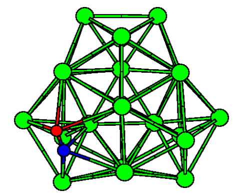
Vorlesung für Masterstudentinnen und –studenten
Modul Nr. 17 W



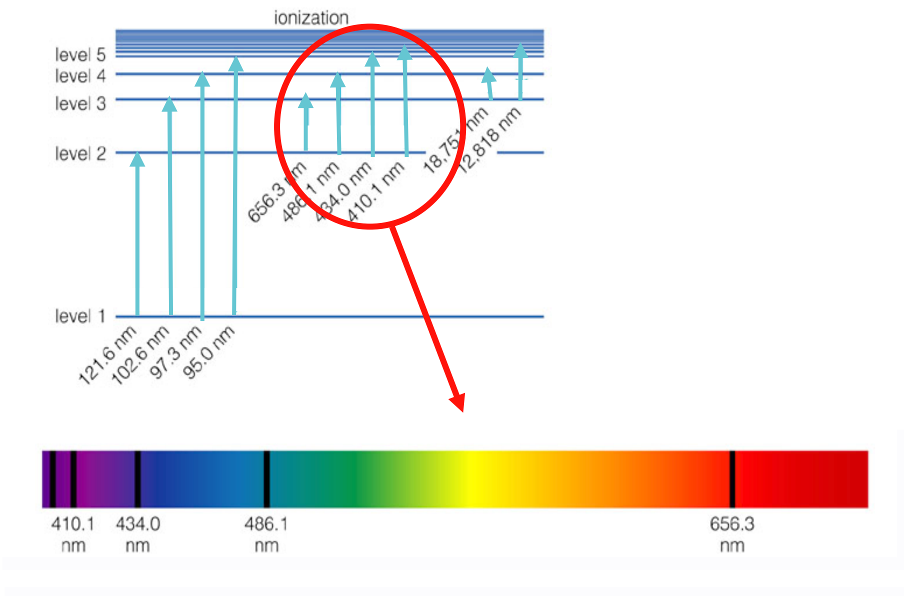
Prof. Dieter Bauer, Quantentheorie und Vielteilchenphysik
Prof. Karl-Heinz Meiwes-Broer, Cluster und Nanostrukturen
Homepage Dieter Bauer: /qtmps teaching WS 10/11 AC

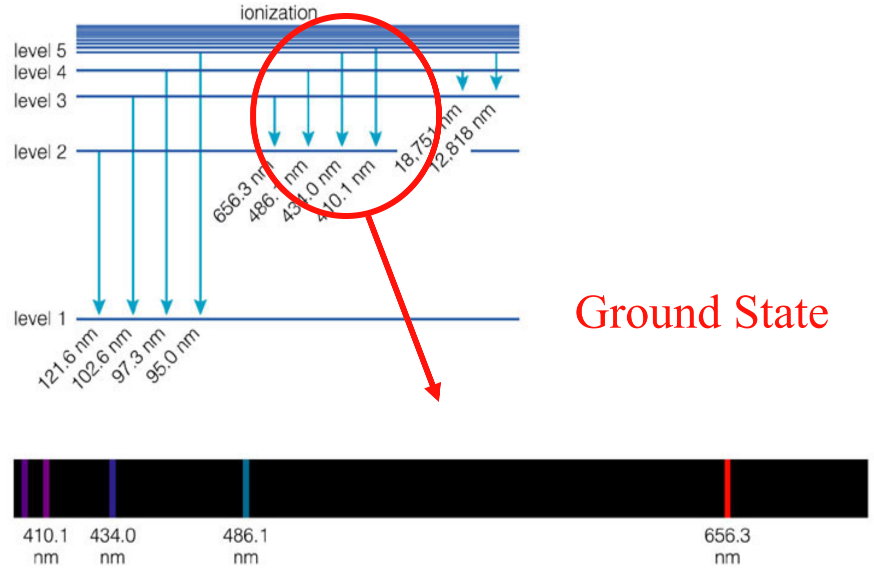
Atome:
Atomare Struktur, Atom-Feld-Wechselwirkung, magnetische und optische Fallen, Bose-Einstein-Kondensate, kalte Fermionen, Atome in starken Feldern, Ionisation, Erzeugung Hoher Harmonischer, Teilchen-beschleunigung mit Lasern, Innerschalen-effekte, Elektronen-korrelationen, relativistische Laser-Atom-Wechsel-wirkung, QED-Effekte

Cluster:
Bindungen, Erzeugung, Schalenmodell, Jellium-Näherung, elektro-nische Struktur, Fullerene, Nichtmetall-Metall-Übergang, Dichtefunk-tionalbeschreibung, Polarisierbarkeit, lineare Antworttheorie, Summenregeln, Resonanzen, Spektroskopie, optische Eigenschaften, Spinordnung, Cluster in He-Tröpfchen, an Oberflächen, in starken Feldern, Nanoplasmen

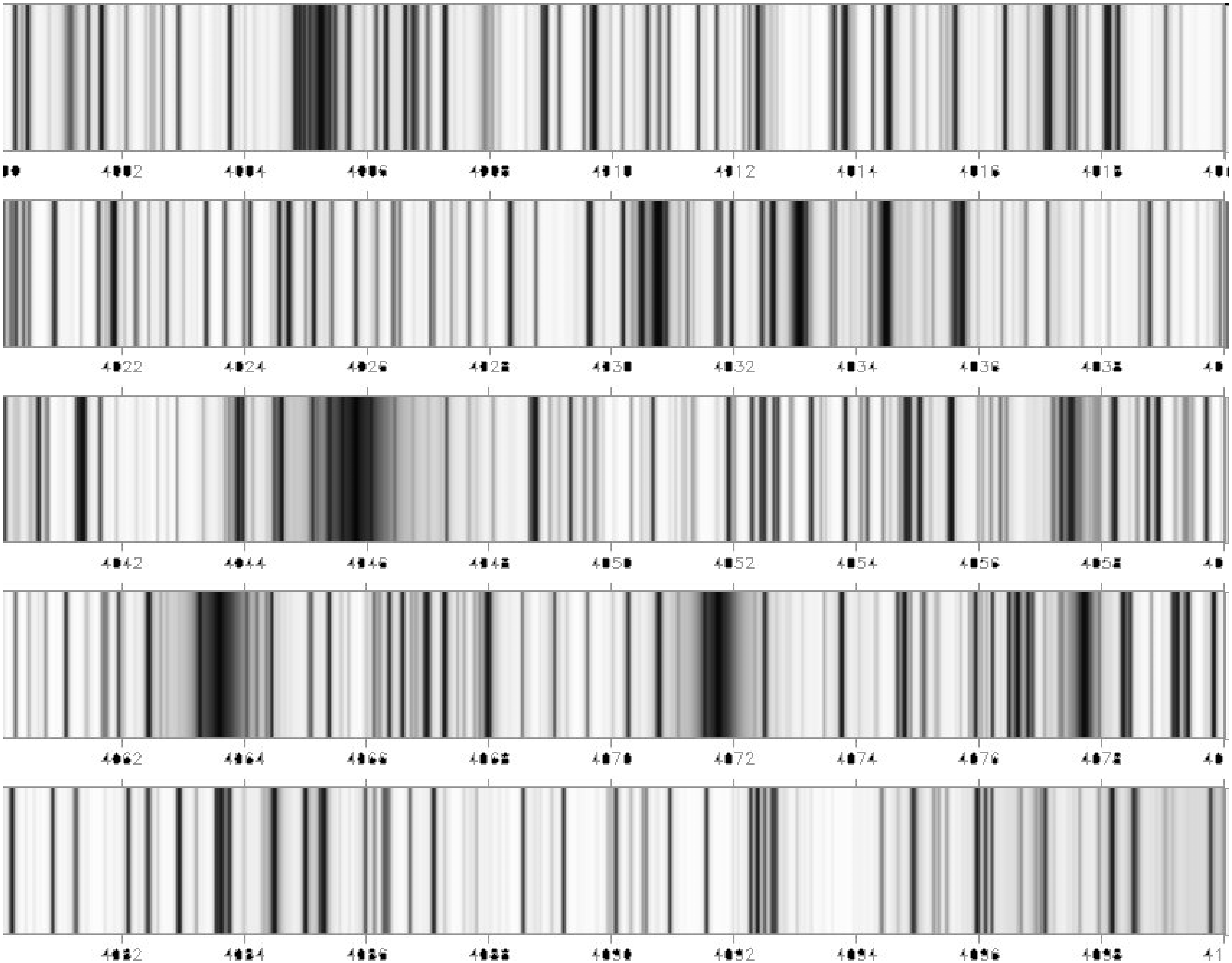
Theorie	Experiment
	Historie Wdhlg 14.10.
Atom-Feld-WW Materie im EM Feld	Präp.methoden Atomstrahl 21.10.
Lichtkräfte auf Teilchen gedresste Atome	Laserkühlung 28.10.
BEC	E + M Fallen 28.10.
Starkfeld-Physik	Koinzidenztechniken, COLTRIMS 4.11.
Starkfeld-Physik II	
Anregung mit hohen Frequenzen	FEL: Funktionsweisen 18.11.
Innerschalen, Augerkaskaden	Einzelschuss-Diffraktion 18.11.
	weitere FEL-Experimente 19.11.
relativistische Laser-Atom-WW, QED	
	Cluster Einf., Bindungstypen 2.12.
MO-Theorie	Erzeugungstechniken 3.12.
Dichtefunktionaltheorie	PES, elektr. Eigenschaften 9.12., 16.12.
Jelliummodell für Cluster- und Kernphysik	
optische Eigensch.: Summenregel, Mie	Photofragmentspektroskopie, opt. Eigenschaften 6.1.
zeitabh. Dichtefunktionaltheorie	Starkfeldanregung 13.1.
	Magnetismus

absorption and emission





Sonnenspektrum 390 nm bis 600 nm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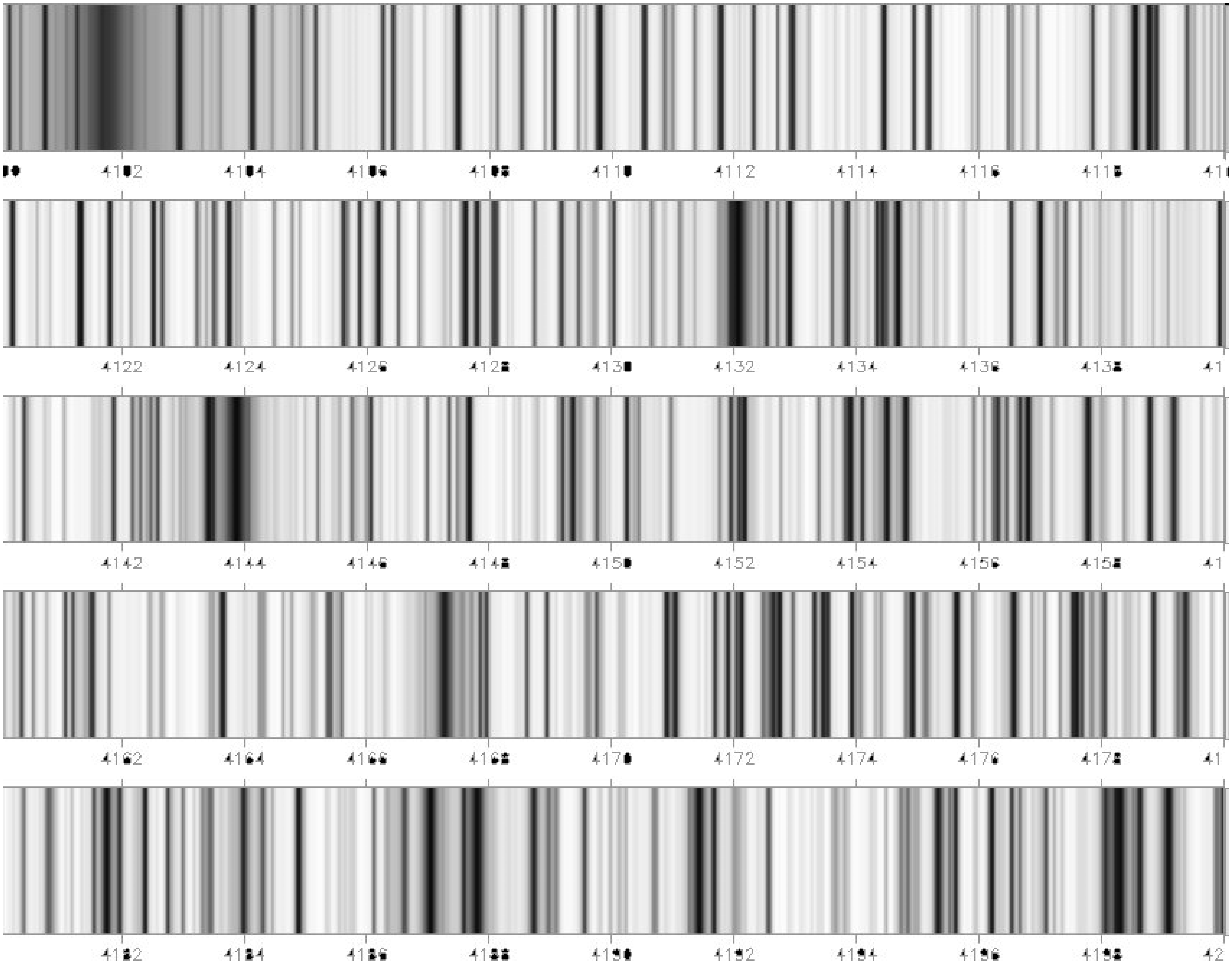

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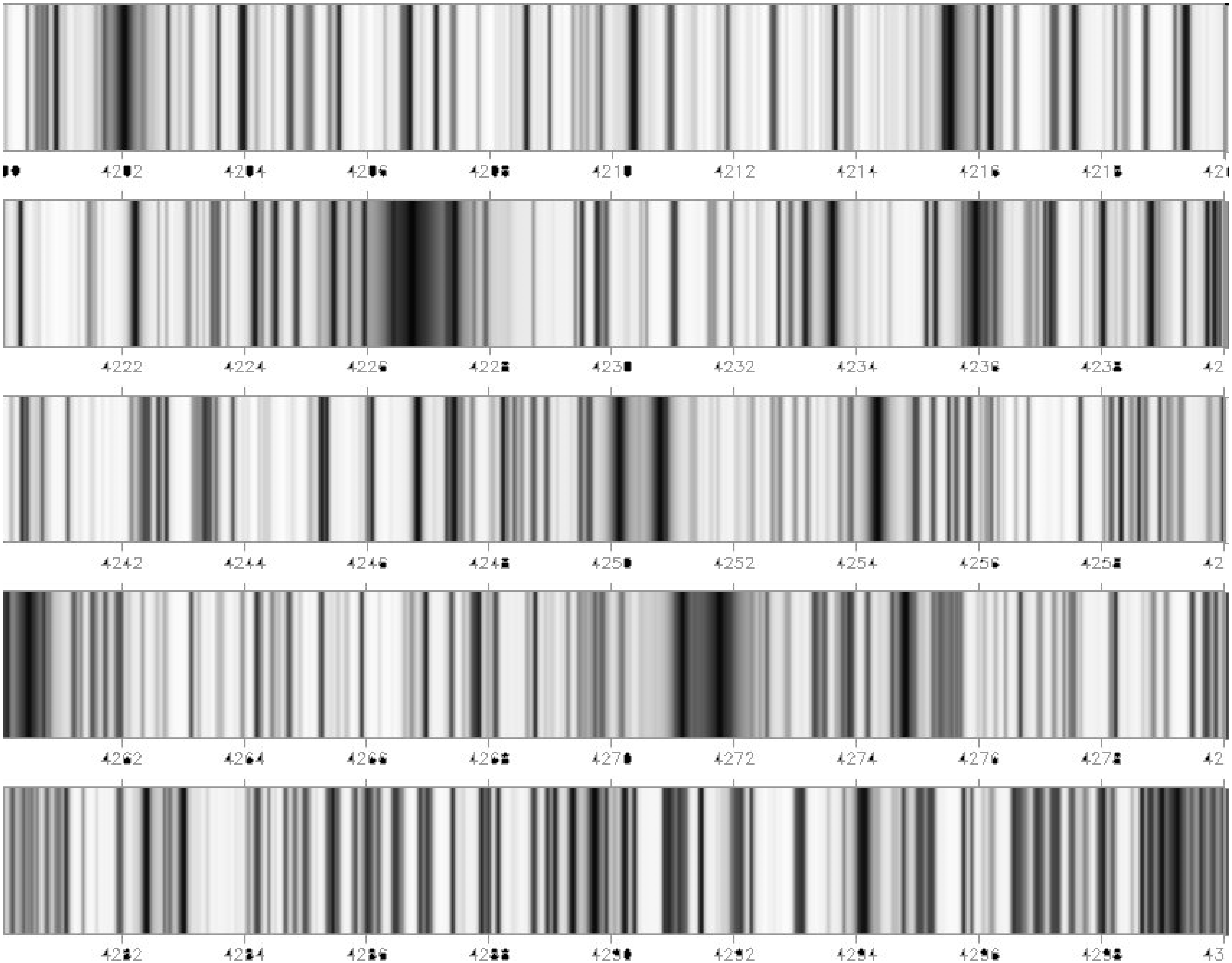
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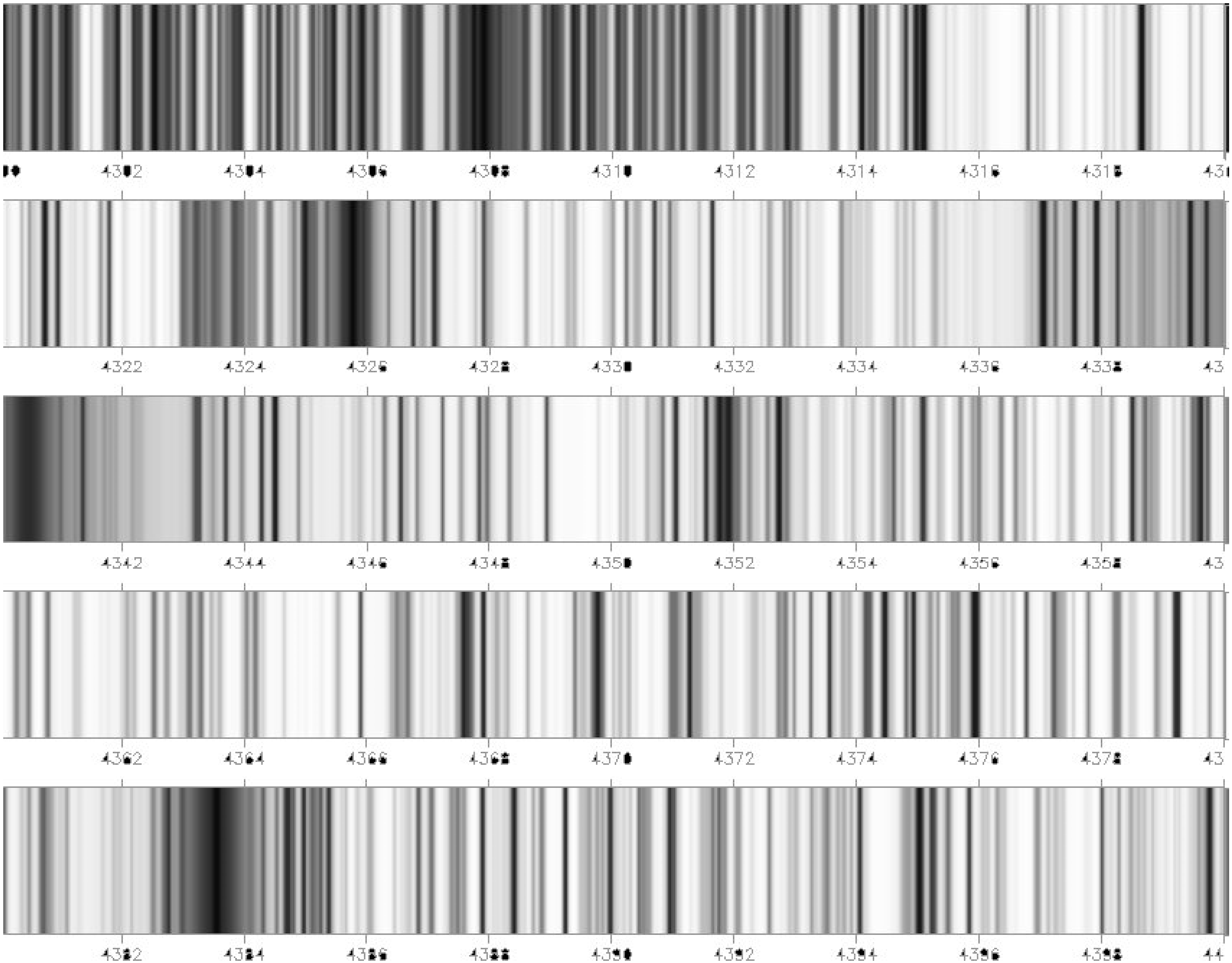
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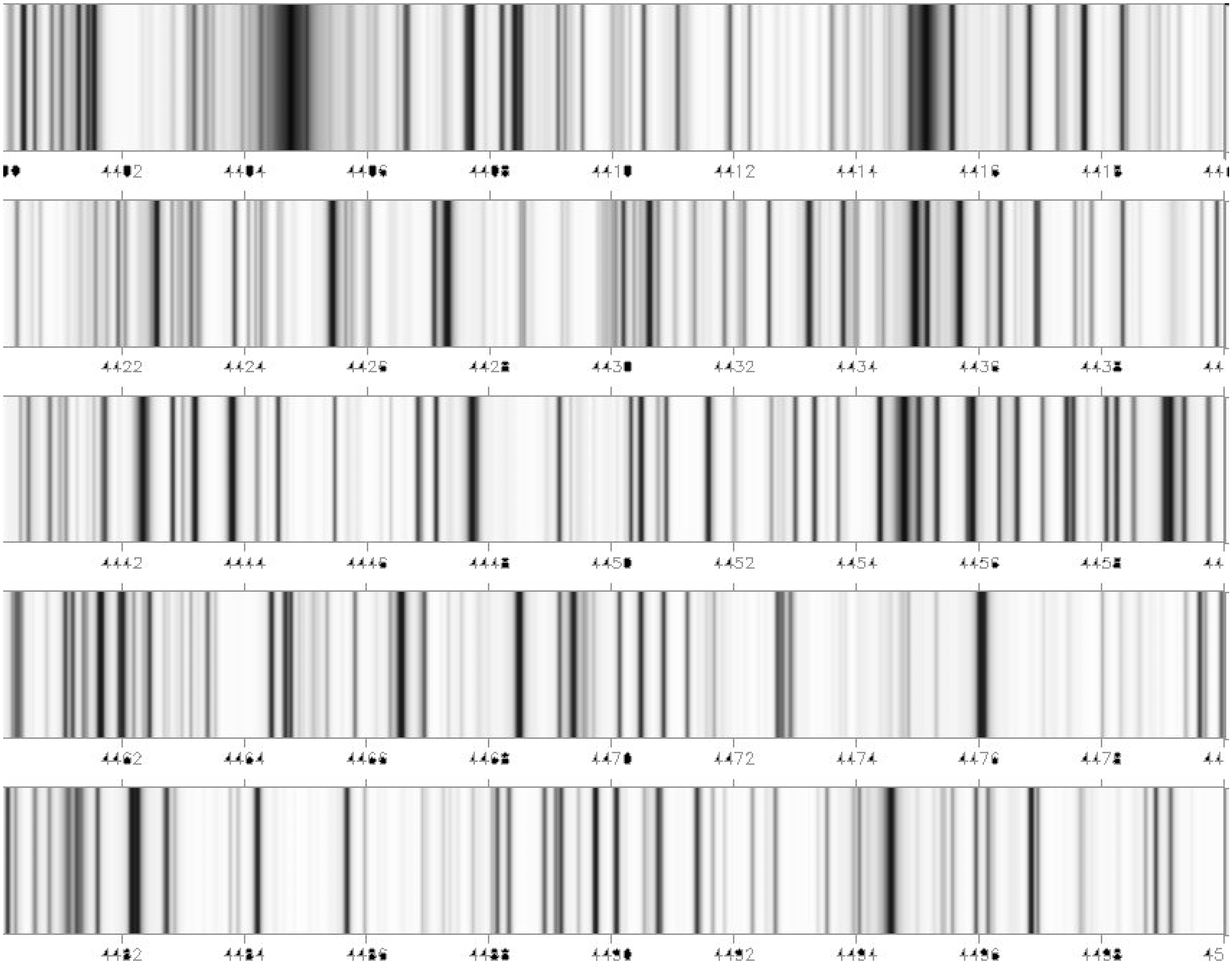

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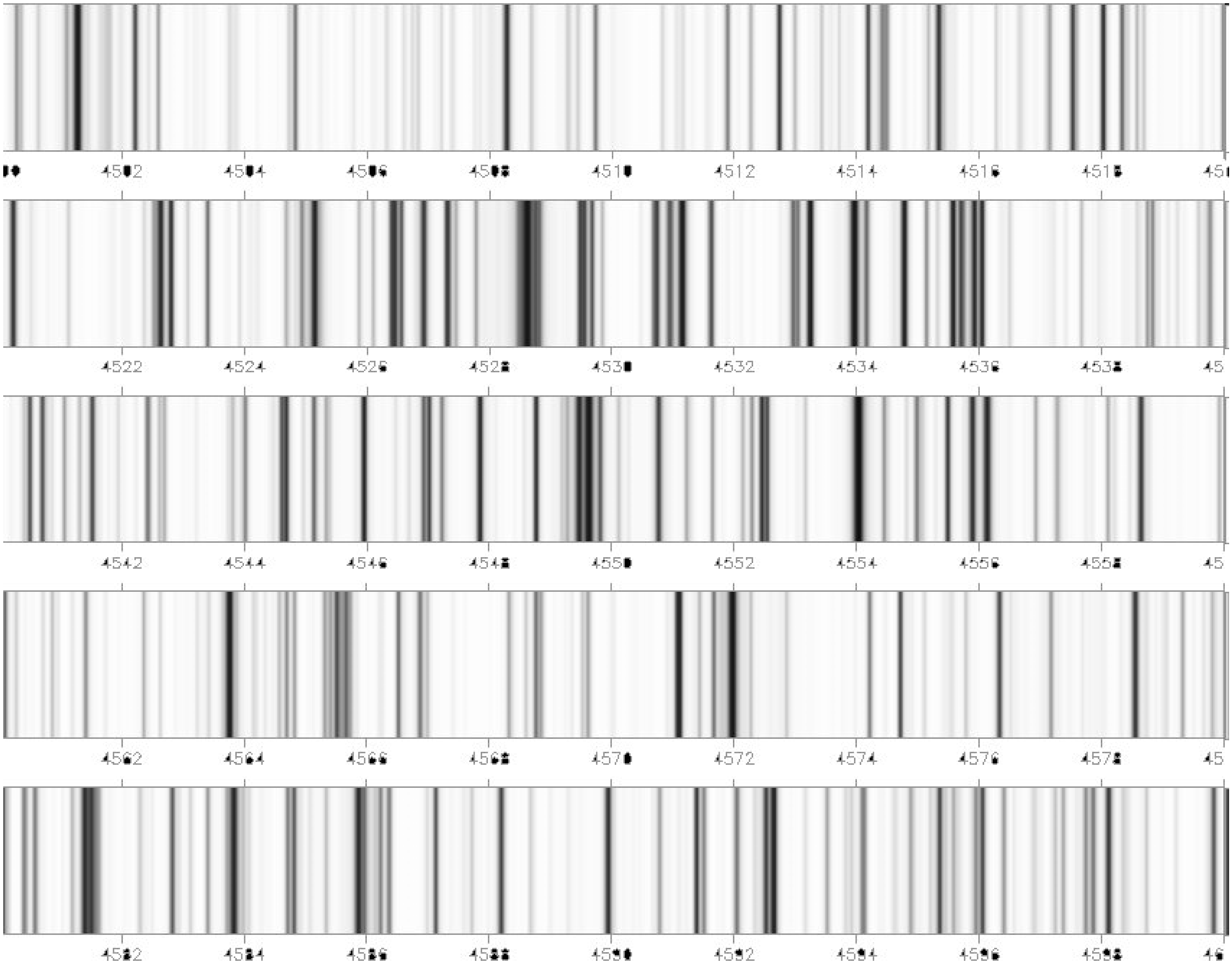
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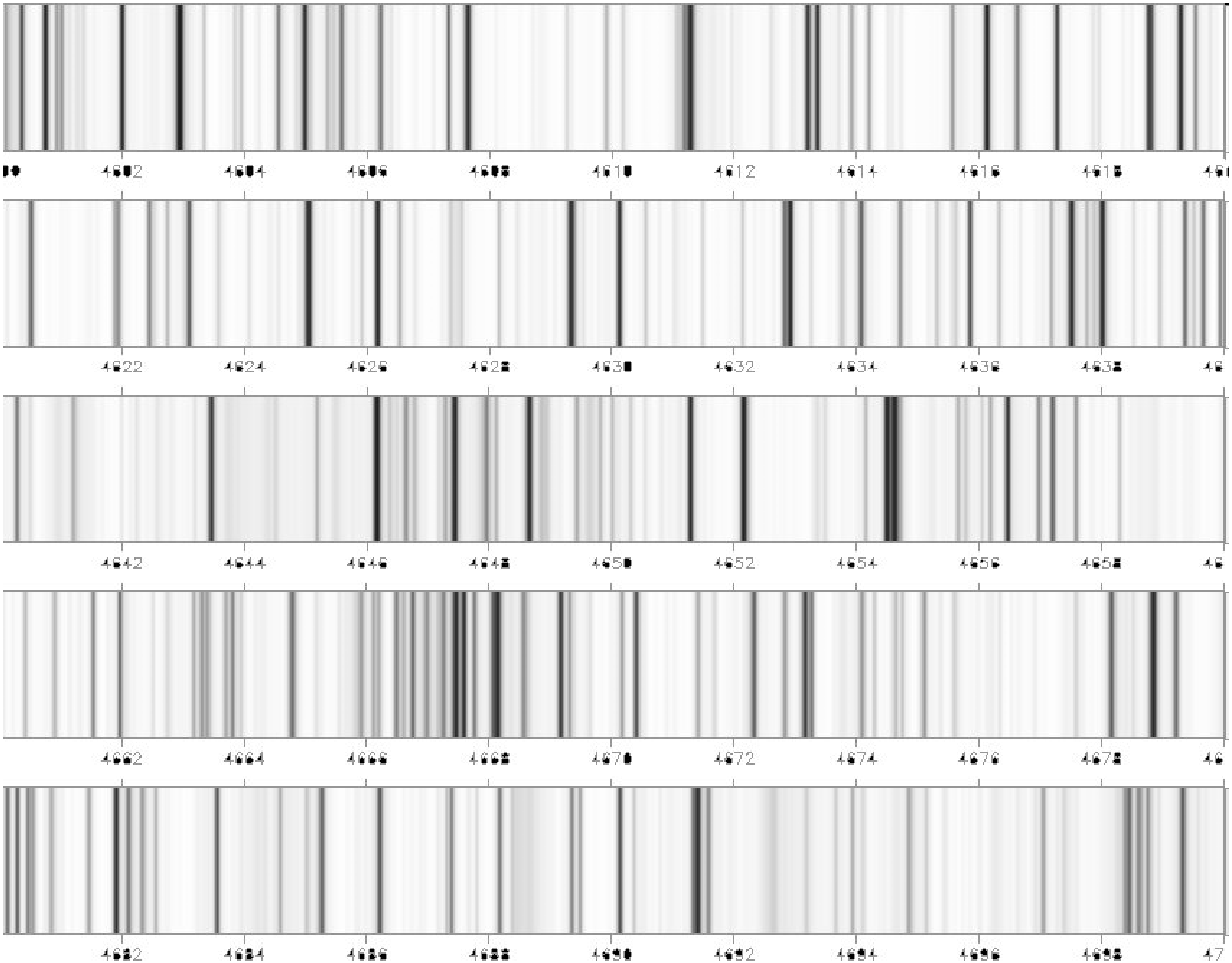

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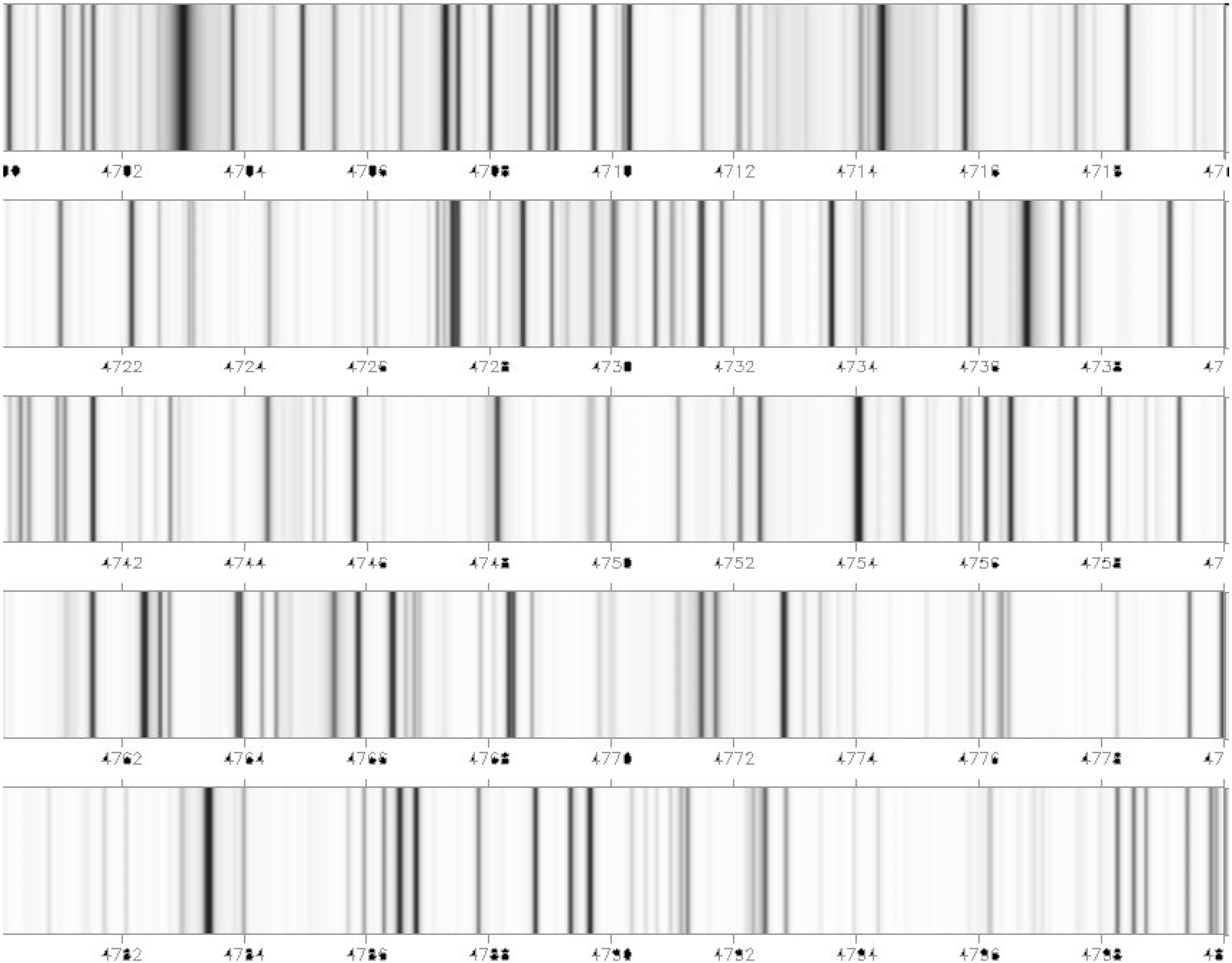
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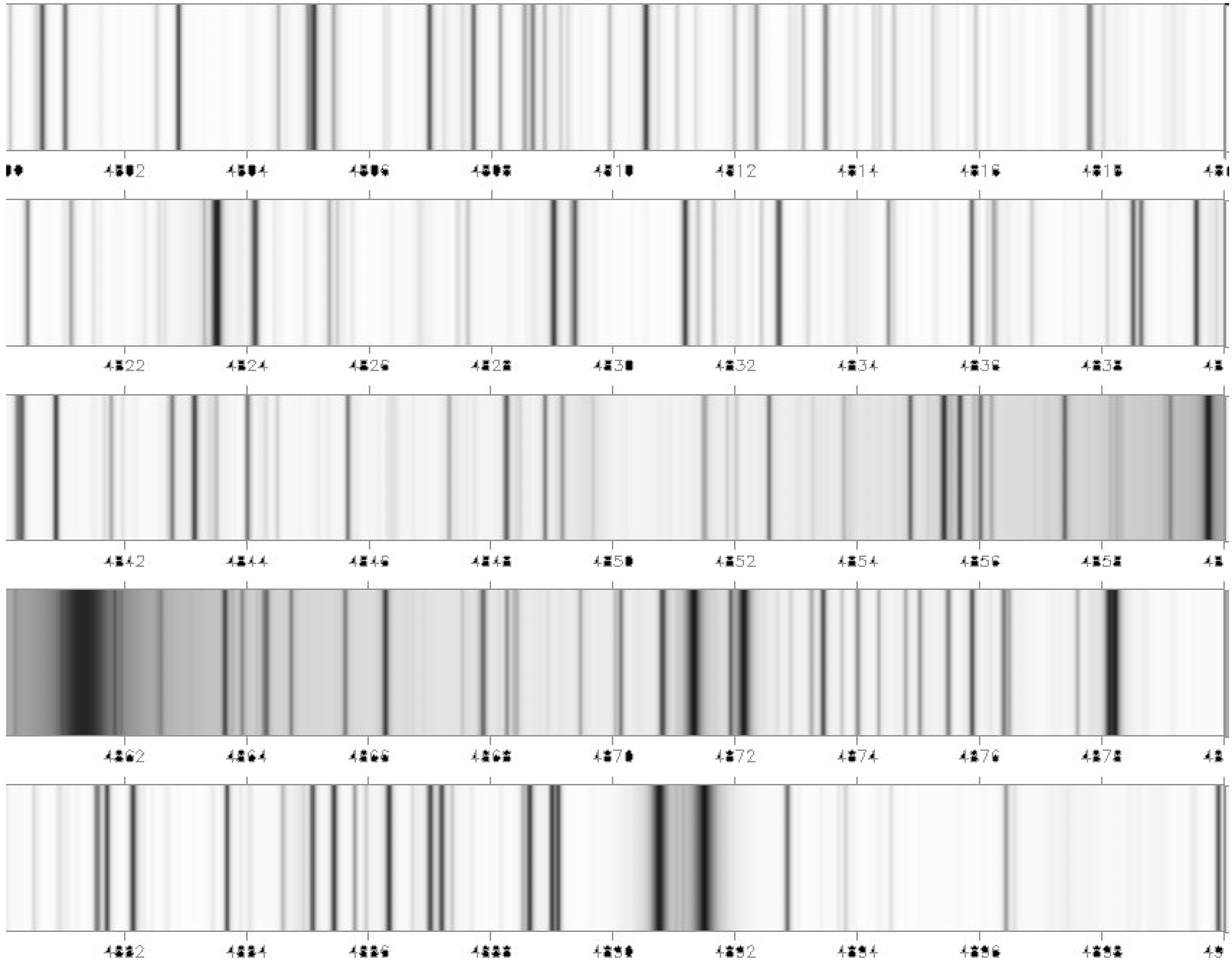

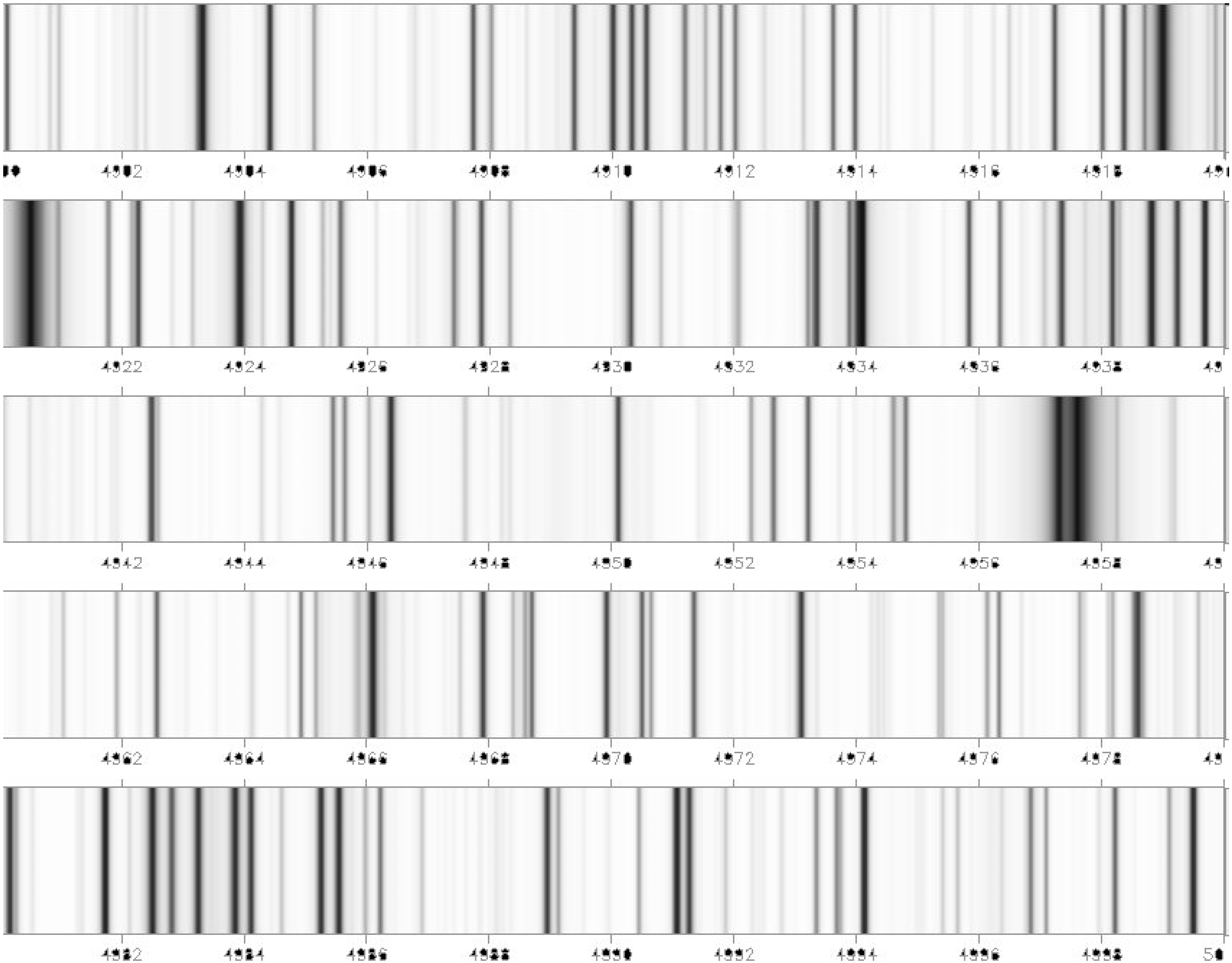
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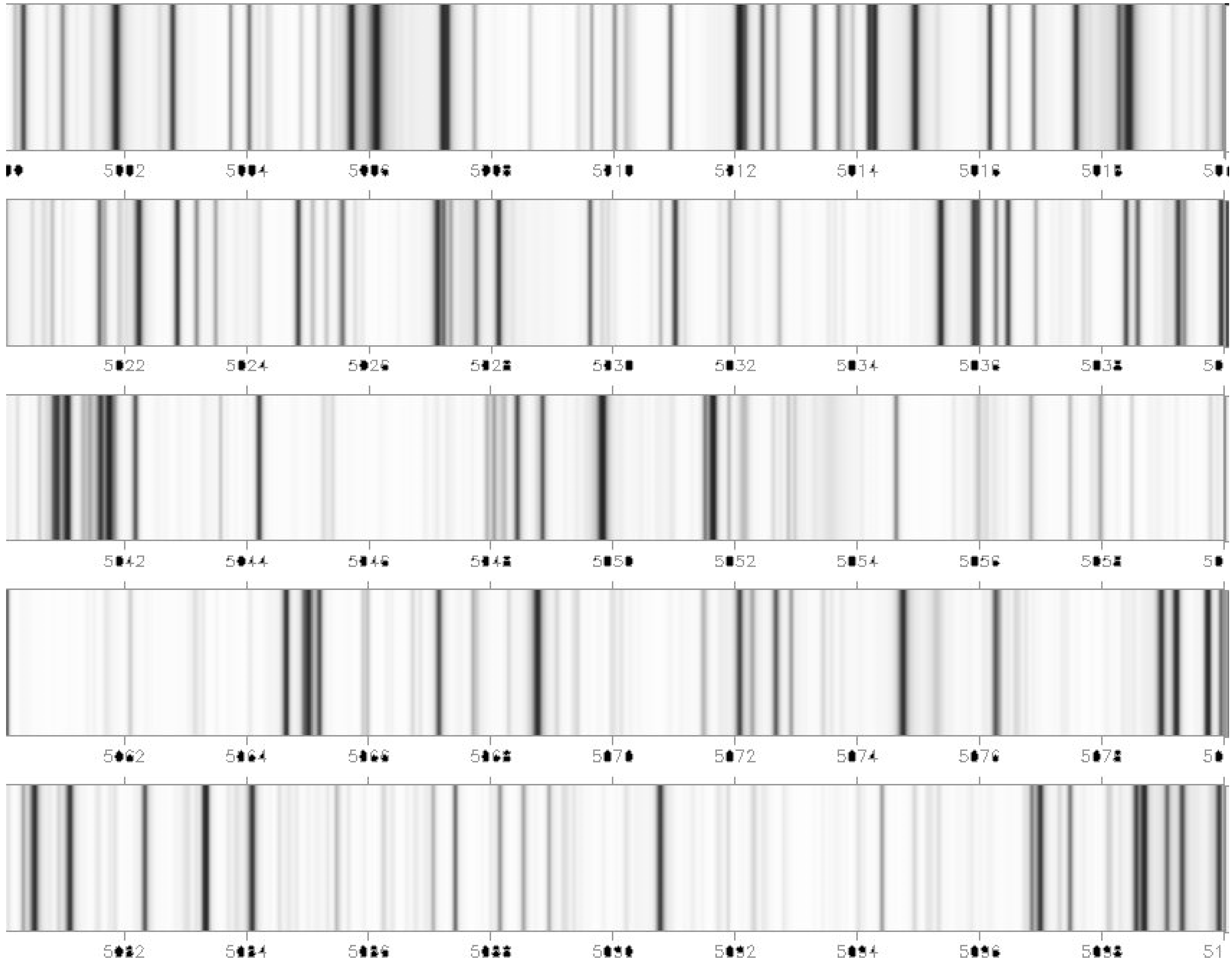

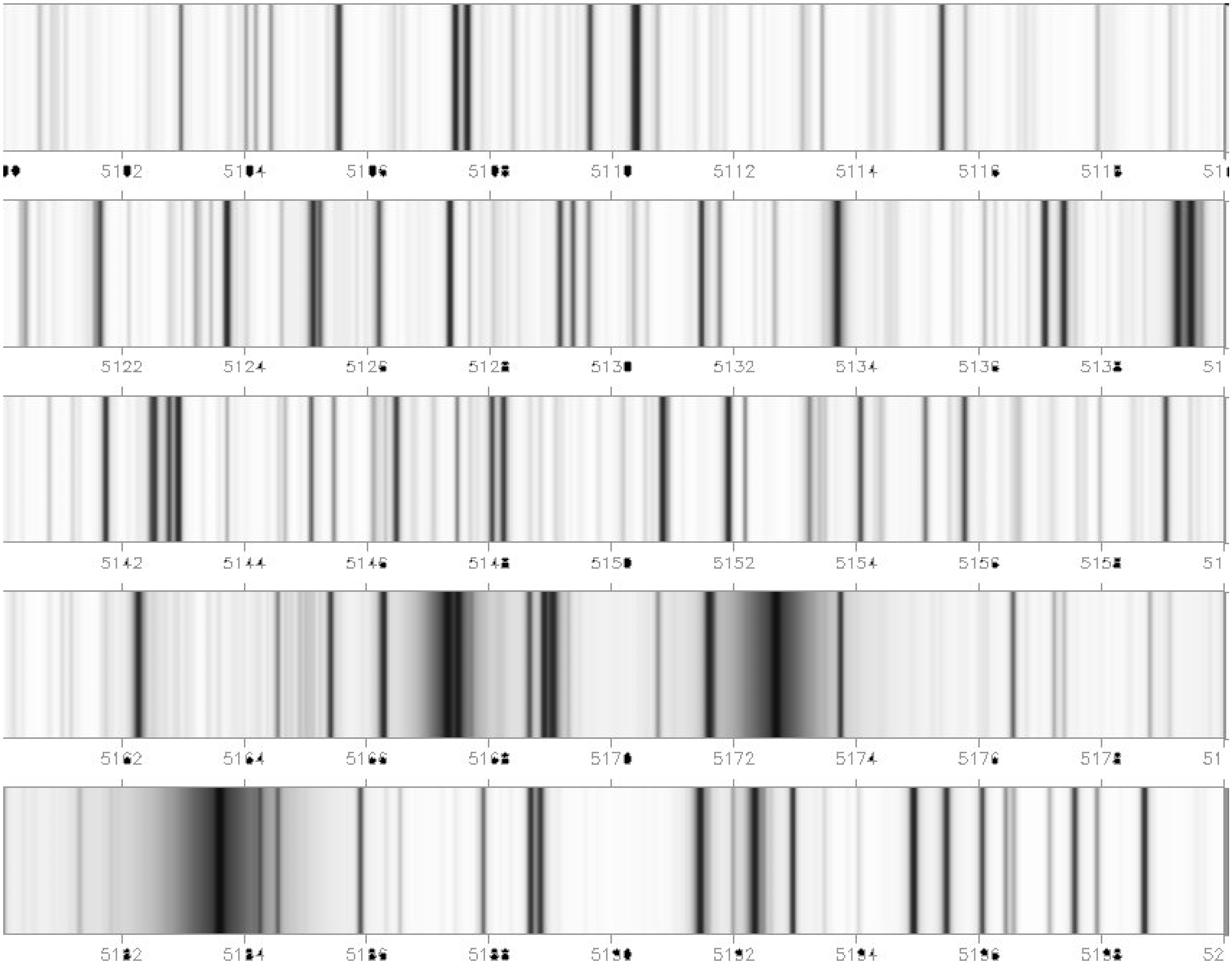
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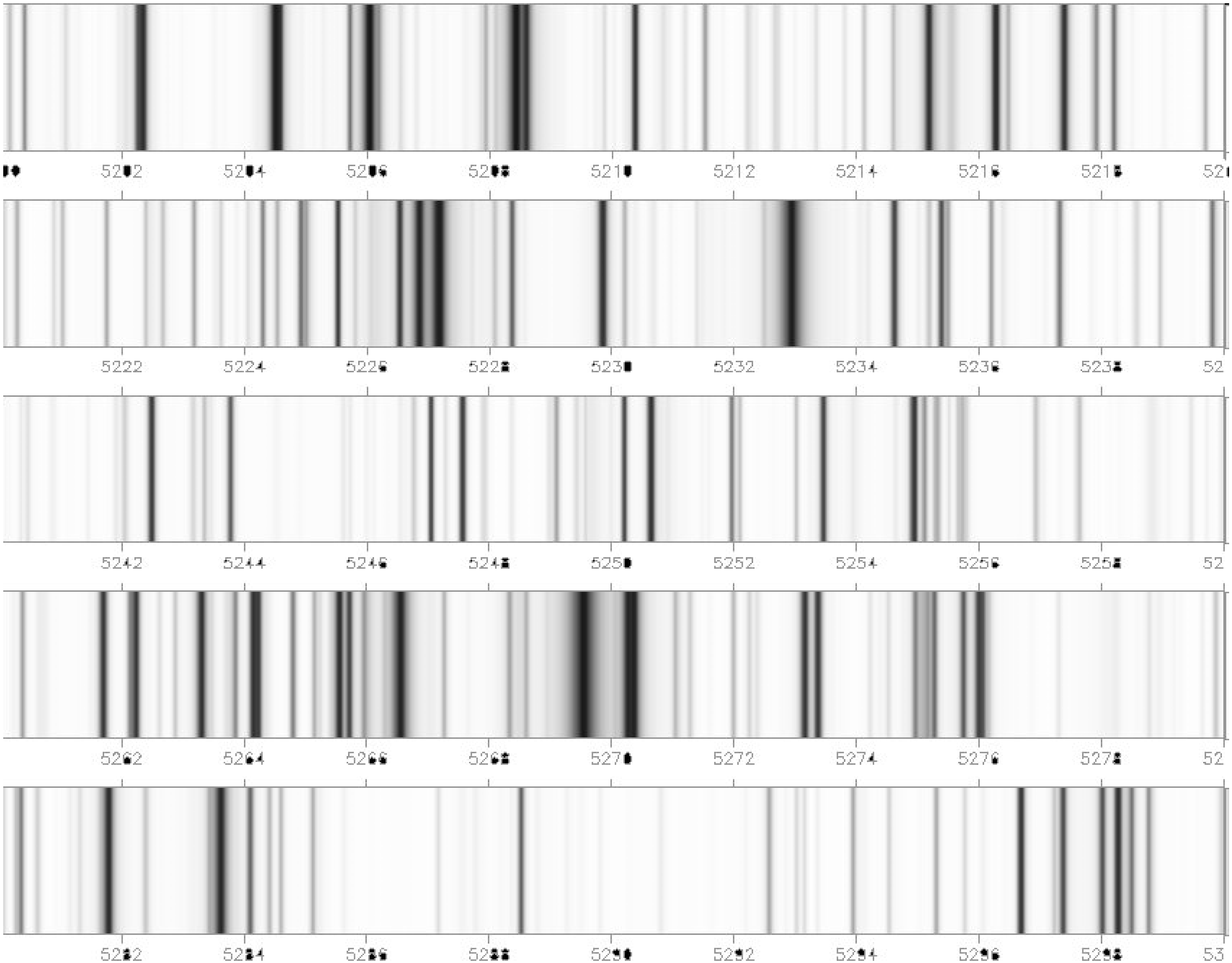
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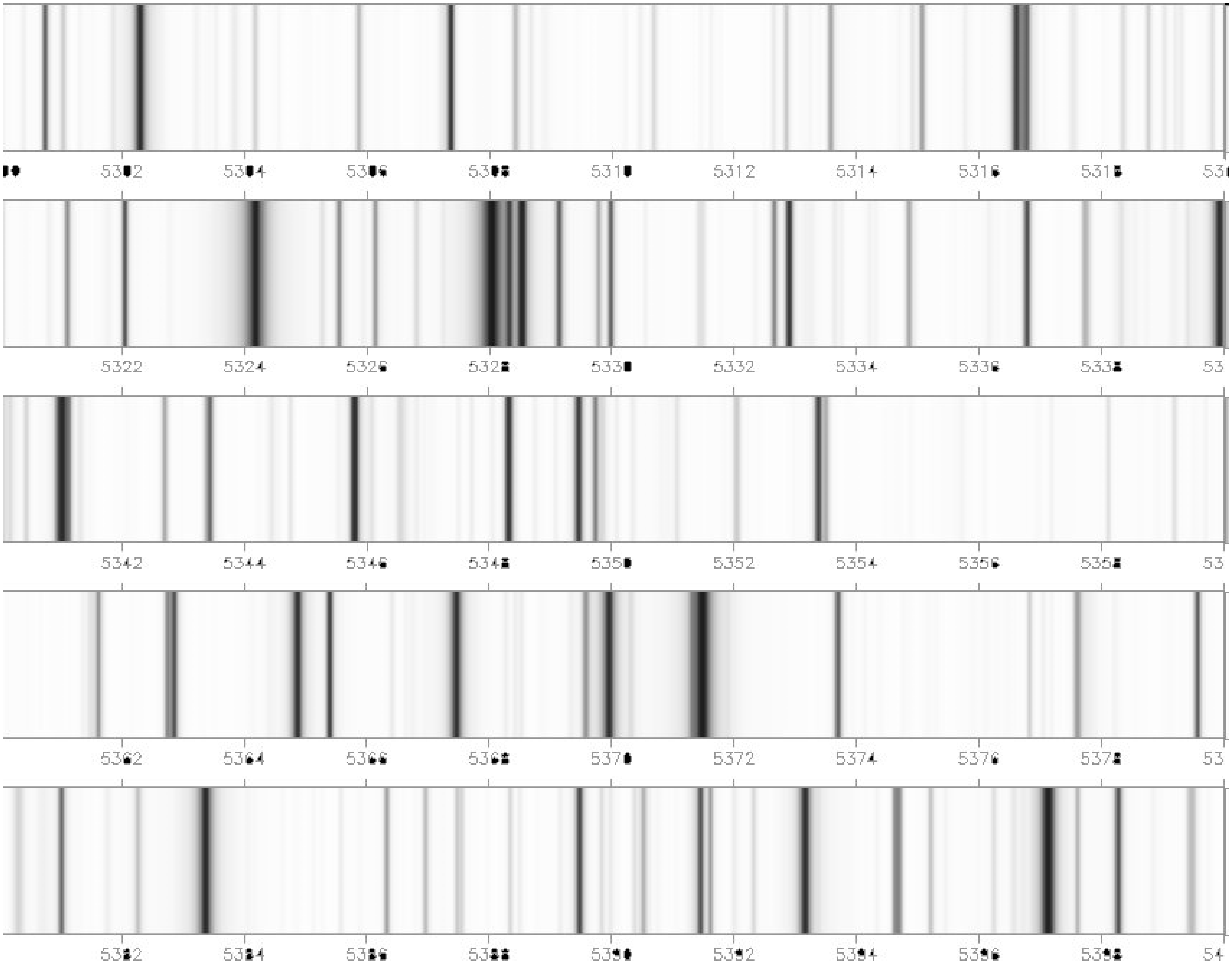
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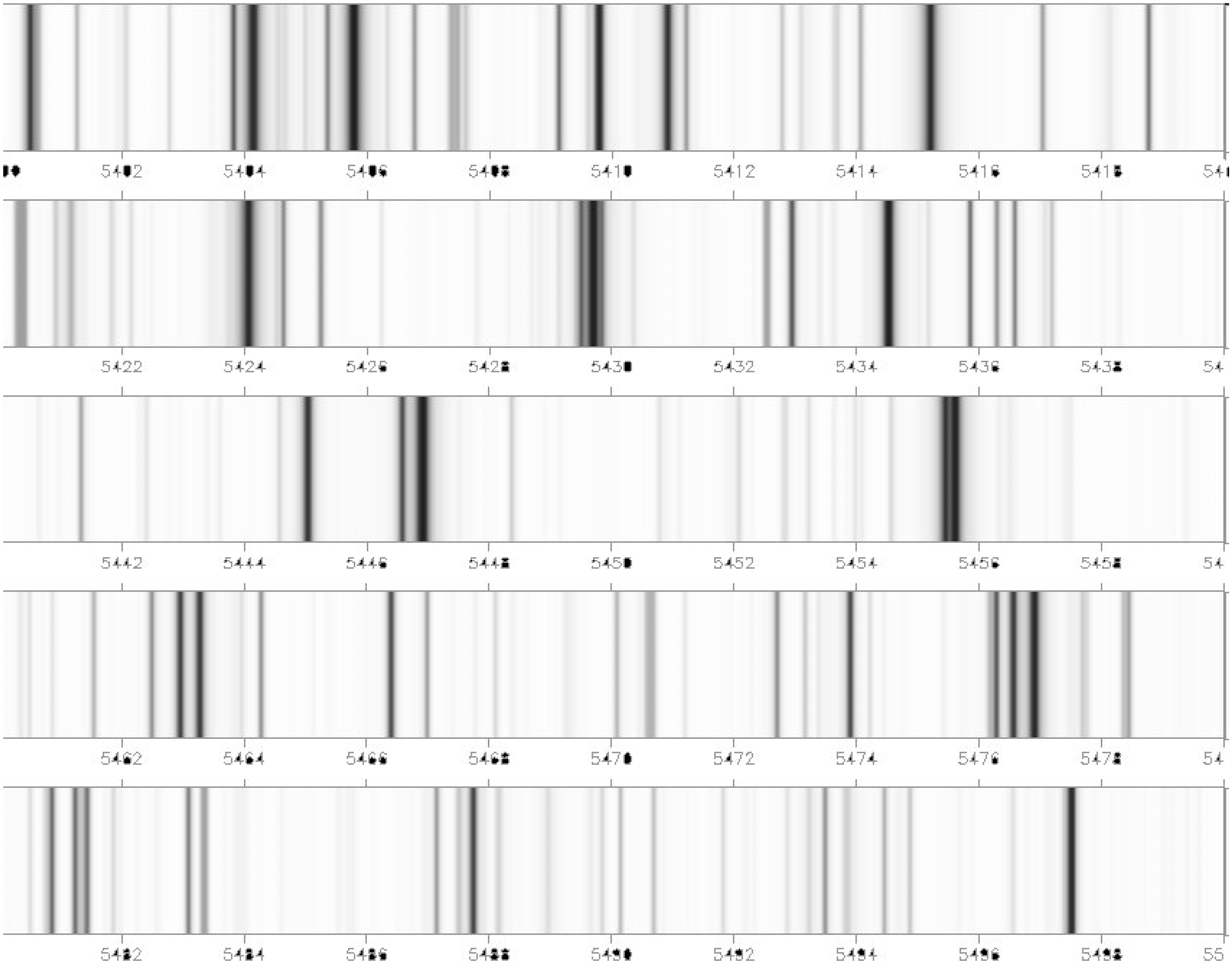
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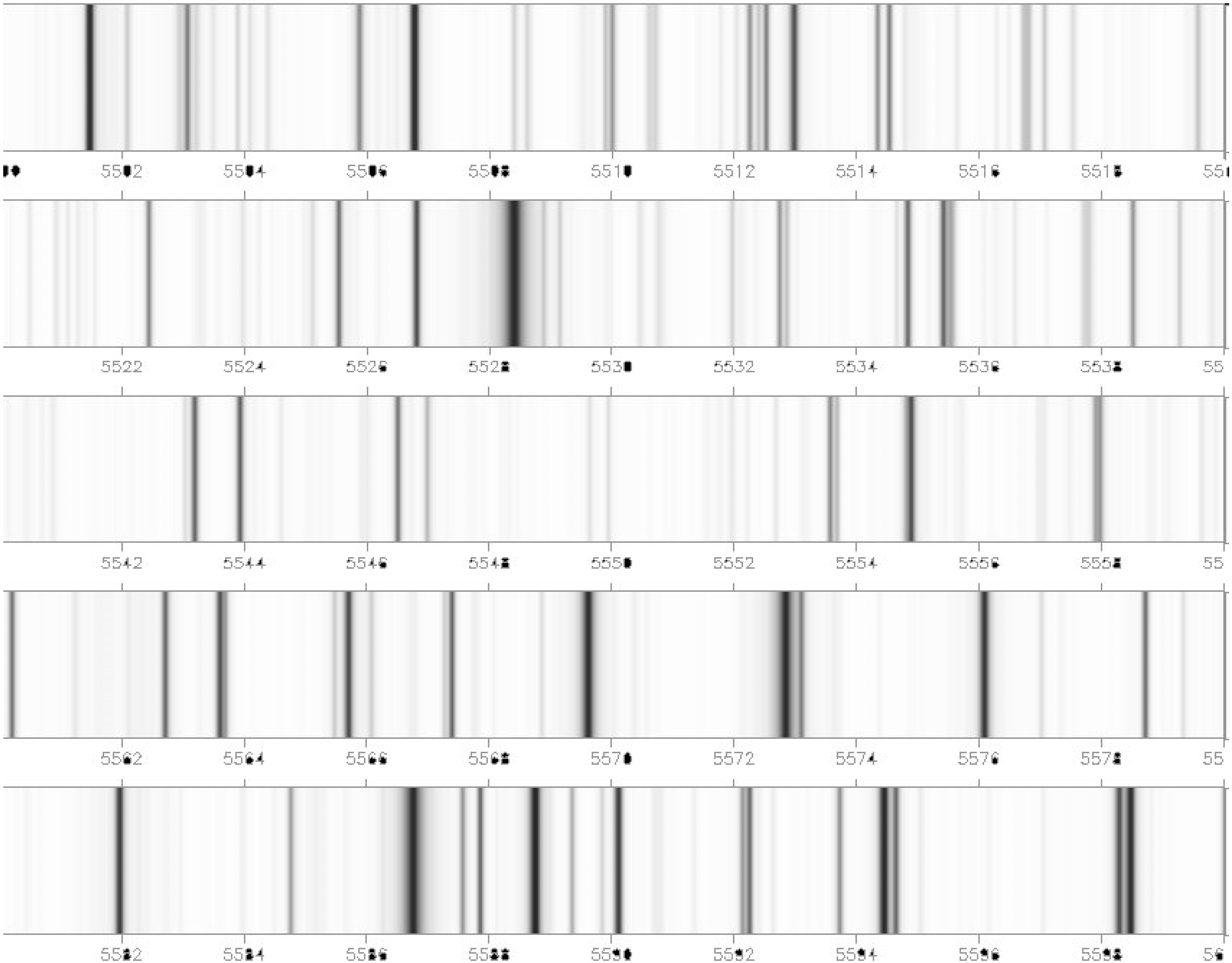
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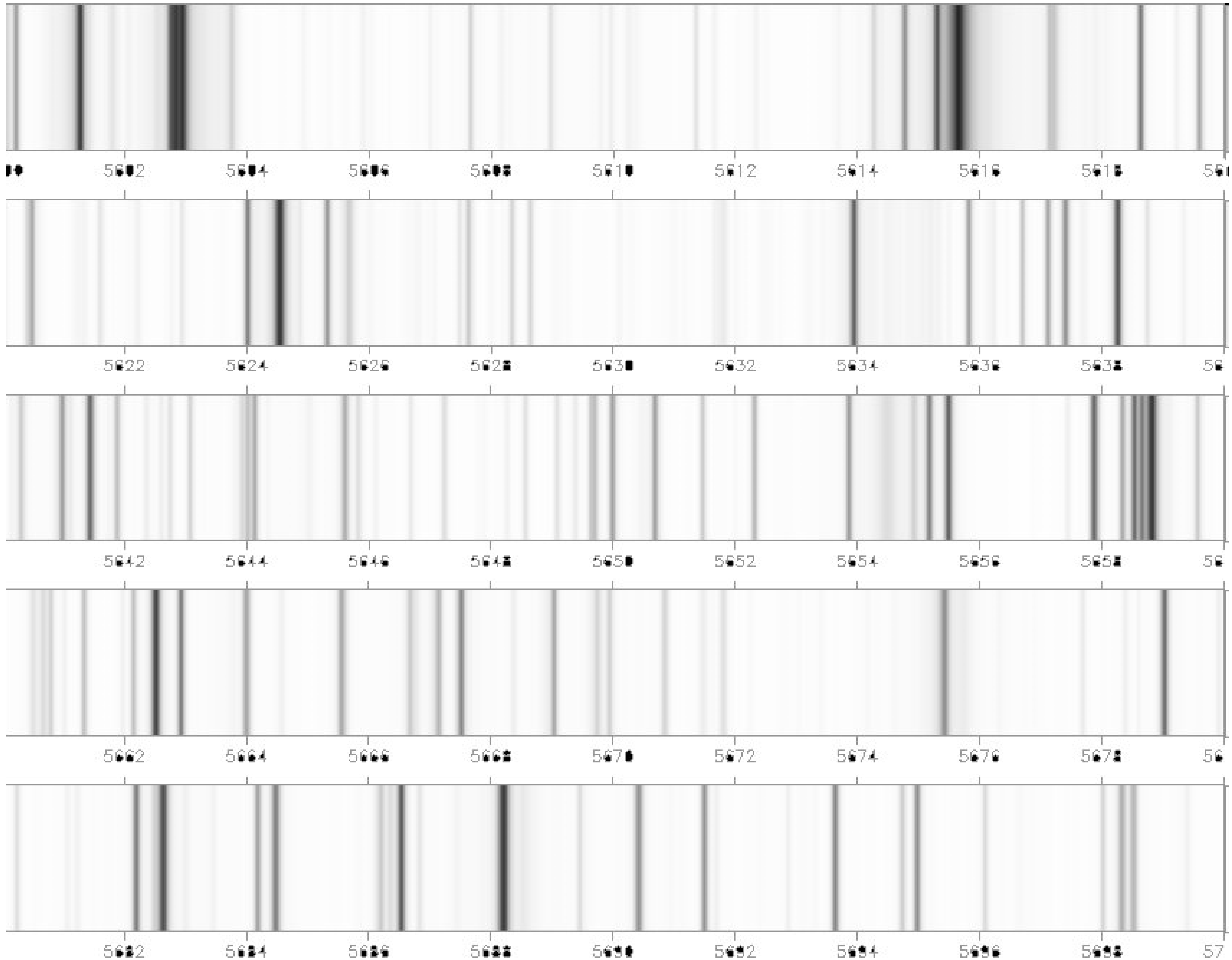

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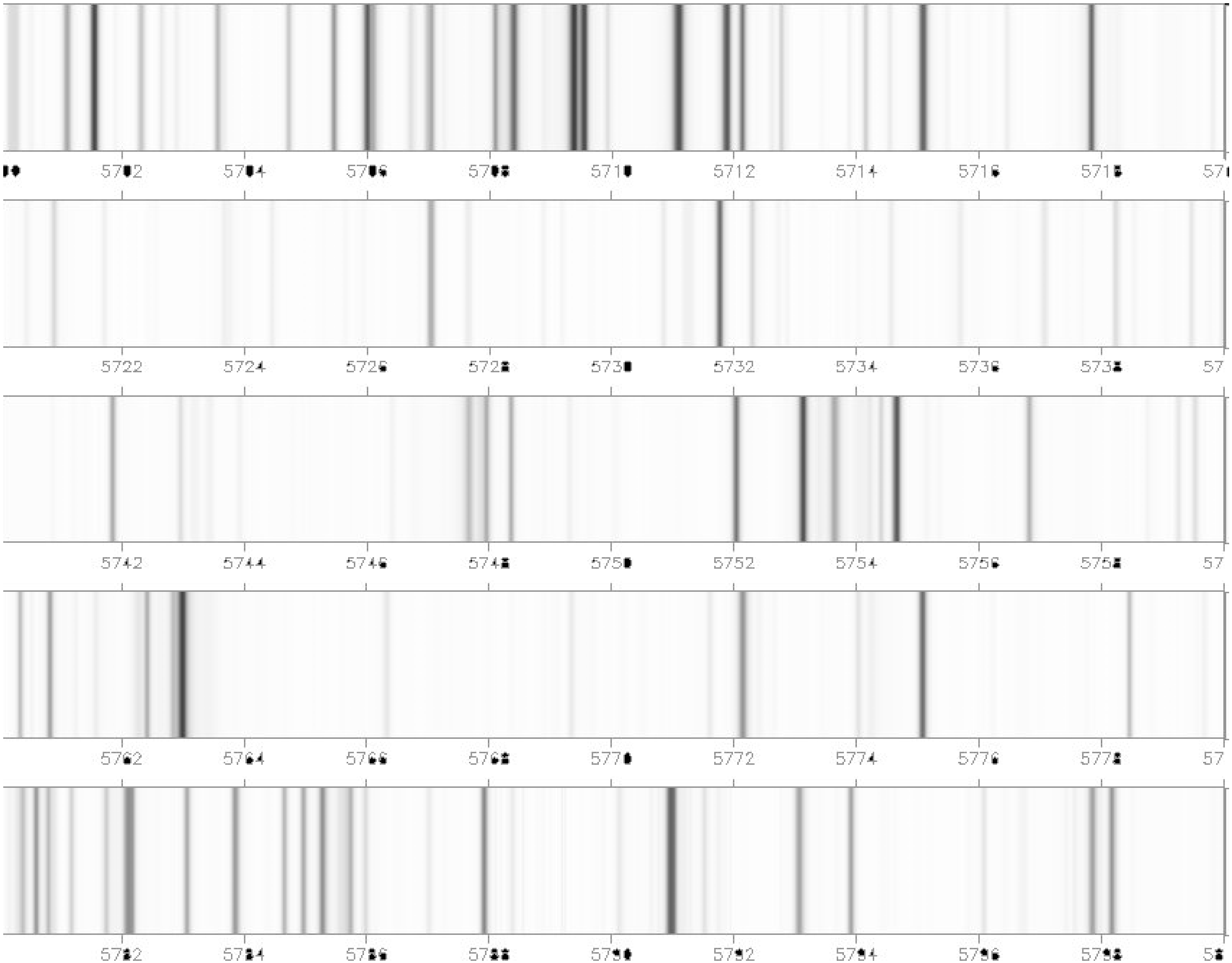

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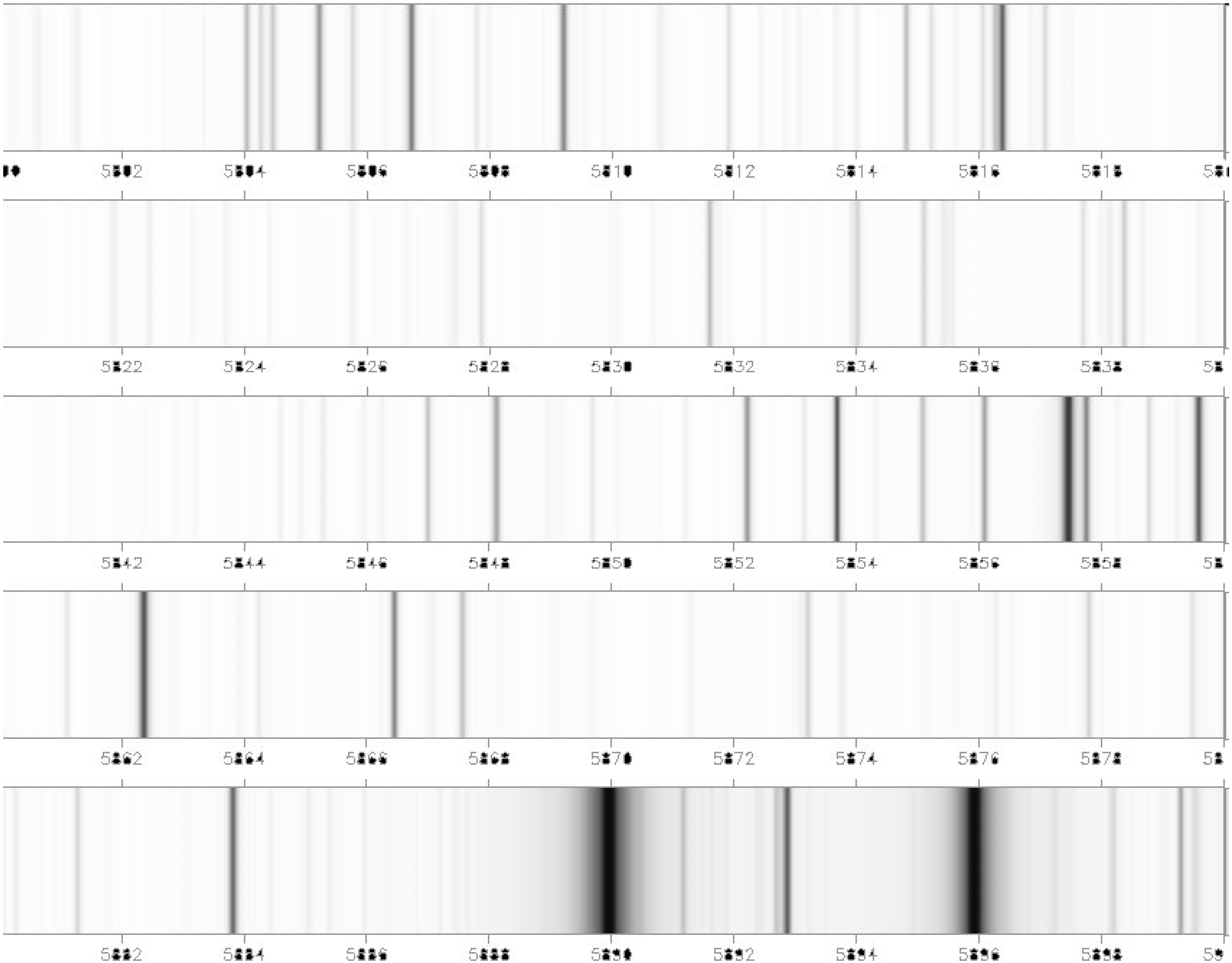

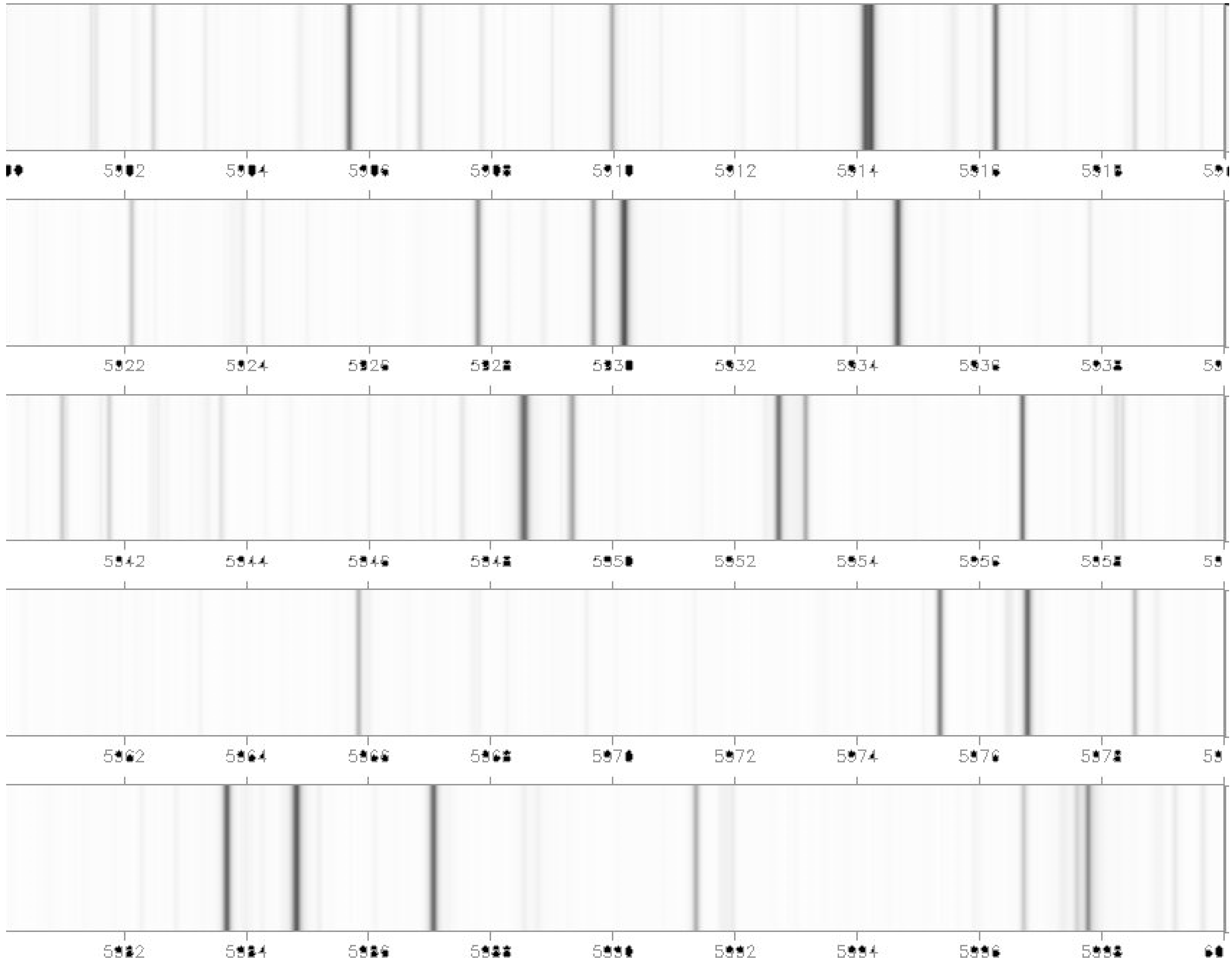
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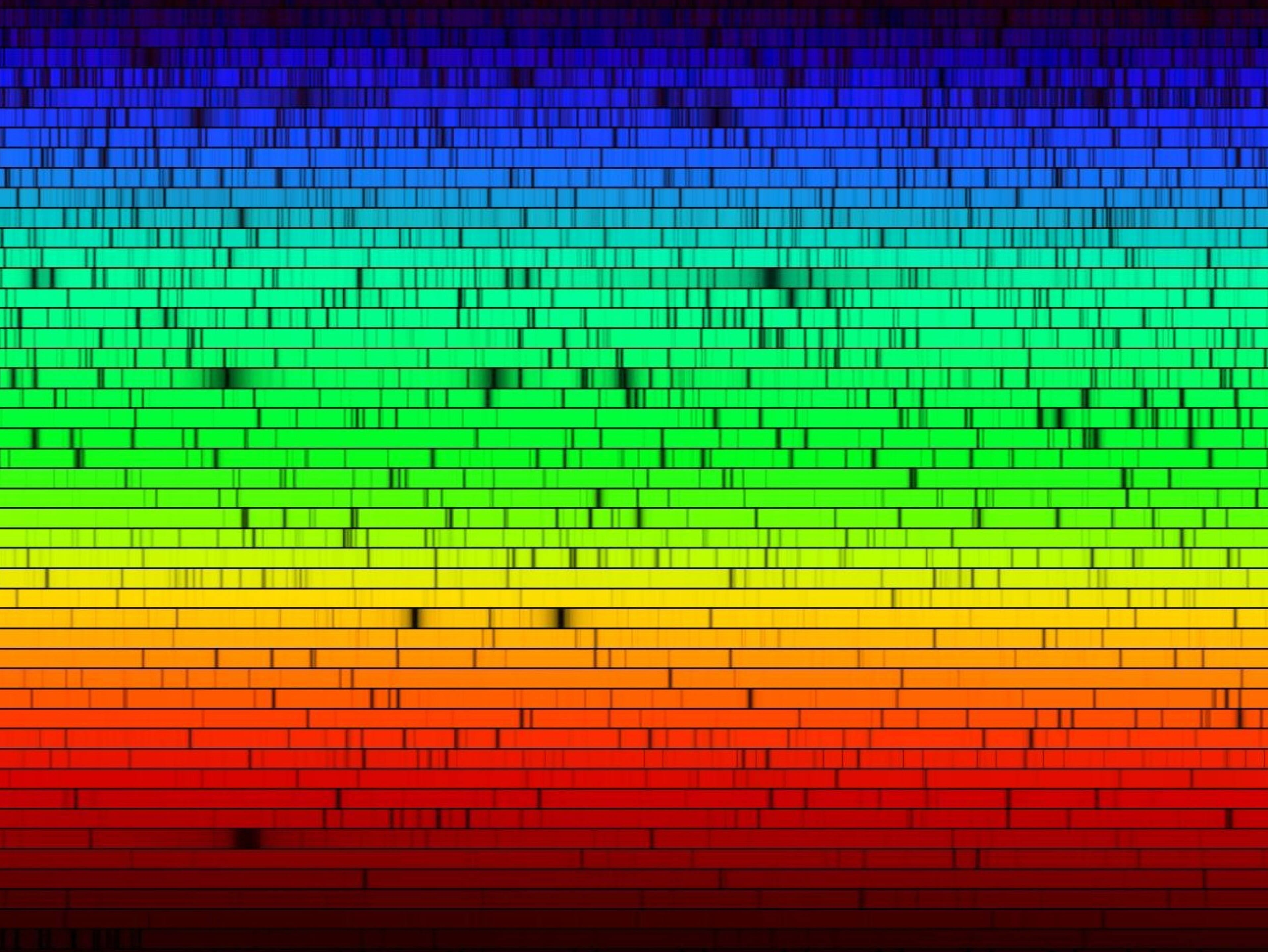


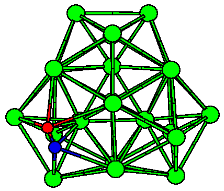
further programme for today:

1. **relevance of atomic physics**
2. **overview cluster physics**

role of atomic physics:

- Astrophysik
- Laserentwicklung
- Prozesse in der oberen Atmosphäre
- Stoßprozesse bei der Kernfusion
- Quantenchemie
- Korrelationsprozesse in starken Feldern (Laser, Magnet)
- Prinzipielle physikalische Fragestellungen wie QED
- Exotische Systeme: Myonium, Positronium, ...

Übersicht Clusterphysik



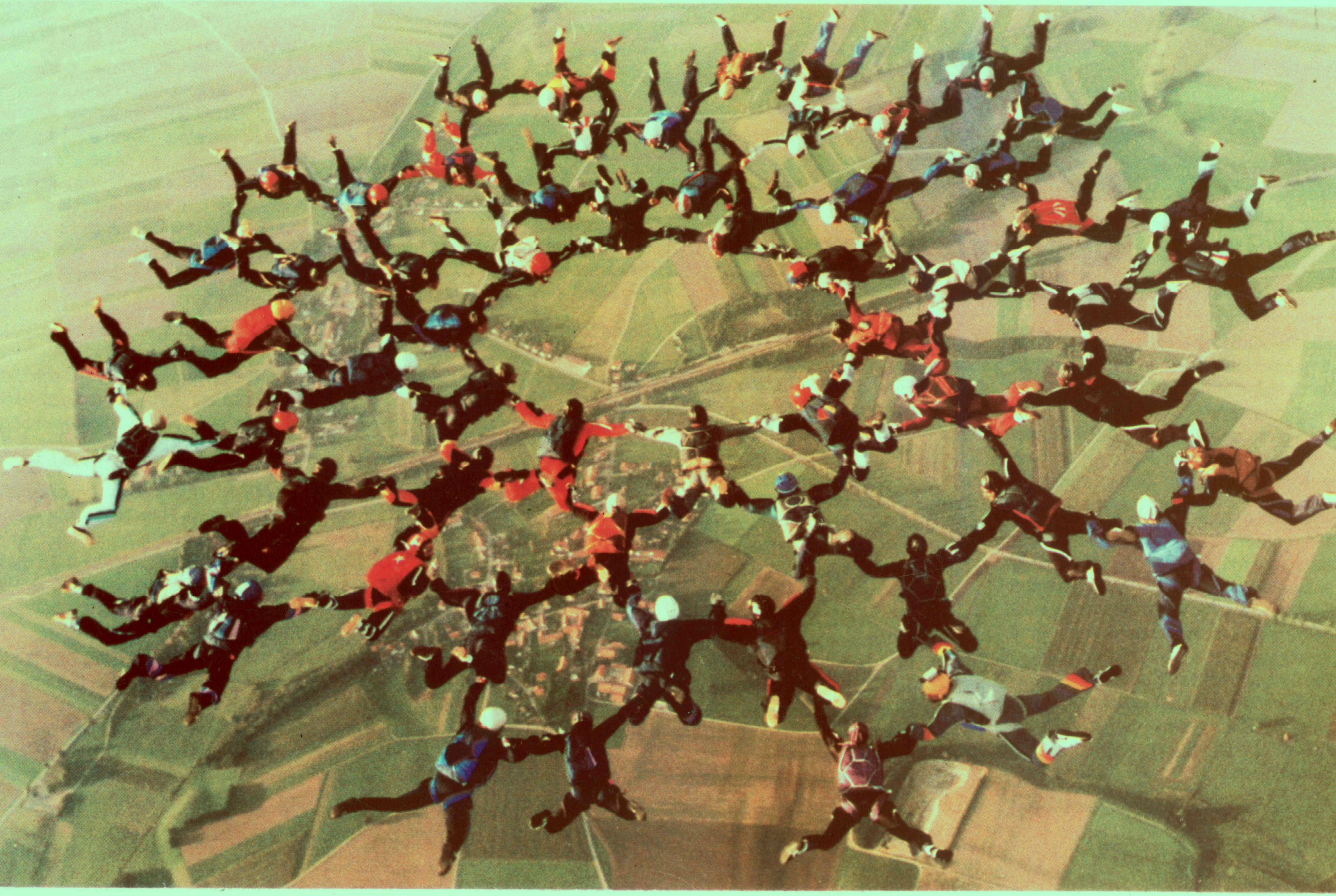
Atomic clusters

or

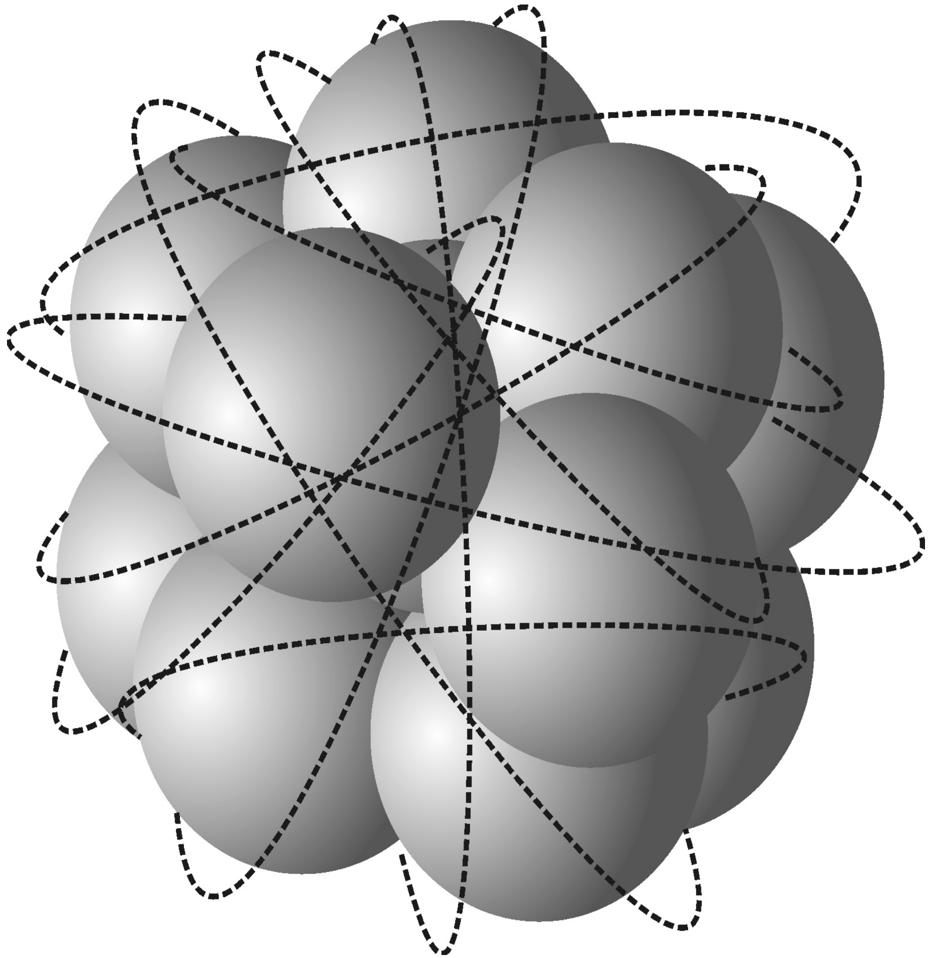
Physics on the 1-nm scale

lectures WS 2010/11

UNIVERSITÄT ROSTOCK



A cluster of simple metal atoms can be considered as a metallic quantum dot. In the corresponding bulk materials the electrons need much more space.



Literature

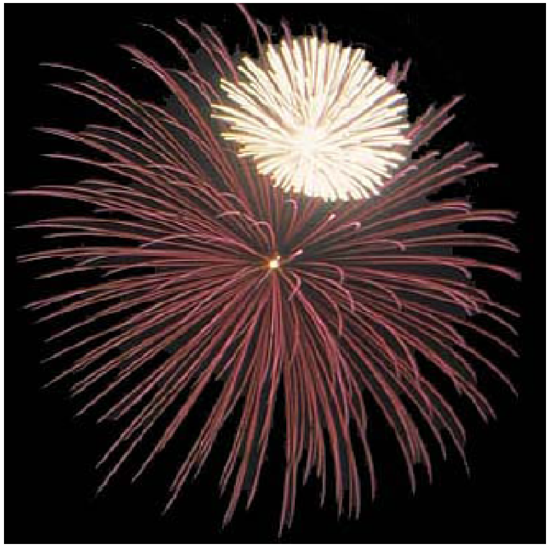
- Sugano/Koizumi *Microcluster Physics* Springer 1998
- Haberland *Clusters of Atoms and Molecules* Springer 1995
- Ekardt *Metal Clusters (Theory)* Wiley 1999
- Kreibig/Vollmer *Optical Properties of Metal Clusters* Springer 1995
- Meiwes-Broer *Metal Clusters at Surfaces* Springer 2000
- Bergmann/Schaefer, Band 5, *Vielteilchensysteme*, S. 549ff

Nano-particles

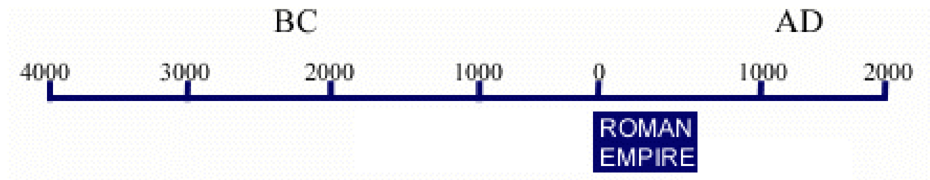
Since long ago man has used the properties of particulate materials in an empirical manner

In the VIIIth century the Chinese discovered the « black powder », which later gave birth to fireworks, then to military uses about the year 1000, well before it was understood that the speed of the combustion was inversely proportional to the grain size.

Man created hand stencils by blowing pigments onto a hand against the wall, which has survived to the ages.(30000 years ago, grotte Chauvet)



Lycurgus-Becher



27 BC bis 5. Jht. AD

British Museum London

The Cup is surrounded by a frieze showing the myth of King Lycurgus. He is seen here being dragged into the underworld by Ambrosia, who has been turned into a vine.

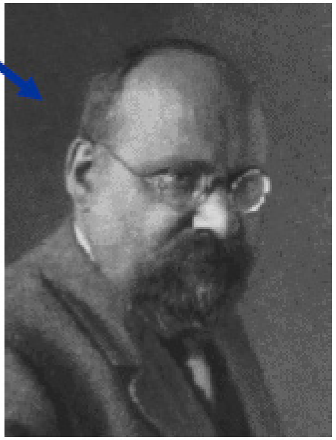
Rubinglas mit eingebetteten Gold- und Silberteilchen lt. Röntgenanalyse

Stained-glass for cathedrals

St Nicolas de Port

The origin of these colours, due to pigmented grains which are insoluble in their surroundings, was invoked by Michael Faraday (1791-1867) in 1853.

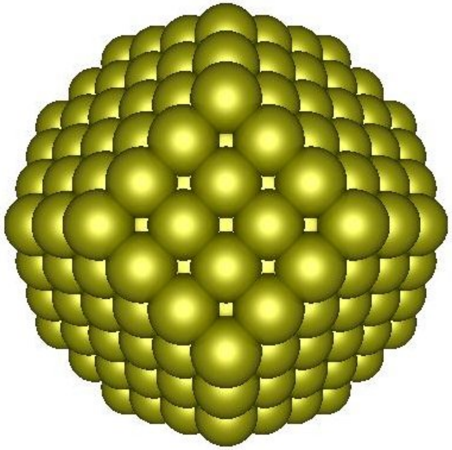
In 1907 Gustav Mie (1868-1957) explained the colours by showing how light in medium gets scattered by particles.



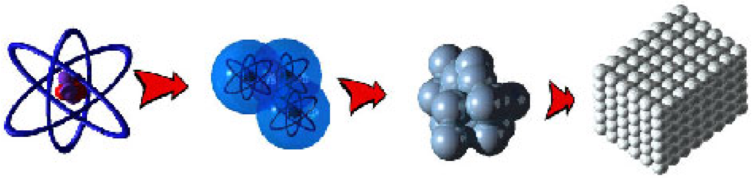

Nano-grains (of carbon) exist in interstellar medium
Horse-head nebula in Orion cloud.
Anglo-Australian observatory

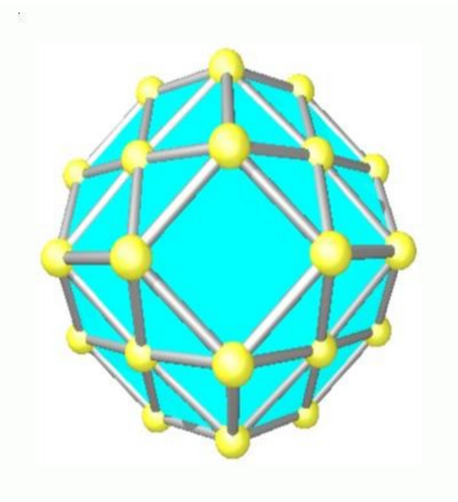
Introduction – What is a cluster ?

Clusters – Intermediate range between atoms and bulk matter



Aggregates of **2–10^{n}** particles
($n \rightarrow 6$ or 7)



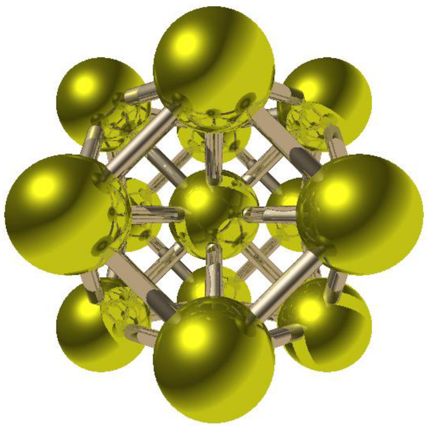


Cluster Size	N	Diameter / nm(Na_N)
Small	$\leq 10^2$	≤ 1.9
Medium	10^2–10^4	1.9–8.6
Large	$> 10^4$	> 8.6

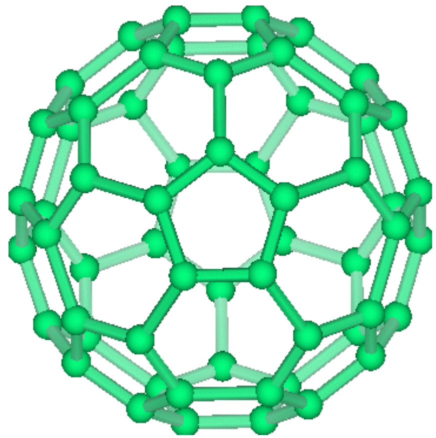
Types of Clusters - 1

Based on the type of constituent particles & type of bonding

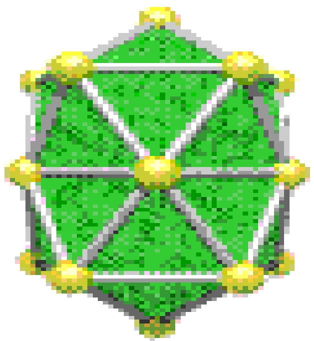
Metal Clusters **Semiconductor Clusters** **Rare gas Clusters**



S block – Metallic bond
(e.g. alkali & alkaline earth)
SP metals – Covalent bond
(e.g. Al)



Bonding – **Covalent**
e.g. C, Si & Ge

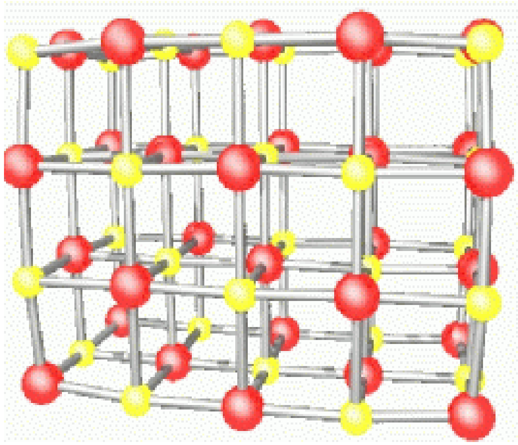


Bonding **-Van der Waals**
Inter-atomic attraction increases with increasing atomic mass (**He→Rn**).

http://www.tc.bham.ac.uk/~roy/Teaching/CHM3T1

Types of Clusters - 2

Ionic Clusters

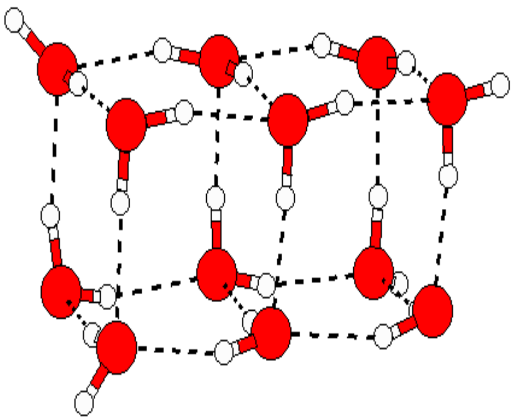


atoms with large difference in electronegativity

Bonding – **Ionic**

e.g. $(NaCl)_n$, $[Mg_xO_y]^{2(x-y)+}$

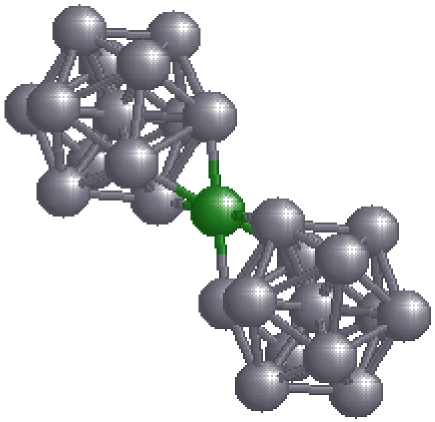
Molecular Clusters



van der Waals,
dipole-dipole interactions, and hydrogen bonding

e.g. $(N_2)_n$, $(C_6H_6)_n$, $(H_2O)_n$

Cluster molecules



thermodynamically and/or kinetically stable with respect to coalescence

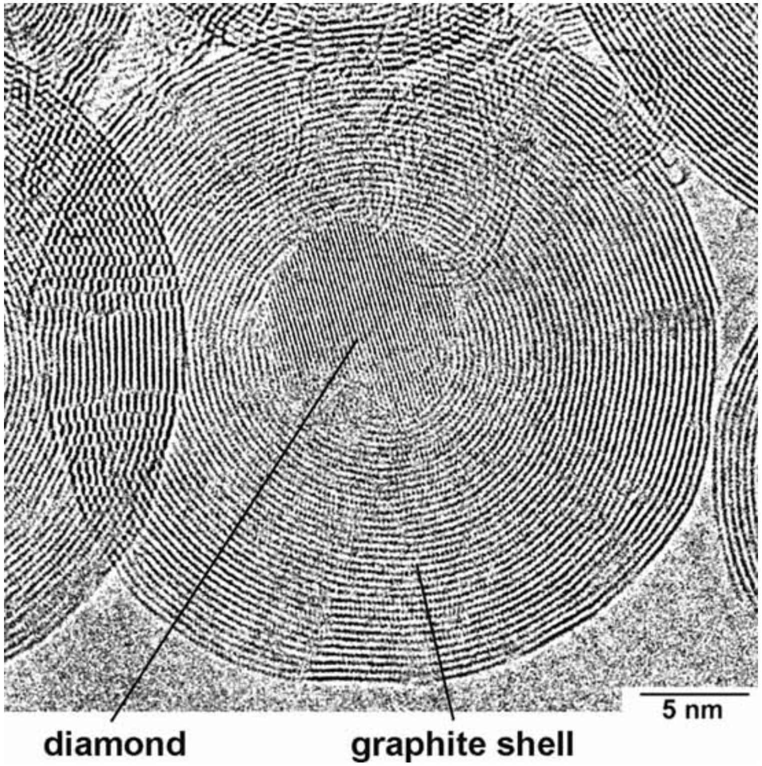
e.g. $Al_{13}MgAl_{13}$

Binding strenghts

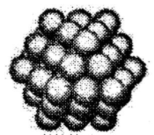
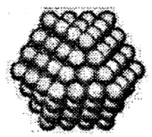
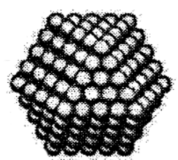
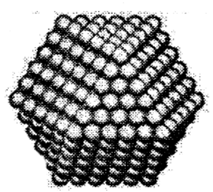
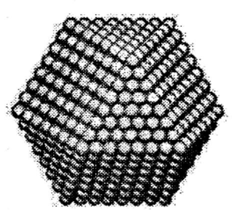
Table 2.1. Classification of clusters according to their binding [Jortner (1984)]

Cluster type	Type of binding	Binding energy [eV]	Examples
van der Waals	Dispersive forces	≤ 0.3	$(Ar)_N$, $(N_2)_N$, $(CO_2)_N$
Molecular	Dispersive forces, weak electrostatic forces	0.3 – 1	$(\text{org.molecules})_N$, $(I_2)_N$
Hydrogen-bonded	Intermolecular hydrogen bridges	0.3 – 0.5	$(HF)_N$, $(H_2O)_N$
Ionic	Heteropolar bonding	2 – 4	$(NaCl)_N$, $(CaF_2)_N$
Valence	Covalent bonding	1 – 4	C_N, S_8, As_4
Metal	Metallic bonding	0.5 – 3	Na_N, Al_N, Cu_N, W_N

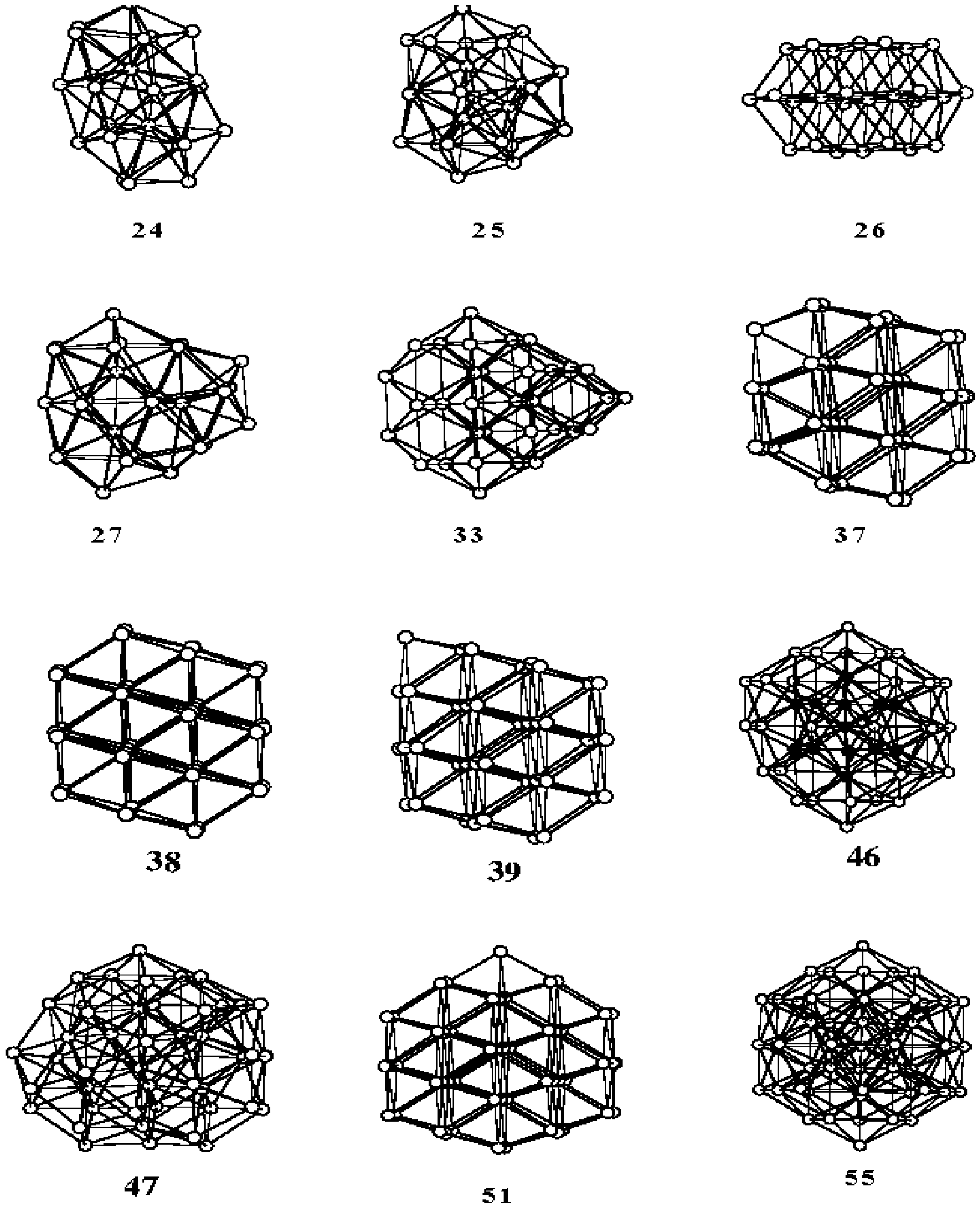
Exotic clusters:
e.g., Carbon nano-onion with enclosed diamond



size-dependence

Full-shell Clusters	Total Number of Atoms	Surface Atoms (%)
1. Shell 	13	92
2 Shells 	55	76
3 Shells 	147	63
4 Shells 	309	52
5 Shells 	561	45
7 Shells 	1415	35

from a compact structure to solid-like structure



Structure of Ni_n

Y. Xiang, X. G. Gong

J. Phys. Chem. (2000)

Size effects : number of atoms/molecules on the surface

Spherical cluster approximation / Hard atomic spheres

Volume of a building block (atomic sphere) : V_a

Volume of cluster : $V_c = \mathrm{n} V_a$ (rough approximation, no filling factor)

Radii of cluster and atom : $$\frac{4\pi}{3} R_c^3 = \mathrm{n} \frac{4\pi}{3} R_a^3$$

$$\boxed{R_c = \mathrm{n}^{1/3} R_a}$$

better: R_c equals the Wigner-Seitz radius

Number of atoms on the surface : $$\mathrm{n}_s = \frac{4\pi R_c^2}{\pi R_a^2} = 4\mathrm{n}^{2/3}$$

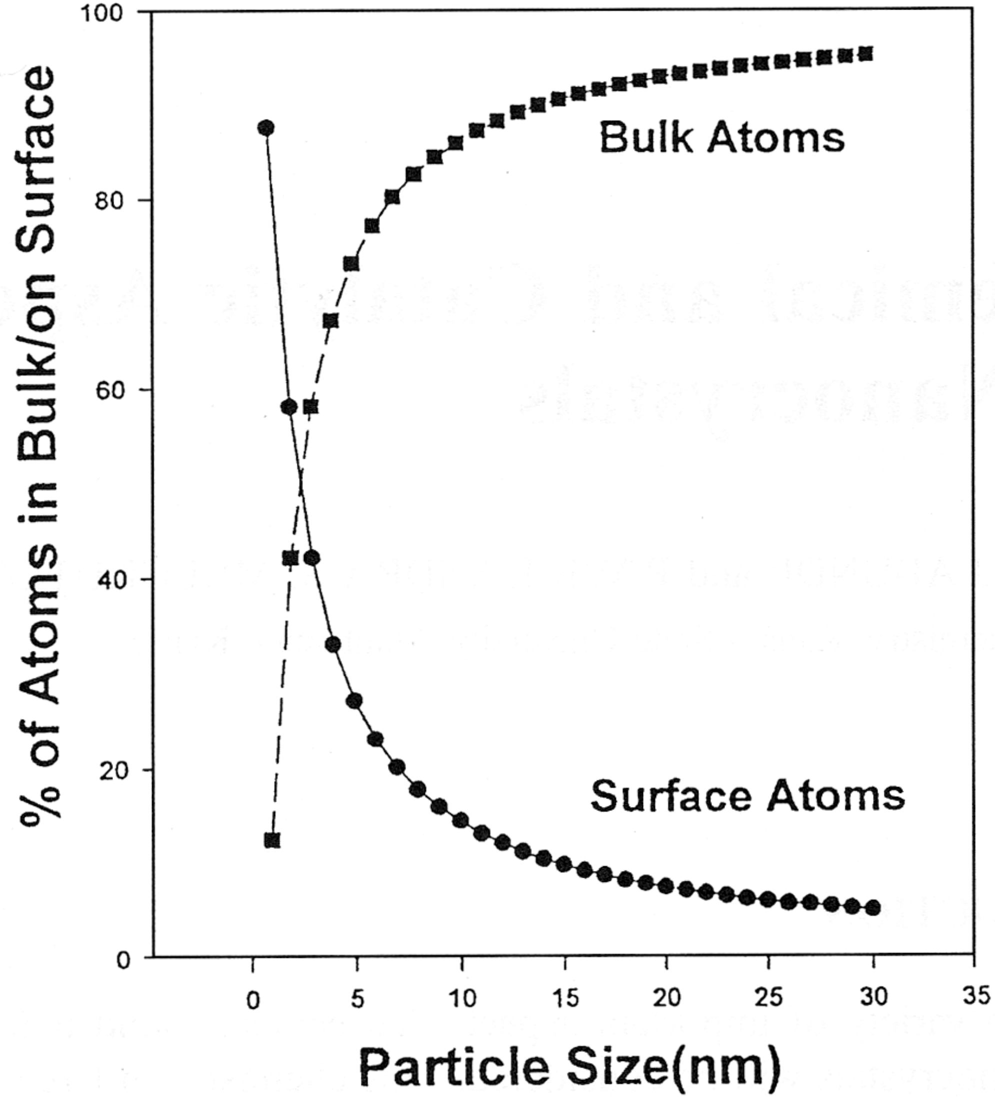
(divide the surface of the cluster sphere by the cross section of an atom)

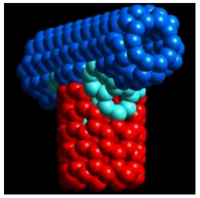
Fraction of atoms on the surface :

$$\boxed{F_s = 4\mathrm{n}^{-1/3}}$$

Surface to bulk atom ratio

- Spherical iron nanocrystals
- J. Phys. Chem. 1996, Vol. 100, p. 12142





Example : Sodium clusters

(average radius of the atomic sphere in the bulk = 0.2 nm)

Small Na clusters : diameter less than 1.9 nm
(**86%** of atoms on surface)

Large Na clusters : diameter larger than 8.6 nm
(**19%** of atoms on surface)

Need to have more than 64 million atoms for 1% of atoms on surface