIST} (Ry)	% Diff	K	Configuration Term	E _{SS} (Ry)	E _{NIST} (Ry)	% Diff
1	1s (² S _{1/2})	0	0	0	9	3d (² D _{5/2})	174.728	174.691	0.02
2	2p (² P ^o _{1/2})	147.352	147.213	0.09	10	4p (² P ^o _{1/2})	184.237	184.199	0.02
3	2p (² P ^o _{3/2})	147.480	147.444	0.02	11	4p (² P ^o _{3/2})	184.252	184.215	0.02
4	2s (² S _{1/2})	147.353	147.320	0.02	12	4s (² S _{1/2})	184.237	184.200	0.02
5	3p (² P ^o _{1/2})	174.678	174.641	0.02	13	4d (² D _{3/2})	184.252	184.215	0.02
6	3p (² P ^o _{3/2})	174.716	174.679	0.02	14	4d (² D _{5/2})	184.258	184.221	0.02
7	3s (² S _{1/2})	174.678	174.642	0.02	15	4f (² F ^o _{5/2})	184.258	184.221	0.02
8	3d (² D _{3/2})	174.716	174.649	0.04	16	4f (² F ^o _{7/2})	184.260	184.223	0.02

Table 5: Comparison between calculated (SS) and measured (NIST) energies of Fe XXIV

K	Configuration Term	E_{SS} (Ry)	E_{NIST} (Ry)	% Diff	K	Configuration Term	E_{SS} (Ry)	E_{NIST} (Ry)	% Diff
1	$1s^2 2s (^2S_{1/2})$	0	0	0	9	$1s^2 4s (^2S_{1/2})$	113.609	113.584	0.02
2	$1s^2 2p (^2P^o_{1/2})$	3.464	3.572	3.0	10	$1s^2 4p (^2P^o_{1/2})$	114.007	113.989	0.02
3	$1s^2 2p (^2P^o_{3/2})$	4.751	4.746	0.1	11	$1s^2 4p (^2P^o_{3/2})$	114.162	114.135	0.02
4	$1s^2 3s (^2S_{1/2})$	84.510	84.497	0.02	12	$1s^2 4d (^2D_{3/2})$	114.319	114.266	0.05
5	$1s^2 3p (^2P^o_{1/2})$	85.479	85.460	0.02	13	$1s^2 4d (^2D_{5/2})$	114.369	114.320	0.04
6	$1s^2 3p (^3P^o_{3/2})$	85.851	85.815	0.04	14	$1s^2 4f (^2F^o_{5/2})$	114.485	114.342	0.1
7	$1s^2 3d (^2D_{3/2})$	86.230	86.197	0.04	15	$1s^2 4f (^2F^o_{7/2})$	114.509	114.379	0.1
8	$1s^2 3d (^2D_{5/2})$	86.350	86.321	0.03	16	$1s^2 5s (^2S_{1/2})$	126.963	[126.898]	0.05

K	Configuration Term	E_{SS} (Ry)	E_{NIST} (Ry)	% Diff	K	Configuration Term	E_{SS} (Ry)	E_{NIST} (Ry)	% Diff
17	$1s^2 5p (^2P^o_{1/2})$	127.272	127.060	0.7	20	$1s^2 5d (^2D_{5/2})$	127.456	127.260	0.2
18	$1s^2 5p (^2P^o_{3/2})$	127.350	127.140	0.2	21	$1s^2 6p (^2P^o_{1/2})$	134.402	134.240	0.1
19	$1s^2 5d (^2D_{3/2})$	127.430	127.220	0.2	22	$1s^2 6p (^2P^o_{3/2})$	134.446	134.280	0.1

Table 6: Comparison between calculated (SS) and measured (NIST) energies of Ni XXVI

K	Configuration Term	E_{SS} (Ry)	E_{NIST} (Ry)	% Diff	K	Configuration Term	E_{SS} (Ry)	E_{NIST} (Ry)	% Diff
1	$1s^2 2s (^2S_{1/2})$	0	0	0	10	$1s^2 4p (^2P^o_{1/2})$	133.672	133.590	0.06
2	$1s^2 2p (^2P^o_{1/2})$	3.802	3.892	2.3	11	$1s^2 4p (^2P^o_{3/2})$	133.880	133.792	0.07
3	$1s^2 2p (^2P^o_{3/2})$	5.557	5.510	0.9	12	$1s^2 4d (^2D_{3/2})$	134.050	133.964	0.06
4	$1s^2 3s (^2S_{1/2})$	99.086	99.020	0.07	13	$1s^2 4d (^2D_{5/2})$	134.118	134.027	0.07
5	$1s^2 3p (^2P^o_{1/2})$	100.155	100.099	0.06	14	$1s^2 5s (^2S_{1/2})$	148.990	148.806	0.1
6	$1s^2 3p (^2P^o_{3/2})$	100.661	100.578	0.08	15	$1s^2 5p (^2P^o_{1/2})$	149.206	149.037	0.1
7	$1s^2 3d (^2D_{3/2})$	101.069	100.987	0.08	16	$1s^2 5p (^2P^o_{3/2})$	149.309	149.141	0.1
8	$1s^2 3d (^2D_{5/2})$	101.232	101.138	0.09	17	$1s^2 5d (^2D_{3/2})$	149.396	149.228	0.1
9	$1s^2 4s (^2S_{1/2})$	133.238	133.1367	0.08	18	$1s^2 5d (^2D_{5/2})$	149.430	149.261	0.1
K	Configuration Term	E_{SS} (Ry)	E_{NIST} (Ry)	% Diff	K	Configuration Term	E_{SS} (Ry)	E_{NIST} (Ry)	% Diff
19	$1s^2 6p (^2P^o_{1/2})$	157.6231	_____	_____	20	$1s^2 6p (^2P^o_{3/2})$	157.682	_____	_____
21	$1s^2 6s (^2S_{1/2})$	157.499	_____	_____					

4.1.2. Transition energies and probabilities (A-values)

The transition energies and probabilities of the identified lines are given in Tables 7–10. The A-values for transitions with around the same energies were added together to give total line strength. There was good agreement between the calculated and observed transition energies. The plasma effect was not included in calculations, so it could shift the data slightly.

Table 7: Transitions in Mg XII

MgXII	Wavelength (Å) NIST/SS	A - value (s ⁻¹)	A - total (s ⁻¹)
$1s\ (^2S_{1/2}) - 4p\ (^2P^o_{1/2})$	6.74	1.381×10^{12}	2.776×10^{12}
$1s\ (^2S_{1/2}) - 4p\ (^2P^o_{3/2})$	6.74	1.395×10^{12}	
$1s\ (^2S_{1/2}) - 5p\ (^2P^o_{1/2})$	6.58	6.840×10^{11}	1.377×10^{12}
$1s\ (^2S_{1/2}) - 5p\ (^2P^o_{3/2})$	6.58	6.929×10^{11}	
$1s\ (^2S_{1/2}) - 6p\ (^2P^o_{1/2})$	6.50	3.829×10^{11}	7.722×10^{12}
$1s\ (^2S_{1/2}) - 6p\ (^2P^o_{3/2})$	6.50	3.893×10^{11}	
$1s\ (^2S_{1/2}) - 7p\ (^2P^o_{1/2})$	6.45	2.244×10^{11}	4.538×10^{11}
$1s\ (^2S_{1/2}) - 7p\ (^2P^o_{3/2})$	6.45	2.294×10^{11}	

Table 8: Transitions in Si

Si XIV	Wavelength (Å)	A - value (s ⁻¹)	A - total (s ⁻¹)
$1s\ (^2S_{1/2})\ to\ 2p\ (^2P_{1/2})$	6.18	2.399×10^{13}	4.798×10^{13}
$1s\ (^2S_{1/2})\ to\ 2p\ (^2P_{3/2})$	6.18	2.399×10^{13}	
Si XIII	Wavelength (Å)	A - value (s ⁻¹)	A - total (s ⁻¹)
$1s^2\ (^1S_0)\ to\ 1s\ 2p\ (^3P^o_0)$	6.69	1.317×10^{11}	3.838×10^{13}
$1s^2\ (^1S_0)\ to\ 2p\ (^1P^o_1)$	6.64	3.825×10^{13}	

Table 9: Transitions in Fe

Fe XXIV	Wavelength (Å)	A - value (s ⁻¹)	A – total (s ⁻¹)
$1s^2 2s (^2S_{1/2})$ to $1s^2 6p (^2P^{\circ}_{1/2})$	6.78	7.035×10^{11}	1.436×10^{12}
$1s^2 2s (^2S_{1/2})$ to $1s^2 6p (^2P^{\circ}_{3/2})$	6.78	7.328×10^{11}	

Table 10: Transitions in Ni and Al

Ni XXVI	Wavelength (Å)	A - value (s ⁻¹)	A – total (s ⁻¹)
1s ² 2s (² S _{1/2}) to 1s ² 4p (² P ^o _{1/2})	6.82	4.261 x 10 ¹²	8.510 x 10 ¹²
1s ² 2s (² S _{1/2}) to 1s ² 4p (² P ^o _{3/2})	6.81	4.249 x 10 ¹²	
1s ² 2s (² S _{1/2}) to 1s ² 5p (² P ^o _{1/2})	6.11	2.039 x 10 ¹²	4.116 x 10 ¹²
1s ² 2s (² S _{1/2}) to 1s ² 5p (² P ^o _{3/2})	6.10	2.077 x 10 ¹²	
1s ² 2s (² S _{1/2}) to 1s ² 6p (² P ^o _{1/2})*	5.78	9.189 x 10 ¹¹	1.8828 x 10 ¹²
1s ² 2s (² S _{1/2}) to 1s ² 6p (² P ^o _{1/2})*	5.78	9.639 x 10 ¹¹	
Table 4.1. Transitions in Al			
*Al XIII 1s to 3p was found to be a better match to the data then Ni XXVI 1s 2s to 1s ² 6p:			
Al XIII	Wavelength (Å)	A - value (s ⁻¹)	A – total (s ⁻¹)
1s (² S _{1/2}) to 3p (² P _{1/2})	6.05	4.684 x 10 ¹²	9.408 x 10 ¹²
1s (² S _{1/2}) to 3p (² P _{3/2})	6.05	4.724 x 10 ¹²	

4.1.3. Overall Results

The previous results have been compiled in Table 11 and Figure 6.

Table 11: An overall look at the identified lines

Ion	Configuration	Wavelength(Å)	Total Probability (s ⁻¹)
Al XIII	3p	6.05	9.408×10^{12}
Ni XXVI	1s ² 5p	6.11	4.116×10^{12}
Ni XXVI	1s ² 4p	6.82	8.510×10^{12}
Si XIV	2p	6.18	4.798×10^{11}
Si XIII	2p	6.69	1.317×10^{11}
Fe XXIV	1s ² 6p	6.78	1.436×10^{12}
Mg XII	7p	6.45	4.538×10^{11}
Mg XII	6p	6.50	7.722×10^{11}
Mg XII	5p	6.58	1.377×10^{12}
Mg XII	4p	6.74	2.776×10^{12}

*Al XIII 1s to 3p was found to better match the data then Ni XXVI 1s2 to 6p

Ion	Configuration	Wavelength(Å)	Total Probability
Ni XXVI	6p	5.78	1.883×10^{12}

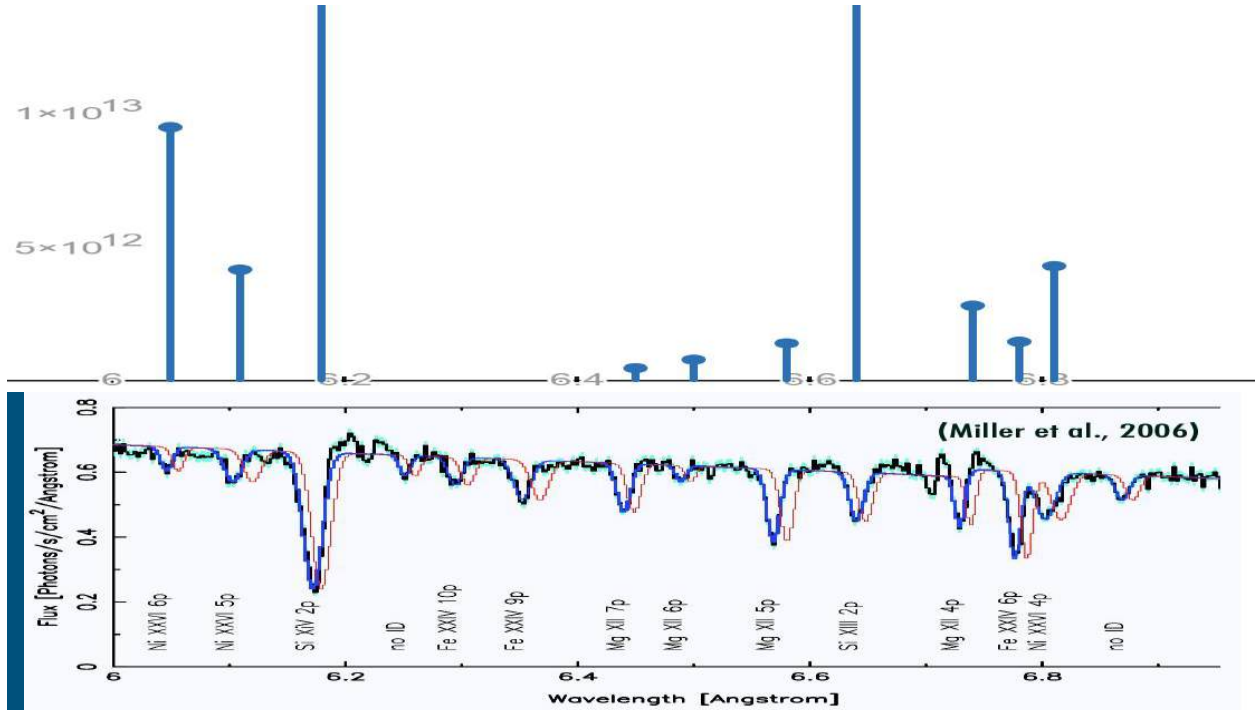


Figure 6: Comparison of the calculated spectrum (top) with the observed spectrum (bottom)

4.2. Al XIII Line

According to the paper, the wavelength of Ni XXVI 6p was 6.05 Å. But our calculations found its wavelength as 5.78 Å. Using trial and error with various ions, we found the wavelength matches Al XIII 3p. It was misidentified by Miller et al. but we have found the correct ion. This identification was found using SUPERSTRUCTURE and compared with values in NIST. Additionally, Anthropic’s AI model Claude was used to corroborate our findings. Claude utilized data of lower levels of Ni XXVI, like 2s to 5p, to extrapolate values for the transition 2s to 6p. These values were then plugged into the quantum-defect (Rydberg-Ritz) formula giving a wavelength of 5.78 Å, which matches our value but not the identified wavelength in the paper’s spectrum. Claude then used the Dirac formula (for relativistic hydrogenic energy levels) to find the wavelength of Al XIII 1s to 3p. This formula gave 6.05 Å, matching our calculated value and fitting with the spectrum data.

5. Conclusions and Future Plan

Our A-values show proportional height of the observed spectrum. We do not expect exact match due to the plasma effect not being included in our calculations. Additionally, our calculated wavelengths for each ion (aside from Ni XXVI 6p) match the corresponding spectrum.

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