Laboratory Spectroscopy for near-Infrared Astrophysics

Solvay Workshop, Brussels november 2019

by

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Collaborators and thanks

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Lars Engström *Physics, Lund University*

Asli Pehlivan Rhodin *Malmö University and Lund Observatory (until 2018)*

Asimina Papoulia *Malmö University and Lund University*

Jörgen Ekman *Malmö University*

Per Jönsson *Malmö University*

LUMCAS, CompAS, Imperial College London, Mons group, NIST and Uppsala university

VETENSKAPSRÅDET
THE SWEDISH RESEARCH COUNCIL

Gyllenstiernska
Krapperupsstiftelsen

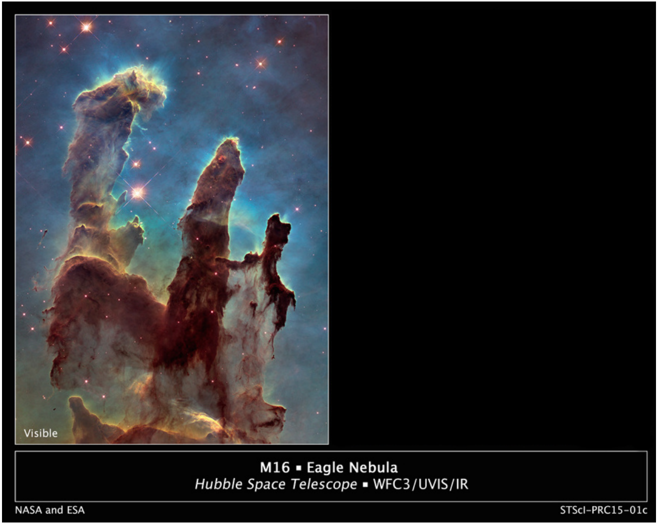
The Crafoord Foundation
ESTABLISHED BY HOLGER CRAFOORD IN 1980

Conclusion

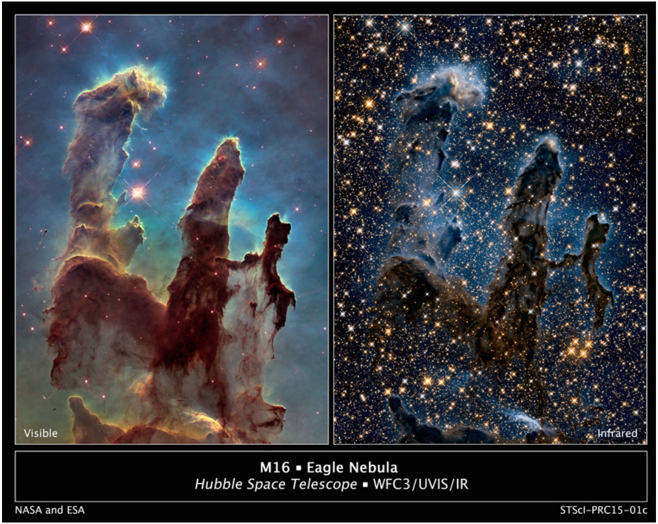
The aim of our program is to provide evaluated sets of transition data with realistic uncertainties for selected atoms and ions with a range in wavelength, strength and excitation potential.

Laboratory measurements and calculations can provide the data needed to analyse the expensively required astronomical observations.

Optical vs near-IR observations



Optical vs near-IR observations



near-IR stellar spectroscopy, 1-5 μm

Motivations for near-infrared observations:

- Several orders of magnitude less extinction
- Atmospheric transmission bands
- Cool stars

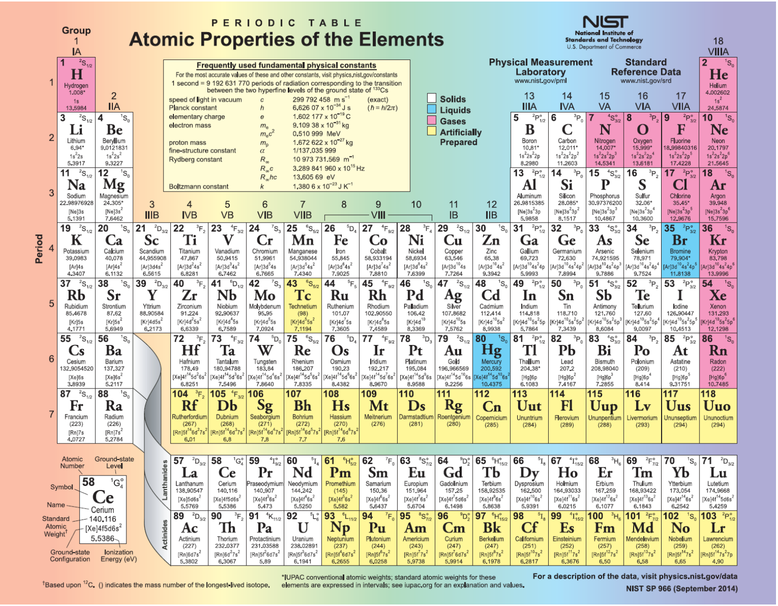
Consequences:

- Astronomical observatories are designed for this region.
- Coming ELTs deigned to observe 1-2.5 μm.
- The atomic data base above 1 micron is sparse.
- Numerous atomic lines in the stellar spectra

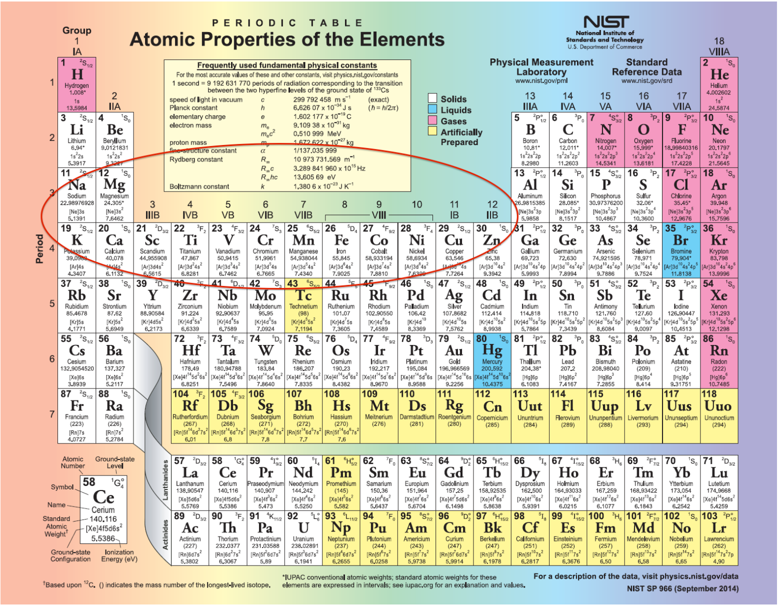
near-IR atomic transitions

near-IR transitions from an atomic physicists point of view:

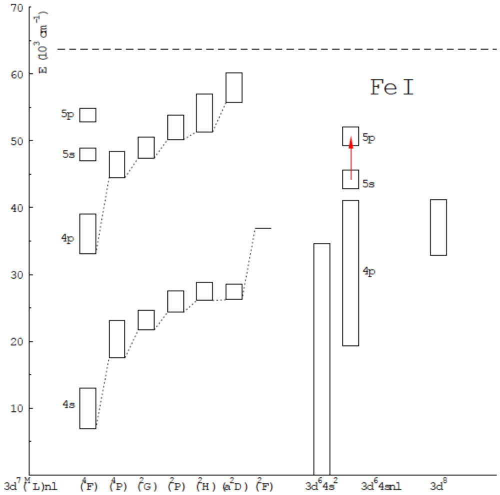
- High-excitation transitions; Rydberg states
- Lower excitation transitions in complex atomic spectra
- Resonance lines in heavier elements, e.g. third spectra of rare-earth elements


PERIODIC TABLE
Atomic Properties of the Elements
NIST National Institute of Standards and Technology U.S. Department of Commerce
Physical Measurement Laboratory www.nist.gov/pml
Standard Reference Data www.nist.gov/srd
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 133Cs
speed of light in vacuum c 299 792 458 m s−1 (exact)
Planck constant h 6.626 07 x 10−34 J s (ħ = h/2π)
elementary charge e 1.602 177 x 10−19 C
electron mass me 9.109 38 x 10−31 kg
mec2 0.510 999 MeV
proton mass mp 1.672 622 x 10−27 kg
fine-structure constant α 1/137.035 999
Rydberg constant R∞ 10 973 731.569 m−1
R∞c 3.289 841 960 x 1015 Hz
R∞hc 13.605 69 eV
Boltzmann constant k 1.380 6 x 10−23 J K−1
Solids
Liquids
Gases
Artificially Prepared
Group
Period
1 H Hydrogen 1.008*
2 He Helium 4.002602
3 Li Lithium 6.94*
4 Be Beryllium 9.0121831
5 B Boron 10.81*
6 C Carbon 12.011*
7 N Nitrogen 14.007*
8 O Oxygen 15.999*
9 F Fluorine 18.99840316
10 Ne Neon 20.1797
11 Na Sodium 22.98976928
12 Mg Magnesium 24.305*
13 Al Aluminum 26.9815385
14 Si Silicon 28.085*
15 P Phosphorus 30.97376200
16 S Sulfur 32.06*
17 Cl Chlorine 35.45*
18 Ar Argon 39.948
19 K Potassium 39.0983
20 Ca Calcium 40.078
21 Sc Scandium 44.955908
22 Ti Titanium 47.867
23 V Vanadium 50.9415
24 Cr Chromium 51.9961
25 Mn Manganese 54.938044
26 Fe Iron 55.845
27 Co Cobalt 58.933194
28 Ni Nickel 58.6934
29 Cu Copper 63.546
30 Zn Zinc 65.38
31 Ga Gallium 69.723
32 Ge Germanium 72.630
33 As Arsenic 74.921595
34 Se Selenium 78.971
35 Br Bromine 79.904*
36 Kr Krypton 83.798
37 Rb Rubidium 85.4678
38 Sr Strontium 87.62
39 Y Yttrium 88.90584
40 Zr Zirconium 91.224
41 Nb Niobium 92.90637
42 Mo Molybdenum 95.95
43 Tc Technetium (98)
44 Ru Ruthenium 101.07
45 Rh Rhodium 102.90550
46 Pd Palladium 106.42
47 Ag Silver 107.8682
48 Cd Cadmium 112.414
49 In Indium 114.818
50 Sn Tin 118.710
51 Sb Antimony 121.760
52 Te Tellurium 127.60
53 I Iodine 126.90447
54 Xe Xenon 131.293
55 Cs Cesium 132.9054520
56 Ba Barium 137.327
72 Hf Hafnium 178.49
73 Ta Tantalum 180.94788
74 W Tungsten 183.84
75 Re Rhenium 186.207
76 Os Osmium 190.23
77 Ir Iridium 192.217
78 Pt Platinum 195.084
79 Au Gold 196.966569
80 Hg Mercury 200.592
81 Tl Thallium 204.38*
82 Pb Lead 207.2
83 Bi Bismuth 208.98040
84 Po Polonium (209)
85 At Astatine (210)
86 Rn Radon (222)
87 Fr Francium (223)
88 Ra Radium (226)
104 Rf Rutherfordium (267)
105 Db Dubnium (268)
106 Sg Seaborgium (271)
107 Bh Bohrium (272)
108 Hs Hassium (270)
109 Mt Meitnerium (276)
110 Ds Darmstadtium (281)
111 Rg Roentgenium (280)
112 Cn Copernicium (285)
113 Uut Ununtrium (284)
114 Fl Flerovium (289)
115 Uup Ununpentium (288)
116 Lv Livermorium (293)
117 Uus Ununseptium (294)
118 Uuo Ununoctium (294)
Lanthanides
57 La Lanthanum 138.90547
58 Ce Cerium 140.116
59 Pr Praseodymium 140.907
60 Nd Neodymium 144.242
61 Pm Promethium (145)
62 Sm Samarium 150.36
63 Eu Europium 151.964
64 Gd Gadolinium 157.25
65 Tb Terbium 158.92535
66 Dy Dysprosium 162.500
67 Ho Holmium 164.93033
68 Er Erbium 167.259
69 Tm Thulium 168.93422
70 Yb Ytterbium 173.054
71 Lu Lutetium 174.9668
Actinides
89 Ac Actinium (227)
90 Th Thorium 232.0377
91 Pa Protactinium 231.03588
92 U Uranium 238.02891
93 Np Neptunium (237)
94 Pu Plutonium (244)
95 Am Americium (243)
96 Cm Curium (247)
97 Bk Berkelium (247)
98 Cf Californium (251)
99 Es Einsteinium (252)
100 Fm Fermium (257)
101 Md Mendelevium (258)
102 No Nobelium (259)
103 Lr Lawrencium (262)
Atomic Number
Ground-state Level
Symbol
Name
Standard Atomic Weight†
Ground-state Configuration
Ionization Energy (eV)
†Based upon 12C. () indicates the mass number of the longest-lived isotope.
*IUPAC conventional atomic weights; standard atomic weights for these elements are expressed in intervals; see iupac.org for an explanation and values.
For a description of the data, visit physics.nist.gov/data
NIST SP 966 (September 2014)

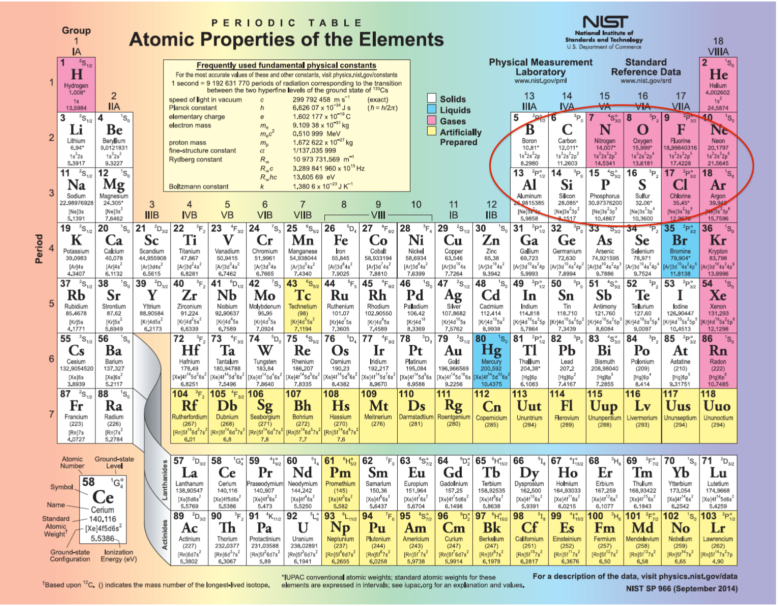
High-excitation transitions



High-excitation transitions- Fe I



p elements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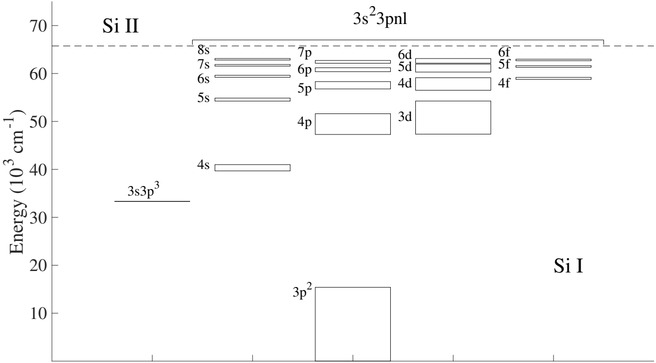
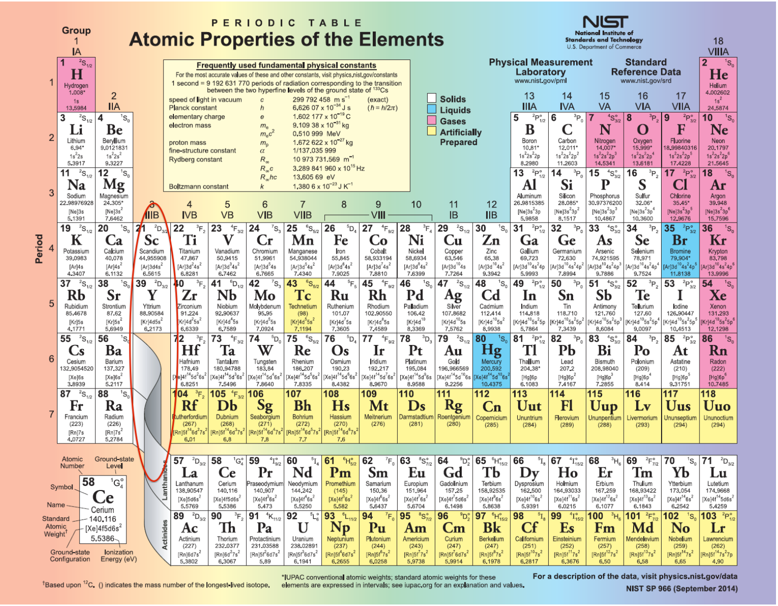
Silicon



Si II
3s²3pnl
70
60
50
40
30
20
10
Energy (10³ cm⁻¹)
8s
7s
6s
5s
4s
7p
6p
5p
4p
6d
5d
4d
3d
6f
5f
4f
3s3p³
3p²
Si I

Low excitation lines - Sc I, Y I, La I



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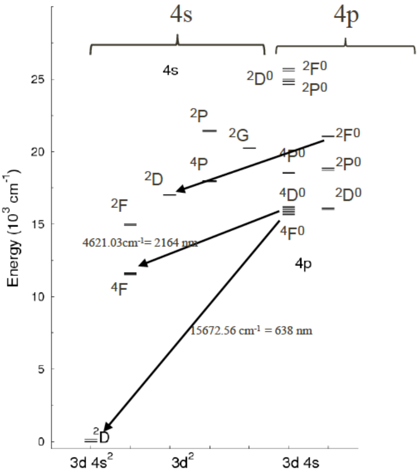

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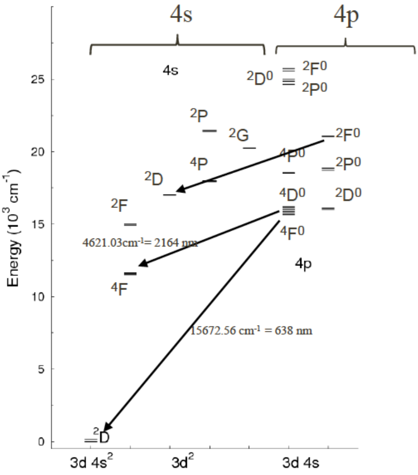

The energy level structure for Sc I, Y I and La I are similar with the energy levels for $nd(n+1)s^2$ and $nd^2(n+1)s$

Sc I : $3d4s^2$, $3d^24s$
Y I : $4d5s^2$, $4d^25s$
La I : $5d6s^2$, $5d^26s$

Infrared transitions between $nd^2(n+1)s$ – $nd(n+1)s(n+1)p$

Experimental transition rates

The A-values is derived from the measured quantities branching fraction (BF) and radiative lifetime (τ) of the upper level.

$$A_{ul} = \frac{BF_{ul}}{\tau_u}$$

where

$$BF_{ul} = \frac{I_{ul}}{\sum_l I_{ul}}$$

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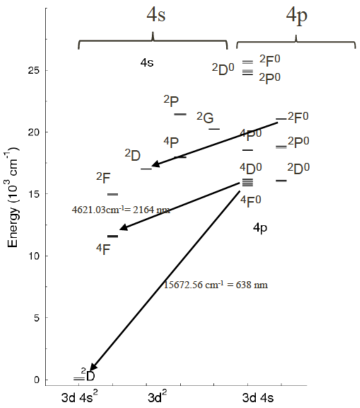

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Decay region	*BF spread*	*lifetime*
only optical	narrow	1-20 ns
optical + nIR	wide	1-20 ns
only nIR	narrow	1-10μs

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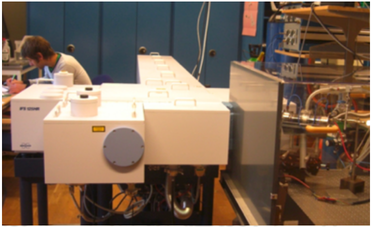
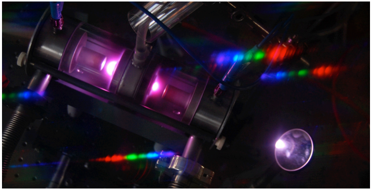
The Edlén laboratory

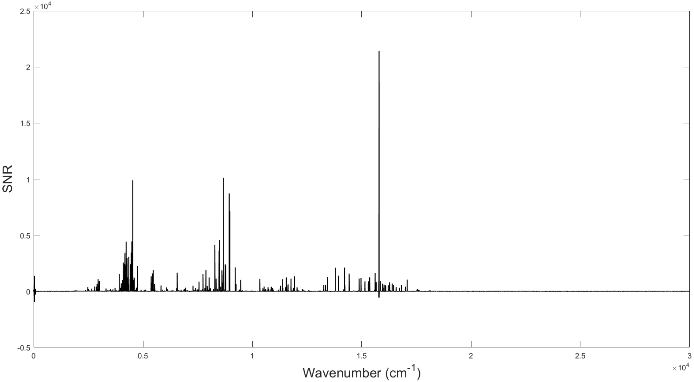




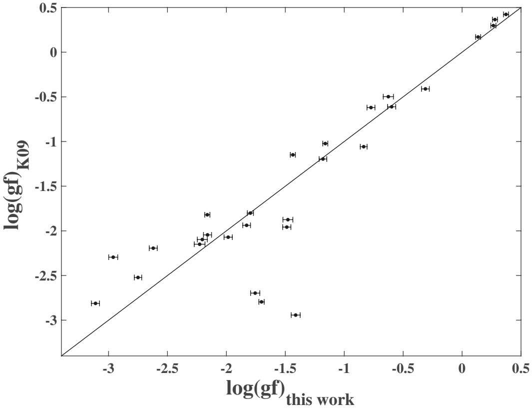
FTS Bruker IFS125
Coverage: 4000 Å- 5 μm
HC lamp produces neutral and singly ionised atoms and ions.
Resolving power 10^6

Lifetimes measured at Lund High Power Laser Facility (closed 2018).

FTS spectrum of Sc I



Results for Sc I

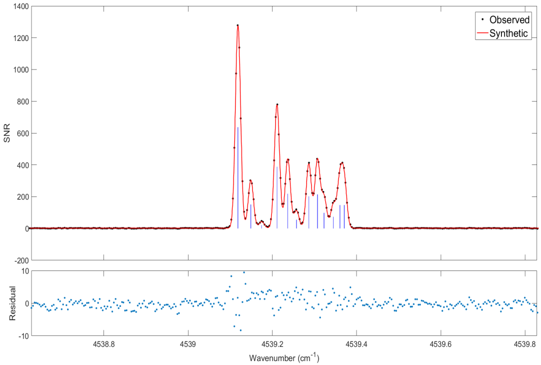


Results from Sc I : Pehlivan et al. (2015)

Lifetimes and branching fraction for Y I and La I have been measured, and are being analysed.

Hyperfine structure

The interaction with the nuclear spin splits the fine structure. More important for near-IR lines.



Spectrum of Sc I observed with the IRFTS at Edlen laboratory, van Deelen 2017.

Hyperfine structure

Physica Scripta. Vol. 53, 28–32, 1996

Hyperfine Structure of Sc I by Infrared Fourier Transform Spectroscopy

A. Aboussaïd,[a] M. Carleer,[a] D. Hurtmans,[a] E. Biémont[b] and M. R. Godefroid[a]*

[a] Laboratoire de Chimie Physique Moléculaire, CP160/09, Université Libre de Bruxelles, 50, av. F.D. Roosevelt, B-1050 Bruxelles, Belgium
[b] Institut d'Astrophysique, Université de Liège, 5, Avenue de Cointe, B-4000 Liège, Belgium

Received March 5, 1995; Accepted in revised form May 29, 1995

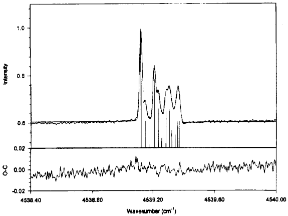


Fig. 1. Observed and fitted hyperfine patterns for the Sc I 3d4s(^{1}D)4p ^{2}D$^o_{3/2}$ – 3d^2(^{3}F)4s ^{4}F$_{5/2}$ at $\tilde{\nu}$ = 4539.227 cm^{-1}. The theoretical components of the profiles with their relative intensities are also shown for comparison. The lower part of the figure shows the (observed–calculated) signal corresponding to the final fit of the line profile.

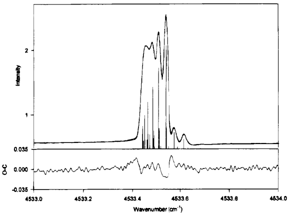
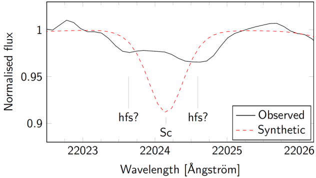


Fig. 2. Observed and fitted hyperfine patterns for the Sc I 3d4s(^{3}D)4p ^{4}D$^o_{7/2}$ – 3d^2(^{3}F)4s ^{4}F$_{9/2}$ at $\tilde{\nu}$ = 4533.502 cm^{-1}. The theoretical components of the profiles with their relative intensities are also shown for comparison. The lower part of the figure shows the (observed–calculated) signal corresponding to the final fit of the line profile.

Hyperfine structure

Omitting the inclusion of the hyperfine structure can result in significant deviations in the abundance.



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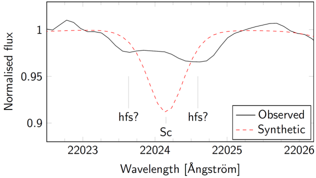
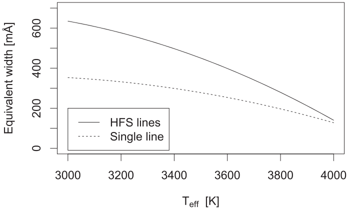
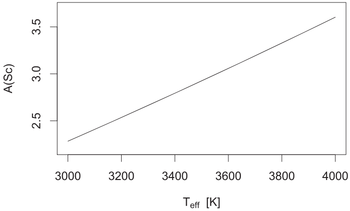






Simulations by Thorsbro+, ApJS (2018).

Approach for Mg, Si and Al

Approach to retrieve an evaluated set of infrared Mg I, Al I and Si I transition data:

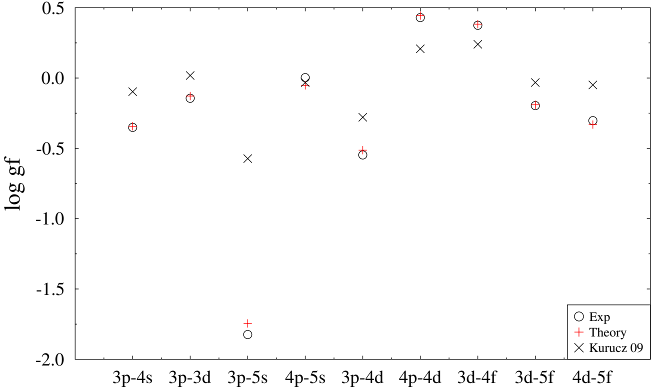
Experimental data
FTS measurements combined with lifetime data

Theoretical data
ATSP2k calculations for additional states

Stellar spectra
For benchmarking and application

Combined with collisional data by P Barklem and J Grumer (Uppsala) to provide *'atomic data to the limit'*. Calculations by P Jönsson, A Papoulia, J Ekman.

Results for Magnesium



Results from Mg I : Pehlivan et al. (2017)

Studies for Silicon (Pehlivan Rhodin et al., in review) and Aluminium (Papoulia et al., 2018 and Burheim et al., in preparation). See Posters.

Note that the uncertainty in the data directly translates to an uncertainty in derived stellar abundance.

Uncertanties

Remember:

$$A_{ul} = \frac{BF_{ul}}{\tau_u}$$

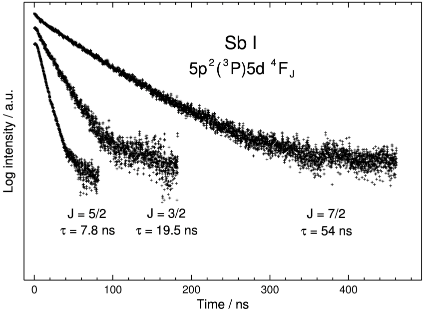
where

$$BF_{ul} = \frac{I_{ul}}{\sum_l I_{ul}}$$

and

$$f \propto \lambda^2 \cdot A$$

Systematic and *statistical* effects contribute to the uncertainty.



Uncertanties

Sources of uncertainties for experimental data:
- *Branching fractions*: calibration, self absorption (radiative transfer), unobserved lines. 0-30%.

- *Radiative lifetime*: statistical and systematic errors. 5-15%

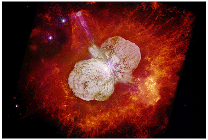
Experimental *f*-values can be obtained with uncertainties down to 5%.

near-IR *forbidden* transitions

An important class of infrared lines are parity forbidden transitions (E2 and M1), observed in nebula and low density plasmas.

- Low transition rates ($\sim 1\ \mathrm{s}^{-1}$)
- Long radiative lifetimes
- Sensitive to collisions

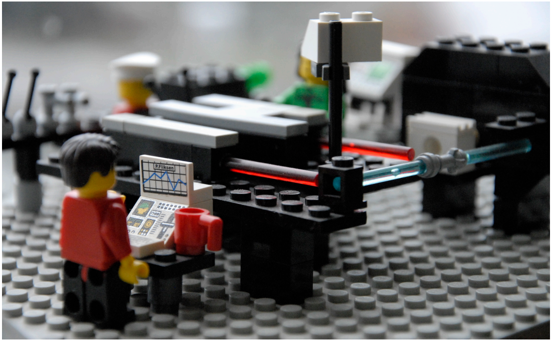
Have relied on calculated transition rates, but can now be measured using selective methods at storage rings (e.g. DESIREE @ Stockholm university, Sweden) combined with astronomical observations of low-density plasmas (Eta Carinae).



http://www.desiree-infrastructure.com

Summary

- near-IR atomic data is crucial to meet the demands from new observatories.
- Lab spectroscopy and calculations can provide evaluated sets of near-infrared atomic data with uncertainties down to 5%



THIS WEEK

EDITORIALS

MENTORING The heavy responsibility to the next generation **p.438**

WORLD VIEW Beware the real risk of World Cup fever **p.439**

POISON Strawberry-frog parents give protection to kids **p.441**

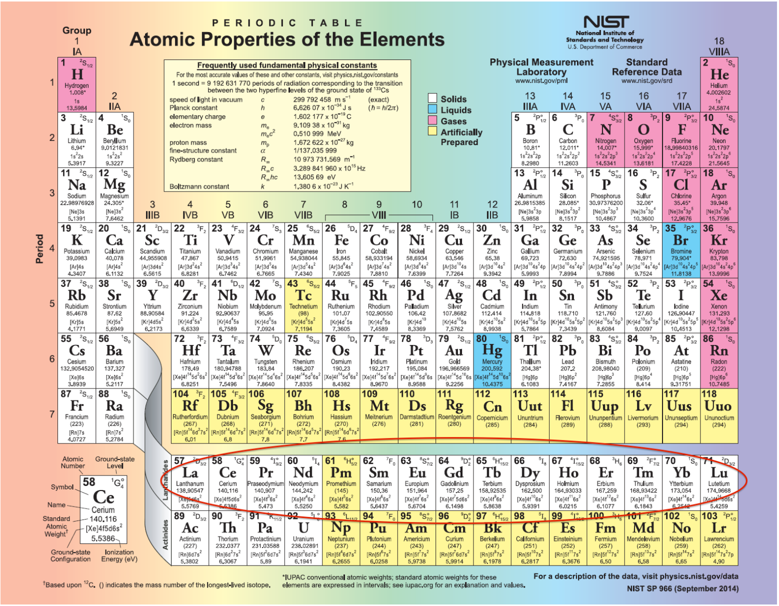
Nailing fingerprints in the stars

Laboratory-based experiments are sorely needed to complement the rapidly proliferating spectral data originating from observations by the latest space telescopes.

What are stars made of? After astronomers detected a bright-yellow, unknown spectral line in sunlight in 1868, they named the new element helium after the Greek Sun god

quantum mechanics. But heavier elements have many electrons that can participate in transitions — iron has 26, making the probabilities of possible transitions between levels too complex to calculate accu-

Periodic table - Rare earth elements



Rare-Earth Elements - La III