CompAS and GRASP for ASOS

Michel GODEFROID, ASOS14, Paris, July 10-14, 2023

CompAS and GRASP for ASOS

Jacek Bieroń, Tomas Brage, Chong Yang Chen, Jörgen Ekman,
Charlotte Froese Fischer, Gediminas Gaigalas, Ian P. Grant, Per Jönsson,
Michel Godefroid, Jon Grumer, Wenxian Li, Yan Ting Li, Jiguang Li,
Ran Si & Kai Wang

Background image of the title slide : OH^- photodetachment microscopy (C. Blondel , private commun.)

ASOS14, Paris, July 10-14, 2023

What is CompAS?

- CompAS is a network for Atomic Structure Theory, based on Multiconfiguration Methods,

$$\Psi(\gamma PJM_J) = \sum_i c_i \, \Phi(\gamma_i PJM_J)$$

- initiated by **Tomas Brage** (Lund, July 2012)
- *Core of CompAS :* consists of groups that are users and developers of the MC(D)HF methods in the form of the ATSP and GRASP packages and successors,
- *The CompAS network* consists of different groups and individuals that are interested in the work of the CompAS core groups.
- More information (including the codes repositories) can be found on github

https://compas.github.io (thanks to Jon Grumer)

The CompAS international collaboration

CompAS is led by a board with at least one representative from each core group. The current composition of the board is

- Jacek Bieroń, Krakow
- Tomas Brage, Lund
- **Charlotte Froese Fischer**, UBC/NIST
- Gediminas Gaigalas, Vilnius
- Michel Godefroid, Brussels
- **Ian Grant**, Oxford
- Jon Grumer, Uppsala
- **Alan Hibbert**, Belfast
- Per Jönsson / Jörgen Ekman, Malmö
- José Marques, Lisboa
- Chongyang Chen / Ran Si, Fudan
- Paweł Syty / Józef Sienkiewicz, Gdansk
- Wenxian Li, Beijing

https://compas.github.io

The CompAS international collaboration

A CompAS meeting has been set up every year to report on further computational and methodological developments for more efficient atomic structure calculations.

- Mölle, Sweden, July 6-9, 2012
- Ystad, Sweden, August 10-12, 2013.
- Malmö, Sweden, Oktober 15-17, 2015.
- Malmö/Lund, Sweden, June 1-4, 2016.
- Malmö/Lund, Sweden, August 18-22, 2017.
- Malmö/Lund, Sweden, June 14-18, 2018.
- Brussels, Belgium, November 22-23, 2019.
- Sopot/Gdańsk, Poland, October 1-3, 2022.
- Uppsala, Sweden, June 6-9, 2023.

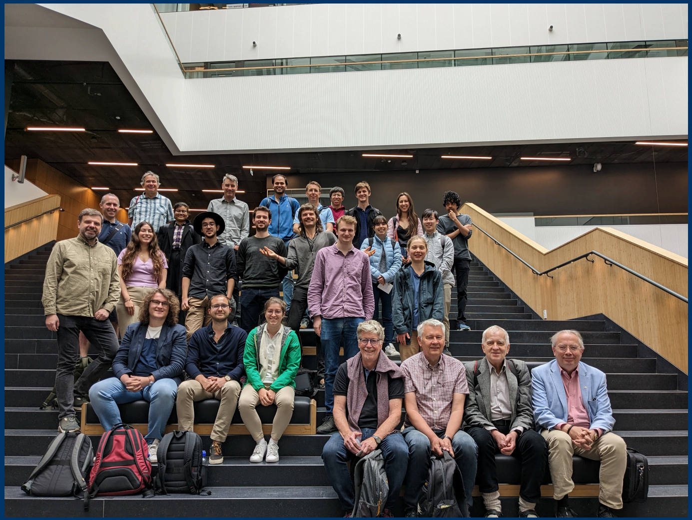
The international collaboration on Computational Atomic Structure (CompAS) https://compas.github.io

2016

2019

2022

2023



The international collaboration on Computational Atomic Structure (CompAS) https://compas.github.io

CompAS, Malmö, , June 1-4, 2016

Charlotte Froese Fischer and Ian P Grant, pioneers of the multiconfiguration methods

The GRASP code

- March 1988: the first **GRASP** manual consisted of a deck of cards describing a single program for the calculation of atomic properties based on **Dirac's theory**, with the following contributing authors *:*

  A. Bar-Shalom, K. G. Dyall, **I. P. Grant**, C. T. Johnson, M. Klapisch, D. F. Mayers, B. J. McKenzie, P. H. Norrington, F. Parpia, E.P. Plummer, N. C. Pyper.

- At the same time, **C. Froese Fischer** concentrated on the problem of electron correlation, in collaboration with A. Hibbert, J. Hansen and M. Godefroid (*Comp. Phys. Rep.* 1986, **3**, 273) and developed the **non-relativistic** Atomic Structure Package **(ATSP).**

- 1996: first extension of the **non-relativistic** HF program to partially filled f-subshells by G. Gaigalas (*CPC* **98** (1996) 255)

Froese Fischer *et al., J. Phys. B* **49** (2016) 182004

Multiconfiguration Hartree-Fock

MCHF wave functions

$$\Psi(\gamma PLSM_LM_S) = \sum_i c_i \, \Phi(\gamma_i PLSM_LM_S)$$

Non-relativistic Hamiltonian

$$H_{NR} = \sum_{i=1}^{N} \left(\frac{\mathrm{p}_i^2}{2m_e} + V(r_i) \right) + \sum_{i<j}^{N} \frac{1}{r_{ij}} \qquad \text{(+BP corrections)}$$

Variational degrees of freedom

$$\{P_{n_i l_i}(r)\}, \{c_k\}$$

$$\psi_{nlm_lm_s}(\mathrm{q}) = \frac{1}{r} P_{nl}(r) Y_{lm_l}(\theta, \phi) \chi_{m_s}(\sigma)$$

Froese Fischer *et al., J. Phys. B* **49** (2016) 182004

Multiconfiguration Dirac-Hartree-Fock

MCDHF wave functions

$$\Psi(\gamma PJM_J) = \sum_i c_i \, \Phi(\gamma_i PJM_J)$$

Dirac-Coulomb-(Breit) Hamiltonian

$$H_{DC} = \sum_{i=1}^{N} (c\boldsymbol{\alpha}_i \cdot \mathrm{p}_i + (\beta_i - 1)c^2 + V(r_i)) + \sum_{i<j}^{N} \frac{1}{r_{ij}} \qquad (+H_{Breit})$$

Variational degrees of freedom

$$\{P_{n_i\kappa_i}(r)\}, \{Q_{n_i\kappa_i}(r)\}, \{c_k\}$$

$$\phi_{n\kappa m}(\mathbf{r}, \sigma) = \frac{1}{r} \begin{pmatrix} P_{n\kappa}(r) \, \chi_{\kappa m}(\theta, \varphi) \\ iQ_{n\kappa}(r) \, \chi_{-\kappa m}(\theta, \varphi) \end{pmatrix}$$

Froese Fischer *et al., J. Phys. B* 49 (2016) 182004

GRASP evolution

- Grant, I.P., McKenzie, B.J., Norrington, P.H., Mayers, D.F. and Pyper, N.C. An atomic multiconfigurational Dirac-Fock package. *CPC* **21 (**1980) 207.
- Dyall, K.G., Grant, I.P., Johnson, C.T., Parpia, F.A. and Plummer, E.P. **GRASP: A general-purpose relativistic atomic structure program.** *CPC* **55** (1989) 425.
- Parpia, F.A., Froese Fischer, C. and Grant, I.P. GRASP92: A package for large-scale relativistic atomic structure calculations, *CPC* **94** (1996) 249.
- Jönsson, P., Gaigalas, G., Bieroń J., Froese Fischer C. and Grant I.P. New version: Grasp2K relativistic atomic structure package, *CPC* **184** (2013) 2197.
- Froese Fischer, C., Gaigalas, G., Jönsson, P. and Bieroń J. GRASP2018—A Fortran 95 version of the General Relativistic Atomic Structure Package. *CPC* **237** (2019) 184.

ATSP, GRASP

- **ATSP** and **GRASP** are both based on the **variational method** applied on **multiconfiguration (Dirac)-Hartree-Fock wave functions** and have many common features.
  Froese Fischer *et al.*, *JPB* **49** (2016) 182004

ATSP, GRASP and MCDFGME

- **ATSP** and **GRASP** are both based on the **variational method** applied on **multiconfiguration (Dirac)-Hartree-Fock wave functions** and have many common features.
  Froese Fischer *et al., JPB* **49** (2016) 182004

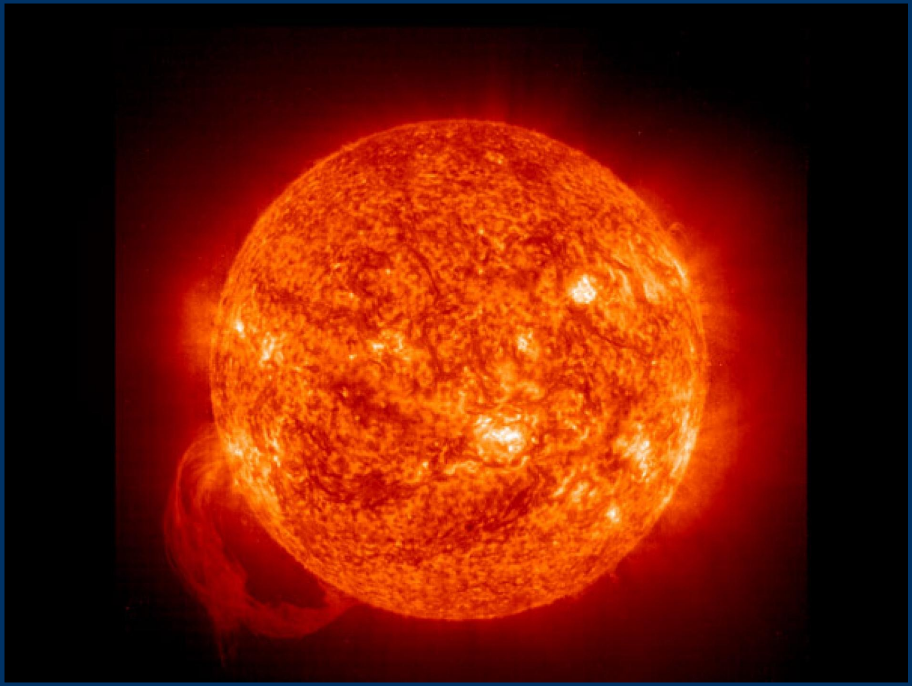
- **Pioneer work of J.-P. Desclaux** in the 70's (in parallel to I.P. Grant)
  Desclaux *et al., JPB* **4** (1971) 631,
  1st MCDF code : Desclaux, *CPC* **9** (1975) 31,
  A longstanding collaboration with Paul Indelicato (MCDFGME).

- For a brief history:
  "An Introduction to Relativistic Theory as Implemented in GRASP"
  Jönsson *et al., Atoms* **11** (2023) 7.

- Code and methodological developments for many different **atomic properties** :

  Radiative transition probabilities, g-factors, hyperfine structures, isotope shifts, Auger transitions, external fields, etc., with advanced evaluation of quantum-electrodynamics (QED) contributions.

CompAS / GRASP for Astrophysics



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CompAS/CIV3 for Astrophysics

Message from Alan Hibbert:

"Do pass on my best wishes to those I might know, and especially to the ASOS scientific committee"

Adam Ritchey (IT16) & Alexander Kramida (IT33)

Accurate oscillator strengths of astrophysical interest for neutral oxygen and nitrogen
Biémont *et al., ApJ* **375** (1991) 818
Hibbert *et al., J. Phys. B* **24** (1991) 3943, *A&A Sup.Series* **88** (1991) 505

Systematic studies of N IV transitions of astrophysical importance
Fleming *et al., ApJ* **455** (1995) 758

log gf values for astrophysically important transitions Fe II
Deb and Hibbert*, A&A* **561** (2014) A32

Successes and Difficulties in Calculating Atomic Oscillator Strengths and Transition Rates
Hibbert, *Galaxies* **6** (2018) 77

CompAS/ATSP/GRASP for Astrophysics

Hyperfine-induced transitions (HITs) for plasma diagnostics

Hyperfine induced transitions as diagnostics of isotopic composittion and densities of low-density plasmas
Brage *et al., ApJ* **500** (1998) 507

Determination of Hyperfine-Induced Transition Rates from Observations of a Planetary Nebulae
Brage T., Judge, P.G. and Proffitt C.R.
Phys. Rev. Lett. **89** (2002) 281101

+ Pritti (IT25) and Sophie Kröger (IT27)

CompAS/ATSP/GRASP for Astrophysics

The MITs in the sun, to monitor the magnetic fields of the corona.

HFSZEEMAN95 - A program for computing weak and intermediate magnetic-field- and hyperfine-induced transition rates
W. Li, J. Grumer, T. Brage & P. Jönsson, *CPC* **253** (2020) 107211

A first spectroscopic measurement of the magnetic-field strength for an active region of the solar corona
R. Si, T. Brage, W. Li, J. Grumer, M. Li & R. Hutton
The Astrophysical Journal Letters **898** (2020) L34

Application of a Magnetic-field-induced Transition in Fe X to Solar and Stellar Coronal Magnetic Field Measurements
Yajie Chen, Wenxian Li *et al.,*
Research in Astronomy and Astrophysics **23** (2023) 022001

Wenxian Li (IT18), Pritti (IT25) and Sophie Kröger (IT27)

CompAS/ATSP/GRASP for Astrophysics

Multiconfiguration Dirac-Hartree-Fock Calculations with **Spectroscopic Accuracy**: Applications to Astrophysics
Jönsson *et al., Atoms* **5** (2017) 16

Experimental and theoretical oscillator strengths of Mg I for **accurate** abundance analysis
Pehlivan Rhodin *et al., A&A* **598** (2017) A102

Multiconfiguration Dirac-Hartree-Fock calculations of **Landé g-factors** for ions of astrophysical interest
W. Li *et al., A&A* **639** (2020) A25

Benchmarking Multiconfiguration Dirac-Hartree-Fock Calculations for Astrophysics: Si-like Ions from Cr XI to Zn XVII
X. H. Zhang, G. Del Zanna, K. Wang *et al., ApJSS* **257** (2021) 56

Uncertainty *Indicators*

Alexander Kramida (IT33)

Evaluating the accuracy of theoretical transition data
Froese Fischer, *Phys. Scr.* **T134** (2009) 014019

Transition probabilities in Te II and Te III spectra (*cancellation factors)*
Zhang *et al., A&A* **551** (2013) A136

Validation and Implementation of Uncertainty Estimates of Calculated Transition Rates
Ekman *et al., Atoms* **2** (2014) 215

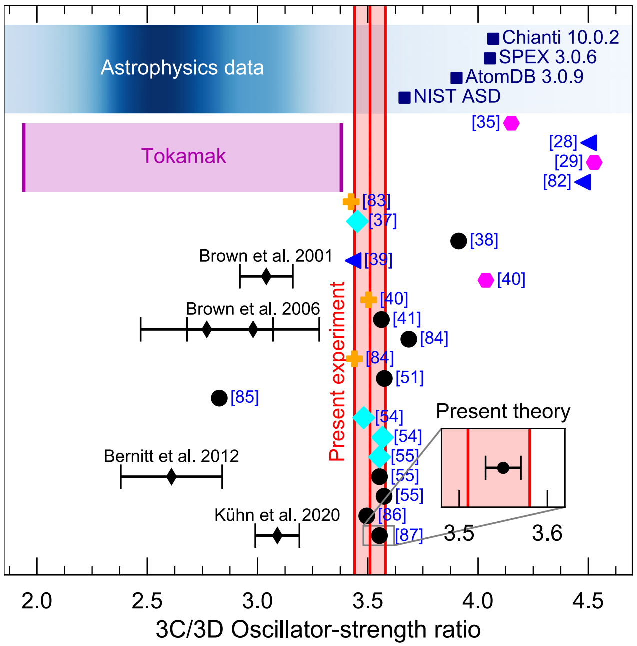
Coulomb (Velocity) Gauge Recommended in Multiconfiguration Calculations of Transition Data Involving Rydberg Series
Papoulia *et al., Atoms* **7** (2019) 106

Extended transition rates and lifetimes in Al I and Al II from systematic multiconfiguration calculations
Papoulia *et al., A&A* **621** (2019) A16

Energy Level Structure and Transition Data of Er^{2+}
Gaigalas *et al., Astron. Astrophys. Suppl. Ser.* **248** (2020) 13

The f3C/f3D ratio in Fe XVII

New Measurement Resolves Key Astrophysical Fe XVII Oscillator Strength Problem, Kühn *et al., PRL* **129** (2022) 245001



Claudio Mendoza (IT34)

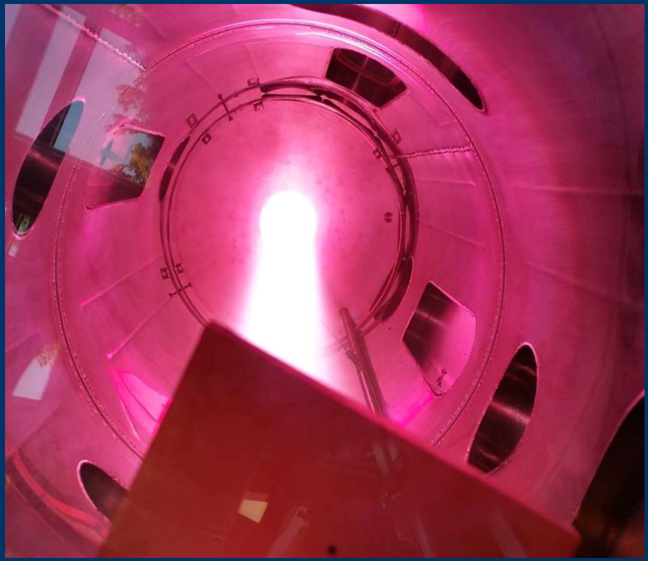
[41] Jönsson *et al., ADNDT* 100, 1 (2014)

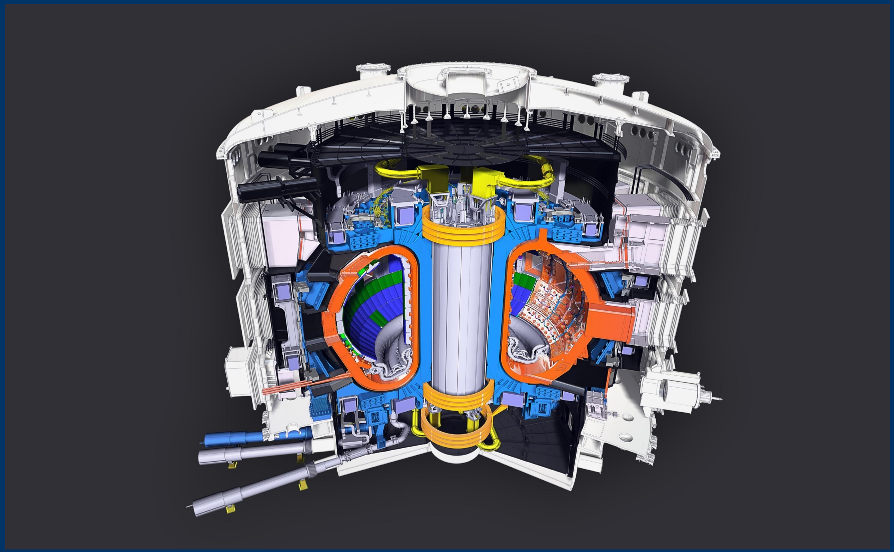
See also Wang *et al., ApJSS* **226** (2016) 14, *PRL* **119** (2017) 189301

Bernitt *et al., Nature* **492** (2012) 225

" In other words, our experiment intimates that quantum mechanics has reached a point where the dominant uncertainties lie in the wavefunctions themselves…" (in my opinion, a nonsense statement)

CompAS / GRASP for Plasma Physics





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CompAS/GRASP for Plasma Physics

Coronal lines and the importance of deep-core-valence correlation in Ag-like ions *(spectroscopic accuracy)*
Grumer *et al., Phys. Rev. A* **89** (2014) 062511

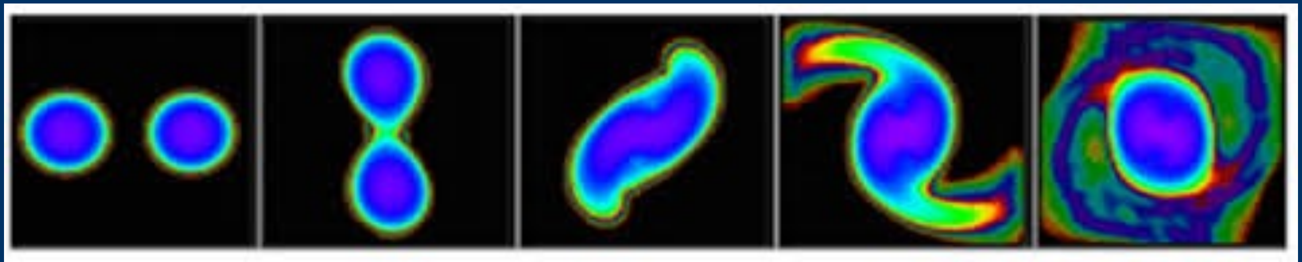
Benchmarking calculations with spectroscopic accuracy of level energies and wavelengths in W LVII–W LXII tungsten ions
Zhang Chun Yu *et al., JQSRT* **269** (2021) 107650 + Jun XIAO's talk (IT22)

Benchmarking calculations of wavelengths and transition rates with spectroscopic accuracy for W XLVIII through W LVI tungsten ions
Zhang Chun Yu *et al., PRA* **105** (2022) 022817

Extended calculations of energy levels, radiative properties, and lifetimes for oxygen-like Zn XXIII
Na Li, Wei Zheng, Kai Wang *et al.*, *JQSRT* **296** (2023) 108429

+ many other works by **Kai Wang** *et al.*

The role of CompAS / GRASP in Nuclear Astrophysics



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Transition data, opacities and line curves

Jérôme Deprince's talk (IT6)

Lanthanide and Actinides in Kilonovae

- Kasen *et al., ApJ* **774** (2013) 25: (Fe, Co, Ni) + (Os, Sn) + Lanthanides(Ce, Nd) / Autostructure
- Gaigalas *et al., ApJS* **240** (2019) 29: Nd II - IV / GRASP
- Fontes *et al., MNRAS* **493** (2020) 4143: All lanthanides / Los Alamos codes
- Even *et al., ApJ* **899** (2020) 24: All lanthanides / Los Alamos codes
- Tanaka *et al., MNRAS* **496** (2020) 1369: All lanthanides I-IV / HULLAC
- Banerjee *et al., A&A* **934** (2022) 117: Nd, Sm, Eu I - XI / HULLAC
- Silva *et al., Atoms* **10** (2022) 18: Nd III & U III / FAC
- Fontes *et al., MNRAS* **519** (2023) 2862: All actinides / Los Alamos codes
- Banerjee *et al.,* arXiv:2304.05810 [astro-ph.HE] (2023): All lanthanides I-XI / HULLAC
- Flörs *et al., MNRAS* **524** (2023) 3083: Nd & U II – III , with FAC // HFR

CompAS/GRASP input

Quinet & Palmeri (Mons) calculations using a multi-platform approach

- Carvajal Gallego *et al. MNRAS* **501** (2021) 1440 : Ce II - IV
  MCDHF
- Maison *et al., Atoms*, 10 (2022) 130 : Lu V
  MCDHF // HFR
- Carvajal Gallego *et al., MNRAS* **509** (2022) 6138 : Ce V – X
  HFR // MCDHF // PH-CI
- Carvajal Gallego *et al., MNRAS* **513** (2022) 2302 : La V – X
  HFR // MCDHF // PH-CI
- Carvajal Gallego *et al. MNRAS* **522** (2023) 312: Sm ions
  HFR // MCDHF
- Carvajal Gallego *et al. MNRAS* **518** (2023) 332: Pr, Nd, Pm X
  HFR // MCDHF // MBPT+CI

CompAS/GRASP for Kilonovae

Gaigalas' Vilnius group contributions

- Tanaka *et al., ApJ* **852** (2018) 109: HULLAC // GRASP
- Gaigalas *et al., ApJ* **240** (2019) 29: Nd II – IV / HULLAC // GRASP
- Gaigalas *et al., ApJSS* **248** (2020) 13: Er III / GRASP
- Radžiūtė *et al., ApJSS* **248** (2020) 17: Pr – Gd II / GRASP
- Radžiūtė *et al., ApJSS* **257** (2021) 29: Tb – Yb II / GRASP
- Rynkun *et al., A&A* **658** (2022) A82: Ce IV / GRASP // HULLAC

NLTE effects (Jon Grumer, Uppsala U.)

- Pognan *et al., MNRAS* **510** (2022), 3806
- Pognan *et al., MNRAS* **513** (2022) 5174

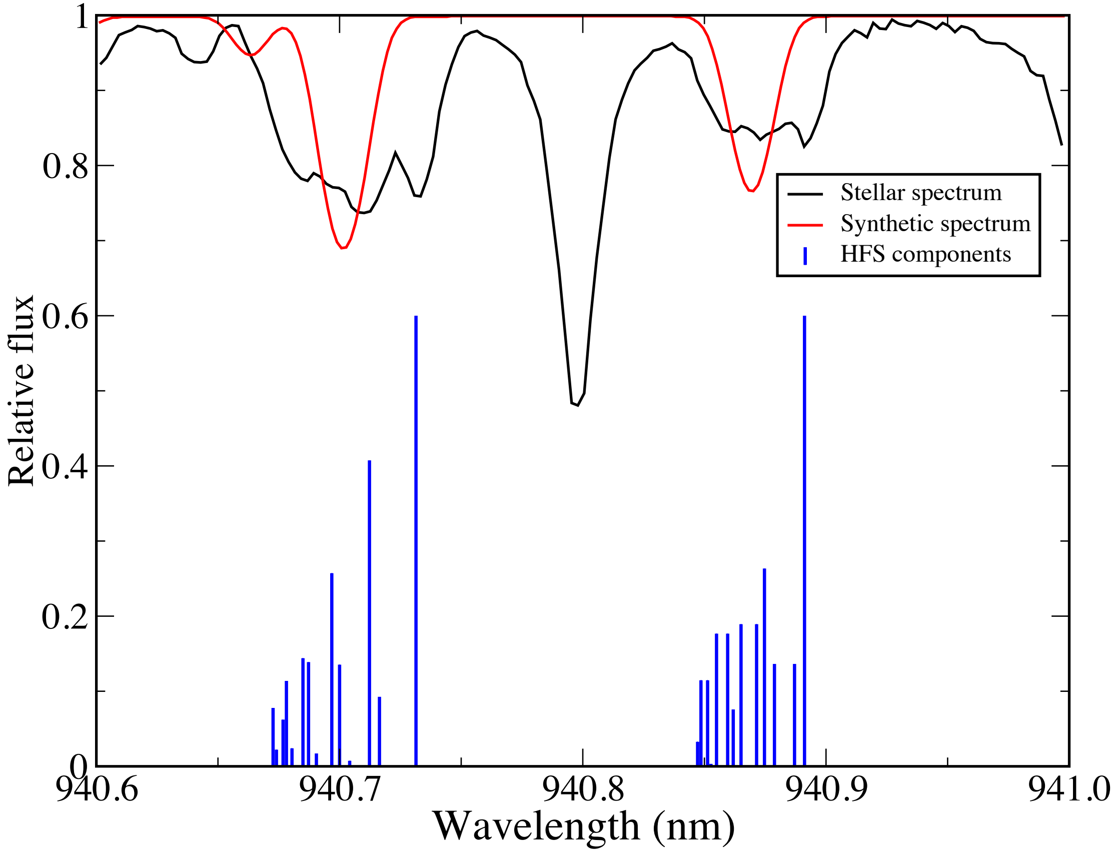
CompAS / GRASP for Nuclear Physics

ASOS14, Paris, July 10-14, 2023

Importance of hyperfine structures and isotope shifts in line profiles

Gillian Nave's talk (ASOS14/IT1)

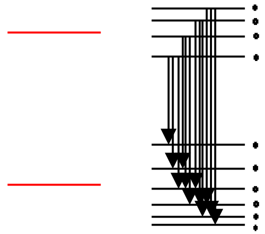
Raies de Mn II



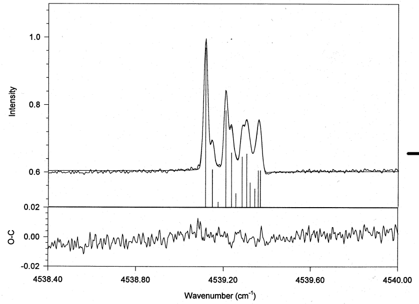
Nave *et al.*, *Can. J. Physics* **95** (2017) 811

Hyperfine structures

$\mathbf{F} = \mathbf{I} + (\mathbf{LS})\mathbf{J}$



$\rightarrow$



$$\rightarrow A, B \xrightarrow[(a_l, a_c, a_{sd}, b_q)]{\text{electronic factors}} \mu_I, I, Q$$

Magnetic dipole interaction

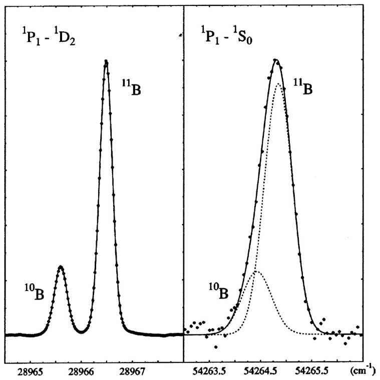
$$A_J \propto \frac{\mu_I}{I} \langle \gamma P J \| T^{(M1)} \| \gamma P J \rangle$$

Electric quadrupole interaction

$$B_J \propto Q \langle \gamma P J \| T^{(E2)} \| \gamma P J \rangle$$

Peter Uylings' talk (ASOS14/IT12)

Isotope shifts



Isotopic Shift **Mass Shift + Field Shift**

$$\delta\nu^{A,A'} = \Delta\tilde{K}^{MS}\,\frac{M'-M}{MM'} + F\,\delta\langle r^2\rangle^{A,A'}$$

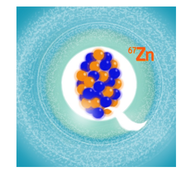
$$\xrightarrow[(\Delta\tilde{K}^{MS},F)]{\text{electronic factors}} \delta\langle r^2\rangle^{A,A'}$$

Julian Berengut's talk (ASOS14/IT14)

CompAS/GRASP for Nuclear Physics

Many papers on **nuclear quadrupole moments** of various nuclei, from Li up to Ra.

Ab initio calculations of the hyperfine structure of zinc and evaluation of the nuclear quadrupole moment of ^{67}Zn
Bieroń *et al., PRA* **97** (2018) 062505



Structural trends in atomic nuclei from laser spectroscopy of tin
Yordanov *et al., Communications Physics* **3** (2020) 107

High-resolution laser spectroscopy of $^{27-32}$Al
Heylen *et al., PRC* **103** (2021) 014318

Large Shape Staggering in Neutron-Deficient Bi Isotopes
Barzakhi *et al., PRL* **127** (2021) 192501

CompAS/GRASP for Atomic Physics

QED-tests Jun XIAO's talk (ASOS14/IT22)

Proposal of highly accurate tests of Breit and QED effects in the ground state $2p^5$ of the F-like isoelectronic sequence
M. C. Li, R. Si, T. Brage, R. Hutton and Y. M. Zou, *PRA* **98** (2018) 020502(R)

Breit and QED effects on the $3d^9$ $^2D_{3/2}$ - $^2D_{5/2}$ transition energy in Co-like ions
R. Si *et al., PRA* **98** (2018) 012504

Negative ions and sympathetic cooling

Candidate for Laser Cooling of a Negative Ion: High-Resolution Photoelectron Imaging of Th−
R Tang, R Si, Z Fei, X Fu, Y Lu, T Brage, H Liu, C Chen, C Ning
Physical Review Letters **123** (2019) 203002

Ab initio multiconfiguration Dirac-Hartree-Fock calculations of the In and Tl electron affinities and their isotope shifts
R. Si *et al., PRA* **104** (2021) 012802

GRASP developments

(present and future)

ASOS14, Paris, July 10-14, 2023

GRASP code developments

The GRASP atomic structure code - current status, the CompAS collaboration and hopes for the future,
Jon Grumer , *CPC Seminar Series* (2022, February 8)
https://cassyni.com/events/UcuYdsoU5WcKvMjD4ixukh

Reducing the computational load - atomic multiconfiguration calculations based on configuration state function generators
Yan Ting Li *et al., CPC* **283** (2023) 108562

Atoms Special Issue: "General Relativistic Atomic Structure Program – GRASP"
Eds: Bieroń, Froese Fischer & Jönsson, *Atoms* **11**(6) (2023) 93

GRASP Manual for Users
Jönsson *et al., Atoms* **11**(4) (2023) 68

An Introduction to Relativistic Theory as Implemented in GRASP
Jönsson *et al., Atoms* **11**(1) (2023) 7

GRASP code developments

RIS4 - A program for relativistic isotope shift calculations
Ekman *et al., CPC* **235** (2019) 433

HFSZEEMAN95 - A program for computing weak and intermediate magnetic-field- and hyperfine-induced transition rates
W. Li, J. Grumer, T. Brage and P. Jönsson *et al., CPC* **253** (2020) 107211

Relativistic radial electron density functions and natural orbitals from GRASP2018
Schiffmann *et al., CPC* **278** (2022) 108403

M3 hyperfine interaction : Re-Evaluation of the Nuclear Magnetic Octupole Moment of ^{209}Bi
Jiguang Li *et al., Atoms* **10** (4) (2022) 132

GRASP code developments

Coupling: The program for searching optimal coupling scheme in atomic theory (a very useful tool !)
Gaigalas, *CPC* **247** (2020) 106960

A Program Library for Computing Pure Spin-Angular Coefficients for One- and Two-Particle Operators in Relativistic Atomic Theory
Gaigalas, *Atoms* **10**(4) (2022) 129

Fine-Tuning of Atomic Energies in Relativistic Multiconfiguration Calculations
Yan Ting Li *et al.*, *Atoms* **11**(4) (2023) 70

JAC: A fresh computational approach to atomic structures, processes and cascades
Fritzsche, *CPC* **240** (2019) 1 + ICAP14/P11

GRASP methodological developments

Biorthonormal transformations for ATSP and GRASP
Transition probability calculations for atoms using non-orthogonal orbitals
Olsen *et al., PRE* **52** (1995) 4499

PCFI: A partitioned correlation function interaction approach for describing electron correlation in atoms
Verdebout *et al., JPB* **46** (2013) 085003

Natural orbitals in multiconfiguration calculations of hyperfine-structure parameters
Schiffmann *et al., PRA* **101** (2020) 062510

Independently Optimized Orbital Sets in GRASP : The Case of Hyperfine Structure in Li I
Yan Ting Li *et al., Atoms* **11**(1) (2023) 4
(see also P24: TO techniques in Au I by Caliskan and Grumer)

GRASP wishing list

QED developments - Current situation: different versions with different implementations

Electron self-energy corrections using the Welton concept for atomic structure calculations
T.V.B. Nguyen, J.A. Lowe, T.L.H. Pham, I.P. Grant & C.T. Chantler, *Radiation Physics and Chemistry* **204** (2023) 110644

QED inclusion in the variational procedure (*done in MCDFGME* !)

Combining MCDHF and perturbation theory
Preliminary (successful) investigations by Gaigalas, Rynkun and Radžiūtė, using the Program Library for Computing Pure Spin–Angular Coefficients for One- and Two-Particle Operators.

The CompAS international collaboration

A CompAS meeting has been set up every year to report on further computational and methodological developments for more efficient atomic structure calculations.

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- Malmö/Lund, Sweden, August 18-22, 2017.
- Malmö/Lund, Sweden, June 14-18, 2018.
- Brussels, Belgium, November 22-23, 2019.
- Sopot/Gdańsk, Poland, October 1-3, 2022.
- Uppsala, Sweden, June 6-9, 2023.
- Lisboa, Portugal, June or July (?), 2024.

The End