NWA 8114 Data Reduction

These notes refer to reduction of xenon isotope data for NWA 8114 samples.

Data are reduced following the steps listed below. Data are reduced in the spreadsheets listed below, and those spreadsheet are available on Figshare, doi: 10.48420/14229269.

Three samples of NWA 8114 were analysed:

- NWA8114_6a_1, mass 2.56 mg,
- NWA8114_6a_2, mass 1.52 mg,
- NWA8114_113, mass 1.33 mg.

Samples were analysed in a single campaign, between 24/02/2014 and 24/03/2014.

All files are in nq15 directories.

A sample for a different meteorite was loaded in the mass spectrometer laser port alongside these samples, and was analysed at the same time. Data for that sample are not included in any of this work, i.e. files nq15_1\File1129 to nq15_1\File1149. The corresponding air calibrations (air cals) and blanks are incorporated into calculations to allow more precise calculations of average values over the entire period of analysis.

Samples were heated using a CW Nd:YAG laser (λ = 1064 nm).

All files for Air Cals, Blanks and Samples were reduced by SAC using **PulsespecXenon_14.xls**.

Data are reduced in the spreadsheet **NWA8114_Xe_Final.xlsm**. Raw data are listed in worksheets labelled with the appropriate directory names. The calculations for air cals, blanks and each individual samples are set out on separate worksheets labelled accordingly.

Initially any air cals and blanks noted in lab book as having problems were excluded – e.g. low air cals because mass spec not tuned up properly, problems with triggering, blanks noted as high or as having high 128 hydrocarbon peak, leaks, build up tests, etc. On further examination of the data, some more air cals and blanks were excluded as outliers, often with high ^{128}Xe peaks due either to the 128 hydrocarbon, or having been run immediately after a sample had released a large amount of gas. The **FileSummary** worksheet lists all data files and indicates which were used and which were excluded, with reasons for excluding individual files.

The following sequence of steps was applied to the data set, with each step being applied to all isotopes and all analyses in that set.

1.1 The summed peak areas, from the first 5 summed spectra (first 50 s) were used in the following calculation.

1.2 From these peak areas, uncorrected ratios relative to ^{132}Xe were calculated for the air cals. The mean ratios of all the separate analyses was also calculated.

1.3 Air cals and blanks were (normally) acquired on the 5mV sensitivity scale, but sample analyses used a range of different scales according to how much gas was extracted from the samples. Therefore the peak areas of all analyses were multiplied by the respective sensitivity scale, so that all analyses could be directly compared regardless of the sensitivity scale used during acquisition.

1.4 The mean ^{132}Xe peak area (as the reference isotope) of the air cals was calculated.

1.5 The numbers of atoms of each isotope were calculated, assuming that an air cal contained 1.2×10^5 atoms ^{132}Xe and had the isotopic composition of atmospheric xenon.

1.5.1 The numbers of atoms in the air cals were calculated simply by multiplying the uncorrected ratios to ^{132}Xe by the number of ^{132}Xe atoms.

1.5.2 The numbers of atoms in blank and sample analyses were calculated by reference to the mean air cal, using the following equation for each isotope, *i*

$$Atoms\ of\ \ i = \frac{peak\ area\ of\ i}{air\ cal\ mean\ ^{132}Xe\ peak\ area} \times 1.2 \times 10^5$$

1.6 The mean number of atoms of each isotope was calculated for the blank analyses, along with the standard deviation of the mean.

1.7 Blank corrected numbers of atoms of each isotope were calculated for the air cals and samples, by subtracting the mean blank values calculated in Step 1.6 from the numbers of atoms calculated in Step 1.5.

1.8 Blank corrected ratios relative to ^{132}Xe were calculated for the air cals. The mean of all the separate analyses was also calculated for each isotope, along with the standard deviation and the standard error of the mean $\left(= standard\ deviation/\sqrt{number\ of\ analyses}\right)$. When the standard deviation of the mean is comparable to (or smaller than) the average error of the analyses contributing to the mean, the standard error can be used as the uncertainty of the mean ratios.

1.9 Delta values were calculated for the mean uncorrected and blank corrected ratios for each isotope *i* of the air cals, using

$$\delta_i = \left(\frac{\left(\frac{^{i}Xe}{^{132}Xe}\right)_{Measured}}{\left(\frac{^{i}Xe}{^{132}Xe}\right)_{Air}} - 1 \right) \times 1000$$

Comparison of the uncorrected and blank corrected ratios illustrated that the blank correction was necessary.

1.10 The ratio of "actual" air to the measured values was also calculated – this is used to apply a correction for instrument dependent mass fractionation to the sample analyses.

1.11 Air corrected numbers of atoms of each isotope were calculated for the samples, by multiplying the blank corrected numbers of atoms from Step 1.7 by the correction factor determined in Step 1.10.

1.12 Corrected ratios to ^{132}Xe were calculated for the sample analyses from the air corrected number of atoms. If ratios to other isotopes are required they should also be calculated at this point from the corrected numbers of atoms.

1.13 The calculations for each sample are in a separate worksheet labelled according to the sample names; the corrected ratios of all samples, and the numbers of atoms of each isotope, are summarised in the **NWA8114Summary** worksheet.

1.14 Xenon isotope data were then modelled using Samaritan[1] to test whether the measured isotope ratios can be accounted for by the components expected to be present in the samples, or whether unanticipated contributions are present.

[1] Gilmour, J.D. (2018) An irrational approach to isotopic analysis. Available online at https://doi.org/10.13140/RG.2.2.27449.01126.