

# GES linelist V4

2013-08-08

Line-lists for the Gaia-ESO Survey

## Citation policy

The line-lists are intended for use within the Gaia-ESO survey. Until further notice, all publications based on these data shall cite (Line-list Group, in prep.) If you wish to use the line-list for non Gaia-ESO related projects, please contact the line-list group.

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Version 4, released 27.07.2013

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## Linelist V4

This new release contains the following files

- 1 ges\_atom\_nohfs-iso\_v4.fits  
Line-list for atoms, no hyper-fine splitting (HFS) or isotopic shifts (ISO)
- 2 ges\_atom\_hfs-iso\_v4.fits  
Line-list for atoms, including HFS and ISO
- 3 ges\_molecule\_v4.fits  
Line-list for molecules, 24 files

The so-called clean line-list forms a subset of the atom\_nohfs-iso and atom\_hfs-iso line-lists. For these 1341 (nohfs-iso) or 2629 (hfs-iso) lines only, assessments of atomic data quality and blending properties are included through flags. **The two atomic lists are complete and mutually exclusive.**

The files are available via the Edinburgh archive.

## 1. Overview of changes in V4

- fits-formatted line-lists
- complete revision of the atomic master line-list in HR21
- homogenization of references in the clean and atomic master line-lists
- Updated transition probabilities for Mg I, Si I, Ti I, Ti II, Fe I and some lines of neutron-capture elements
- new flag (EW\_FLAG) indicating the usefulness of a line for the EW analysis, based on statistical analysis of 400 UVES iDR1 spectra
- All lines synthesized in Arcturus with central line depth indicated in DEPTH-parameter. Can be used e.g. to discard weak lines in synthesis.
- reported bugs in v3 fixed
- Spectral atlases are provided on the line-list wiki.
- New ABO theory van der Waals values for nine Fe I lines in the clean line list (U.Heiter, P. Barklem)

## 2. Description of the FITS-format

The new fits-format has been implemented for convenient verification of all data and simple addition of flags (see Table 1). The files can e.g. be read into IDL structures with the command MRDFITS of the NASA IDL library. A line-list for a given purpose can then be created by filtering the information, in e.g. wavelength, relative depth, and/or flags. Some of the information, including log gf\_flag, syn\_flag, ew\_flag, and labels are only included for the clean subset of lines.

**Table 1.** FITS format

NAME	STRING (3)	E.g. [Ti, O] or Ca
ION	INT	Ionisation stage of atom or molecule, e.g. 1 for neutral, 2 for singly ionized
ISOTOPE	LONG (3)	Isotope information for NAME, e.g. [46, 0]; 0 if only one isotope present in list
LAMBDA	DOUBLE	Wavelength Å
LAMBDA_REF	STRING	Reference for LAMBDA
LOG_GF	FLOAT	Logarithm of gf-value
LOG_GF_ERR	FLOAT	Experimental error in LOG_GF if applicable
LOG_GF_REF	STRING	Reference for LOG_GF
LOG_GF_FLAG	STRING	Flag indicating relative quality of LOG_GF <sup>a</sup>
LABEL_LOW	STRING	Lower level electron configuration
LABEL_UP	STRING	Upper level electron configuration
E_LOW	FLOAT	Lower level energy [eV]
E_LOW_REF	STRING	Reference for E_LOW
J_LOW	FLOAT	Lower level J-value
E_UP	FLOAT	Upper level energy [eV]
E_UP_REF	FLOAT	Reference for E_UP
J_UP	FLOAT	Upper level J-value
LANDE_LOW	FLOAT	Lower level Lande factor
LANDE_UP	FLOAT	Upper level Lande factor
LANDE_MEAN	FLOAT	Mean Lande factor
LANDE_REF	FLOAT	Reference for Lande factors
RAD_DAMP	FLOAT	Radiation damping : $\log(\text{FWHM} [\text{rad/s}])$
RAD_DAMP_REF	STRING	Reference for RAD_DAMP
STARK_DAMP	FLOAT	Stark broadening per perturber at 10000K, $\log(\text{FWHM} [\text{rad/s/cm}^3])$
STARK_DAMP_REF	STRING	Reference for STARK_DAMP
VDW_DAMP	FLOAT	Broadening by H I <sup>b</sup>
VDW_DAMP_REF	STRING	Reference for VDW_DAMP
DEPTH	FLOAT	Central line depth in Arcturus <sup>c</sup>
SYN_FLAG	STRING	Blending quality for synthesis <sup>d</sup>
EW_FLAG	FLOAT (4)	Usefulness for EW - analysis

<sup>a</sup> log gf: Y: Recommended, U: Un-decided, N: Not recommended

<sup>b</sup> > 0: int(sigma).alpha ABO theory; < 0: Van der Waals broad. per perturber at 10000K,  $\log(\text{FWHM} [\text{rad/s/cm}^3])$

<sup>c</sup> Computed assuming 4247/1.59/-0.54 and scaled solar, 0.2 dex alpha-enhanced composition. For all H I lines, depth is set to 0.999

<sup>d</sup> Y: relatively unblended, U: maybe useful in some stars, N: badly blended, not recommended

### 3. LOG\_GF\_FLAG and SYN\_FLAG

The flags are either Y (Yes), N (No), or U (un-decided). They shall be interpreted as follows:

LOG\_GF\_FLAG: Quality of transition probability listed as log gf

- Y - Data come from a trusted source (mainly laboratory measurements with excellent accuracy)
- U - Quality of data is not decided (advanced theoretical calculations and lower accuracy laboratory data)
- N - Data are expected to have low accuracy

SYN\_FLAG: Blending properties for the Sun and Arcturus

- Y - Line is particularly un-blended or only blended with line of same species in both stars

- U - Line may be inappropriate in at least one of the stars
- N - Line is strongly blended with line(s) of different species in both stars

We have been more selective with Y-flags for elements with more spectral lines, such as Fe, compared to e.g. O, with very few lines. We have not considered whether the strength of the line is appropriate for analysis in a specific star, since this will vary much between the targets. The blending assessment of a line should thus be seen relative to other lines of the same species and line strength. In the spectral atlases available on the wiki, the titles read: LOG\_GF\_FLAG/SYN\_FLAG ABO (indicating presence of ABO data) EW\_FLAG

#### 4. Hyperfine splitting and isotopic shifts

HFS and ISO were added for Sc I, V I Mn I, Co I, Cu I, Ba II, Eu II, La II, Pr II, Nd II, Sm II. The gf-values are NOT scaled to isotopic abundances. Line-lists with scaled gf-values can be also provided upon request.

#### 5. Atomic line-lists

An updated extraction of VALD3 data has been used as basis, covering the wavelengths from 4750 to 6850 Å and 8450 to 8950 Å. This includes the Paschen series that previously were missing.

- Mg I gf values updated for 2 lines (Chang & Tang 1990)
- Si I gf-values updated for 6 lines (Nahar 1993)
- Fe I gf-values updated for many Y/ lines. Average values of several sources now account for measurement uncertainties
- Ti I and Ti II gf values updated for 74 and 16 lines, respectively (Lawler et al. 2013, Wood et al. 2013)
- 28 lines of neutron-capture elements (Y, Zr, La, Ce, Nd, Sm, Eu, Gd) have been added.
- Upper cutoff on lower level excitation potential, 50 eV, enforced
- For the lines not in the clean linelist, upper cutoff of 10 eV if  $\log gf < -3$ .
- The previous VALD3 extraction contained some duplicate transitions for some Sr I lines with Elow 0.5eV and some CrI lines that are not present in the new lists
- Several spurious lines, including the Fe I line at 523.8 nm, have been removed.

#### 6. Molecular line-lists

The recommended partition functions ( $Q$ ) are given on polynomial form such that:

$$\log(Q) = \sum_1^6 a_i \ln(T)^i$$

The data are given in Tables 2 and 3.

#### 7. Flag for EW analysis

The EW\_FLAG is computed on the basis of a statistical analysis of two sample of stars: i) the benchmark sample which includes all stars proposed in the paper by Paula Jofre and Ulrike Heiter, whose spectra have been re-sampled at UVES580 resolution; ii) The DR1 sample, which includes the 421 stars with WG11 recommended parameters.

EWs have been measured in a homogeneous way with an automatic version of Daospec (DOOp, Cantat-Gaudin et al. 2013, A&A submitted), and the abundances have been with FAMA (Magrini et al 2013 arXiv:1307.2367), considering the HFS when necessary, for lines in the EW range: 15-100 mÅ (to avoid faint lines affected by noise and saturated lines). The distribution of the deviation from the average (computed with Y/Y lines whenever possible, or including also Y/U, /UY, and U/U for elements without Y/Y lines) has been built. The sigma corresponding to the 68.2% percentile has been computed.

The results of the statistical analysis are reported in the following way:

1. Number of times (in percentage) the line has been detected in the benchmark sample
2. Sigma of the line at the 68.2 percentile for the benchmark sample
3. Number of times (in percentage) the line has been detected in the DR1 sample
4. Sigma of the line at the 68.2 percentile for the DR1 sample

Thus, a "good" line is a line with a small value of 2 and 4, and high values of the detection percentages (1. and 3.). These two percentiles are usually in good agreement when the % of detection is above 20% in the two sample. For poorly detected lines the percentile values should be considered with some warnings.

The EW\_FLAG should be used to exclude from the analysis some lines which are in most cases very far from the average of the other lines of the same element. For example, the iron line at 6089.59 Å is 2.555 dex above the average in the benchmark sample, and 2.492 dex from the average in the DR1 sample, hence it is highly recommended its exclusion from any EW based analysis. On the other hand, the iron line at 6220.78 Å is 0.361/0.369 dex from the average, and its exclusion is arguable.

#### 8. Van der Waals damping

We recommend all nodes to comply with the Anstee, Barklem & O'Mara theory for collisional broadening by hydrogen (ABO theory). The column for van der Waals damping data contains the cross-sections and temperature dependence of this theory in a compact notation that we encourage all nodes to adapt directly in their codes. For a detailed description, see <http://www.astro.uu.se/~barklem/howto.html>. For transitions lacking ABO data, the column contains the value 0.000. Negative values for Sc II, Ti II, and Y II lines are logarithmic line widths at

**Table 2.** Summary of data for molecular transitions

Molecule	Isotope	Dissociation energy (eV)	Reference
C2	12C12C 12C13C 13C13C	6.371	T. Masseron (positions: Tanabashi et al. 2007a,b; intensities: Brooke et al. 2013; D00: Luo 2007)
CaH		1.700	Weck et al. 2003
CH	12C 13C	3.466	T.Masseron (positions: Zachwieja 1995, 1997; intensities: Luque & Crosley 1999; D00: Kumar et al. 1998)
CN	12C14N 13C14N	7.738	T. Masseron (positions: Ram et al. 2006; intensities: Knowles et al. 1998; D00: Huan et al. 1992)
FeH		1.590	Dulick et al. 2003
MgH		1.285	T. Masseron (positions: Shayesteh & Bernath 2011; intensities: Saxon et al. 1978; D00: Shayesteh & Bernath 2006)
NH		3.420	T. Masseron (positions: Ram et al. 2010a; intensities: Cantarella et al. 1992; D00: Tarroni et al. 1997)
OH		4.392	T. Masseron (positions: Bernath & Colin 2009; intensities: Goldman et al. 1998a)
SiH		3.060	Kurucz database
TiO	46Ti 47Ti 48Ti 49Ti 50Ti	6.870	B. Plez (1998)
VO		6.437	B. Plez (private comm.)
ZrO	90Zr 91Zr 92Zr 94Zr 96Zr	7.890	B. Plez (private comm.)

**Table 3.** Partition functions for molecules

Mol	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>	a <sub>6</sub>
C2	-1.37611619D+02	7.52473987D+01	-1.60701760D+01	1.72410801D+00	-9.08948951D-02	1.90678635D-03
CaH	1.57677958D+03	-9.82846806D+02	2.44267425D+02	-3.01777064D+01	1.85392515D+00	-4.52292569D-02
CH	-4.91887806D+02	3.09155097D+02	-7.70038741D+01	9.57241011D+00	-5.93380866D-01	1.47420199D-02
CN	6.81165938D+02	-4.46981105D+02	1.17584738D+02	-1.53931948D+01	1.00366669D+00	-2.60084236D-02
FeH	0.1552109D0	0.3983233D0	0.6073527D0	-0.198406D0	2.47056D-02	-9.90570D-04
MgH	6.53454485D+02	-4.13828321D+02	1.04888640D+02	-1.32317730D+01	8.31982710D-01	-2.07967780D-02
NH	-2.70001339D+02	1.77303226D+02	-4.62157841D+01	6.04541228D+00	-3.95886800D-01	1.04339634D-02
OH	-4.56875469D+02	2.87960316D+02	-7.20525364D+01	9.01193168D+00	-5.62538083D-01	1.40661068D-02
SiH	9.01120422D+01	-4.42299680D+01	8.35706604D+00	-6.74290104D-01	1.83429417D-02	1.99216485D-04
TiO	5.92027276D+02	-3.65351492D+02	9.03939514D+01	-1.10869716D+01	6.75722876D-01	-1.63144071D-02
VO	6.62090157D+02	-4.03350494D+02	9.82836218D+01	-1.18526504D+01	7.08429905D-01	
ZrO	4.27195765D+02	-2.51905561D+02	5.85682500D+01	-6.63032743D+00	3.67462428D-01	-7.92597014D-03

10000K (Kurucz data); they shall be scaled to the local temperature (see the GES document). In the absence of ABO data (available, in particular, for Ba II), one shall use the Unsöld approximation with an enhancement factor of 1.5 for the line width.

The dedicated document is available on the GES wiki<sup>1</sup>.

<sup>1</sup> <http://great.ast.cam.ac.uk/GESwiki/GesWg/GesWg11/Linelists?>

## 9. References codes

Note that **some** references are ordered by **year** and appear in the first part of each list; other references are ordered by **author** and come thereafter.

### 9.0.1. References to the HFS and ISO data in the clean linelist

#### by year

Wagner (1955) Fischer et al. (1967) Handrich et al. (1969) Davis et al. (1971) Childs (1971) Childs (1971) Luc & Gerstenkorn (1972) Zeiske et al. (1976) Ertmer & Hofer (1976) Childs et al. (1979a) Childs et al. (1979b) Dembczyński et al. (1979) Johann et al. (1981) Becker et al. (1981b) Becker et al. (1981a) Höhle et al. (1982) Silverans et al. (1986) Brodzinski et al. (1987) Ginibre (1989) Unkel et al. (1989) Bergström et al. (1989) Villemoes et al. (1992b) El-Kashef & Ludwig (1992) Villemoes et al. (1992a) Hermann (1993) Villemoes et al. (1993) Möller et al. (1993) Palmeri et al. (1995) Pickering (1996) Nakhate et al. (1997) Cochrane et al. (1998) Li et al. (2001a) Rivest et al. (2002) Lefèbvre et al. (2003) Masterman et al. (2003) Başar et al. (2003) Ma & Yang (2004) Başar et al. (2004) Blackwell-Whitehead et al. (2005a) Rosner et al. (2005) Öztürk et al. (2007) Kurucz (2013b)

### 9.0.2. References in the clean linelist

#### by year

Wolnik et al. (1968) Garz & Kock (1969) Richter & Wulff (1970) Wolnik et al. (1970) Whaling et al. (1977) Kuehne et al. (1978) Biemont & Godefroid (1980) Kerkhoff et al. (1980) Cardon et al. (1982) Blackwell et al. (1982b) Blackwell et al. (1982a) Blackwell et al. (1983) Blackwell et al. (1984) Booth et al. (1984) Kock et al. (1984) Whaling et al. (1985) Doerr & Kock (1985) Duquette et al. (1986) Blackwell et al. (1986) Grevesse et al. (1989) Carlsson et al. (1989) Chang & Tang (1990) Hibbert et al. (1991) Davidson et al. (1992) Hibbert et al. (1993) Butler et al. (1993) Nahar (1993) Mendoza et al. (1995) Volz et al. (1996) Yan et al. (1998) Nitz et al. (1999) Storey & Zeppen (2000) Johansson et al. (2003) Fuhr & Wiese (2006) Zatsarinny & Bartschat (2006) Blackwell-Whitehead & Bergemann (2007) Li et al. (2007) Meléndez & Barbuy (2009) Wiese & Fuhr (2009) Kułaga-Egger & Migdałek (2009)

Lawler et al. (2013) Wood et al. (2013)

#### by author

Aldenius et al. (2007) Barklem & Aspelund-Johansson (2005) Biémont et al. (2011) Biemont et al. (1981a) Bizzarri et al. (1993) Blackwell et al. (1979a) Bard et al. (1991) Bridges & Kornblith (1974) Bard & Kock (1994) O'brian & Lawler (1991) Barklem et al. (2000) O'Brian et al. (1991) Corliss & Bozman (1962a) Cowley & Corliss (1983a) Cocke et al. (1973) Drozdowski et al. (1997) Den Hartog et al. (2006) Den Hartog et al. (2011) Fuhr et al. (1988) Garz (1973) García & Campos (1988) Blackwell et al. (1979b) Blackwell et al. (1982c) Blackwell et al. (1982d) Blackwell et al. (1995) Grevesse (2012) Froese Fischer & Tachiev (2012) Saraph & Storey (2012) Ruffoni & Pickering (2012) Hannaford et al. (1982) Den Hartog et al. (2003) Ivarsson et al. (2001) Kurucz (2006) Kurucz (2007) Kurucz (2008) Kurucz (2009) Kurucz (2010) Kurucz (2011) Kock & Richter (1968) Lawler et al. (2001a) Lawler et al. (2006) Lawler & Dakin (1989) Ljung et al. (2006) Lawler et al. (2009) Lawler et al. (2001c) Lennard et al. (1975) Meggers et al. (1975) Martin et al. (1988) May et al. (1974) Nitz et al. (1998) Pinnington et al. (1993) Pitts & Newsom (1986) Palmeri et al. (2000) Pickering et al. (2001) Raassen & Uylings (1998) Smith & Kuehne (1978) Sobeck et al. (2007) Smith & O'Neill (1975) Smith & Raggett (1981) Smith (1988) Vaeck et al. (1988) Wolnik et al. (1971) Whaling & Brault (1988) Werij et al. (1992) Wickliffe et al. (2000) Wickliffe & Lawler (1997b) Wickliffe et al. (1994)

### 9.0.3. References in the atomic masterline list

#### by year

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