

High-Precision Determination of Oxygen-K α Transition Energy Excludes Incongruent Motion of Interstellar Oxygen: Supplemental Material

I. EVALUATION OF THE BESSY II U49-2/PGM-1 ENERGY SCALE CALIBRATION STABILITY

We evaluate the stability of the energy scale calibration of BESSY II beamline U49-2/PGM-1 in four ways: we consider how stable the energy scale is from one scan point to the next during a single scan by examining jitter in the flux of the $1s - 3p$ transition of atomic Ne gas measured in the gas cell; we compare consecutive scans of $1s - np$ transitions in He-like ions; we compare non-consecutive scans of $1s - np$ transitions in He-like ions separated by an intervening scan of a different energy range; and we compare multiple scans of the O $_2$ Rydberg series to test the relative stability of the energy scale over single extended scans spanning ~ 2 eV.

A. Point-to-point jitter

We scanned the $1s - 3p$ transition of atomic Ne in the gas cell, and we fit it with a Voigt model added to a linear term to account for background from residual gases and other terms in the Ne absorption cross section, as shown in Figure 1. In the bottom panel we show the fractional residuals as a percentage of the model value. We also show the product of the derivative of the model multiplied by 1 meV; this corresponds to the amplitude of point-to-point flux variability that would be expected if there were a 1 meV jitter in the energy compared with the reported energy. The error bars on each point correspond to the uncertainties from counting statistics only. While there are non-negligible residuals, the shape of the residuals as a function of energy indicates that there is a small systematic error in the model of the peak shape. The scatter of the points in the energy range where the derivative is highest is consistent with an energy calibration jitter of no more than 1 meV. Note that other effects, such as intrinsic fluctuations in the source flux, could contribute to flux jitter, and the 1 meV energy calibration jitter is thus an upper limit.

B. Repeatability of consecutive scans

To evaluate the stability of the beamline energy scale on timescales of tens of minutes and when not moving the monochromator optics to very different positions, we compared consecutive scans of the same $1s - np$ lines in N $^{5+}$, O $^{6+}$, or O $^{5+}$. In Figure 2 we show the centroid shift of each measurement in the series relative to the first measurement as a function of the time lag after the first measurement. We find typical shifts of order ± 5 -

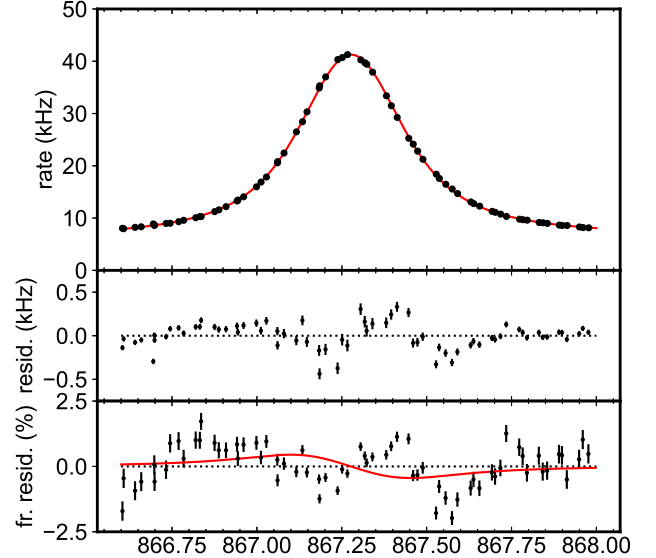


FIG. 1. $1s - 3p$ transition of atomic Ne in the gas cell, with the data and model shown in the top panel, the absolute residuals in the middle panel, and percent residuals shown in the bottom panel. Solid black circles with error bars represent the data. The solid red curve in the top panel shows the best-fit Voigt plus linear model. The solid red curve in the bottom panel is the derivative of the best-fit model times 1 meV, and corresponds to the flux jitter amplitude expected for an energy scale jitter of 1 meV.

10 meV, with a largest shift of -27 meV after 52 minutes.

C. Repeatability of non-consecutive scans

To test the effect of larger motions of the monochromator, we evaluated the energy shifts of many scans of the $1s - 5p$ transition of N $^{5+}$ and the $1s - 2p$ transition of O $^{6+}$ throughout our experimental campaign. We show these measurements in Figure 3. We express the measured line positions as an energy shift relative to the nominal energy of the beamline (right y-axes), and as an angular shift in the source, equivalent to a shift in the incident angle α on the grating relative to the nominal angle (left y-axis)[1]. These are reported as a function of time during the experiment campaign, and the points are grouped by whether a lower or higher energy scan precedes the measurement. We found that scans preceded by a higher energy tended to be offset to higher correction angles relative to those preceded by a lower energy. We speculate that this could be due to a hysteresis effect

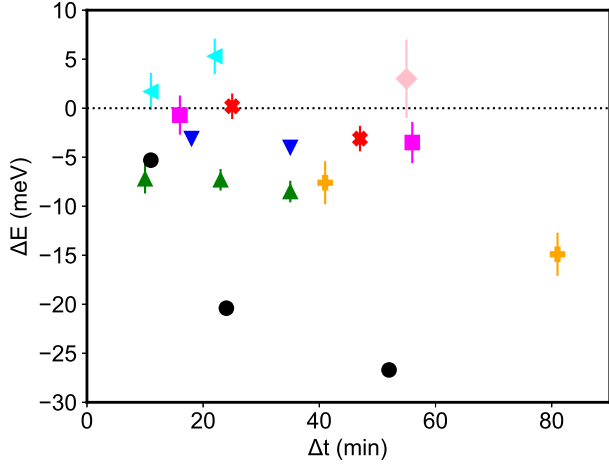


FIG. 2. Relative shifts of repeated consecutive centroid measurements of the same transition as a function of lag after the first measurement in the series. Different symbols refer to different transitions: black circles are $O^{6+} 1s - 2p$; magenta squares are $O^{5+} q(1s - 2p)$; red Xes are $O^{6+} 1s - 3p$; orange plus signs are $O^{6+} 1s - 4p$; pink diamonds are $O^{6+} 1s - 5p$; blue downward pointing triangles are $N^{5+} 1s - 2p$; green upward pointing triangles are $N^{5+} 1s - 3p$; and cyan left pointing triangles are $N^{5+} 1s - 4p$.

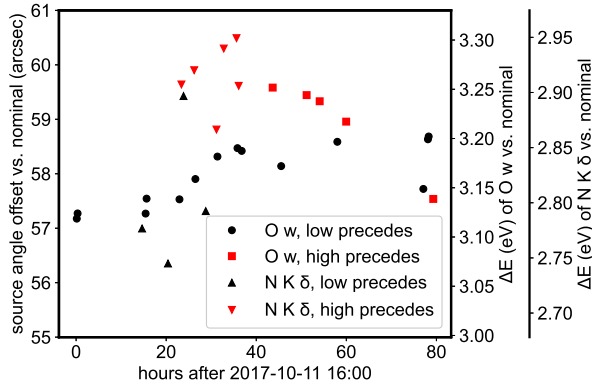


FIG. 3. Offset in angle relative to nominal (left y-axis) and offset in calibrated energy relative to nominal (right y-axes) for $N^{5+} 1s - 5p$ and $O^{6+} 1s - 2p$, shown as a function of time during the experiment campaign. (Note that the large offset of ~ 3 eV in the *nominal* energy scale is a known issue for this beamline, and that recalibrating against a known standard is routine.) The data points are also segregated into two groups depending on the state of the monochromator immediately preceding the measurement: “high precedes” refers to scans preceded by monochromator scans at a higher energy, while “low precedes” are preceded by monochromator scans at a lower energy.

in the motions of the monochromator, or that it could be due to a time-variable heatload effect in the monochromator optics. A more careful and systematic study would be required to distinguish between these possibilities.

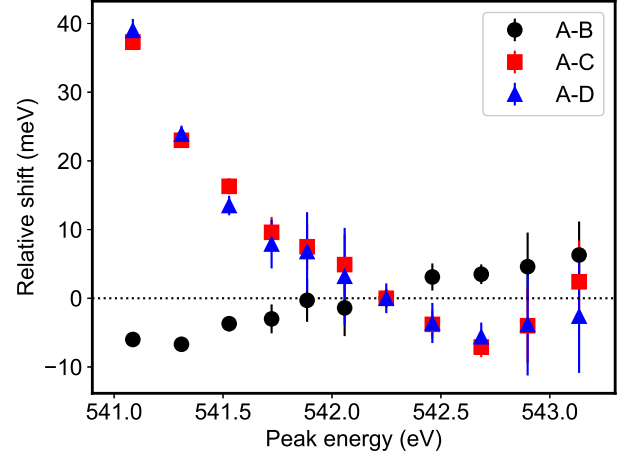


FIG. 4. Relative shift of lines in the O_2 Rydberg series for four scans (labeled A-D). All scans are calibrated to set peak s12 to 542.249 eV, the value derived in this work. Scans A and B were both preceded by scans at lower energies, while scans C and D were both preceded by scans at higher energies. We speculate that the pattern of relative shifts may be due to a differential thermal relaxation effect.

D. Drift during scans over a broad energy range

We tested the stability of the energy scale during scans over a broad energy range (~ 2 eV) by comparing repeated scans of the O_2 Rydberg series, labeled A-D in chronological order, as shown in Figure 4. Scans A and B were used together with the $1s - 7p$ line of N^{5+} to produce the absolute measurements of the Rydberg series reported in this article. During scans C and D the EBIT did not produce lines from N^{7+} because of an issue with the sample injection system, so we can only use scans C and D by calibrating them against scans A and B. We thus used peak s12 as a reference for all four scans, and assessed the drift by comparing the relative shifts of the other peaks in the Rydberg series.

We found that scans A and B agree quite well over the whole Rydberg series, with no shifts larger than ± 10 meV. On the other hand, scans C and D have a larger offset of almost 40 meV at the beginning of the scan (near 541 eV). Scans C and D were immediately preceded by scans at higher energies, while scans A and B were immediately preceded by scans at lower energies. Given the results of Section IC, we speculate that the same thermal or hysteresis effect is present here, and that the effect gradually relaxes over the course of the scan.

E. Conclusions regarding energy scale stability

Based on the measurements shown in Sections IA-ID, we reach the following conclusions: first, large energy shifts of $\sim$ tens of meV are usually associated with large relative motions of the monochromator energy from scan

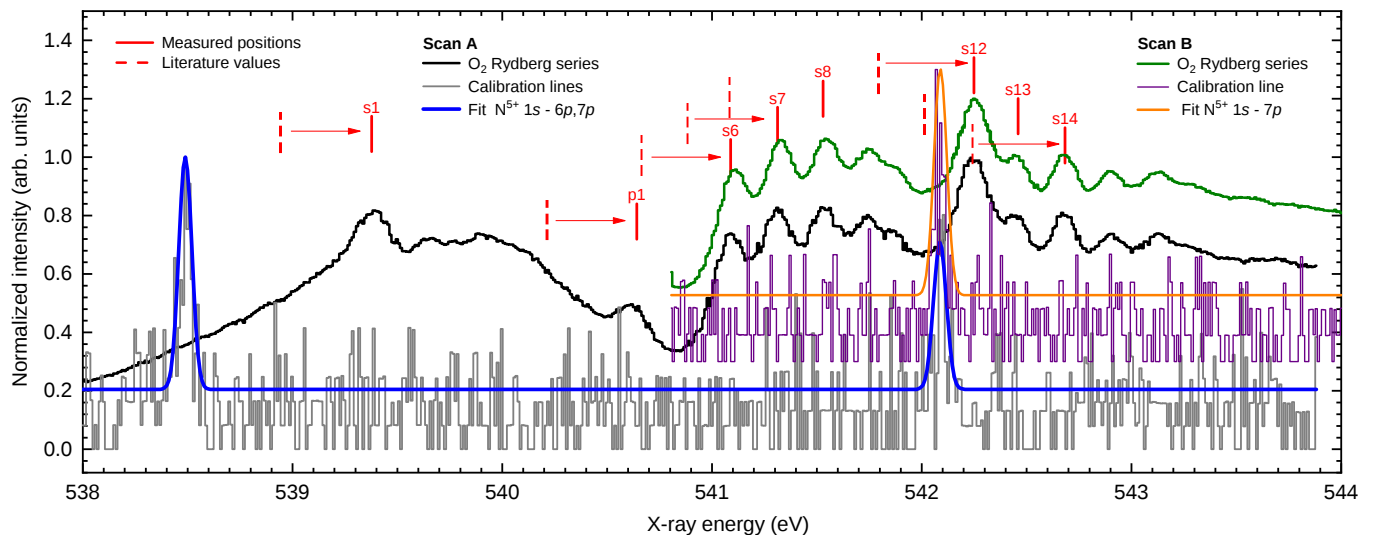


FIG. 5. O_2 Rydberg series, showing energy range where two calibration scans were performed.

to scan; second, shifts or distortions during a scan are typically not large, with possible shifts up to 40 meV per eV, which may however be associated with differences in the state of the monochromator in the preceding measurement. We therefore assign a systematic uncertainty to each peak in the Rydberg spectrum of O_2 of 40 meV per eV of shift relative to the closest calibration line of N^{6+} .

II. COMPARISON OF O_2 RYDBERG SERIES SCAN DATA

For clarity, Figure 3 of the main article shows only the Rydberg series data from scan A. In Figure 5 we show both scans A and B over the energy range where they overlap.

The two scans were aligned using peak s12, and the $1s - 7p$ transition of N^{5+} was fit jointly for the two data sets, fixing the absolute energy scale calibration. We used this technique instead of calibrating each scan on its own best fit value of $N^{5+} 1s - 7p$ because of the relatively smaller statistical uncertainty on centroid positions in the O_2 Rydberg series.

[1] Note that at a single energy point a shift in energy can be expressed equally well as a shift in source position, exit slit position, or a combination of the two. We have chosen

in Figure 3 to follow the convention of a pure source angle displacement.