

Supplementary material for :
Limits of detection in elemental analysis of food via laser-induced breakdown
spectroscopy

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1. Apparatus response function

The apparatus response function was measured using a deuterium arc (Optronic Laboratories, model OL UV-40) and a tungsten filament lamp (Optronic Laboratories, model OL 220M) for the ultraviolet and visible/near infrared spectral ranges, respectively. Both the spectral and the intensity calibration were checked regularly using a procedure based on the simulation of the LIBS spectrum of steel [1].

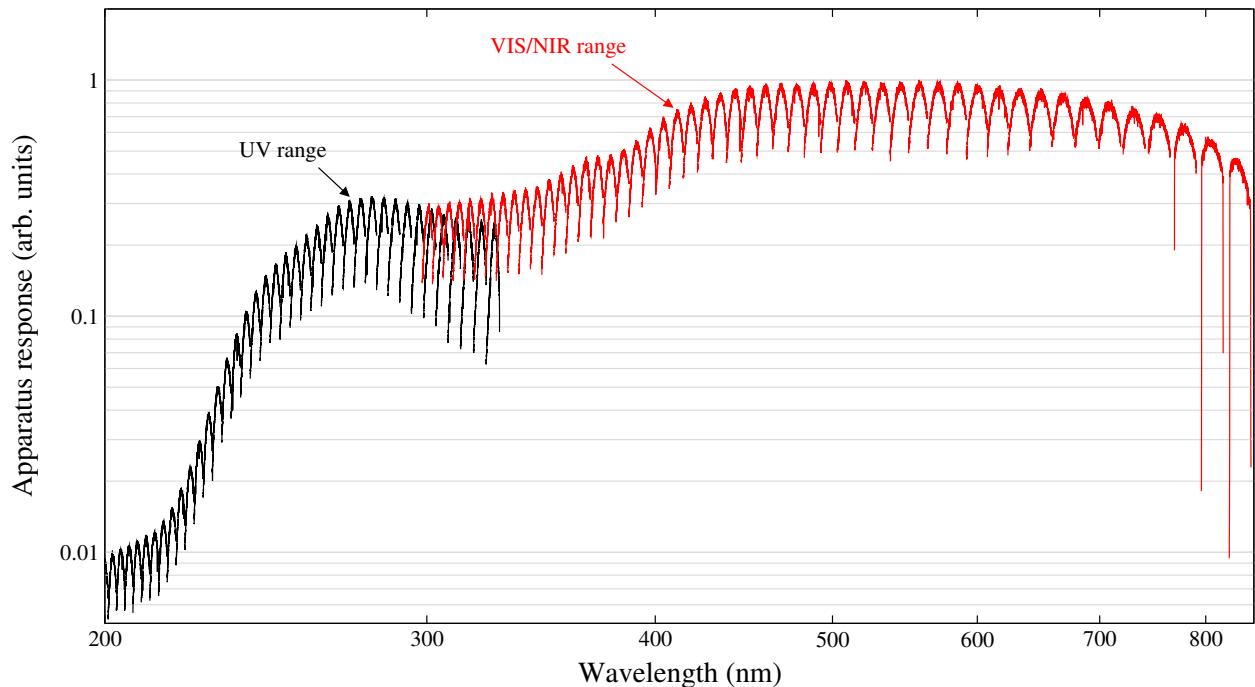


Figure 1: Apparatus response function for the ultraviolet and visible/near infrared spectral ranges of the used echelle spectrometer (Lasertechnik Berlin, model Aryelle Butterfly).

2. Analysis of background signal

The measured spectrum (black) and the spectrum obtained after smoothing (red) are displayed in Fig. 1(a) for the spectral range of the As I 234.98 nm transition. The noise function that characterizes the data point fluctuation associated to the background signal is obtained by subtracting the smoothen spectrum from the original measured one [see Fig. 1(b)]. The displayed spectral range includes 345 data points that were found to present a sufficiently large data size for reliable statistical analysis, enabling thus the accurate determination of the sample standard deviation of the background signal.

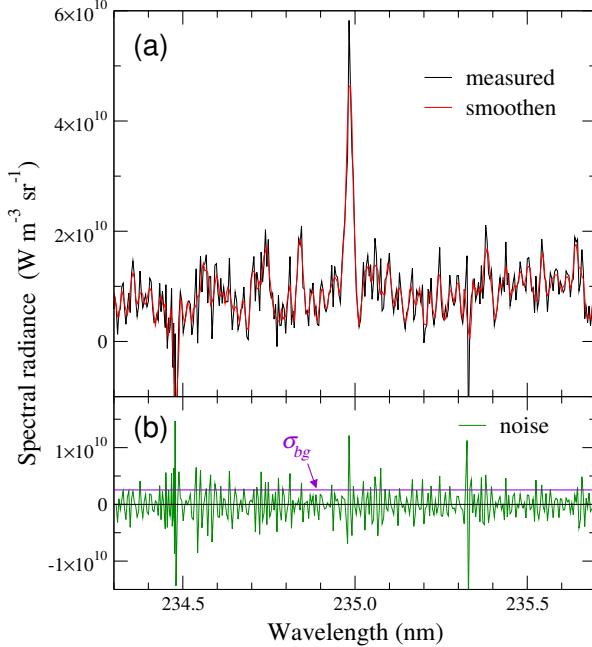


Figure 2: (a) Measured spectrum before and after smoothing with an appropriate procedure. (b) Noise function obtained by subtracting the smoothen spectrum from the original measured one. The standard deviation of the noise σ_{bg} is indicated by the purple colored line.

3. Analytical transitions with corresponding LOD

The analytical transitions were chosen according to the signal-to-noise ratio and the interferences with transitions emitted by atomic or molecular species that originate from the organic matrix or from the most abundant minerals. The most sensitive transitions are presented in Table 1 for each element together with alternative transitions of equal or close sensitivity that may be used for analytical measurements in case of interferences with transitions from other minor or trace elements listed in the last column.

Most of the transitions have been previously observed in calibration-free LIBS analyses of various materials [2, 3, 4, 5, 6, 7]. For these lines, the Stark broadening parameters are given in Table 5. The limits of detection of the corresponding elements can thus be considered as validated. Moreover, a high level of confidence can be attributed to all LOD-values obtained with transitions for which reliable spectroscopic data are available in the NIST database.

The previous validation of the here applied sensitivity-improved calibration-free approach showed that trace element concentrations can be quantified with an uncertainty better than 50% for most elements. This value of confidence can be safely applied to the C_{LOD} -values of all elements that have been previously quantified in food or other sample materials, indicated by the filled and empty red circles in Fig. 7, respectively. For the other elements, the expected uncertainty ΔC_{LOD} is the same if the spectroscopic data required for the spectral line intensity calculation are reliable. For some elements, and in particular those of largest atomic number, the uncertainty of the Einstein coefficients of spontaneous emission is not reported (see Table 5) and the uncertainty of the corresponding C_{LOD} -value is therefore unknown.

Table 1: Limit of detection C_{LOD} in mass fraction units, analytical transition, apparatus response R_{app} , possibly interfering lines, and material for which the analytical transition was measured. All C_{LOD} -values are given with a single significant digit according to the estimated uncertainty of 50%. If available, C_{LOD} -values are given for alternative transitions with similar analytical performance. The spectroscopic data of the transitions are given in Table 5.

| Element | | C_{LOD} (ppm) | Transition | R_{app} | possibly interfering transitions | validation |
|---------|-----------|-----------------|---------------|-----------|---|------------|
| Ac | Actinium | 0.5 | Ac II 315.308 | 0.23 | | - |
| | | 0.5 | Ac II 299.416 | 0.14 | | - |
| Ag | Silver | 0.2 | Ag I 328.068 | 0.20 | | alloy |
| | | 0.5 | Ag I 338.288 | 0.26 | | alloy |
| Al | Aluminum | 1 | Al I 396.152 | 0.57 | | food |
| | | 2 | Al I 394.400 | 0.40 | Ce II 394.388, U II 394.413 | food |
| | | 2 | Al I 308.215 | 0.09 | Gd II 308.199 | food |
| As | Arsenic | 10 | As I 234.984 | 0.055 | | food |
| | | 10 | As I 228.811 | 0.031 | Cd I 228.801 | food |
| At | Astatine | 20 | At I 216.225 | 0.010 | | - |
| | | 100 | At I 224.401 | 0.022 | | - |
| Au | Gold | 1 | Au I 267.593 | 0.24 | Ta II 267.590 | - |
| | | 1 | Au I 242.794 | 0.10 | Os II 242.789 | - |
| B | Boron | 0.2 | B I 249.772 | 0.11 | | food |
| | | 0.5 | B I 249.676 | 0.062 | Hf II 249.699 | food |
| Ba | Barium | 0.2 | Ba II 233.527 | 0.062 | | glass |
| | | 0.5 | Ba II 230.424 | 0.050 | | glass |
| Be | Beryllium | 0.01 | Be II 313.042 | 0.30 | | alloy |
| | | 0.02 | Be II 313.106 | 0.30 | Tm II 313.125 | alloy |
| | | 1 | Be I 234.860 | 0.051 | | alloy |
| Bi | Bismut | 2 | Bi I 306.770 | 0.25 | | alloy |
| | | 2 | Bi I 293.868 | 0.24 | | alloy |
| Br | Bromine | 5000 | Br I 827.241 | 0.43 | Ag I 827.348, Nd II 827.279 | thin film |
| Ca | Calcium | 0.02 | Ca II 393.366 | 0.39 | | food |
| | | 0.05 | Ca II 396.846 | 0.60 | | food |
| | | 0.5 | Ca I 422.672 | 0.53 | | food |
| Cd | Cadmium | 0.2 | Cd I 228.801 | 0.031 | As I 228.811 | food |
| Ce | Cerium | 5 | Ce II 320.171 | 0.27 | | glass |
| | | 10 | Ce II 265.100 | 0.26 | Be I 265.062, Ge I 265.117, Ta II 265.123 | glass |
| Cl | Chlorine | 10000 (1%) | Cl I 837.594 | 0.43 | Gd I 837.473, Nd II 837.516, Sc II 837.706 | polymer |
| | | 50000 (5%) | Cl I 725.661 | 0.68 | Fe I 725.612, Mn I 725.573, Ni I 725.658, Sc I 725.758, Sm II 725.710, Ti I 725.727 | polymer |

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Table 1 – continued from previous page

| Element | | <i>C_{LOD}</i> (ppm) | Transition | <i>R_{app}</i> | possibly interfering transitions | validation |
|---------|------------|------------------------------|---------------|------------------------|---|------------------|
| Co | Cobalt | 2 | Co I 340.511 | 0.30 | Dy II 340.498 | alloy |
| | | 2 | Co I 252.136 | 0.15 | Hf II 252.148, W I 252.131 | alloy |
| | | 2 | Co I 240.725 | 0.084 | | alloy |
| Cr | Chromium | 1 | Cr II 283.563 | 0.29 | | alloy |
| | | 1 | Cr II 276.653 | 0.29 | | alloy |
| Cs | Cesium | 1000 | Cs I 455.528 | 0.63 | Ce II 455.543, Cr I 455.408, Dy I 455.522, Gd II 455.498, Nd II 455.513, Ti I 455.548, U II 455.509, Zr II 455.512 | thin film |
| Cu | Copper | 0.1 | Cu I 324.753 | 0.29 | | food |
| | | 0.2 | Cu I 327.395 | 0.22 | | food |
| Dy | Dysprosium | 1 | Dy II 353.170 | 0.27 | | - |
| | | 2 | Dy II 340.779 | 0.29 | | - |
| Er | Erbium | 1 | Er II 337.275 | 0.19 | Ti II 337.279 | - |
| | | 2 | Er II 323.058 | 0.16 | | - |
| | | 2 | Er II 291.036 | 0.20 | V II 291.038 | - |
| Eu | Europium | 0.5 | Eu II 397.197 | 0.60 | | - |
| | | 1 | Er II 390.710 | 0.54 | | - |
| F | Fluorine | 200000 (20%) | F I 685.603 | 0.80 | Ce I 685.655, Cr I 685.625, Dy I 685.646, Fe I 685.516, Nd I 685.698, Sc II 685.653, Si I 685.603, Sm II 685.601, Ti II 685.573, Tm I 685.688, V II 685.648 | CaF ₂ |
| Fe | Iron | 1 | Fe II 259.939 | 0.16 | | food |
| | | 2 | Fe II 238.203 | 0.082 | | food |
| Fr | Francium | 50 | Fr I 717.986 | 0.58 | | - |
| | | 100 | Fr I 816.941 | 0.41 | | - |
| Ga | Galium | 1 | Ga I 294.363 | 0.12 | | - |
| | | 1 | Ga I 287.423 | 0.26 | | - |
| | | 2 | Ga I 403.297 | 0.65 | Mn I 403.306, Tb II 403.302 | - |
| Gd | Gadolinium | 2 | Gd II 342.246 | 0.20 | | - |
| | | 2 | Gd II 310.050 | 0.20 | | - |
| Ge | Germanium | 1 | Ge I 265.117 | 0.26 | Ta II 265.123 | thin film |
| | | 2 | Ge I 303.906 | 0.12 | U II 303.913 | thin film |
| Hf | Hafnium | 2 | Hf II 264.141 | 0.23 | | alloy |
| | | 2 | Hf II 277.335 | 0.24 | | alloy |
| Hg | Mercury | 20 | Hg I 296.728 | 0.27 | Cr I 296.764, Fe I 296.689, Hf I 296.723, Re I 296.724, Ti I 296.722, W I 296.755 | - |
| | | 100 | Hg I 365.015 | 0.39 | Er II 365.040, La II 365.017, Sm II 365.017 | - |

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| Element | | <i>C_{LOD}</i> (ppm) | Transition | <i>R_{app}</i> | possibly interfering transitions | validation |
|---------|------------|------------------------------|---|------------------------------|---|----------------------------------|
| Ho | Holmium | 0.1 1 | Ho II 341.644 Ho II 339.895 | 0.24 0.34 | | - - |
| I | Iodine | 5000 | I I 206.163 | 0.010 | Bi I 206.162, Cr II 206.157, Os I 206.170 | - |
| In | Indium | 5 10 | In I 325.607 In I 303.934 | 0.32 0.12 | | thin film thin film |
| Ir | Iridium | 5 10 | Ir I 263.970 Ir I 284.972 | 0.22 0.28 | Cr II 284.983 | - - |
| K | Potassium | 200 200 | K I 769.896 K I 404.414 | 0.51 0.69 | | food food |
| La | Lanthanum | 1 2 | La II 394.910 La II 398.851 | 0.45 0.56 | | glass glass |
| Li | Lithium | 0.1 | Li I 670.776 | 0.83 | | food |
| Lu | Lutetium | 0.2 0.5 | Lu II 261.541 Lu II 290.030 | 0.24 0.13 | | - - |
| Mg | Magnesium | 0.02 0.05 0.1 | Mg II 279.552 Mg II 280.270 Mg I 285.212 | 0.30 0.31 0.27 | | food food food |
| Mn | Manganese | 0.2 0.2 0.5 2 | Mn II 259.372 Mn II 260.568 Mn II 294.920 Mn I 403.075 | 0.11 0.21 0.16 0.62 | | alloy alloy alloy alloy |
| Mo | Molybdenum | 1 1 2 | Mo I 313.259 Mo II 281.615 Mo I 317.034 | 0.29 0.13 0.30 | Er II 313.251 Er II 281.617, U II 281.598 | alloy alloy alloy |
| N | Nitrogen | 50000 (5%) | N I 746.831 | 0.59 | Ru I 746.893, S I 746.858, Ta I 746.772, V I 746.831, Zr I 746.754 | food |
| Na | Sodium | 2 1 | Na I 589.592 Na I 588.995 | 0.84 0.85 | | food food |
| Nb | Niobium | 1 2 | Nb II 313.078 Nb II 316.339 | 0.29 0.29 | Be II 313.042 | alloy alloy |
| Nd | Neodymium | 5 10 | Nd II 404.079 Nd II 397.326 | 0.67 0.59 | Ce II 404.075 | glass glass |
| Ni | Nickel | 2 2 2 | Ni I 232.003 Ni I 300.248 Ni I 305.081 | 0.038 0.19 0.20 | Er II 300.240 Er II 305.085 | alloy alloy alloy |

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| Element | | <i>C_{LOD}</i> (ppm) | Transition | <i>R_{app}</i> | possibly interfering transitions | validation |
|---------|--------------|------------------------------|---------------|------------------------|--|------------|
| Os | Osmium | 2 | Ni I 341.476 | 0.26 | Ho II 341.490, Zr II 341.467 | alloy |
| | | 1 | Os II 248.624 | 0.15 | | - |
| | | 1 | Os II 253.798 | 0.17 | Ta II 253.795 | - |
| | | 1 | Os II 321.331 | 0.31 | | - |
| P | Phosphorus | 20 | P I 253.561 | 0.16 | Co I 253.596, Fe I 253.560, Ru II 253.559, Ti II 253.587 | food |
| | | 50 | P I 214.914 | 0.012 | | food |
| | | 50 | P I 255.326 | 0.17 | Co I 255.333, Re II 255.360, W I 255.315 | food |
| Pb | Lead | 2 | Pb I 283.305 | 0.27 | | glass |
| | | 5 | Pb I 261.417 | 0.23 | Hf II 261.429 | glass |
| Pd | Palladium | 0.5 | Pd I 340.457 | 0.32 | | - |
| | | 1 | Pd I 342.122 | 0.19 | | - |
| | | 1 | Pd I 324.269 | 0.27 | Y II 324.227 | - |
| Pm | Promethium | 10 | Pm II 429.778 | 0.47 | Pr II 429.776 | - |
| Po | Polonium | 5 | Po I 255.800 | 0.14 | Ta II 255.880 | - |
| | | 10 | Po I 300.320 | 0.21 | Gd II 300.286, Ta II 300.299 | - |
| Pr | Praseodymium | 2 | Pr II 406.280 | 0.57 | U II 406.254 | glass |
| | | 5 | Pr II 390.842 | 0.54 | Ce II 390.840 | glass |
| Pt | Platinum | 2 | Pt I 306.471 | 0.26 | Hf II 306.468 | - |
| | | 2 | Pt I 265.945 | 0.22 | Ta II 265.940 | - |
| Ra | Radium | 1 | Ra II 270.896 | 0.22 | Ta II 270.926 | - |
| Rb | Rubidium | 5 | Rb I 780.027 | 0.62 | | - |
| Re | Rhenium | 1 | Re II 260.849 | 0.22 | | - |
| | | 1 | Re II 273.303 | 0.25 | | - |
| | | 2 | Re II 256.863 | 0.17 | | - |
| Rh | Rhodium | 1 | Rh I 343.488 | 0.29 | | - |
| | | 2 | Rh I 339.681 | 0.35 | Lu II 339.706 | - |
| Ru | Ruthenium | 1 | Ru II 267.875 | 0.26 | Ta II 267.880, Zr II 267.864 | - |
| | | 2 | Ru II 273.434 | 0.24 | | - |
| S | Sulfur | 10000 (1%) | S I 675.715 | 0.69 | Co I 675.806 | pyrite |
| Sb | Antimony | 5 | Sb I 276.993 | 0.27 | Er II 277.001, Gd II 276.980 | - |
| | | 10 | Sb I 302.980 | 0.22 | | - |
| | | 10 | Sb I 267.063 | 0.20 | Er II 267.026 | - |
| Sc | Scandium | 0.2 | Sc II 361.382 | 0.40 | | - |
| | | 0.2 | Sc II 424.682 | 0.72 | | - |
| Se | Selenium | 50 | Se I 203.985 | 0.010 | | - |

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Table 1 – continued from previous page

| Element | | <i>C_{LOD}</i> (ppm) | Transition | <i>R_{app}</i> | possibly interfering transitions | validation |
|---------|------------|------------------------------|---------------|------------------------|--|------------|
| | | 100 | Se I 206.278 | 0.010 | | - |
| Si | Silicium | 0.5 | Si I 251.611 | 0.17 | | food |
| | | 1 | Si I 288.157 | 0.30 | | food |
| | | 2 | Si I 252.850 | 0.11 | Co II 252.861, Sb I 252.850 | food |
| | | | | | | |
| Sm | Samarium | 5 | Sm II 330.638 | 0.32 | U II 330.589, Zr II 330.627 | - |
| | | 5 | Sm II 360.949 | 0.42 | Pd I 360.954, Th II 360.944, Tm II 360.953 | - |
| Sn | Tin | 2 | Sn I 283.997 | 0.31 | U II 283.989 | alloy |
| | | 2 | Sn I 326.233 | 0.30 | Os I 326.228 | alloy |
| | | 2 | Sn I 317.503 | 0.29 | | alloy |
| Sr | Strontium | 0.02 | Sr II 407.770 | 0.44 | | food |
| Ta | Tantalum | 0.5 | Ta II 301.254 | 0.26 | | - |
| | | 0.5 | Ta II 268.518 | 0.28 | | - |
| | | 1 | Ta II 240.063 | 0.081 | | - |
| Tb | Terbium | 1 | Tb II 350.914 | 0.34 | U II 350.884 | - |
| | | 2 | Tb II 400.546 | 0.36 | | - |
| Tc | Technetium | 0.5 | Tc II 260.999 | 0.23 | | - |
| | | 0.5 | Tc II 264.701 | 0.27 | | - |
| Te | Tellurium | 10 | Te I 238.579 | 0.098 | | glass |
| | | 10 | Te I 238.327 | 0.091 | | glass |
| | | 20 | Te I 317.514 | 0.29 | Dy II 317.488, Sn I 317.503 | glass |
| Th | Thorium | 5 | Th II 283.729 | 0.30 | U II 283.719 | - |
| | | 10 | Th II 326.266 | 0.31 | Er II 326.280, Sn I 326.233 | - |
| | | 10 | Th II 325.627 | 0.32 | Dy II 325.625, In I 325.607 | - |
| Ti | Titanium | 0.2 | Ti II 334.940 | 0.33 | | glass |
| | | 0.2 | Ti II 323.451 | 0.19 | | glass |
| Tl | Thallium | 5 | Tl I 276.790 | 0.28 | | - |
| | | 50 | Tl I 291.830 | 0.25 | W I 291.824, Zr II 291.824 | - |
| Tm | Thulium | 0.5 | Tm II 313.125 | 0.29 | Be II 313.106 | - |
| | | 1 | Tm II 286.922 | 0.22 | | - |
| U | Uranium | 0.5 | U II 288.962 | 0.28 | | - |
| | | 0.5 | U II 294.191 | 0.22 | | - |
| | | 1 | U II 268.328 | 0.29 | | - |
| V | Vanadium | 1 | V II 290.881 | 0.19 | Os I 290.905 | alloy |
| | | 1 | V II 311.071 | 0.25 | | alloy |
| W | Tungsten | 10 | W I 289.644 | 0.25 | Er II 289.657 | alloy |

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Table 1 – continued from previous page

| Element | C_{LOD} (ppm) | Transition | R_{app} | possibly interfering transitions | validation |
|--------------|-----------------|---------------|-----------|--|------------|
| Y Yttrium | 20 | W I 294.698 | 0.14 | Dy II 294.706, Er II 294.661, Hf II 294.713, Nb II 294.688 | alloy |
| | 20 | W I 272.435 | 0.30 | | alloy |
| | 0.5 | Y II 324.227 | 0.25 | | glass |
| | 0.5 | Y II 360.073 | 0.41 | | glass |
| Yb Ytterbium | 0.1 | Yb II 328.936 | 0.26 | | - |
| | 0.5 | Yb II 369.419 | 0.28 | | - |
| Zn Zinc | 1 | Zn I 213.857 | 0.0095 | | food |
| | 5 | Zn I 334.501 | 0.33 | Ce II 334.476, La II 334.456, Th II 334.487 Zr II 334.478 | food |
| | 5 | Zn I 481.053 | 0.80 | | food |
| Zr Zirconium | 0.5 | Zr II 339.198 | 0.32 | Er II 339.198 | alloy |
| | 1 | Zr II 343.822 | 0.30 | Hf II 343.828 | alloy |

4. Food content and safety regulations

4.1. Minerals, oligo- and toxic elements in foodstuff

Table 2: Average fractions of minerals and oligo-elements measured for different foodstuffs on the French marked [8]. The values given in ppm mass fractions refer to the original food including moisture.

| Foodstuff | Ca | Co | Cr | Cu | Li | Mg | Mn | Mo | Na | Ni | Se | Zn |
|-------------------|------|-------|------|------|-------|-----|------|-------|------|------|-------|------|
| Breakfast cereals | 1800 | 0.008 | 0.13 | 2.5 | 0.009 | 480 | 11 | 0.37 | 3300 | 0.55 | 0.025 | 12 |
| Pasta | 200 | 0.025 | 0.04 | 1.1 | 0.002 | 120 | 2.5 | 0.034 | 2500 | 0.02 | 0.011 | 3.8 |
| Rize semoline | 220 | 0.010 | 0.06 | 1.2 | 0.004 | 230 | 4.4 | 0.11 | 3400 | 0.02 | 0.011 | 4.7 |
| Milk | 1400 | 0.001 | 0.02 | 0.12 | 0.006 | 140 | 0.09 | 0.039 | 450 | 0.07 | 0.015 | 5.1 |
| Oils | 19 | 0.017 | 0.04 | 0.05 | 0.002 | 45 | 0.06 | 0.011 | 60 | 0.02 | 0.011 | 0.19 |
| Meat | 150 | 0.008 | 0.05 | 0.78 | 0.002 | 290 | 0.13 | 0.14 | 1300 | 0.02 | 0.095 | 37 |
| Fish | 350 | 0.007 | 0.08 | 0.41 | 0.030 | 260 | 0.30 | 0.065 | 2100 | 0.05 | 0.17 | 5.5 |
| Crustaceans | 750 | 0.046 | 0.09 | 7.1 | 0.12 | 510 | 2.7 | 0.13 | 5400 | 0.23 | 0.011 | 66 |
| Vegetables | 450 | 0.006 | 0.05 | 0.89 | 0.014 | 170 | 1.8 | 0.17 | 810 | 0.08 | 0.017 | 2.5 |
| Fruits | 99 | 0.009 | 0.01 | 0.65 | 0.007 | 100 | 2.1 | 0.010 | 12 | 0.03 | 0.016 | 0.73 |
| Chocolate | 1400 | 0.050 | 0.34 | 2.4 | 0.021 | 370 | 2.4 | 0.17 | 980 | 0.63 | 0.17 | 8.6 |

Table 3: Average content of toxic elements in different foodstuffs on the French marked [8]. The values given in ppm mass fraction units refer to the original food including moisture.

| Foodstuff | Al | As | Cd | Hg | Pb | Sb |
|-------------------|------|-------|--------|-------|-------|--------|
| Breakfast cereals | 3.0 | 0.004 | 0.0017 | 0.015 | 0.010 | 0.0003 |
| Pasta | 0.39 | 0.003 | 0.0022 | 0.012 | 0.003 | 0.0003 |
| Rize semoline | 0.42 | 0.016 | 0.0032 | 0.005 | 0.005 | 0.0003 |
| Milk | 0.19 | 0.003 | 0.0004 | 0.003 | 0.003 | 0.0003 |
| Oils | 0.05 | 0.045 | 0.0004 | 0.003 | 0.005 | 0.0003 |
| Meat | 0.21 | 0.009 | 0.0010 | 0.003 | 0.004 | 0.0017 |
| Fish | 0.51 | 2.2 | 0.0016 | 0.062 | 0.023 | 0.0003 |
| Crustaceans | 17 | 1.9 | 0.083 | 0.017 | 0.098 | 0.0018 |
| Vegetables | 3.2 | 0.012 | 0.011 | 0.005 | 0.015 | 0.0018 |
| Fruits | 0.41 | 0.076 | 0.0018 | 0.003 | 0.010 | 0.0024 |
| Chocolate | 3.7 | 0.007 | 0.0004 | 0.042 | 0.028 | 0.0003 |

4.2. Food safety regulations

Table 4: Maximum content of toxic elements recommended by European and Turkish safety regulations [9, 10]. The values given in ppm mass fraction units refer to the original food including moisture.

| Foodstuff | Al | As | Cd | Hg | Pb | Sb |
|---------------------|-----|------|-----|------|----|----|
| Breakfast cereales | | 0.1 | | 0.20 | | |
| Meat | | 0.05 | | 0.10 | | |
| Muscle meat of fish | | 0.05 | 0.5 | 0.30 | | |
| Breakfast cereales | | 0.1 | | 0.20 | | |
| Crustaceans | | 0.50 | | 0.50 | | |
| Rize | 0.2 | 0.2 | | | | |
| Breakfast cereales | | 0.1 | | 0.20 | | |
| Milk | | | | 0.02 | | |
| fruits & vegetables | | 0.05 | | 0.10 | | |
| Breakfast cereales | | 0.1 | | 0.20 | | |
| Fungi | | 1 | | 0.10 | | |
| fat & oils | | | | 3.0 | | |
| Breakfast cereales | | 0.1 | | 0.20 | | |
| honey | | | | 0.10 | | |
| Food supplements | 1 | 0.1 | | 3.0 | | |

5. LOD with sensitivity-improved LIBS apparatus

The apparatus used in the present experiment was designed for calibration-free LIBS measurement under controlled atmospheric conditions. It is therefore equipped with an echelle spectrometer and an observation geometry of large focusing distance. The solid angle of observation is given by

$$\Omega = \frac{\pi r^2}{f^2}, \quad (1)$$

where r is the radius and f is the focusing distance of the lens used for capturing the plasma emission. The solid angle, and thus the number of captured photons, could be increased by almost one order of magnitude by using the lens of 3 times shorter focusing length ($f = 50$ mm instead of $f = 150$ mm). Moreover, the captured plasma emission is transported via an optical fiber of $600\text{ }\mu\text{m}$ core diameter to the echelle spectrometer. According to its entrance hole of $50 \times 50\text{ }\mu\text{m}^2$, a fraction $\approx 1\%$ of the captured plasma photons enters into the spectrometer. This loss can be avoided by using an optimized optical detection system. Both improvements would thus increase the number of detected photons by a factor of 10^3 .

Another significant improvement of sensitivity is possible when using a spectrometer equipped with gratings of appropriate of blazing wavelength and a detector of optimized efficiency at the wavelength of interest. Assuming a detection system that leads to an apparatus response (see Fig 1) close to unity, the further enhancement of sensitivity scales as $1/R_{app}$. Thus, for a spectral line in the UV close to 200 nm, where $R_{app} \approx 0.01$, the number of detected photons would increase by a factor of 10^5 . According to Eqs 1 and 2 (see manuscript), the limit of detection would be reduced by $1/\sqrt{10^5} \approx 1/300$. The limits of detection being achievable with such a sensitivity-improved LIBS apparatus are displayed in Fig. 3.

| | | | | | | | | | | | | | | | | | |
|-------------|-----------|---------|----------|-----------|----------|-----------|-----------|-----------|----------|----------|-----------|-----------|----------|-----------|-----------|-------------|---------|
| H - | | | | | | | | | | | | | | He - | | | |
| Li 2 | Be 0.2 | | | | | | | | | | | | | | | | |
| Na 20 | Mg 0.2 | | | | | | | | | | | | | | | | |
| K 5000 | Ca 0.5 | Sc 5 | Ti 5 | V 10 | Cr 20 | Mn 2 | Fe 10 | Co 50 | Ni 10 | Cu 2 | Zn 2 | Ga 10 | Ge 20 | As 100 | Se 200 | Br 0.01% | Kr - |
| Rb 100 | Sr 0.5 | Y 10 | Zr 10 | Nb 20 | Mo 20 | Tc 10 | Ru 20 | Rh 20 | Pd 10 | Ag 2 | Cd 1 | In 100 | Sn 50 | Sb 100 | Te 100 | I 20000 | Xe - |
| Cs 20000 | Ba 2 | | Hf 20 | Ta 10 | W 200 | Re 20 | Os 10 | Ir 100 | Pt 50 | Au 20 | Hg 200 | Tl 100 | Pb 50 | Bi 20 | Po 50 | At 50 | Rn - |
| Fr 1000 | Ra 20 | | La 20 | Ce 100 | Pr 50 | Nd 100 | Pm 200 | Sm 100 | Eu 10 | Gd 20 | Tb 20 | Dy 20 | Ho 2 | Er 20 | Tm 10 | Yb 2 | Lu 2 |
| | | | Ac 10 | Th 100 | Pa ? | U 10 | Np ? | Pu ? | Am ? | Cm ? | Bk ? | Cf ? | Es ? | Fm ? | Md ? | No ? | Lr ? |

Figure 3: Limits of detection in ppb mass fraction units being achievable with a sensitiviy-improved LIBS apparatus.

6. Spectroscopic data

The spectroscopic data were taken in priority from the NIST database [11], and completed with data from the Kurucz database [12]. For a few transitions, data were unavailable in both databases and therefore taken from literature.

Table 5: Wavelength λ , transition probability A_{ul} , accuracy ΔA_{ul} , energy E , configuration, term and total angular momentum quantum number J of lower (index l) and upper (index u) electronic states, Stark broadening width w and shift d for $n_e = 1 \times 10^{17} \text{ cm}^{-3}$. The superscripts a , b , c and d indicate that the data were taken from the references [13], [12], [14], and [15], respectively. All other data were taken from the NIST database.

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| | λ (nm) | A_{ul} (μs^{-1}) | ΔA_{ul} (%) | E_l (eV) | E_u (eV) | config | lower level term | J_l | config | upper level term | J_u | w (pm) | d (pm) |
|-------|-------------------|------------------------------------|------------------------|---------------|---------------|-------------------|---------------------|-------|-------------------|---------------------|-------|-------------|-------------|
| Ac II | 315.308 | 269 | 20 | 0.65 | 4.58 | $6d7s$ | 3D | 2 | $6d7p$ | $^3D^\circ$ | 3 | - | - |
| Ac II | 299.416 | 282 | 20 | 0.00 | 4.14 | $7s^2$ | 1S | 0 | $6d7p$ | $^3D^\circ$ | 1 | - | - |
| Ag I | 328.068 | 140 | - | 0.00 | 3.78 | $4d^{10}5s$ | 2S | 1/2 | $4d^{10}5p$ | $^2P^\circ$ | 3/2 | 16 | 0.0 |
| Ag I | 338.288 | 130 | - | 0.00 | 3.66 | $4d^{10}5s$ | 2S | 1/2 | $4d^{10}5p$ | $^2P^\circ$ | 1/2 | 40 | 3.9 |
| Al I | 396.152 | 98.5 | 10 | 0.01 | 3.14 | $3s^23p$ | $^2P^\circ$ | 3/2 | $3s^24s$ | 2S | 1/2 | 42 | 24 |
| Al I | 394.400 | 49.9 | 10 | 0.00 | 3.14 | $3s^23p$ | $^2P^\circ$ | 1/2 | $3s^24s$ | 2S | 1/2 | 42 | 24 |
| Al I | 308.215 | 58.7 | 10 | 0.00 | 4.02 | $3s^23p$ | $^2P^\circ$ | 1/2 | $3s^23d$ | 2D | 3/2 | 76 | 18 |
| As I | 234.984 | 310 | 40 | 1.31 | 6.59 | $4s^24p^3$ | $^2D^\circ$ | 3/2 | $4s^24p^2(^3P)5s$ | 2P | 1/2 | 14 | 0.0 |
| As I | 228.811 | 280 | 40 | 1.35 | 6.77 | $4s^24p^3$ | $^2D^\circ$ | 5/2 | $4s^24p^2(^3P)5s$ | 2P | 3/2 | 14 | 0.0 |
| At I | 216.225 | 313 ^a | - | 0.00 | 5.73 | $6p^5$ | $^2P^\circ$ | 3/2 | $6p^4(^3P)7s$ | 4P | 3/2 | - | - |
| At I | 224.401 | 27.8 ^a | - | 0.00 | 5.52 | $6p^5$ | $^2P^\circ$ | 3/2 | $6p^4(^3P)7s$ | 4P | 5/2 | - | - |
| Au I | 267.593 | 164 | 5 | 0.00 | 4.63 | $5d^{10}6s$ | 2S | 1/2 | $5d^{10}6p$ | $^2P^\circ$ | 1/2 | 1.4 | 5.6 |
| Au I | 242.794 | 198 | 10 | 0.00 | 5.11 | $5d^{10}6s$ | 2S | 1/2 | $5d^{10}6p$ | $^2P^\circ$ | 3/2 | 1.4 | 5.6 |
| B I | 249.772 | 168 | 7 | 0.00 | 4.96 | $2s^22p$ | $^2P^\circ$ | 3/2 | $2s^23s$ | 2S | 1/2 | 12 | 7.0 |
| B I | 249.676 | 84.0 | 7 | 0.00 | 4.96 | $2s^22p$ | $^2P^\circ$ | 1/2 | $2s^23s$ | 2S | 1/2 | 12 | 7.0 |
| Ba II | 233.526 | 2655 | - | 0.70 | 6.01 | $5d$ | 2D | 5/2 | $4f$ | $^2F^\circ$ | 7/2 | 17 | -1.5 |
| Ba II | 230.424 | 3316 | - | 0.60 | 5.98 | $5d$ | 2D | 3/2 | $4f$ | $^2F^\circ$ | 5/2 | 17 | -1.4 |
| Be II | 313.042 | 113 | 1 | 0.00 | 3.96 | $1s^22s$ | 2S | 1/2 | $1s^22p$ | $^2P^\circ$ | 3/2 | - | - |
| Be II | 313.106 | 113 | 1 | 0.00 | 3.96 | $1s^22s$ | 2S | 1/2 | $1s^22p$ | $^2P^\circ$ | 1/2 | - | - |
| Be I | 234.860 | 552 | 7 | 0.00 | 5.28 | $1s^22s^2$ | 1S | 0 | $1s^22s2p$ | $^1P^\circ$ | 1 | - | - |
| Bi I | 306.770 | 167 | - | 0.00 | 4.04 | $6p^3$ | $^4S^\circ$ | 3/2 | $6p^2(^3P_0)7s$ | $^2[0]$ | 1/2 | 23 | 12 |
| Bi I | 293.829 | 123 | - | 1.91 | 6.13 | $6p^3$ | $^2D^\circ$ | 5/2 | $6p^2(^3P_2)7s$ | $^2[2]$ | 3/2 | 100 | 30 |
| Br I | 827.241 | 35.0 | 20 | 7.87 | 9.36 | $4s^24p(^3P_2)5s$ | $^2[2]$ | 5/2 | $4s^24p(^3P_2)5p$ | $^2[3]^\circ$ | 7/2 | 140 | 35 |
| Ca II | 393.366 | 147 | 25 | 0.00 | 3.15 | $3p^64s$ | 2S | 1/2 | $3p^64p$ | $^2P^\circ$ | 3/2 | 20 | -4.0 |
| Ca II | 396.846 | 140 | 25 | 0.00 | 3.12 | $3p^64s$ | 2S | 1/2 | $3p^64p$ | $^2P^\circ$ | 1/2 | 20 | -4.0 |
| Ca I | 422.672 | 218 | 10 | 0.00 | 2.93 | $3p^64s^2$ | 1S | 0 | $3p^64s4p$ | $^1P^\circ$ | 1 | 20 | 2.9 |
| Cd I | 228.802 | 530 | 25 | 0.00 | 5.42 | $4d^{10}5s^2$ | 1S | 0 | $4d^{10}5s5p$ | $^1P^\circ$ | 1 | 3.0 | 0.0 |

continued on next page

Table 5 – continued from previous page

| | λ (nm) | A_{ul} (μs^{-1}) | ΔA_{ul} (%) | E_l (eV) | E_u (eV) | config | lower level term | J_l | config | upper level term | J_u | w (pm) | d (pm) |
|-------|-------------------|------------------------------------|------------------------|---------------|---------------|--------------------------------------|---------------------|-------|--------------------------------------|----------------------|-------|-----------|-----------|
| Ce II | 320.171 | 349 ^b | - | 0.86 | 4.73 | $4f5d(^3H^{\circ})6s$ | $^4H^{\circ}$ | 13/2 | $4f6s(^3F^{\circ})6p$ | 4G | 11/2 | - | - |
| Ce II | 265.100 | 2079 ^b | - | 1.21 | 5.89 | $4f(^2F^{\circ})6s^2$ | $^2F^{\circ}$ | 5/2 | $5d^2(^1G)6s$ | 2G | 7/2 | - | - |
| Cl I | 837.594 | 28.0 | 40 | 8.92 | 10.40 | $3s^23p^4(^3P)4s$ | 4P | 5/2 | $3s^23p^4(^3P)4p$ | $^4D^{\circ}$ | 7/2 | 154 | 0.0 |
| Cl I | 725.661 | 15.0 | 40 | 8.92 | 10.63 | $3s^23p^4(^3P)4s$ | 4P | 5/2 | $3s^23p^4(^3P)4p$ | $^4S^{\circ}$ | 3/2 | - | - |
| Co I | 340.511 | 100 | 20 | 0.43 | 4.07 | $3d^8(^3F)4s$ | b 4F | 9/2 | $3d^8(^3F)4p$ | y $^4F^{\circ}$ | 9/2 | - | - |
| Co I | 252.136 | 300 | 40 | 0.00 | 4.92 | $3d^74s^2$ | a 4F | 9/2 | $3d^7(^4F)4s4p(^1P^{\circ})$ | x $^4D^{\circ}$ | 7/2 | - | - |
| Co I | 240.725 | 360 | 25 | 0.00 | 5.15 | $3d^74s^2$ | a 4F | 9/2 | $3d^7(^4F)4s4p(^1P^{\circ})$ | x $^4G^{\circ}$ | 11/2 | 5.0 | 2.0 |
| Cr II | 283.563 | 200 | 25 | 1.55 | 5.92 | $3d^4(^5D)4s$ | a 6D | 9/2 | $3d^4(^5D)4p$ | z $^6F^{\circ}$ | 11/2 | 10 | 0.0 |
| Cr II | 276.653 | 222 | - | 1.55 | 6.03 | $3d^4(^5D)4s$ | a 6D | 9/2 | $3d^4(^5D)4p$ | z $^6P^{\circ}$ | 7/2 | 4.0 | 0.0 |
| Cs I | 455.528 | 1.84 | 2 | 0.00 | 2.72 | $5p^66s$ | 2S | 1/2 | $5p^67p$ | $^2P^{\circ}$ | 3/2 | 500 | 200 |
| Cu I | 324.753 | 140 | 2 | 0.00 | 3.82 | $3d^{10}4s$ | 2S | 1/2 | $3d^{10}4p$ | $^2P^{\circ}$ | 3/2 | 7.0 | 3.0 |
| Cu I | 327.395 | 138 | 2 | 0.00 | 3.79 | $3d^{10}4s$ | 2S | 1/2 | $3d^{10}4p$ | $^2P^{\circ}$ | 1/2 | 7.0 | 3.0 |
| Dy II | 353.170 | 156 | - | 0.00 | 3.51 | $4f^{10}(^5I_8)6s_{1/2}$ | (8,1/2) | 17/2 | $4f^{10}(^5I_6)6p$ | $^6K^{\circ}$ | 19/2 | - | - |
| Dy II | 340.779 | 48.8 | - | 0.00 | 3.64 | $4f^{10}(^5I_8)6s_{1/2}$ | (8,1/2) | 17/2 | $4f^{10}(^5I_6)6p$ | $^6I^{\circ}$ | 17/2 | - | - |
| Er II | 337.275 | 130 | - | 0.00 | 3.68 | $4f^{12}(^3H_6)6s_{1/2}$ | (6,1/2) | 13/2 | $4f^{12}(^3H_6)6p_{3/2}$ | (6,3/2) ^o | 15/2 | - | - |
| Er II | 323.058 | 150 | - | 0.05 | 3.89 | $4f^{12}(^3H_6)6s_{1/2}$ | (6,1/2) | 11/2 | | | 11/2 | - | - |
| Er II | 291.036 | 366 | - | 0.85 | 5.11 | $4f^{11}6s^2$ | $^4I^{\circ}$ | 15/2 | | | 15/2 | - | - |
| Eu II | 397.197 | 89.0 | - | 0.21 | 3.33 | $4f^7(^8S^{\circ})6s$ | a $^7S^{\circ}$ | 3 | $4f^7(^8S_{7/2})6p_{3/2}$ | (7/2,3/2) | 4 | - | - |
| Eu II | 390.710 | 137 | - | 0.21 | 3.38 | $4f^7(^8S^{\circ})6s$ | a $^7S^{\circ}$ | 3 | $4f^7(^8S_{7/2})6p_{3/2}$ | (7/2,3/2) | 2 | - | - |
| F I | 685.603 | 48.7 | 20 | 12.70 | 14.50 | $2s^22p^4(^3P)3s$ | 4P | 5/2 | $2s^22p^4(^3P)3p$ | $^4D^{\circ}$ | 7/2 | - | - |
| Fe II | 259.939 | 235 | 10 | 0.00 | 4.77 | $3d^6(^5D)4s$ | a 6D | 9/2 | $3d^6(^5D)4p$ | z $^6D^{\circ}$ | 9/2 | 3.0 | 0.0 |
| Fe II | 238.203 | 313 | 10 | 0.00 | 5.20 | $3d^6(^5D)4s$ | a 6D | 9/2 | $3d^6(^5D)4p$ | z $^6F^{\circ}$ | 11/2 | 10 | 0.0 |
| Fr I | 717.986 | 47.8 | - | 0.00 | 1.73 | 7s | 2S | 1/2 | 7p | $^2P^{\circ}$ | 3/2 | - | - |
| Fr I | 816.941 | 32.2 | - | 0.00 | 1.52 | 7s | 2S | 1/2 | 7p | $^2P^{\circ}$ | 1/2 | - | - |
| Ga I | 294.363 | 134 | 10 | 0.10 | 4.31 | $3d^{10}4s^24p$ | $^2P^{\circ}$ | 3/2 | $4s^24d$ | 2D | 5/2 | - | - |
| Ga I | 287.423 | 117 | 10 | 0.00 | 4.31 | $3d^{10}4s^24p$ | $^2P^{\circ}$ | 1/2 | $4s^24d$ | 2D | 3/2 | - | - |
| Ga I | 403.298 | 48.5 | 10 | 0.00 | 3.07 | $3d^{10}4s^24p$ | $^2P^{\circ}$ | 1/2 | $4s^25s$ | 2S | 1/2 | - | - |
| Gd II | 342.246 | 118 ^b | - | 0.24 | 3.86 | $4f^7(^8S^{\circ})5d(^9D^{\circ})6s$ | $^{10}D^{\circ}$ | 13/2 | $4f^7(^8S^{\circ})5d(^9D^{\circ})6p$ | ^{10}F | 15/2 | - | - |
| Gd II | 310.050 | 169 ^b | - | 0.24 | 4.24 | $4f^7(^8S^{\circ})5d(^9D^{\circ})6s$ | $^{10}D^{\circ}$ | 13/2 | $4f^7(^8S^{\circ})5d(^9D^{\circ})6p$ | ^{10}P | 11/2 | - | - |
| Ge I | 265.117 | 200 | - | 0.17 | 4.85 | $4s^24p^2$ | 3P | 2 | $4s^24p5s$ | $^3P^{\circ}$ | 2 | - | - |
| Ge I | 303.906 | 280 | - | 0.88 | 4.96 | $4s^24p^2$ | 1D | 2 | $4s^24p5s$ | $^1P^{\circ}$ | 1 | 17 | 11 |
| Hf II | 264.141 | 372 ^b | - | 1.04 | 5.73 | $5d^2(^3F)6s$ | a 4F | 9/2 | $5d^2(^3F)6p$ | $z ^4G^{\circ}$ | 11/2 | 14 | 2.2 |
| Hf II | 277.335 | 141 ^b | - | 0.79 | 5.26 | $5d^2(^3F)6s$ | a 4F | 7/2 | $5d^2(^3F)6p$ | $z ^4G^{\circ}$ | 9/2 | 12 | 2.2 |

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Table 5 – continued from previous page

| | λ (nm) | A_{ul} (μs^{-1}) | ΔA_{ul} (%) | E_l (eV) | E_u (eV) | config | lower level term | J_l | config | upper level term | J_u | w (pm) | d (pm) |
|-------|-------------------|------------------------------------|------------------------|---------------|---------------|-------------------------------|---------------------|-------|-------------------------------|---------------------|-------|-----------|-----------|
| Hg I | 296.728 | 46.0 | 40 | 4.67 | 8.84 | $5d^{10}6s6p$ | $^3P^\circ$ | 0 | $5d^{10}6s6d$ | 3D | 1 | - | - |
| Hg I | 365.484 | 18.4 | 15 | 5.46 | 8.85 | $5d^{10}6s6p$ | $^3P^\circ$ | 2 | $5d^{10}6s6d$ | 3D | 2 | - | - |
| Ho II | 341.644 | 974 ^b | - | 0.08 | 3.71 | $4f^{11}(^4I_{15/2})6s_{1/2}$ | $(15/2,1/2)^\circ$ | 7 | $4f^{11}(^4I_{15/2})6p_{3/2}$ | $(15/2,3/2)$ | 7 | - | - |
| Ho II | 339.895 | 63.5 ^b | - | 0.00 | 3.65 | $4f^{11}(^4I_{15/2})6s_{1/2}$ | $(15/2,1/2)^\circ$ | 8 | $4f^{11}(^4I_{15/2})6p_{3/2}$ | $(15/2,3/2)$ | 8 | - | - |
| I I | 206.162 | 3.0 | - | 0.94 | 6.95 | $5s^25p^5$ | $^2P^\circ$ | 1/2 | $5s^25p(^3P_2)6s$ | $^2[2]$ | 3/2 | - | - |
| In I | 325.607 | 130 | - | 0.27 | 4.08 | $5s^25p$ | $^2P^\circ$ | 3/2 | $5s^25d$ | 2D | 5/2 | 134 | -17 |
| In I | 303.934 | 111 | - | 0.00 | 4.08 | $5s^25p$ | $^2P^\circ$ | 1/2 | $5s^25d$ | 2D | 3/2 | 100 | -13 |
| Ir I | 263.970 | 46.9 | 7 | 0.00 | 4.70 | $5d^76s^2$ | a 4F | 9/2 | $5d^76s(^5F)6p$ | $z \ ^4F^\circ$ | 9/2 | - | - |
| Ir I | 284.972 | 22.6 | 10 | 0.00 | 4.35 | $5d^76s^2$ | a 4F | 9/2 | $5d^76s(^5F)6p$ | $z \ ^6G^\circ$ | 9/2 | - | - |
| K I | 769.896 | 37.5 | 5 | 0.00 | 1.61 | $3p^64s$ | 2S | 1/2 | $3p^64p$ | $^2P^\circ$ | 1/2 | 105 | 24 |
| K I | 404.414 | 1.16 | - | 0.00 | 3.06 | $3p^64s$ | 2S | 1/2 | $3p^65p$ | $^2P^\circ$ | 3/2 | 124 | 47 |
| La II | 394.910 | 147 | 10 | 0.40 | 3.54 | $5d6s$ | a 3D | 3 | $5d6p$ | $x \ ^3F^\circ$ | 4 | 17 | 0.0 |
| La II | 398.851 | 97.0 | 15 | 0.40 | 3.51 | $5d6s$ | a 3D | 3 | $5d6p$ | $y \ ^3D^\circ$ | 3 | - | - |
| Li I | 670.776 | 36.9 | 1 | 0.00 | 1.85 | $1s^22s$ | 2S | 1/2 | $1s^22p$ | $^2P^\circ$ | 3/2 | 39 | -2.7 |
| Lu II | 261.541 | 453 | - | 0.00 | 4.74 | $6s^2$ | 1S | 0 | $6s6p$ | $^1P^\circ$ | 1 | - | - |
| Lu II | 290.030 | 380 ^b | - | 1.54 | 5.82 | $5d6s$ | 3D | 2 | $5d6p$ | $^3D^\circ$ | 2 | - | - |
| Mg II | 279.552 | 260 | 5 | 0.00 | 4.43 | $2p^63s$ | 2S | 1/2 | $2p^63p$ | $^2P^\circ$ | 3/2 | 4.0 | 0.0 |
| Mg II | 280.270 | 257 | 5 | 0.00 | 4.42 | $2p^63s$ | 2S | 1/2 | $2p^63p$ | $^2P^\circ$ | 1/2 | 4.0 | 0.0 |
| Mg I | 285.212 | 491 | 7 | 0.00 | 4.35 | $2p^63s^2$ | 1S | 0 | $3s3p$ | $^1P^\circ$ | 1 | 11 | 4.2 |
| Mn II | 259.372 | 276 | 5 | 0.00 | 4.78 | $3d^5(^6S)4s$ | a 7S | 3 | $3d^5(^6S)4p$ | $z \ ^7P^\circ$ | 3 | 4.5 | -1.0 |
| Mn II | 260.568 | 269 | 5 | 0.00 | 4.76 | $3d^5(^6S)4s$ | a 7S | 3 | $3d^5(^6S)4p$ | $z \ ^7P^\circ$ | 2 | 2.1 | 1.7 |
| Mn II | 294.920 | 196 | 5 | 1.17 | 5.38 | $3d^5(^6S)4s$ | a 5S | 2 | $3d^5(^6S)4p$ | $z \ ^5P^\circ$ | 3 | 4.4 | 1.6 |
| Mn I | 403.075 | 17.0 | 20 | 0.00 | 3.08 | $3d^54s^2$ | a 6S | 5/2 | $3d^5(^6S)4s4p(^3P^\circ)$ | $z \ ^6P^\circ$ | 7/2 | 12 | 0.0 |
| Mo I | 313.259 | 179 | 10 | 0.00 | 3.96 | $4d^5(^6S)5s$ | a 7S | 3 | $4d^45s(^6D)5p$ | $y \ ^7P^\circ$ | 4 | 5.0 | 0.0 |
| Mo II | 281.615 | 227 ^b | - | 1.67 | 6.07 | $4d^4(^5D)5s$ | a 6D | 9/2 | $4d^4(^5D)5p$ | $z \ ^6F^\circ$ | 11/2 | 4.0 | 0.0 |
| Mo I | 317.034 | 137 | 10 | 0.00 | 3.91 | $4d^5(^6S)5s$ | a 7S | 3 | $4d^45s(^6D)5p$ | $y \ ^7P^\circ$ | 3 | 5.0 | 0.0 |
| N I | 746.831 | 19.6 | 10 | 10.34 | 12.00 | $2s^22p^2(^3P)3s$ | 4P | 5/2 | $2s^22p^2(^3P)3p$ | $^4S^\circ$ | 3/2 | 106 | 32 |
| Na I | 589.592 | 61.4 | 2 | 0.00 | 2.10 | $2p^63s$ | 2S | 1/2 | $2p^63p$ | $^2P^\circ$ | 1/2 | 44 | 13 |
| Na I | 588.995 | 61.6 | 2 | 0.00 | 2.10 | $2p^63s$ | 2S | 1/2 | $2p^63p$ | $^2P^\circ$ | 3/2 | 44 | 13 |
| Nb II | 313.078 | 159 ^b | - | 0.44 | 4.40 | $4d^3(^4F)5s$ | a 5F | 4 | $4d^3(^4F)5p$ | $z \ ^5G^\circ$ | 5 | 10 | 0.0 |
| Nb II | 316.339 | 135 ^b | - | 0.38 | 4.29 | $4d^3(^4F)5s$ | a 5F | 3 | $4d^3(^4F)5p$ | $z \ ^5G^\circ$ | 4 | 5.0 | 0.0 |
| Nd II | 404.079 | 38.2 ^b | - | 0.18 | 3.25 | $4f^4(^5I)6s$ | 6I | 11/2 | $4f^4(^5I)6p$ | | 13/2 | - | - |
| Nd II | 397.326 | 54.0 ^b | - | 0.63 | 3.75 | $4f^4(^5I)6s$ | 6I | 17/2 | $4f^4(^5I)6p$ | $^6I^\circ$ | 17/2 | - | - |

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Table 5 – continued from previous page

| | λ (nm) | A_{ul} (μs^{-1}) | ΔA_{ul} (%) | E_l (eV) | E_u (eV) | config | lower level term | J_l | config | upper level term | J_u | w (pm) | d (pm) |
|-------|-------------------|------------------------------------|------------------------|---------------|---------------|----------------------------|---------------------|-------|----------------------------|---------------------|-------|-----------|-----------|
| Ni I | 232.003 | 690 | 25 | 0.00 | 5.34 | $3d^8(^3F)4s^2$ | 3F | 4 | $3d^8(^3F)4s4p(^1P^\circ)$ | ${}^3G^\circ$ | 5 | 3.5 | 1.5 |
| Ni I | 300.248 | 80.0 | 20 | 0.03 | 4.15 | $3d^9(^2D)4s$ | 3D | 3 | $3d^8(^3F)4s4p(^3P^\circ)$ | ${}^3D^\circ$ | 3 | 7.0 | 0.0 |
| Ni I | 305.081 | 60.0 | 20 | 0.03 | 4.09 | $3d^9(^2D)4s$ | 3D | 3 | $3d^8(^3F)4s4p(^3P^\circ)$ | ${}^3F^\circ$ | 4 | 2.0 | 0.0 |
| Ni I | 341.476 | 55.0 | 25 | 0.03 | 3.66 | $3d^9(^2D)4s$ | 3D | 3 | $3d^9(^2D)4p$ | ${}^3F^\circ$ | 4 | 7.6 | 0.4 |
| Os II | 248.624 | 2816 ^b | - | 0.45 | 5.43 | $5d^6(^5D)6s$ | $a {}^6D$ | 7/2 | $5d^6(^5D)6p$ | $z {}^6D^\circ$ | 7/2 | - | - |
| Os II | 253.798 | 1235 ^b | - | 0.00 | 4.88 | $5d^6(^5D)6s$ | $a {}^6D$ | 9/2 | $5d^5 6s6p$ | ${}^8P^\circ$ | 7/2 | - | - |
| Os II | 321.331 | 1230 ^b | - | 1.64 | 5.49 | $5d^7$ | 4F | 7/2 | $5d^6(^3D)6p$ | $z {}^6D^\circ$ | 9/2 | - | - |
| P I | 253.561 | 95.0 | 25 | 2.32 | 7.21 | $3s^23p^3$ | ${}^2P^\circ$ | 3/2 | $3s^23p^2(^3P)4s$ | 2P | 3/2 | 10 | 2.0 |
| P I | 214.914 | 318 | 25 | 1.41 | 7.18 | $3s^23p^3$ | ${}^2D^\circ$ | 3/2 | $3s^23p^2(^3P)4s$ | 2P | 1/2 | - | - |
| P I | 255.326 | 71.0 | 25 | 2.32 | 7.18 | $3s^23p^3$ | ${}^2P^\circ$ | 1/2 | $3s^23p^2(^3P)4s$ | 2P | 1/2 | 10 | 2.0 |
| Pb I | 283.305 | 49.0 | 20 | 0.00 | 4.38 | $6s^26p^2$ | $(1/2,1/2)$ | 0 | $6s^26p7s$ | $(1/2,1/2)^\circ$ | 1 | 18 | 10 |
| Pb I | 261.417 | 198 | 20 | 0.97 | 5.71 | $6s^26p^2$ | $(3/2,1/2)$ | 1 | $6s^26p(^2P)_{1/2}6d$ | ${}^2[3/2]^\circ$ | 2 | 40 | -4.1 |
| Pd I | 340.457 | 134 | - | 0.81 | 4.45 | $4d^9(^2D_{5/2})5s$ | ${}^2[5/2]$ | 3 | $4d^9(^2D_{5/2})5p$ | ${}^2[7/2]^\circ$ | 4 | 42 | -4.2 |
| Pd I | 342.122 | 168 ^b | - | 0.96 | 4.58 | $4d^9(^2D_{5/2})5s$ | ${}^2[5/2]$ | 2 | $4d^9(^2D_{5/2})5p$ | ${}^2[5/2]^\circ$ | 2 | 40 | 0.0 |
| Pd I | 324.269 | 77.0 | - | 0.81 | 4.64 | $4d^9(^2D_{5/2})5s$ | ${}^2[5/2]$ | 3 | $4d^9(^2D_{5/2})5p$ | ${}^2[5/2]^\circ$ | 3 | 40 | 0.0 |
| Pm II | 429.778 | 68.8 ^c | - | 0.00 | 2.88 | $4f^5(^6H)6s$ | ${}^7H^\circ$ | 2 | $4f^5(^6H)6p$ | 7I | 3 | - | - |
| Po I | 255.800 | 71.8 ^d | - | 0.00 | 4.85 | $6p^4$ | 3P | 2 | $6p^3(^4S^\circ)7s$ | ${}^5S^\circ$ | 2 | - | - |
| Po I | 300.320 | 37.9 ^d | - | 0.93 | 5.06 | $6p^4$ | 3P | 0 | $6p^3(^4S^\circ)7s$ | ${}^3S^\circ$ | 1 | - | - |
| Pr II | 406.280 | 100 ^b | - | 0.42 | 3.47 | $4f^3(^4I_{13/2})6s_{1/2}$ | $(13/2,1/2)^\circ$ | 6 | $4f^3(^4I^\circ)6p$ | 3I | 7 | - | - |
| Pr II | 390.842 | 89.3 ^b | - | 0.00 | 3.17 | $4f^3(^4I_{9/2})6s_{1/2}$ | $(9/2,1/2)^\circ$ | 4 | $4f^3(^4I^\circ)6p$ | 5H | 3 | - | - |
| Pt I | 306.471 | 65.9 | 10 | 0.00 | 4.04 | $5d^96s$ | 3D | 3 | $5d^96p$ | $a {}^3P^\circ$ | 2 | - | - |
| Pt I | 265.945 | 99.0 | 10 | 0.00 | 4.66 | $5d^96s$ | 3D | 3 | $5d^96p$ | ${}^3F^\circ$ | 4 | - | - |
| Ra II | 270.896 | 370 | 2 | 1.50 | 6.07 | $6d$ | 2D | 3/2 | $5f$ | ${}^2F^\circ$ | 5/2 | - | - |
| Rb I | 780.027 | 38.1 | - | 0.00 | 1.59 | $4p^65s$ | 2S | 1/2 | $4p^65p$ | ${}^2P^\circ$ | 3/2 | 200 | 0.0 |
| Re II | 260.849 | 4386 ^b | - | 1.78 | 6.53 | $5d^46s^2$ | $a {}^5D$ | 2 | $5d^5(^6S)6p$ | $z {}^4P^\circ$ | 2 | - | - |
| Re II | 273.303 | 3431 ^b | - | 2.14 | 6.67 | $5d^5(^6S)6s$ | $a {}^5S$ | 2 | $5d^5(^6S)6p$ | $z {}^5P^\circ$ | 3 | - | - |
| Re II | 256.863 | 2626 ^b | - | 1.85 | 6.67 | $5d^46s^2$ | $a {}^5D$ | 4 | $5d^5(^6S)6p$ | $z {}^5P^\circ$ | 3 | - | - |
| Rh I | 343.488 | 133 ^b | - | 0.00 | 3.61 | $4d^8(^3F)5s$ | $a {}^4F$ | 9/2 | $4d^8(^3F)5p$ | $z {}^4G^\circ$ | 11/2 | - | - |
| Rh I | 339.681 | 65.0 ^b | - | 0.00 | 3.65 | $4d^8(^3F)5s$ | $a {}^4F$ | 9/2 | $4d^8(^3F)5p$ | $z {}^4F^\circ$ | 9/2 | - | - |
| Ru II | 267.875 | 1507 ^b | - | 1.13 | 5.76 | $4d^6(^5D)5s$ | 6D | 9/2 | $4d^6(^5D)5p$ | ${}^6D^\circ$ | 9/2 | - | - |
| Ru II | 273.434 | 927 ^b | - | 1.26 | 5.79 | $4d^6(^5D)5s$ | 6D | 7/2 | $4d^6(^5D)5p$ | ${}^6D^\circ$ | 7/2 | - | - |
| S I | 675.715 | 7.2 | 30 | 7.87 | 9.70 | $3s^23p^3(^4S^\circ)4p$ | 5P | 3 | $3s^23p^3(^4S^\circ)5d$ | ${}^5D^\circ$ | 4 | 500 | 0.0 |
| Sb I | 276.993 | 189 ^b | - | 1.22 | 5.70 | $5p^3$ | ${}^2D^\circ$ | 5/2 | $5p^2(^3P)6s$ | 4P | 3/2 | - | - |

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Table 5 – continued from previous page

| | λ (nm) | A_{ul} (μs^{-1}) | ΔA_{ul} (%) | E_l (eV) | E_u (eV) | config | lower level term | J_l | config | upper level term | J_u | w (pm) | d (pm) |
|-------|-------------------|------------------------------------|------------------------|---------------|----------------------|-------------------------------------|---------------------|----------------------|-----------------------------------|-------------------------|-------|-----------|-----------|
| Sb I | 302.980 | 262 ^b | - | 2.03 | 6.12 | $5p^3$ | $^2\text{P}^\circ$ | 1/2 | $5p^2(^3\text{P})6s$ | ^2P | 3/2 | 165 | 76 |
| Sb I | 267.063 | 75.6 ^b | - | 1.06 | 5.70 | $5p^3$ | $^2\text{D}^\circ$ | 3/2 | $5p^2(^3\text{P})6s$ | ^4P | 3/2 | - | - |
| Sc II | 361.382 | 148 | 10 | 0.02 | 3.45 | $3p^63d4s$ | ^3D | 3 | $3p^63d4p$ | $^3\text{F}^\circ$ | 4 | - | - |
| Sc II | 424.682 | 129 | 7 | 0.32 | 3.23 | $3p^63d4s$ | ^1D | 2 | $3p^63d4p$ | $^1\text{D}^\circ$ | 2 | - | - |
| Se I | 203.985 | 414 ^b | - | 0.25 | 6.32 | $4p^4$ | ^3P | 1 | $4p^3(^4\text{S}^\circ)5s$ | $^3\text{S}^\circ$ | 1 | - | - |
| Se I | 206.278 | 158 ^b | - | 0.31 | 6.32 | $4p^4$ | ^3P | 0 | $4p^3(^4\text{S}^\circ)5s$ | $^3\text{S}^\circ$ | 1 | - | - |
| Si I | 251.611 | 168 | 15 | 0.03 | 4.95 | $3s^23p^2$ | ^3P | 2 | $3s^23p4s$ | $^3\text{P}^\circ$ | 2 | 11 | 7.0 |
| Si I | 288.157 | 217 | 15 | 0.78 | 5.08 | $3s^23p^2$ | ^1D | 2 | $3s^23p4s$ | $^1\text{P}^\circ$ | 1 | 14 | 9.8 |
| Si I | 252.850 | 90.4 | 15 | 0.03 | 4.93 | $3s^23p^2$ | ^3P | 2 | $3s^23p4s$ | $^3\text{P}^\circ$ | 1 | 11 | 7.0 |
| Sm II | 330.638 | 50.5 ^b | - | 0.48 | 4.23 | $4f^6(^7\text{F})6s$ | ^8F | 13/2 | $4f^55d6s?$ | | 13/2 | - | - |
| Sm II | 360.949 | 58.0 | - | 0.28 | 3.71 | $4f^6(^7\text{F})6s$ | ^8F | 9/2 | $4f^55d6s?$ | | 11/2 | - | - |
| Sn I | 283.997 | 170 | - | 0.42 | 4.79 | $5s^25p^2$ | ^3P | 2 | $5s^25p6s$ | $^3\text{P}^\circ$ | 2 | 23 | 9.8 |
| Sn I | 326.233 | 270 | - | 1.07 | 4.87 | $5s^25p^2$ | ^1D | 2 | $5s^25p6s$ | $^1\text{P}^\circ$ | 1 | 20 | 7.4 |
| Sn I | 317.503 | 100 | - | 0.42 | 4.33 | $5s^25p^2$ | ^3P | 2 | $5s^25p6s$ | $^3\text{P}^\circ$ | 1 | 23 | 12 |
| Sr II | 407.770 | 141 | 2 | 0.00 | 3.04 | $4p^65s$ | ^2S | 1/2 | $4p^65p$ | $^2\text{P}^\circ$ | 3/2 | 41 | -3.4 |
| Ta II | 301.254 | 1648 ^b | - | 0.66 | 4.78 | $5d^26s^2$ | a ^3P | 1 | $5d^4$ | $^5\text{F}^\circ$ | 2 | - | - |
| Ta II | 268.518 | 4063 ^b | - | 0.51 | 5.13 | $5d^26s^2$ | a ^3P | 0 | $5d^4$ | $^\circ$ | 1 | - | - |
| Ta II | 240.063 | 3974 ^b | - | 0.77 | 5.93 | $5d^3(^4\text{F})6s$ | a ^5F | 5 | $5d^4$ | $^\circ$ | 6 | - | - |
| Tb II | 350.914 | 53.7 | - | 0.00 | 3.53 | $4f^9(^6\text{H}_{15/2})6s_{1/2}$ | $(15/2, 1/2)^\circ$ | 8 | $4f^9(^6\text{H}_{15/2})6p_{3/2}$ | $(15/2, 3/2)$ | 9 | - | - |
| Tb II | 400.546 | 90.8 ^b | - | 0.13 | 3.22 | $4f^9(^6\text{H}_{15/2})6s_{1/2}$ | $(15/2, 1/2)^\circ$ | 7 | $4f^9(^6\text{H}_{15/2})6p_{3/2}$ | $(15/2, 1/2)$ | 8 | - | - |
| Tc II | 260.999 | 380 | 0.00 | 4.75 | $4d^5(^6\text{S})5s$ | a ^7S | 3 | $4d^5(^6\text{S})5p$ | $z \, ^7\text{P}^\circ$ | 3 | - | - | |
| Tc II | 264.701 | 370 | - | 0.00 | 4.68 | $4d^5(^6\text{S})5s$ | a ^7S | 3 | $4d^5(^6\text{S})5p$ | $z \, ^7\text{P}^\circ$ | 2 | - | - |
| Te I | 238.579 | 270 ^b | - | 0.59 | 5.78 | $5p^4$ | ^3P | 1 | $5p^3(^4\text{S}^\circ)6s$ | $^3\text{S}^\circ$ | 1 | - | - |
| Te I | 238.327 | 215 ^b | - | 0.58 | 5.78 | $5p^4$ | ^3P | 0 | $5p^3(^4\text{S}^\circ)6s$ | $^3\text{S}^\circ$ | 1 | - | - |
| Te I | 317.514 | 206 ^b | - | 2.88 | 6.78 | $5p^4$ | ^1S | 0 | $5p^3(^2\text{D}^\circ)6s$ | $^3\text{D}^\circ$ | 1 | - | - |
| Th II | 283.729 | 166 ^b | - | 0.77 | 5.14 | $6d^2(^3\text{F})7s$ | ^4F | 9/2 | $6d^2(^3\text{F})7p$ | $^4\text{G}^\circ$ | 11/2 | - | - |
| Th II | 326.266 | 58.7 ^b | - | 0.76 | 4.56 | $5f6d(^3\text{H}^\circ)7s$ | $^4\text{H}^\circ$ | 7/2 | $5f6d(^1\text{G}^\circ)7p$ | | 7/2 | - | - |
| Th II | 325.627 | 94.5 ^b | - | 1.15 | 4.95 | $5f6d(^1\text{G}^\circ)7s$ | | 9/2 | $5f^2(^3\text{F})6d$ | | 11/2 | - | - |
| Ti II | 334.940 | 168 | 20 | 0.05 | 3.75 | $3d^2(^3\text{F})4s$ | a ^4F | 9/2 | $3d^2(^3\text{F})4p$ | $z \, ^4\text{G}^\circ$ | 11/2 | 11 | 0.1 |
| Ti II | 323.451 | 171 | 10 | 0.05 | 3.88 | $3d^2(^3\text{F})4s$ | a ^4F | 9/2 | $3d^2(^3\text{F})4p$ | $z \, ^4\text{F}^\circ$ | 9/2 | 12 | 0.0 |
| Tl I | 276.790 | 126 | 25 | 0.00 | 4.48 | $6s^26p$ | $^2\text{P}^\circ$ | 1/2 | $6s^26d$ | ^2D | 3/2 | - | - |
| Tl I | 291.830 | 42.0 | 25 | 0.97 | 5.21 | $6s^26p$ | $^2\text{P}^\circ$ | 3/2 | $6s^27d$ | ^2D | 5/2 | - | - |
| Tm II | 313.125 | 106 | - | 0.00 | 3.96 | $4f^{13}(^2\text{F}_{7/2})6s_{1/2}$ | $(7/2, 1/2)^\circ$ | 4 | $4f^{12}5d6s$ | | 5 | - | - |

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Table 5 – continued from previous page

| | λ (nm) | A_{ul} (μs^{-1}) | ΔA_{ul} (%) | E_l (eV) | E_u (eV) | config | lower level term | J_l | config | upper level term | J_u | w (pm) | d (pm) |
|-------|-------------------|------------------------------------|------------------------|---------------|---------------|---------------------------|----------------------|-------|----------------------|-------------------------|-------|-----------|-----------|
| Tm II | 286.922 | 491 ^b | - | 1.54 | 5.86 | $4f^{12}(^3\text{H})6s^2$ | ${}^3\text{H}$ | 6 | $4f^{12}5d6p$ | ${}^\circ$ | 7 | - | - |
| U II | 288.962 | 62.5 ^b | - | 0.04 | 4.33 | $5f^36d^2$ | ${}^6\text{L}$ | 11/2 | | | 11/2 | - | - |
| U II | 294.191 | 190 ^b | - | 0.69 | 4.90 | $5f^36d7s$ | ${}^6\text{K}$ | 13/2 | | | 15/2 | - | - |
| U II | 268.328 | 392 ^b | - | 1.03 | 5.65 | $5f^36d7s$ | ${}^4\text{I}$ | 13/2 | | | 13/2 | - | - |
| V II | 290.881 | 177 | 10 | 0.39 | 4.65 | $3d^3(^4\text{F})4s$ | $a\ {}^5\text{F}$ | 5 | $3d^3(^4\text{F})4p$ | $z\ {}^5\text{D}^\circ$ | 4 | - | - |
| V II | 311.071 | 158 | 10 | 0.35 | 4.33 | $3d^3(^4\text{F})4s$ | $a\ {}^5\text{F}$ | 3 | $3d^3(^4\text{F})4p$ | $z\ {}^5\text{G}^\circ$ | 4 | 10 | 0.0 |
| W I | 289.644 | 130 | 40 | 0.37 | 4.65 | $5d^5(^6\text{S})6s$ | ${}^7\text{S}$ | 3 | | ${}^\circ$ | 2 | - | - |
| W I | 294.698 | 82.0 | 15 | 0.37 | 4.57 | $5d^5(^6\text{S})6s$ | ${}^7\text{S}$ | 3 | | ${}^\circ$ | 3 | - | - |
| W I | 272.435 | 105 | 15 | 0.37 | 4.92 | $5d^5(^6\text{S})6s$ | ${}^7\text{S}$ | 3 | | ${}^\circ$ | 3 | - | - |
| Y II | 324.227 | 203 | 10 | 0.18 | 4.00 | $4d5s$ | $a\ {}^3\text{D}$ | 3 | $4d5p$ | $y\ {}^3\text{P}^\circ$ | 2 | 8.0 | 0.0 |
| Y II | 360.073 | 138 | 10 | 0.18 | 3.62 | $4d5s$ | $a\ {}^3\text{D}$ | 3 | $4d5p$ | $z\ {}^3\text{D}^\circ$ | 3 | 7.0 | 0.0 |
| Yb II | 328.936 | 162 | - | 0.00 | 3.77 | $4f^{14}6s$ | ${}^2\text{S}$ | 1/2 | $4f^{14}6p$ | ${}^2\text{P}^\circ$ | 3/2 | - | - |
| Yb II | 369.419 | 123 | - | 0.00 | 3.36 | $4f^{14}6s$ | ${}^2\text{S}$ | 1/2 | $4f^{14}6p$ | ${}^2\text{P}^\circ$ | 1/2 | - | - |
| Zn I | 213.857 | 714 | 7 | 0.00 | 5.80 | $3d^{10}4s^2$ | ${}^1\text{S}$ | 0 | $3d^{10}4s4p$ | ${}^1\text{P}^\circ$ | 1 | 2.0 | 0.0 |
| Zn I | 334.501 | 170 | 15 | 4.08 | 7.78 | $3d^{10}4s4p$ | ${}^3\text{P}^\circ$ | 2 | $3d^{10}4s4d$ | ${}^3\text{D}$ | 3 | 96 | -11 |
| Zn I | 481.053 | 70.0 ^b | - | 4.08 | 6.65 | $3d^{10}4s4p$ | ${}^3\text{P}^\circ$ | 2 | $3d^{10}4s5s$ | ${}^3\text{S}$ | 1 | 64 | 38 |
| Zr II | 339.198 | 140 ^b | - | 0.16 | 3.82 | $4d^2(^3\text{F})5s$ | $a\ {}^4\text{F}$ | 9/2 | $4d^2(^3\text{F})5p$ | $z\ {}^4\text{G}^\circ$ | 11/2 | 12 | 1.0 |
| Zr II | 343.822 | 115 ^b | - | 0.09 | 3.70 | $4d^2(^3\text{F})5s$ | $a\ {}^4\text{F}$ | 7/2 | $4d^2(^3\text{F})5p$ | $z\ {}^4\text{G}^\circ$ | 9/2 | 12 | 1.0 |

References

- [1] A. Taleb, C. Shen, D. Mory, K. Cieślik, S. Merk, M. R. Aziz, A. P. Caricato, C. Gerhard, F. Pelascini, J. Hermann, Echelle spectrometer calibration by means of laser plasma, *Spectrochim. Acta Part B: Atom. Spectrosc.* 178 (2021) 106144 1–13.
- [2] E. Axente, J. Hermann, G. Socol, L. Mercadier, S. A. Beldjilali, M. Cirisan, C. R. Luculescu, C. Ristoscu, I. N. Mihailescu, V. Craciun, Accurate analysis of indium-zinc oxide thin films via laser-induced breakdown spectroscopy based on plasma modeling, *J. Anal. At. Spectrom.* 29 (2014) 553–564.
- [3] C. Gerhard, J. Hermann, L. Mercadier, L. Loewenthal, E. Axente, C. R. Luculescu, T. Sarnet, M. Sentis, W. Viöl, Quantitative analyses of glass via laser-induced breakdown spectroscopy in argon, *Spectrochim. Acta Part B: Atom. Spectrosc.* 101 (2014) 32–45.
- [4] M. Boudhib, J. Hermann, C. Dutouquet, Compositional analysis of aerosols using calibration-free laser-induced breakdown spectroscopy, *Anal. Chem.* 88 (2016) 4029–4035.
- [5] J. Hermann, E. Axente, F. Pelascini, V. Craciun, Analysis of multi-elemental thin films via calibration-free laser-induced breakdown spectroscopy, *Anal. Chem.* 91 (2019) 2544–2550.
- [6] C. Gerhard, A. Taleb, F. Pelascini, J. Hermann, Quantification of surface contamination on optical glass via sensitivity-improved calibration-free laser-induced breakdown spectroscopy, *Appl. Surf. Sci.* 537 (2021) 147984 1–7.
- [7] J. Hermann, C. Gerhard, M. Burger, V. Craciun, F. Pelascini, Progress in calibration-free laser-induced breakdown spectroscopy, *Spectrochim. Acta Part B: Atom. Spectrosc.* 200 (2023) 106595 1–12.
- [8] J.-C. Leblanc, Etude de l'alimentation totale française : Mycotoxines, minéraux, et éléments de trace, Tech. rep., Institut National de la Recherche Agronomique (2004).
URL http://www.nord-nature.org/info_veille/2004/200409062.pdf
- [9] European Comission, Commission regulation (ec) no 1881/2006 of 19 december 2006, Tech. rep., European Union, <https://faolex.fao.org/docs/pdf/eur68134.pdf> (2006).
- [10] Turkish Food Codex, Contaminants Regulation. No:28157/26 December 2011, Tech. rep., Turkish Government, <https://www.resmigazete.gov.tr/eskiler/2011/12/20111229M3-8-1.pdf> (2011).
- [11] A. Kramida, Y. Ralchenko, J. Reader, NIST Atomic Spectra Database (version 5.10), National Institute of Standards and Technology, Gaithersburg, MD (2022).
URL <http://physics.nist.gov/PhysRefData/ASD/>
- [12] P. L. Smith, C. Heise, J. R. Esmond, R. L. Kurucz, Atomic spectral line database built from atomic data files from R. L. Kurucz CD-ROM 23 (2011).
URL www.pmp.uni-hannover.de/cgi-bin/ssi/test/_kurucz/sekur.html
- [13] P. Quinet, G. Sicorello, Newly identified energy levels and calculated transition rates in astatine atom, the rarest element on earth, *J. Quant. Spectrosc. Radiat. Transf.* 204 (2018) 120–130.
- [14] V. Fivet, P. Quinet, E. Biémont, A. Jorissen, A. V. Yushchenko, S. V. Eck, Transition probabilities in singly ionized promethium and the identification of Pm II lines in Przybylski's star and HR 465, *Mon. Not. R. Astr. Soc.* 380 (2007) 771–780.
- [15] P. Quinet, Investigation of intravalance, core-valence and core-core electron correlation effects in polonium atomic structure calculations, *J. Quant. Spectrosc. Radiat. Transf.* 145 (2014) 153–159.