Supporting Information for:

Electronic structure studies reveal 4f/5d mixing and its effect on bonding characteristics in Ce-imido and -oxo complexes

Liane M. Moreau,Ekaterina Lapsheva,Jorge I. Amaro-Estrada,Michael R. Gau,Patrick J. Carroll,Brian C. Manor,Yusen Qiao,Qiaomu Yang,Wayne W. Lukens,Dimosthenis Sokaras,Eric J. Schelter,Laurent Maron, and Corwin H. Booth

1 Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States
2 Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104, United States
3 LPCNO, UMR 5215, CNRS, INSA, UPS, Université de Toulouse, 31000 Toulouse, France
4 Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, United States

Table of Contents:

Figure S1. Monomeric unit of (2-Cs)$_4$.................................................................S3

Synthetic details and characterization........................................................................S4

Data for (2-K)$_4$ ........................................................................................................S4

Figure S2. $^1$H NMR spectrum for (2-K)$_4$............................................................S4
Figure S3. $^{13}$C NMR spectrum for (2-K)$_4$............................................................S4
Figure S4. UV-Vis spectrum for (2-K)$_4$..................................................................S5
Figure S5. IR spectrum for (2-K)$_4$........................................................................S5
Figure S6. Cyclic voltammogram for (2-K)$_4$..........................................................S6

Data for (2-Cs)$_4$ ........................................................................................................S7

Figure S7. $^1$H NMR spectrum for (2-Cs)$_4$ .............................................................S7
Figure S8. $^{13}$C NMR spectrum for (2-Cs)$_4$.............................................................S8
Figure S9. UV-Vis spectrum for (2-Cs)$_4$.................................................................S8
Figure S10. IR spectrum for (2-Cs)$_4$........................................................................S9
Figure S11. Cyclic voltammogram for (2-Cs)$_4$.........................................................S9

Further details of XANES methods and results ......................................................S10

XANES sample holder integrity ..............................................................................S10
Figure S12. Standard XANES spectra ................................................................. S10

Temperature-dependent XANES spectra .......................................................... S11

Figure S13. L_{III} edge XANES spectra at varying temperatures ....................... S11

Figure S14. HERFD spectra of (2-Cs)_4 at varying temperatures ....................... S12

XANES fitting methods .................................................................................... S12

Results from XANES fitting used to determine n(f^0) ........................................ S13

Figure S15a-e. Fits of XANES data ................................................................. S14-S18

Table S1. XANES fitting parameter results ...................................................... S18

XANES fitting using a 3-peak vs. 2-peak model .............................................. S19

Figure S16. Simulation of (2-K)_4 using 3-peak model vs. 2-peak model ............ S19

Table S2. f^{1,2} and f^0 peak energies from XANES data .................................... S20

Raw XANES and HERFD data ........................................................................... S20

Table S3. Anilide XANES ................................................................................ S20

Table S4. Imido XANES (1-Li, 1-K, and 1-Rb) .................................................. S24

Table S5. Imido XANES (1-Cs and 1') ............................................................. S28

Table S6. Oxo XANES .................................................................................... S37

Table S7. Anilide HERFD ............................................................................... S45

Table S8. Imido HERFD ............................................................................... S52

Table S9. Oxo HERFD ................................................................................... S60

Additional HERFD and FDMNES results ......................................................... S69

Figure S17. 1-H HERFD spectrum ................................................................. S69

Figure S18. 1-H FDMNES simulation and LDOS ............................................. S69

Figure S19. 1' HERFD spectrum ................................................................. S70

Figure S20. 1' FDMNES simulation and LDOS .............................................. S70

Further details of magnetism results ............................................................... S71

Figure S21a-i. Magnetic susceptibility curves and fitting ............................... S72-S80

Evans method analysis .................................................................................. S81

Further details of computational results ......................................................... S81
Figure S22. Restricted open-shell Hartree-Fock molecular orbitals for (CAS)..........................S81-S82

Cartesian coordinates of all optimized structures .................................................................S83-S95

References ..........................................................................................................................S96

Figure S1. A fragment of (2-Cs)$_4$ structure showing the monomeric [Ce(TriNOx)═O]$^-$ unit. Thermal ellipsoids are shown at 30% probability. Hydrogen atoms have been omitted for clarity. Tert-butyl groups are depicted using the wireframe model.
Synthetic details and characterization

*Data for (2-K)₄*

Figure S2. ¹H NMR spectrum for (2-K)₄ in THF-ᵈ8. * - proteo solvent peaks.

Figure S3. ¹³C NMR spectrum for (2-K)₄ in THF-ᵈ8. * - solvent peaks.
Figure S4. UV-Vis spectrum for (2-K)₄ (in THF). $\lambda_{\text{max}} = 299 \text{ nm}, 380 \text{ nm}$.

Figure S5. IR spectrum for (2-K)₄.
Figure S6. Full scan cyclic voltammogram for (2-K)$_4$ in THF, red trace. Scan rate = 100 mV/s, supporting electrolyte [aPr$_4$N][BArF$_{24}$] (0.1 M). Solvent background, black trace. Experimental details can be found in the main text.
**Data for (2-Cs)$_4$**

![NMR Spectrum](image)

**Figure S7.** $^1$H NMR spectrum for (2-Cs)$_4$ in THF-$d_8$. * - proteo solvent peaks.
**Figure S8.** $^{13}$C NMR spectrum for (2-Cs)$_4$ in THF-$d_8$. * - solvent peaks. # - solvent impurity peaks.

**Figure S9.** UV-Vis spectrum for (2-Cs)$_4$ (in THF). $\lambda_{\text{max}} = 298$ nm, 379 nm.
Figure S10. IR spectrum for $\text{(2-Cs)}_4$.

Figure S11. Full scan cyclic voltammogram for $\text{(2-Cs)}_4$ in THF, red trace. Scan rate = 100 mV/s, supporting electrolyte $[^7\text{Pr}_4\text{N}][\text{BArF}_{24}]$ (0.1 M). Solvent background, black trace. Experimental details can be found in the main text.
Further details of XANES Methods and Results

XANES Sample Holder Integrity

Figure S12. Standard XANES spectra. CeCp^{tet}_3 (Ce(III)) and CeO_{2} (Ce(IV)) standards are shown to demonstrate the features expected for formal Ce(III) vs. formal Ce(IV) compounds. CeCp^{tet}_3 shows the typical single peak characteristic of Ce(III) and CeO_{2} shows the double-peak signature characteristic of Ce(IV). CeCp^{tet}_3 was used as a canary sample, to ensure that the samples were not compromised by air or water before or during measurement. Namely, if it began to show a second peak characteristic of formal Ce(IV), the data was discarded.
Temperature-dependent XANES spectra

From the plots below in Figures S9 and S10, no temperature dependence in the XANES or HERFD spectra was observed, suggesting no changes in electronic structure of the Ce TriNOx complexes as a function of temperature. XANES data were available for all samples except for (2-Cs)$_4$, so the HERFD data are instead displayed here.

Figure S13. L$_{III}$ edge XANES spectra of TriNO$_x$ complexes at varying temperatures. None of the complexes exhibit temperature dependent spectral differences at 50 K (dotted lines) versus 300 K (solid lines in 1-H, 1-Li, 1-Rb, 1, (2-K)$_4$, and (2-Rb)$_4$) or 200 K (solid lines in 1-K and 1-Cs).
Figure S14. HERFD spectra of \((2-\text{Cs})_4\) show no temperature-dependent differences between 50 K and 200 K. HERFD data were shown instead of XANES, as temperature-dependent XANES data on this sample was not collected.

XANES fitting methods

XANES data were fit in order to extract \(n(f^0)\) according to previously described methods.\textsuperscript{1-3} The fits consisted of a sum of a step-like function to model the absorption edge and two Gaussians to fit peaks associated with \(f^{1,2}\) and \(f^0\) configurations, in addition to a third Gaussian fit to a shoulder in the EXAFS region. The step-like function (integrated Gaussian) models excitations into the continuum whose position is given by a weighted average of the \(f^{1,2}\) and \(f^0\) peak energies, rather than using two step-like functions, in order to reduce the number of parameters in the fit and to control correlations between the fit parameters. This edge step is defined according to the expression:

\[
I_{\text{edge}}(E) = \int_{-\infty}^{E} C_{\text{edge}} e^{-\frac{(E'-E_0)^2}{2\sigma^2}} dE',
\]

and the Gaussians defined according to the expression:

\[
I_i(E) = \frac{A_i}{\sqrt{2\pi} \sigma_i} e^{-\frac{(E-e_i)^2}{2\sigma_i^2}},
\]
where $E$ is the incident energy, $e_i$ is the peak energy, $\sigma_i$ is the half-width of the Gaussian and $I_i$ is the intensity of peak $i$. $E_0$ is constrained to be the average of the peak energies of $f^{1,2}$ and $f^0$ weighted by the area under each associated Gaussian, $A_i$. The Gaussian widths of the $f^{1,2}$ and $f^0$ peaks were held equal. The calculation of error bars for fitting parameters was achieved using a covariance matrix assuming normal distributions for variances in the data. Normally, the $f$-occupancy $n_f$ is calculated via:

$$n_f = \frac{A_{III}}{A_{III} + A_{IV}},$$

where $A_{III}$ and $A_{IV}$ are the areas for the so-called Ce(III) and Ce(IV) features in the spectra, as described below. However it is possible that any $f^2$ contribution will affect the area of the A(III) peak. This issue has been noted for Yb edges. To avoid this issue, we instead report here the $f^0$ contribution:

$$n(f^0) = \frac{A_{IV}}{A_{III} + A_{IV}}.$$

Error bars on calculated $n(f^0)$ values determined from the $f^{1,2}$ and $f^0$ peak areas are estimated to be about 0.03 normalized units. Parameters reported without error bars were held fixed or constrained during the fit.

**Results from XANES fitting used to determine $n(f^0)$**

The following figures and tables show representative results from XANES fitting. In some cases, more than one data set per sample was collected, in which case the numbers in Table 1 of the manuscript represent average $n(f^0)$ values, where the error bars encompass any variation from data set to data set, which was small. Note that the fit quality, especially for the (2-M)$_4$ samples, is not as high as has previously been reported in other formal Ce(IV) complexes. This is due to increased splitting of the 5d manifold. Despite this difference in the model, the $4f/5d$ feature was not used in determining $n(f^0)$, given the correlation with other parameters in the fitting procedure. A 3-peak fit was also attempted that uses a third peak fit to the $4f/5d$ feature and is shown in figure 10 and described below. We demonstrate, however, that the overall integrated intensity ratios between $f^{1,2}$ and $f^0$ are conserved regardless of using a 3 vs. 2-peak fitting model, and therefore the $n(f^0)$ results are deemed reliable to within the estimated errors. The pre-edge feature at ~5715 eV which is thought to arise from either 2p-4f quadrupole excitation or from mixed d- and f-states was not included in the fit due to its small contribution and high correlation with other parameters.
Figure S15a. Fit of XANES data for a) 1-H and b) 1-Li samples.
**Figure S15b.** Fit of XANES data for a) 1-K and b) 1-Rb samples.
Figure S15c. Fit of XANES data for a) 1-Cs and b) 1- samples.
Figure S15d. Fit of XANES data for a) (2-K)$_4$ and b) (2-Rb)$_4$ samples.
Figure S15e. Fit of XANES data for (2-Cs)$_4$ sample.

Table S1. Fit parameter results for $f^{1,2}$ and $f^0$ integrated peak areas. Error estimates are determined from the covariance matrix and data errors determined by assuming the fitted $\chi^2$ parameter equals the degrees of freedom in the fit.

| Sample   | $f^{1,2}$ peak area | $f^0$ peak area | $R(\%)$ from Fit |
|----------|---------------------|-----------------|------------------|
| 1-H      | 11.4(2)             | 9.3(2)          | 2.6              |
| 1-Li     | 10.2(2)             | 7.5(2)          | 2.4              |
| 1-K      | 11.6(3)             | 7.1(2)          | 2.7              |
| 1-Rb     | 11.7(2)             | 6.7(2)          | 3.0              |
| 1-Cs     | 10.6(3)             | 7.3(3)          | 3.6              |
| 1-        | 10.5(3)             | 6.1(3)          | 3.5              |
| (2-K)$_4$| 10.3(4)             | 7.1(4)          | 4.4              |
| (2-Rb)$_4$| 10.3(3)           | 6.8(3)          | 4.3              |
| (2-Cs)$_4$| 10.4(4)           | 7.3(3)          | 4.3              |
XANES fitting using a 3-peak vs. 2-peak model

In order to estimate the error introduced into the n(f₀) fits as a result of using a 2-peak model that cannot account for the “middle peak” which results from d-state broadening, a 3-peak simulation was used. Figure 10a shows a 3 peak simulation to the (2-K)₄ XANES spectrum. As with the 2-peak fits, an EXAFS shoulder at higher energy is also included. The position of the middle peak was fixed to the weighted average of the energies of the f¹,² and f⁰ peaks. The simulation appears to match the experimental spectrum well, with an n(f₀) value of 0.395. Through fitting the standard 2-peak model introduced earlier to this 3-peak simulation, the n(f₀) value from the fit could be compared to a “known” n(f₀) value from the simulation. The 2-peak model fit to the 3-peak simulation from Figure 10a is shown in Figure 10b. Interestingly, the n(f₀) result from the 2-peak fit was nearly identical to that from the 3-peak simulation 0.4(3). Therefore, the error bar reported for the n(f₀) values extracted from the 2-peak fits presented above should accurately encompass any error that would result from using a 2-peak vs. 3-peak model.

Figure S16. a) A simulation of (2-K)₄ using 3 peaks (f¹,², f⁰ and an additional middle peak (red)) with a known n(f₀) value of 0.395 matched well with the (2-K)₄ experimental XANES data in comparison to the 2-peak fits to the (2-M)₄ sample spectra. When the simulation was fit with a 2-
peak model (b) the resulting $n(f^0)$ value extracted was 0.4(3). Therefore, the 2-peak model was shown to still result in a representative value for $n(f^0)$ and legitimizes its use.

**Table S2.** $f^{1,2}$ and $f^0$ peak energies from XANES data

| Sample     | $f^{1,2}$ peak energy (eV) | $f^0$ peak energy (eV) |
|------------|---------------------------|------------------------|
| CeCp$^{3+}$ | 5724.6                    | N/A                    |
| CeO$_2$    | 5729.4                    | 5736.2                 |
| 1-H        | 5726.5                    | 5735.8                 |
| 1-Li       | 5726.1                    | 5735.7                 |
| 1-K        | 5725.7                    | 5735.7                 |
| 1-Rb       | 5725.0                    | 5735.2                 |
| 1-Cs       | 5725.2                    | 5736.0                 |
| 1           | 5725.7                    | 5735.4                 |
| (2-K)$_4$  | 5725.7                    | 5735.7                 |
| (2-Rb)$_4$ | 5725.8                    | 5735.9                 |
| (2-Cs)$_4$ | 5725.9                    | 5735.7                 |

**Raw XANES and HERFD data**

**Table S3.** Anilide XANES

| E(eV) | Normalized XANES |
|-------|------------------|
| 5553.5| 0.000481         |
| 5566.833| 0.002966        |
| 5576.833| 0.005604        |
| 5586.834| 0.007039        |
| 5596.833| 0.007           |
| 5606.833| 0.006929        |
| 5616.833| 0.006451        |
| 5626.834| 0.006129        |
| 5636.834| 0.004889        |
| 5646.835| 0.003433        |
| 5656.834| 0.000932        |
| 5666.833| -0.001792       |
| 5676.833| -0.001545       |
| 5686.833| 0.00028         |
| 5696.834| 0.003316        |
| 5703.617| 0.009956        |
| Value   | Probability |
|---------|-------------|
| 5703.964 | 0.011102    |
| 5704.311 | 0.010352    |
| 5704.659 | 0.010904    |
| 5705.007 | 0.012871    |
| 5705.355 | 0.013837    |
| 5705.704 | 0.014111    |
| 5706.052 | 0.015545    |
| 5706.399 | 0.01651     |
| 5706.746 | 0.018068    |
| 5707.094 | 0.018233    |
| 5707.443 | 0.019766    |
| 5707.791 | 0.020643    |
| 5708.137 | 0.021283    |
| 5708.486 | 0.022957    |
| 5708.834 | 0.025452    |
| 5709.181 | 0.026372    |
| 5709.529 | 0.027495    |
| 5709.877 | 0.029257    |
| 5710.225 | 0.031167    |
| 5710.572 | 0.032342    |
| 5710.919 | 0.035095    |
| 5711.268 | 0.037873    |
| 5711.615 | 0.040291    |
| 5711.963 | 0.042984    |
| 5712.311 | 0.046231    |
| 5712.659 | 0.050087    |
| 5713.007 | 0.053348    |
| 5713.355 | 0.058176    |
| 5713.703 | 0.062971    |
| 5714.052 | 0.067511    |
| 5714.398 | 0.073225    |
| 5714.746 | 0.07902     |
| 5715.095 | 0.087418    |
| 5715.441 | 0.09506     |
| 5715.79  | 0.10492     |
| 5716.138 | 0.11722     |
| 5716.485 | 0.131803    |
| 5716.833 | 0.147728    |
| 5717.181 | 0.168203    |
| 5717.53  | 0.188218    |
| 5717.877 | 0.210187    |
| 5718.224 | 0.228434    |
| 5718.571 | 0.242698    |
| Value  | Another Value |
|--------|---------------|
| 5718.92 | 0.256569      |
| 5719.269| 0.270628      |
| 5719.617| 0.28775       |
| 5719.964| 0.31018       |
| 5720.312| 0.340786      |
| 5720.659| 0.380806      |
| 5721.007| 0.431403      |
| 5721.355| 0.495774      |
| 5721.703| 0.574725      |
| 5722.051| 0.668475      |
| 5722.398| 0.776662      |
| 5722.747| 0.897776      |
| 5723.095| 1.022846      |
| 5723.443| 1.145683      |
| 5723.791| 1.262972      |
| 5724.139| 1.372017      |
| 5724.486| 1.475514      |
| 5724.833| 1.571992      |
| 5725.181| 1.65861       |
| 5725.529| 1.727437      |
| 5725.877| 1.773039      |
| 5726.225| 1.798312      |
| 5726.572| 1.804183      |
| 5726.92 | 1.796729      |
| 5727.269| 1.781707      |
| 5727.617| 1.765805      |
| 5727.963| 1.750555      |
| 5728.312| 1.734741      |
| 5728.66 | 1.720109      |
| 5729.007| 1.708143      |
| 5729.355| 1.69787       |
| 5729.702| 1.687599      |
| 5730.051| 1.67686       |
| 5730.399| 1.666961      |
| 5730.746| 1.65865       |
| 5731.095| 1.651292      |
| 5731.442| 1.647412      |
| 5731.791| 1.646258      |
| 5732.138| 1.650859      |
| 5732.486| 1.660676      |
| 5732.833| 1.676766      |
| 5733.181| 1.700457      |
| 5733.529| 1.728757      |
|     |       |
|-----|-------|
| 5733.877 | 1.760414 |
| 5734.226 | 1.794063 |
| 5734.572 | 1.826808 |
| 5734.92 | 1.852781 |
| 5735.269 | 1.869534 |
| 5735.616 | 1.877196 |
| 5735.964 | 1.875827 |
| 5736.313 | 1.861838 |
| 5736.66 | 1.832887 |
| 5737.007 | 1.789297 |
| 5737.354 | 1.730023 |
| 5737.703 | 1.659579 |
| 5738.052 | 1.58366 |
| 5738.399 | 1.50933 |
| 5738.747 | 1.437427 |
| 5739.094 | 1.37487 |
| 5739.441 | 1.318939 |
| 5739.789 | 1.272277 |
| 5740.137 | 1.232819 |
| 5740.484 | 1.199632 |
| 5740.832 | 1.172625 |
| 5741.18 | 1.150441 |
| 5741.528 | 1.131442 |
| 5741.875 | 1.115151 |
| 5742.224 | 1.101622 |
| 5742.572 | 1.088529 |
| 5742.92 | 1.077195 |
| 5743.268 | 1.066392 |
| 5743.787 | 1.05265 |
| 5744.958 | 1.023991 |
| 5746.771 | 0.989744 |
| 5748.658 | 0.971235 |
| 5750.62 | 0.966871 |
| 5752.655 | 0.972926 |
| 5754.764 | 0.987667 |
| 5756.945 | 1.00882 |
| 5759.2 | 1.029886 |
| 5761.528 | 1.045707 |
| 5763.931 | 1.060137 |
| 5766.406 | 1.072855 |
| 5768.957 | 1.081318 |
| 5771.581 | 1.086399 |
| 5774.277 | 1.084931 |
| E(eV) | Normalized XANES | E(eV) | Normalized XANES | E(eV) | Normalized XANES |
|-------|-----------------|-------|-----------------|-------|-----------------|
| 5553.40049 | -5.34E-02 | 5553.4005 | 1.59E-02 | 5552.5005 | -0.06784484 |
| 5566.73252 | -4.96E-02 | 5566.7325 | 1.11E-02 | 5565.8325 | -0.04607055 |
| 5576.73301 | -4.91E-02 | 5576.733 | 7.61E-03 | 5575.833 | -0.02800729 |
| 5586.7335 | -3.81E-02 | 5586.7335 | 5.14E-03 | 5585.8335 | -0.01482073 |
| 5596.73252 | -3.03E-02 | 5596.7325 | 3.95E-03 | 5595.8325 | -0.00751829 |
| 5606.73252 | -2.67E-02 | 5606.7325 | -3.64E-05 | 5605.8325 | -0.00329756 |
| 5616.73301 | -2.27E-02 | 5616.733 | -5.54E-03 | 5615.833 | 0.001737218 |
| 5626.73398 | -8.08E-03 | 5626.734 | 1.79E-03 | 5625.834 | 0.001650672 |
| 5636.73398 | 1.17E-03 | 5636.734 | 2.48E-03 | 5635.834 | 0.003519306 |
| 5646.73496 | 2.94E-03 | 5646.735 | 2.93E-03 | 5645.835 | 0.001773595 |
| 5656.73447 | -6.36E-04 | 5656.7345 | -8.60E-04 | 5655.8345 | 0.001068324 |

**Table S4.** Imido XANES (1-Li, 1-K, and 1-Rb)
| 5666.73301 | 8.79E-04 | 5666.733 | -7.49E-04 | 5665.833 | 0.000144824 |
| 5676.73301 | 5.27E-05 | 5676.733 | -1.95E-03 | 5675.833 | -0.00258339 |
| 5686.73301 | -1.21E-03 | 5686.733 | -1.07E-03 | 5685.833 | -0.00210925 |
| 5696.73398 | 9.62E-04 | 5696.734 | 4.17E-03 | 5695.834 | 0.002397203 |
| 5703.51719 | 8.01E-04 | 5703.517 | 9.74E-03 | 5702.617 | 0.009599048 |
| 5703.86436 | 2.42E-03 | 5703.864 | 8.67E-03 | 5702.964 | 0.0010533163 |
| 5704.21055 | 4.97E-03 | 5704.210 | 9.66E-03 | 5703.310 | 0.0010493236 |
| 5704.55869 | 4.59E-03 | 5704.558 | 1.27E-02 | 5703.658 | 0.010897409 |
| 5704.90684 | 7.61E-04 | 5704.907 | 1.29E-02 | 5704.007 | 0.01233446 |
| 5705.25498 | 3.82E-03 | 5705.255 | 1.24E-02 | 5704.355 | 0.012625537 |
| 5705.60361 | 6.69E-03 | 5705.603 | 1.26E-02 | 5704.703 | 0.013335417 |
| 5705.95176 | 6.67E-03 | 5705.951 | 1.10E-02 | 5705.051 | 0.014874729 |
| 5706.29941 | 6.47E-03 | 5706.299 | 1.16E-02 | 5705.399 | 0.016908407 |
| 5706.64561 | 7.65E-03 | 5706.646 | 1.46E-02 | 5705.746 | 0.015821073 |
| 5706.99424 | 1.16E-02 | 5706.994 | 2.04E-02 | 5706.094 | 0.015282807 |
| 5707.34287 | 1.28E-02 | 5707.343 | 1.87E-02 | 5706.443 | 0.015645305 |
| 5707.69053 | 1.13E-02 | 5707.690 | 1.79E-02 | 5706.790 | 0.017109644 |
| 5708.03721 | 1.32E-02 | 5708.037 | 2.13E-02 | 5707.137 | 0.018950167 |
| 5708.38584 | 1.46E-02 | 5708.386 | 2.21E-02 | 5707.486 | 0.021117362 |
| 5708.7335 | 1.67E-02 | 5708.733 | 2.55E-02 | 5707.833 | 0.024025889 |
| 5709.08066 | 1.81E-02 | 5709.081 | 2.86E-02 | 5708.181 | 0.023742725 |
| 5709.4293 | 2.03E-02 | 5709.429 | 3.02E-02 | 5708.529 | 0.025471943 |
| 5709.77744 | 2.11E-02 | 5709.777 | 3.11E-02 | 5708.877 | 0.027865789 |
| 5710.12461 | 2.24E-02 | 5710.125 | 3.32E-02 | 5709.224 | 0.030027706 |
| 5710.47227 | 2.46E-02 | 5710.472 | 3.48E-02 | 5709.572 | 0.031827123 |
| 5710.81943 | 2.66E-02 | 5710.819 | 3.70E-02 | 5709.919 | 0.033903461 |
| 5711.16807 | 2.87E-02 | 5711.168 | 4.19E-02 | 5710.268 | 0.03566014 |
| 5711.51523 | 3.29E-02 | 5711.515 | 4.55E-02 | 5710.615 | 0.038179196 |
| 5711.86338 | 3.74E-02 | 5711.863 | 4.56E-02 | 5710.963 | 0.040484586 |
| 5712.21104 | 3.83E-02 | 5712.211 | 5.20E-02 | 5711.311 | 0.043209022 |
| 5712.55918 | 4.16E-02 | 5712.559 | 5.75E-02 | 5711.659 | 0.046016885 |
| 5712.90684 | 4.58E-02 | 5712.906 | 6.19E-02 | 5712.006 | 0.049411983 |
| 5713.25547 | 4.90E-02 | 5713.255 | 6.39E-02 | 5712.355 | 0.053570552 |
| 5713.60312 | 5.71E-02 | 5713.603 | 6.90E-02 | 5712.703 | 0.05814318 |
| 5713.95176 | 6.50E-02 | 5713.951 | 7.43E-02 | 5713.051 | 0.062734261 |
| 5714.29844 | 7.02E-02 | 5714.298 | 8.18E-02 | 5713.398 | 0.067103288 |
| 5714.64609 | 7.62E-02 | 5714.646 | 9.25E-02 | 5713.746 | 0.073176169 |
| 5714.99473 | 8.49E-02 | 5714.995 | 1.01E-01 | 5714.094 | 0.079197078 |
| 5715.34141 | 9.45E-02 | 5715.341 | 1.09E-01 | 5714.441 | 0.085935403 |
| 5715.68955 | 0.1067537 | 5715.689 | 1.22E-01 | 5714.789 | 0.095101873 |
| 5716.03818 | 0.1190924 | 5716.038 | 1.35E-01 | 5715.138 | 0.104395747 |
| 5716.38535 | 0.1341301 | 5716.385 | 1.52E-01 | 5715.485 | 0.116598877 |
| 5716.73252 | 0.1541431 | 5716.732 | 1.71E-01 | 5715.832 | 0.128940019 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|5717.08066|0.1793683|5717.0807|1.94E-01|5716.1807|0.142930258|
|5717.42979|0.2005443|5717.4298|2.18E-01|5716.5298|0.160206827|
|5717.77695|0.2228482|5717.777|2.41E-01|5716.877|0.17958385|
|5718.12412|0.2508308|5718.1241|2.66E-01|5717.2241|0.200603618|
|5718.47129|0.2723683|5718.4713|2.93E-01|5717.5713|0.223119435|
|5718.81992|0.2905191|5718.8199|3.17E-01|5717.9199|0.247587751|
|5719.16904|0.309051|5719.169|3.38E-01|5718.269|0.27091598|
|5719.5167|0.3272207|5719.5167|3.68E-01|5718.6167|0.292495028|
|5719.86436|0.3501892|5719.8644|4.03E-01|5718.9644|0.314692557|
|5720.21152|0.3811402|5720.2115|4.42E-01|5719.3115|0.340917734|
|5720.55918|0.4265558|5720.5592|4.96E-01|5719.6592|0.3748292|
|5720.90732|0.4785726|5720.9073|5.66E-01|5720.0073|0.412588905|
|5721.25498|0.5421402|5721.255|6.48E-01|5720.355|0.461579507|
|5721.60264|0.6244491|5721.6026|7.45E-01|5720.7026|0.524590557|
|5721.95078|0.7164172|5721.9508|8.50E-01|5721.0508|0.599230853|
|5722.29844|0.8175204|5722.2984|9.61E-01|5721.3984|0.685766447|
|5722.6458|0.9337112|5722.6466|1.08E+00|5721.7466|0.787800875|
|5722.99473|1.051497|5722.9947|1.21E+00|5722.0947|0.895812457|
|5723.34287|1.1641839|5723.3429|1.34E+00|5722.4429|1.011448018|
|5723.69102|1.2698321|5723.691|1.46E+00|5722.791|1.135332264|
|5724.03916|1.365004|5724.0392|1.56E+00|5723.1392|1.2576722|
|5724.38633|1.4434252|5724.3863|1.65E+00|5723.4863|1.367462655|
|5724.7325|1.5092675|5724.7325|1.71E+00|5723.8325|1.465307255|
|5725.08066|1.5608332|5725.0807|1.75E+00|5724.1807|1.544490291|
|5725.4293|1.598173|5725.4293|1.77E+00|5724.5293|1.603626227|
|5725.77744|1.6201855|5725.7774|1.78E+00|5724.8774|1.641510945|
|5726.1251|1.6271222|5726.1251|1.76E+00|5725.2251|1.661825936|
|5726.47178|1.6252412|5726.4718|1.74E+00|5725.5718|1.667103445|
|5726.82041|1.6182307|5726.8204|1.72E+00|5725.9204|1.658356409|
|5727.16904|1.6136583|5727.169|1.69E+00|5726.269|1.639585491|
|5727.5167|1.6043952|5727.5167|1.66E+00|5726.6167|1.6173418|
|5727.86338|1.5941909|5727.8634|1.64E+00|5726.9634|1.5927745|
|5728.21201|1.5868623|5728.212|1.61E+00|5727.312|1.568079864|
|5728.56016|1.5750226|5728.5602|1.59E+00|5727.6602|1.546464509|
|5728.90684|1.5678893|5728.9068|1.58E+00|5728.0068|1.526462927|
|5729.25498|1.5567477|5729.255|1.56E+00|5728.355|1.506218473|
|5729.60215|1.552158|5729.6022|1.54E+00|5728.7022|1.488730145|
|5729.95078|1.5461416|5729.9508|1.53E+00|5729.0508|1.472476291|
|5730.29893|1.5353957|5730.2989|1.52E+00|5729.3989|1.454215155|
|5730.64609|1.5261346|5730.6461|1.51E+00|5729.7461|1.437455955|
|5730.99473|1.5196094|5730.9947|1.50E+00|5730.0947|1.423360109|
|5731.34189|1.5149781|5731.3419|1.49E+00|5730.4419|1.407603355|
|5731.69053|1.5104522|5731.6905|1.48E+00|5730.7905|1.393866536|
|   |     |     |     |     |
|---|-----|-----|-----|-----|
|   | 5732.0377 | 5732.0377 | 1.48E+00 | 5731.1377 | 1.384461573 |
|   | 5732.3863 | 5732.3863 | 1.48E+00 | 5731.4863 | 1.382561273 |
|   | 5732.73301 | 5732.73301 | 1.48E+00 | 5731.8333 | 1.3784608 |
|   | 5733.08066 | 5733.08066 | 1.49E+00 | 5732.1807 | 1.37857409 |
|   | 5733.4293 | 5733.4293 | 1.50E+00 | 5732.5293 | 1.379987218 |
|   | 5733.77695 | 5733.77695 | 1.51E+00 | 5732.8777 | 1.383969027 |
|   | 5734.12559 | 5734.12559 | 1.52E+00 | 5733.2256 | 1.395395018 |
|   | 5734.47227 | 5734.47227 | 1.54E+00 | 5733.5723 | 1.406279582 |
|   | 5734.81992 | 5734.81992 | 1.55E+00 | 5733.9199 | 1.4198365 |
|   | 5735.16904 | 5735.16904 | 1.56E+00 | 5734.269 | 1.432140527 |
|   | 5735.51572 | 5735.51572 | 1.57E+00 | 5734.6157 | 1.449408527 |
|   | 5735.86387 | 5735.86387 | 1.57E+00 | 5734.9639 | 1.463851064 |
|   | 5736.21299 | 5736.21299 | 1.55E+00 | 5735.313 | 1.471506573 |
|   | 5736.55967 | 5736.55967 | 1.53E+00 | 5735.6597 | 1.470626809 |
|   | 5736.90684 | 5736.90684 | 1.51E+00 | 5736.0068 | 1.465484009 |
|   | 5737.254 | 5737.254 | 1.47E+00 | 5736.354 | 1.451225609 |
|   | 5737.60264 | 5737.60264 | 1.43E+00 | 5736.7026 | 1.424205518 |
|   | 5737.95176 | 5737.95176 | 1.39E+00 | 5737.0518 | 1.393372364 |
|   | 5738.29893 | 5738.29893 | 1.34E+00 | 5737.3989 | 1.355901955 |
|   | 5738.64658 | 5738.64658 | 1.30E+00 | 5737.7466 | 1.313872336 |
|   | 5738.99375 | 5738.99375 | 1.26E+00 | 5738.0938 | 1.271022018 |
|   | 5739.34141 | 5739.34141 | 1.22E+00 | 5738.4414 | 1.226511109 |
|   | 5739.68906 | 5739.68906 | 1.19E+00 | 5738.7891 | 1.187335255 |
|   | 5740.03672 | 5740.03672 | 1.16E+00 | 5739.1367 | 1.151579509 |
|   | 5740.38438 | 5740.38438 | 1.13E+00 | 5739.4844 | 1.120019718 |
|   | 5740.73203 | 5740.73203 | 1.12E+00 | 5739.832 | 1.092563973 |
|   | 5741.07969 | 5741.07969 | 1.10E+00 | 5740.1797 | 1.070961627 |
|   | 5741.42783 | 5741.42783 | 1.08E+00 | 5740.5278 | 1.050553209 |
|   | 5741.77549 | 5741.77549 | 1.07E+00 | 5740.8755 | 1.034964755 |
|   | 5742.12363 | 5742.12363 | 1.06E+00 | 5741.2236 | 1.021826918 |
|   | 5742.47178 | 5742.47178 | 1.05E+00 | 5741.5718 | 1.0117908 |
|   | 5742.81992 | 5742.81992 | 1.04E+00 | 5741.9199 | 1.001076809 |
|   | 5743.16807 | 5743.16807 | 1.03E+00 | 5742.2681 | 0.991689618 |
|   | 5743.68711 | 5743.68711 | 1.02E+00 | 5742.7871 | 0.984460982 |
|   | 5744.585801 | 5744.585801 | 1.01E+00 | 5743.958 | 0.966827109 |
|   | 5746.67148 | 5746.67148 | 9.90E-01 | 5745.7715 | 0.946072555 |
|   | 5748.5582 | 5748.5582 | 9.78E-01 | 5747.6582 | 0.936159764 |
|   | 5750.51963 | 5750.51963 | 9.80E-01 | 5749.6196 | 0.935912027 |
|   | 5752.55479 | 5752.55479 | 9.84E-01 | 5751.6548 | 0.940623282 |
|   | 5754.66367 | 5754.66367 | 9.93E-01 | 5753.7637 | 0.950101936 |
|   | 5756.84482 | 5756.84482 | 1.00E+00 | 5755.9448 | 0.961079164 |
|   | 5759.1002 | 5759.1002 | 1.01E+00 | 5758.2002 | 0.970588273 |
|   | 5761.42783 | 5761.42783 | 1.01E+00 | 5760.5278 | 0.976875909 |
| E(eV)   | Normalized XANES | E(eV)   | Normalized XANES |
|--------|------------------|--------|------------------|
| 5580.8 | 0.309392482      | 5553.40049 | -7.77E-02       |
| 5590.79951 | 0.313898236      | 5566.73252 | -6.68E-02       |
| 5600.80049 | 0.304259926      | 5576.73301 | -5.20E-02       |
| 5610.79951 | 0.259761661      | 5586.7335 | -3.86E-02       |
| 5620.8 | 0.233820677      | 5596.73252 | -3.33E-02       |
| 5630.80049 | 0.212604538      | 5606.73252 | -2.44E-02       |
| 5640.8 | 0.222777367      | 5616.73301 | -1.88E-02       |

**Table S5.** Imido XANES (1-Cs and 1')

1-Cs

| E(eV) | Normalized XANES | E(eV) | Normalized XANES |
|-------|------------------|--------|------------------|
| 5563.83066 | 1.0019296       | 5763.8307 | 1.02E+00 |
| 5766.30625 | 1.0037667       | 5766.3063 | 1.00E+00 |
| 5768.85703 | 1.00496969      | 5768.857  | 1.00E+00 |
| 5771.48057 | 1.0053344       | 5771.4806 | 1.00E+00 |
| 5774.17734 | 1.0037667       | 5774.1773 | 1.00E+00 |
| 5776.94736 | 0.9966806       | 5776.9474 | 0.983634755 |
| 5779.916   | 0.9784971       | 5779.916  | 0.969608 |
| 5782.70811 | 0.9630728       | 5782.7081 | 0.95433245 |
| 5785.69834 | 0.9482784       | 5785.6983 | 0.921748 |
| 5788.76328 | 0.9354794       | 5788.7633 | 0.9041236 |
| 5791.90195 | 0.924174        | 5791.902  | 0.8849686 |
| 5795.11387 | 0.9113269       | 5795.1139 | 0.8692564 |
| 5798.4     | 0.8999259       | 5798.4   | 0.8702564 |
| 5801.75986 | 0.8890821       | 5801.7599 | 0.8392564 |
| 5805.19297 | 0.8789557       | 5805.193  | 0.8092564 |
| 5808.69834 | 0.8691413       | 5808.6983 | 0.7892564 |
| 5812.27744 | 0.8571719       | 5812.2774 | 0.7692564 |
| 5815.93233 | 0.8479618       | 5815.9322 | 0.7492564 |
| 5819.65853 | 0.8338478       | 5819.6583 | 0.7392564 |
| 5823.45957 | 0.8272676       | 5823.4596 | 0.7392564 |
| 5827.33048 | 0.8173204       | 5827.3341 | 0.7392564 |
| 5831.28232 | 0.8138697       | 5831.2823 | 0.7392564 |
| 5835.30381 | 0.8176108       | 5835.3038 | 0.7392564 |
| 5839.39854 | 0.8082248       | 5839.3985 | 0.7392564 |
| 5843.56748 | 0.7989965       | 5843.5675 | 0.7392564 |
| 5847.80869 | 0.7905131       | 5847.8087 | 0.7392564 |
| 5852.12607 | 0.7793599       | 5852.1261 | 0.7392564 |
| 5856.51426 | 0.7663467       | 5856.5143 | 0.7392564 |
| 5860.97812 | 0.7441254       | 5860.9781 | 0.7392564 |
| 5865.51523 | 0.7195885       | 5865.5152 | 0.7392564 |
| Value  | Column1     | Column2     | Column3     |
|--------|-------------|-------------|-------------|
| 5650.8 | 0.216378227 | 5626.73398  | -9.50E-03   |
| 5660.8 | 0.219338581 | 5636.73398  | 2.45E-04    |
| 5670.8 | 0.171896383 | 5646.73496  | 4.45E-03    |
| 5680.80049 | 0.14043206 | 5656.73447  | 1.56E-03    |
| 5681.80049 | 0.129954383 | 5666.73301  | -1.03E-03   |
| 5682.8 | 0.124737829 | 5676.73301  | -3.81E-03   |
| 5683.79951 | 0.118943684 | 5686.73301  | -5.53E-04   |
| 5684.8 | 0.101963937 | 5696.73398  | 5.30E-03    |
| 5685.8 | 0.094915144 | 5703.51719  | 1.41E-02    |
| 5686.8 | 0.090352796 | 5703.86436  | 2.18E-02    |
| 5687.79951 | 0.084419012 | 5704.21055  | 1.78E-02    |
| 5688.8 | 0.070879377 | 5704.55869  | 1.76E-02    |
| 5689.80049 | 0.076527089 | 5704.90684  | 1.70E-02    |
| 5690.80049 | 0.057188522 | 5705.25498  | 2.38E-02    |
| 5691.79951 | 0.049757455 | 5705.60361  | 2.63E-02    |
| 5692.79951 | 0.045594912 | 5705.95176  | 2.58E-02    |
| 5693.8 | 0.03387424  | 5706.29941  | 2.56E-02    |
| 5694.79951 | 0.027203396 | 5706.64561  | 2.70E-02    |
| 5695.8 | 0.030833313 | 5706.99424  | 2.82E-02    |
| 5696.80049 | 0.015712734 | 5707.34287  | 3.74E-02    |
| 5697.79951 | 0.018769098 | 5707.69053  | 4.29E-02    |
| 5698.8 | 0.00917671  | 5708.03721  | 4.16E-02    |
| 5699.8 | 0.00659235  | 5708.38584  | 4.31E-02    |
| 5700.80049 | -0.00207253 | 5708.7335   | 4.82E-02    |
| 5701.8 | -0.00156069 | 5709.08066  | 4.96E-02    |
| 5702.80049 | -0.00930035 | 5709.4293   | 5.20E-02    |
| 5703.8 | -0.01590575 | 5709.77744  | 5.59E-02    |
| 5704.80049 | -0.01695128 | 5710.12461  | 6.18E-02    |
| 5705.8 | -0.02280265 | 5710.47227  | 6.83E-02    |
| 5706.8 | -0.01326754 | 5710.81943  | 7.44E-02    |
| 5707.80049 | -0.01181218 | 5711.16807  | 7.88E-02    |
| 5708.8 | -0.01186572 | 5711.51523  | 8.27E-02    |
| 5709.80049 | 0.00560458  | 5711.86338  | 9.53E-02    |
| 5710.8 | 0.009620191 | 5712.21104  | 0.1102704   |
| 5711.80049 | 0.048906311 | 5712.55918  | 0.1192734   |
| 5712.8 | 0.056853738 | 5712.90684  | 0.1290536   |
| 5713.8 | 0.106925525 | 5713.25547  | 0.1492835   |
| 5714.80049 | 0.183904514 | 5713.60312  | 0.167489    |
| 5714.89961 | 0.187141359 | 5713.95176  | 0.1863802   |
| 5715.00029 | 0.193100095 | 5714.29844  | 0.2028608   |
| 5715.10029 | 0.198375776 | 5714.64609  | 0.2187945   |
| 5715.19941 | 0.205624402 | 5714.99473  | 0.2379926   |
| 5715.3 | 0.209690407 | 5715.34141  | 0.2552378   |
|       |         |         |         |
|-------|---------|---------|---------|
| 5715.4001 | 0.214966312 | 5715.68955 | 0.2748935 |
| 5715.50068 | 0.230179861 | 5716.03818 | 0.298223  |
| 5715.59932 | 0.23742342  | 5716.38535 | 0.3185287 |
| 5715.6999   | 0.243283018 | 5716.73252 | 0.3427659 |
| 5715.80049 | 0.251344651 | 5717.08066 | 0.3595758 |
| 5715.89961 | 0.253774881 | 5717.42979 | 0.3808123 |
| 5716.0002   | 0.261501819 | 5717.77695 | 0.4069308 |
| 5716.10029  | 0.273052543 | 5718.12412 | 0.4289525 |
| 5716.19941  | 0.275747567 | 5718.47129 | 0.448635  |
| 5716.3      | 0.285443038 | 5718.81992 | 0.473795  |
| 5716.40059  | 0.295432717 | 5719.16904 | 0.5063353 |
| 5716.49971  | 0.299446076 | 5719.5167  | 0.5376182 |
| 5716.5998   | 0.308333427 | 5719.86436 | 0.570718  |
| 5716.70039  | 0.31137225  | 5720.21152 | 0.6136792 |
| 5716.79951  | 0.320736647 | 5720.55918 | 0.6737393 |
| 5716.9001   | 0.324037552 | 5720.90732 | 0.7409493 |
| 5717.00068  | 0.334425777 | 5721.25498 | 0.8184614 |
| 5717.0998   | 0.342340112 | 5721.60264 | 0.8926835 |
| 5717.1999   | 0.345438004 | 5721.95078 | 0.9852142 |
| 5717.29951  | 0.354740888 | 5722.29844 | 1.0804772 |
| 5717.4001   | 0.36235559  | 5722.64658 | 1.1770638 |
| 5717.50068  | 0.36531958  | 5722.99473 | 1.2871255 |
| 5717.59932  | 0.37386316  | 5723.34287 | 1.3941501 |
| 5717.6999   | 0.377993733 | 5723.69102 | 1.4921398 |
| 5717.80049  | 0.382371277 | 5724.03916 | 1.5722889 |
| 5717.9001   | 0.388617188 | 5724.38633 | 1.6326327 |
| 5718.00068  | 0.397048384 | 5724.73252 | 1.6651584 |
| 5718.09932  | 0.396039575 | 5725.08066 | 1.6805487 |
| 5718.1999   | 0.40319851  | 5725.4293  | 1.681316  |
| 5718.29951  | 0.409281135 | 5725.77744 | 1.668518  |
| 5718.4001   | 0.41178298  | 5726.1251  | 1.6473641 |
| 5718.50068  | 0.424908519 | 5726.47178 | 1.6149554 |
| 5718.5998   | 0.428850502 | 5726.82041 | 1.5772694 |
| 5718.70039  | 0.437625885 | 5727.16904 | 1.5449256 |
| 5718.79951  | 0.435445398 | 5727.5167  | 1.5182161 |
| 5718.9001   | 0.440721422 | 5727.86338 | 1.4908981 |
| 5718.99971  | 0.443488508 | 5728.21201 | 1.4638424 |
| 5719.0998   | 0.448266119 | 5728.56016 | 1.4515438 |
| 5719.20039  | 0.459315926 | 5728.90684 | 1.4346134 |
| 5719.3      | 0.459327668 | 5729.25498 | 1.4217011 |
| 5719.40059  | 0.458854675 | 5729.60215 | 1.4078709 |
| 5719.5002   | 0.468288422 | 5729.95078 | 1.3984538 |
| 5719.60029  | 0.478925109 | 5730.29893 | 1.3914032 |
| Value 1 | Value 2 | Value 3 | Value 4 |
|--------|--------|--------|--------|
| 5719.6999 | 0.482789606 | 5730.64609 | 1.3848524 |
| 5719.80049 | 0.490297556 | 5730.99473 | 1.3755417 |
| 5719.9001 | 0.496398717 | 5731.34189 | 1.36479 |
| 5720.00068 | 0.502095222 | 5731.69053 | 1.3679162 |
| 5720.09932 | 0.511559248 | 5732.0377 | 1.3578601 |
| 5720.20039 | 0.523370564 | 5732.38633 | 1.3558459 |
| 5720.29951 | 0.53346616 | 5732.73301 | 1.3628339 |
| 5720.40059 | 0.540799558 | 5733.08066 | 1.364082 |
| 5720.5002 | 0.560021579 | 5733.4293 | 1.3679162 |
| 5720.60029 | 0.563241899 | 5733.77695 | 1.3754467 |
| 5720.6999 | 0.578378439 | 5734.12559 | 1.3858581 |
| 5720.80049 | 0.588643312 | 5734.47227 | 1.399251 |
| 5720.9001 | 0.605754077 | 5734.81992 | 1.4147973 |
| 5721.00068 | 0.61965853 | 5735.16904 | 1.4206557 |
| 5721.0998 | 0.635289967 | 5735.51572 | 1.4178466 |
| 5721.19941 | 0.654179871 | 5735.86387 | 1.4092881 |
| 5721.3 | 0.673237026 | 5736.21299 | 1.3956556 |
| 5721.39961 | 0.688828409 | 5736.55967 | 1.3746733 |
| 5721.5002 | 0.710366488 | 5736.90684 | 1.3449186 |
| 5721.59932 | 0.735416412 | 5737.254 | 1.310313 |
| 5721.70039 | 0.752966821 | 5737.60264 | 1.2800552 |
| 5721.8 | 0.778972626 | 5737.95176 | 1.244063 |
| 5721.90059 | 0.803634882 | 5738.29893 | 1.2099751 |
| 5722.0002 | 0.825638294 | 5738.64658 | 1.1726369 |
| 5722.09932 | 0.852842152 | 5738.99375 | 1.1361259 |
| 5722.1999 | 0.883112907 | 5739.34141 | 1.1138599 |
| 5722.29951 | 0.907142937 | 5739.68906 | 1.090803 |
| 5722.40059 | 0.927799881 | 5740.03672 | 1.0686368 |
| 5722.5002 | 0.966260374 | 5740.38438 | 1.0571676 |
| 5722.59932 | 0.994932473 | 5740.73203 | 1.0413772 |
| 5722.6999 | 1.01783264 | 5741.07969 | 1.0255916 |
| 5722.79951 | 1.05625618 | 5741.42783 | 1.0158135 |
| 5722.90059 | 1.08451641 | 5741.77549 | 1.0117108 |
| 5723.0002 | 1.11342466 | 5742.12363 | 1.0030488 |
| 5723.09932 | 1.1475383 | 5742.47178 | 0.9984958 |
| 5723.20039 | 1.1837647 | 5742.81992 | 0.9917546 |
| 5723.3 | 1.20494795 | 5743.16807 | 0.9892382 |
| 5723.39961 | 1.23859012 | 5743.68711 | 0.9866204 |
| 5723.5002 | 1.27262723 | 5744.85801 | 0.9783494 |
| 5723.5998 | 1.30123723 | 5746.67148 | 0.9708158 |
| 5723.70039 | 1.33492339 | 5748.5582 | 0.9665663 |
| 5723.8 | 1.36476958 | 5750.51963 | 0.9681707 |
| 5723.89961 | 1.38933647 | 5752.55479 | 0.9839451 |
| S32   | 5724.00068 | 1.41343963 | 5754.66367 | 0.9947466  |
|-------|------------|------------|------------|------------|
|       | 5724.0998  | 1.44764709 | 5756.84482 | 1.0036501  |
|       | 5724.19941 | 1.47221601 | 5759.1002  | 1.009203   |
|       | 5724.30049 | 1.49960279 | 5761.42783 | 1.0085888  |
|       | 5724.4001  | 1.52747285 | 5763.83066 | 1.0047473  |
|       | 5724.5002  | 1.54460621 | 5766.30625 | 0.9991045  |
|       | 5724.60029 | 1.56731331 | 5768.85703 | 0.9945289  |
|       | 5724.6999  | 1.58073056 | 5771.48057 | 0.9863971  |
|       | 5724.8     | 1.59867895 | 5774.17734 | 0.9810573  |
|       | 5724.89961 | 1.61521375 | 5776.94736 | 0.9760618  |
|       | 5725.00068 | 1.63429499 | 5779.7916  | 0.9783381  |
|       | 5725.0998  | 1.65808058 | 5782.70811 | 0.9773257  |
|       | 5725.19941 | 1.66159332 | 5785.69834 | 0.9783736  |
|       | 5725.30049 | 1.67466366 | 5788.76328 | 0.9787685  |
|       | 5725.4001  | 1.69056559 | 5791.90195 | 0.9803028  |
|       | 5725.5002  | 1.69020224 | 5795.11387 | 0.9818565  |
|       | 5725.59932 | 1.6945926  | 5798.4     | 0.9730932  |
|       | 5725.70039 | 1.70378578 | 5801.75986 | 0.9737753  |
|       | 5725.8     | 1.70343554 | 5805.19297 | 0.9707429  |
|       | 5725.9001  | 1.69690478 | 5808.69834 | 0.9710169  |
|       | 5725.99971 | 1.69270766 | 5812.27744 | 0.9711415  |
|       | 5726.10029 | 1.69002903 | 5815.93223 | 0.9698167  |
|       | 5726.1999  | 1.68732035 | 5819.6583  | 0.9637923  |
|       | 5726.3     | 1.69391191 | 5823.45957 | 0.9676976  |
|       | 5726.39961 | 1.69487941 | 5827.33408 | 0.9897082  |
|       | 5726.50068 | 1.68231523 | 5831.28232 | 0.9985261  |
|       | 5726.5998  | 1.67312849 | 5835.30381 | 0.9987197  |
|       | 5726.6999  | 1.66447067 | 5839.39854 | 0.995077   |
|       | 5726.79951 | 1.65497017 | 5843.56748 | 0.9993772  |
|       | 5726.89961 | 1.64929783 | 5847.80869 | 1.0042126  |
|       | 5727.00068 | 1.64629936 | 5852.12607 | 1.0114734  |
|       | 5727.0998  | 1.63169897 | 5856.51426 | 1.004903   |
|       | 5727.1999  | 1.62719262 | 5860.97812 | 0.9988036  |
|       | 5727.29951 | 1.62789869 | 5865.51523 | 0.9970074  |
|       | 5727.39961 | 1.61279964 |             |             |
|       | 5727.50068 | 1.60584104 |             |             |
|       | 5727.5998  | 1.60266292 |             |             |
|       | 5727.6999  | 1.59585249 |             |             |
|       | 5727.8     | 1.59011304 |             |             |
|       | 5727.89961 | 1.58529532 |             |             |
|       | 5728.00068 | 1.57739937 |             |             |
|       | 5728.10029 | 1.56742668 |             |             |
|       | 5728.1999  | 1.56838512 |             |             |
| Value     | 1.56657934 |   |   |   |
|-----------|------------|---|---|---|
| 5728.3    | 1.56657934 |   |   |   |
| 5728.4001 | 1.55174208 |   |   |   |
| 5728.49971| 1.54753006 |   |   |   |
| 5728.59932| 1.54925978 |   |   |   |
| 5728.70039| 1.53962791 |   |   |   |
| 5728.80049| 1.53682649 |   |   |   |
| 5728.9001 | 1.53729212 |   |   |   |
| 5729.0002 | 1.52904212 |   |   |   |
| 5729.0998 | 1.52236331 |   |   |   |
| 5729.1999 | 1.52329826 |   |   |   |
| 5729.29951| 1.51590598 |   |   |   |
| 5729.39961| 1.50968349 |   |   |   |
| 5729.50068| 1.50893974 |   |   |   |
| 5729.60029| 1.5004648  |   |   |   |
| 5729.70039| 1.49304903 |   |   |   |
| 5729.8    | 1.49557436 |   |   |   |
| 5729.9001 | 1.49606407 |   |   |   |
| 5730.0002 | 1.48646736 |   |   |   |
| 5730.0998 | 1.47872066 |   |   |   |
| 5730.1999 | 1.47889149 |   |   |   |
| 5730.3    | 1.47174108 |   |   |   |
| 5730.39961| 1.46604192 |   |   |   |
| 5730.49971| 1.46723711 |   |   |   |
| 5730.59932| 1.45552814 |   |   |   |
| 5730.69941| 1.45110166 |   |   |   |
| 5730.79951| 1.45618773 |   |   |   |
| 5730.90059| 1.45226467 |   |   |   |
| 5731.00068| 1.44344747 |   |   |   |
| 5731.10029| 1.44661474 |   |   |   |
| 5731.20039| 1.44309986 |   |   |   |
| 5731.30049| 1.43804896 |   |   |   |
| 5731.40059| 1.4372077  |   |   |   |
| 5731.50068| 1.43989992 |   |   |   |
| 5731.60029| 1.43438876 |   |   |   |
| 5731.70039| 1.4348613  |   |   |   |
| 5731.80049| 1.43321431 |   |   |   |
| 5732.00068| 1.4266609  |   |   |   |
| 5732.20039| 1.42920732 |   |   |   |
| 5732.40059| 1.43107283 |   |   |   |
| 5732.60029| 1.43037558 |   |   |   |
| 5732.80049| 1.4270674  |   |   |   |
| 5732.99971| 1.43488467 |   |   |   |
| 5733.19941| 1.43571246 |   |   |   |
| 5733.4001 | 1.43542469 |
| 5733.5998 | 1.4415368 |
| 5733.8 | 1.45544779 |
| 5734.0006 | 1.45514357 |
| 5734.20039 | 1.46591485 |
| 5734.39961 | 1.47270787 |
| 5734.5998 | 1.47828484 |
| 5734.8 | 1.48874557 |
| 5735.00068 | 1.50004017 |
| 5735.19941 | 1.50462198 |
| 5735.4001 | 1.51627159 |
| 5735.60029 | 1.51250517 |
| 5735.79951 | 1.52053821 |
| 5736.0002 | 1.5218035 |
| 5736.20039 | 1.51670134 |
| 5736.39961 | 1.51532984 |
| 5736.5998 | 1.50053215 |
| 5736.79951 | 1.49271429 |
| 5737.0002 | 1.48734045 |
| 5737.20039 | 1.47107828 |
| 5737.4001 | 1.44932973 |
| 5737.60029 | 1.42646992 |
| 5737.8 | 1.40311587 |
| 5738.00068 | 1.38047886 |
| 5738.1999 | 1.35471058 |
| 5738.40059 | 1.3357892 |
| 5738.5998 | 1.30475712 |
| 5738.79951 | 1.28031647 |
| 5739.0002 | 1.25974834 |
| 5739.1999 | 1.23551023 |
| 5739.40059 | 1.21495771 |
| 5739.5998 | 1.19998038 |
| 5739.79951 | 1.17548096 |
| 5740.00068 | 1.15898418 |
| 5740.1999 | 1.15079391 |
| 5740.4001 | 1.13008273 |
| 5740.59932 | 1.11556482 |
| 5740.80049 | 1.10880148 |
| 5741.0002 | 1.09604895 |
| 5741.1999 | 1.08570802 |
| 5741.39961 | 1.07161641 |
| 5741.59932 | 1.06466782 |
| 5741.80049 | 1.05167198 |
| Price   | Value   |
|---------|---------|
| 5742.0002 | 1.0508939 |
| 5742.1999 | 1.04476821 |
| 5742.4001 | 1.03275359 |
| 5742.5998 | 1.02946353 |
| 5742.8 | 1.02871394 |
| 5742.99971 | 1.01788425 |
| 5743.19941 | 1.02016675 |
| 5743.39961 | 1.01533735 |
| 5743.59932 | 1.00645471 |
| 5743.79951 | 1.00620663 |
| 5745.79951 | 0.989976108 |
| 5747.80049 | 0.977128208 |
| 5749.79951 | 0.968251884 |
| 5749.90059 | 0.967899024 |
| 5750.0002 | 0.96755904 |
| 5750.0998 | 0.96723108 |
| 5750.19941 | 0.96690011 |
| 5750.30049 | 0.966580093 |
| 5750.40059 | 0.966271222 |
| 5750.5002 | 0.9659729 |
| 5750.5998 | 0.965677083 |
| 5750.69941 | 0.965394795 |
| 5750.80049 | 0.96514892 |
| 5750.90059 | 0.96484524 |
| 5751.0002 | 0.964586198 |
| 5751.0998 | 0.964328706 |
| 5751.19941 | 0.964084625 |
| 5751.30049 | 0.963843524 |
| 5751.40059 | 0.96361208 |
| 5751.5002 | 0.963388741 |
| 5751.5998 | 0.963168442 |
| 5751.6999 | 0.962959766 |
| 5751.79951 | 0.96275826 |
| 5751.89961 | 0.96256274 |
| 5752.00068 | 0.962371886 |
| 5752.0998 | 0.962188423 |
| 5752.1999 | 0.962013543 |
| 5752.3 | 0.961845458 |
| 5752.4001 | 0.961684167 |
| 5752.49971 | 0.961530626 |
| 5752.59932 | 0.961379051 |
| 5752.70039 | 0.961235702 |
| 5752.80049 | 0.961100042 |
| Time       | Value    |
|------------|----------|
| 5752.9001  | 0.96097213 |
| 5753.0002  | 0.960849524 |
| 5753.0998  | 0.960728884 |
| 5753.1999  | 0.960618794 |
| 5753.29951 | 0.960514605 |
| 5753.39961 | 0.960416794 |
| 5753.49971 | 0.960324109 |
| 5753.59932 | 0.960234463 |
| 5753.70039 | 0.960152566 |
| 5753.80049 | 0.960076809 |
| 5753.90059 | 0.960007489 |
| 5754.00068 | 0.959942877 |
| 5754.0998  | 0.959881246 |
| 5754.1999  | 0.95982784 |
| 5754.3     | 0.959780693 |
| 5754.4001  | 0.959737837 |
| 5756.4001  | 0.964720428 |
| 5758.40059 | 0.965539157 |
| 5760.39961 | 0.960518599 |
| 5762.39961 | 0.967659235 |
| 5767.4001  | 0.970997572 |
| 5772.4001  | 0.966919899 |
| 5777.4001  | 0.962209046 |
| 5782.40059 | 0.953148305 |
| 5787.4001  | 0.942896545 |
| 5792.39961 | 0.951727808 |
| 5797.39961 | 0.959930599 |
| 5802.40059 | 0.973468959 |
| 5812.39961 | 1.00078452 |
| 5822.39961 | 1.0082165 |
| 5832.4001  | 1.00416362 |
| 5842.4001  | 0.981871188 |
| 5852.39961 | 0.952466309 |
| 5862.4001  | 0.917500317 |
| 5872.4001  | 0.907691956 |
| 5882.39961 | 0.913750112 |
| 5892.4001  | 0.897524059 |
| E(eV) | [2-K]₄ Normalized XANES | E(eV) | [2-Rb]₄ Normalized XANES | E(eV) | [2-Cs]₄ Normalized XANES |
|-------|------------------------|-------|---------------------------|-------|--------------------------|
| 5553.4 | 0.000476               | 5552.8 | -0.080109                 | 5580.8 | 0.005732                 |
| 5566.733 | -0.002077            | 5566.133 | -0.055195               | 5594.133 | 0.017919                 |
| 5576.733 | -0.003133            | 5576.133 | -0.037129               | 5604.134 | 0.008316                 |
| 5586.734 | -0.004066            | 5586.134 | -0.022134               | 5614.133 | -0.002494                |
| 5596.733 | -0.005338            | 5596.133 | -0.011923               | 5624.134 | -0.019095                |
| 5606.733 | -0.007347            | 5606.133 | -0.003561               | 5634.134 | -0.025827                |
| 5616.733 | -0.007811            | 5616.133 | 0.001686                | 5644.134 | -0.008683                |
| 5626.734 | -0.001829            | 5626.134 | 0.001543                | 5654.134 | 0.01791                  |
| 5636.734 | 0.00139               | 5636.134 | 0.003969                | 5664.134 | 0.011979                 |
| 5646.735 | 0.000844             | 5646.135 | 0.003169                | 5674.134 | -0.009776                |
| 5656.734 | -0.000417            | 5656.134 | 0.001949                | 5681.134 | -0.015569                |
| 5666.733 | 0.000335             | 5666.133 | -0.00019                | 5682.134 | -0.016407                |
| 5676.733 | 0.001041             | 5676.133 | -0.002941               | 5683.133 | -0.012074                |
| 5686.733 | -0.001787            | 5686.133 | -0.002296               | 5684.133 | -0.005491                |
| 5696.734 | 0.002336             | 5696.134 | 0.001261                | 5685.134 | -0.008989                |
| 5703.517 | 0.006991             | 5702.917 | 0.007171                | 5686.134 | -0.004935                |
| 5703.864 | 0.007857             | 5703.264 | 0.006378                | 5687.133 | -0.00686                 |
| 5704.211 | 0.009321             | 5703.611 | 0.006408                | 5688.133 | 0.00323                  |
| 5704.559 | 0.00818              | 5703.959 | 0.008331                | 5689.134 | 0.005849                 |
| 5704.907 | 0.008227             | 5704.307 | 0.009291                | 5690.134 | 0.005295                 |
| 5705.255 | 0.011128             | 5704.655 | 0.009587                | 5691.134 | 0.008426                 |
| 5705.604 | 0.010938             | 5705.004 | 0.009073                | 5692.133 | 0.006598                 |
| 5705.952 | 0.01104              | 5705.352 | 0.009993                | 5693.133 | 0.005928                 |
| 5706.299 | 0.011727             | 5705.699 | 0.011424                | 5694.133 | 0.001985                 |
| 5706.646 | 0.01239              | 5706.046 | 0.012566                | 5695.133 | -0.001176                |
| 5706.994 | 0.014905             | 5706.394 | 0.011103                | 5696.134 | 0.002399                 |
| 5707.343 | 0.017406             | 5706.743 | 0.011637                | 5697.134 | 0.006703                 |
| 5707.691 | 0.017381             | 5707.091 | 0.015389                | 5698.133 | 0.003797                 |
| 5708.037 | 0.017481             | 5707.437 | 0.017343                | 5699.134 | 0.006204                 |
| 5708.386 | 0.020215             | 5707.786 | 0.01665                 | 5700.134 | 0.011486                 |
| 5708.734 | 0.020929             | 5708.134 | 0.018457                | 5701.134 | 0.018906                 |
| 5709.081 | 0.021407             | 5708.481 | 0.020048                | 5702.134 | 0.026016                 |
| 5709.429 | 0.020995             | 5708.829 | 0.020593                | 5703.134 | 0.019247                 |
| 5709.777 | 0.022814             | 5709.177 | 0.023218                | 5704.134 | 0.021831                 |
| 5710.125 | 0.026519             | 5709.525 | 0.024199                | 5705.134 | 0.023488                 |
| 5710.472 | 0.028737             | 5709.872 | 0.02663                 | 5706.134 | 0.028648                 |
| 5710.819 | 0.030651             | 5710.219 | 0.028873                | 5707.134 | 0.040452                 |
| 5711.168 | 0.034009             | 5710.568 | 0.031253                | 5708.134 | 0.037461                 |

Table S6. Oxo XANES
|      | 0.036013  | 5710.915  | 0.032693  | 5709.134  | 0.048357  |
|------|-----------|-----------|-----------|-----------|-----------|
| 5711.515 | 0.037325  | 5711.263  | 0.034605  | 5710.134  | 0.067114  |
| 5711.863 | 0.040576  | 5711.611  | 0.036422  | 5711.134  | 0.080663  |
| 5712.211 | 0.045114  | 5711.959  | 0.039193  | 5712.134  | 0.106996  |
| 5712.559 | 0.049056  | 5712.307  | 0.04152   | 5713.134  | 0.130847  |
| 5712.907 | 0.053285  | 5712.655  | 0.046082  | 5714.134  | 0.176037  |
| 5713.255 | 0.057392  | 5713.003  | 0.050807  | 5714.834  | 0.213753  |
| 5713.603 | 0.062567  | 5713.352  | 0.053557  | 5714.933  | 0.221367  |
| 5713.952 | 0.068287  | 5713.698  | 0.057936  | 5715.033  | 0.22624   |
| 5714.298 | 0.074742  | 5714.046  | 0.063567  | 5715.134  | 0.237909  |
| 5714.646 | 0.082088  | 5714.395  | 0.068532  | 5715.233  | 0.238908  |
| 5715.341 | 0.089547  | 5714.741  | 0.074754  | 5715.333  | 0.250808  |
| 5715.69  | 0.099113  | 5715.09   | 0.082258  | 5715.434  | 0.262725  |
| 5716.038 | 0.110665  | 5715.438  | 0.091794  | 5715.533  | 0.258143  |
| 5716.385 | 0.125418  | 5715.785  | 0.101741  | 5715.633  | 0.260582  |
| 5716.733 | 0.142086  | 5716.133  | 0.11263   | 5715.734  | 0.268208  |
| 5717.081 | 0.164001  | 5716.481  | 0.126743  | 5715.834  | 0.276092  |
| 5717.43  | 0.186346  | 5716.83   | 0.144007  | 5715.933  | 0.278345  |
| 5717.777 | 0.21269   | 5717.177  | 0.163557  | 5716.033  | 0.277782  |
| 5718.124 | 0.239447  | 5717.524  | 0.187004  | 5716.134  | 0.287019  |
| 5718.471 | 0.263634  | 5717.871  | 0.213096  | 5716.233  | 0.288367  |
| 5718.82  | 0.281787  | 5718.22   | 0.24094   | 5716.334  | 0.29884   |
| 5719.169 | 0.295115  | 5718.569  | 0.268787  | 5716.434  | 0.307243  |
| 5719.517 | 0.308481  | 5718.917  | 0.290553  | 5716.533  | 0.303298  |
| 5719.864 | 0.324451  | 5719.264  | 0.306966  | 5716.634  | 0.315755  |
| 5720.212 | 0.340368  | 5719.612  | 0.320071  | 5716.734  | 0.327543  |
| 5720.559 | 0.369942  | 5719.959  | 0.33412   | 5716.833  | 0.327922  |
| 5720.907 | 0.410598  | 5720.307  | 0.350776  | 5716.934  | 0.335042  |
| 5721.255 | 0.463915  | 5720.655  | 0.374837  | 5717.034  | 0.340224  |
| 5721.603 | 0.531464  | 5721.003  | 0.414294  | 5717.133  | 0.344308  |
| 5721.951 | 0.608729  | 5721.351  | 0.464011  | 5717.233  | 0.356106  |
| 5722.298 | 0.702486  | 5721.698  | 0.526454  | 5717.333  | 0.367595  |
| 5722.647 | 0.815706  | 5722.047  | 0.602908  | 5717.434  | 0.371824  |
| 5722.995 | 0.950403  | 5722.395  | 0.692135  | 5717.533  | 0.376879  |
| 5723.343 | 1.099569  | 5722.743  | 0.794062  | 5717.633  | 0.376941  |
| 5723.691 | 1.25883   | 5723.091  | 0.918674  | 5717.734  | 0.380509  |
| 5724.039 | 1.412268  | 5723.439  | 1.060228  | 5717.834  | 0.388629  |
| 5724.386 | 1.551092  | 5723.786  | 1.211113  | 5717.934  | 0.396659  |
| 5724.733 | 1.658202  | 5724.133  | 1.360502  | 5718.033  | 0.409822  |
| 5725.081 | 1.731318  | 5724.481  | 1.500445  | 5718.133  | 0.410405  |
| 5725.429 | 1.762056  | 5724.829  | 1.611737  | 5718.233  | 0.420074  |
| 5725.777 | 1.769419  | 5725.177  | 1.68977   | 5718.333  | 0.432472  |
| 5726.125 | 1.757159  | 5725.525  | 1.735255  | 5718.434  | 0.438113  |
| 5726.472 | 1.730071 | 5725.872 | 1.747001 | 5718.534 | 0.443873 |
| 5726.82  | 1.697215 | 5726.22  | 1.737201 | 5718.634 | 0.447098 |
| 5727.169 | 1.66005  | 5726.569 | 1.714112 | 5718.734 | 0.450978 |
| 5727.517 | 1.627344 | 5726.917 | 1.684017 | 5718.833 | 0.457269 |
| 5727.863 | 1.602185 | 5727.263 | 1.650517 | 5718.933 | 0.457001 |
| 5728.212 | 1.581861 | 5727.612 | 1.618511 | 5719.033 | 0.459791 |
| 5728.56  | 1.56983  | 5727.96  | 1.590784 | 5719.134 | 0.466647 |
| 5728.907 | 1.564195 | 5728.307 | 1.569069 | 5719.234 | 0.470765 |
| 5729.255 | 1.561617 | 5728.655 | 1.554449 | 5719.334 | 0.483204 |
| 5729.602 | 1.562024 | 5729.002 | 1.54656  | 5719.434 | 0.481171 |
| 5729.951 | 1.563073 | 5729.351 | 1.544293 | 5719.533 | 0.487569 |
| 5730.299 | 1.561921 | 5729.699 | 1.544436 | 5719.634 | 0.49563  |
| 5730.646 | 1.561921 | 5730.046 | 1.544728 | 5719.734 | 0.495784 |
| 5730.995 | 1.561939 | 5730.395 | 1.545029 | 5719.834 | 0.501219 |
| 5731.342 | 1.563581 | 5730.742 | 1.546556 | 5719.934 | 0.507296 |
| 5731.691 | 1.564645 | 5731.091 | 1.548702 | 5720.033 | 0.507547 |
| 5732.038 | 1.564179 | 5731.438 | 1.546247 | 5720.133 | 0.511991 |
| 5732.386 | 1.564028 | 5731.786 | 1.546534 | 5720.234 | 0.520364 |
| 5732.733 | 1.565904 | 5732.133 | 1.546886 | 5720.333 | 0.530392 |
| 5733.081 | 1.569206 | 5732.481 | 1.54731  | 5720.434 | 0.537387 |
| 5733.429 | 1.573127 | 5732.829 | 1.544732 | 5720.533 | 0.549662 |
| 5733.777 | 1.576962 | 5733.177 | 1.544918 | 5720.634 | 0.558647 |
| 5734.126 | 1.581876 | 5733.526 | 1.547623 | 5720.734 | 0.564413 |
| 5734.472 | 1.587765 | 5733.872 | 1.54779  | 5720.834 | 0.581314 |
| 5734.82  | 1.595114 | 5734.22  | 1.552415 | 5720.934 | 0.59673  |
| 5735.169 | 1.601591 | 5734.569 | 1.558968 | 5721.034 | 0.605524 |
| 5735.516 | 1.605913 | 5734.916 | 1.565097 | 5721.133 | 0.618695 |
| 5735.864 | 1.602207 | 5735.264 | 1.57179  | 5721.233 | 0.638519 |
| 5736.213 | 1.589301 | 5735.613 | 1.577896 | 5721.333 | 0.650069 |
| 5736.56  | 1.570351 | 5735.96  | 1.578688 | 5721.433 | 0.667079 |
| 5736.907 | 1.541588 | 5736.307 | 1.572904 | 5721.533 | 0.690135 |
| 5737.254 | 1.502679 | 5736.654 | 1.56041  | 5721.633 | 0.706928 |
| 5737.603 | 1.45811  | 5737.003 | 1.537252 | 5721.734 | 0.729489 |
| 5737.952 | 1.410862 | 5737.352 | 1.503571 | 5721.834 | 0.749473 |
| 5738.299 | 1.364077 | 5737.699 | 1.465102 | 5721.934 | 0.768547 |
| 5738.647 | 1.322997 | 5738.047 | 1.422101 | 5722.033 | 0.790766 |
| 5738.994 | 1.28447  | 5738.394 | 1.378496 | 5722.133 | 0.819031 |
| 5739.341 | 1.247682 | 5738.741 | 1.337031 | 5722.233 | 0.842396 |
| 5739.689 | 1.214985 | 5739.089 | 1.300914 | 5722.333 | 0.867387 |
| 5740.037 | 1.18511  | 5739.437 | 1.264432 | 5722.434 | 0.893155 |
| 5740.384 | 1.158366 | 5739.784 | 1.230975 | 5722.533 | 0.919407 |
| 5740.732 | 1.136298 | 5740.132 | 1.204698 | 5722.633 | 0.94916  |
| 5741.08  | 1.117085 | 5740.48  | 1.178449 | 5722.733 | 0.987932 |
|       |       |       |       |       |
|-------|-------|-------|-------|-------|
| 5741.428 | 1.100967 | 5740.828 | 1.155834 | 5722.833 | 1.018716 |
| 5741.775 | 1.086725 | 5741.175 | 1.136491 | 5722.934 | 1.039835 |
| 5742.124 | 1.075088 | 5741.524 | 1.120043 | 5723.033 | 1.072076 |
| 5742.472 | 1.065626 | 5741.872 | 1.10674  | 5723.133 | 1.109362 |
| 5742.82  | 1.055723 | 5742.22  | 1.096278 | 5723.234 | 1.135922 |
| 5743.168 | 1.048049 | 5742.568 | 1.086616 | 5723.333 | 1.171017 |
| 5743.687 | 1.039913 | 5743.087 | 1.076034 | 5723.433 | 1.202678 |
| 5744.858 | 1.023532 | 5744.258 | 1.059987 | 5723.533 | 1.242282 |
| 5746.671 | 1.000406 | 5746.071 | 1.040727 | 5723.634 | 1.282989 |
| 5748.558 | 0.982379 | 5747.958 | 1.022846 | 5723.734 | 1.316873 |
| 5750.52  | 0.972974 | 5749.92  | 1.007486 | 5723.833 | 1.35731  |
| 5752.555 | 0.971075 | 5751.955 | 1.005119 | 5723.933 | 1.383112 |
| 5754.664 | 0.977331 | 5754.064 | 1.010212 | 5724.034 | 1.419658 |
| 5756.845 | 0.987532 | 5756.245 | 1.018039 | 5724.133 | 1.455518 |
| 5759.1   | 0.993945 | 5758.5   | 1.026913 | 5724.233 | 1.476097 |
| 5761.428 | 0.992466 | 5760.828 | 1.030277 | 5724.334 | 1.506149 |
| 5763.831 | 0.986057 | 5763.231 | 1.029534 | 5724.433 | 1.538888 |
| 5766.306 | 0.981637 | 5765.706 | 1.028663 | 5724.533 | 1.565221 |
| 5768.857 | 0.980636 | 5768.257 | 1.029393 | 5724.634 | 1.585618 |
| 5771.481 | 0.976972 | 5770.881 | 1.030893 | 5724.733 | 1.613667 |
| 5774.177 | 0.972305 | 5773.577 | 1.029657 | 5724.833 | 1.629822 |
| 5776.947 | 0.965034 | 5776.347 | 1.025287 | 5724.933 | 1.648904 |
| 5779.792 | 0.960408 | 5779.192 | 1.022876 | 5725.034 | 1.675938 |
| 5782.708 | 0.956648 | 5782.108 | 1.021424 | 5725.133 | 1.689323 |
| 5785.698 | 0.9539  | 5785.098 | 1.01983  | 5725.233 | 1.696712 |
| 5788.763 | 0.948948 | 5788.163 | 1.017985 | 5725.334 | 1.714897 |
| 5791.902 | 0.941102 | 5791.302 | 1.015634 | 5725.433 | 1.720275 |
| 5795.114 | 0.933381 | 5794.514 | 1.016316 | 5725.533 | 1.71421  |
| 5798.4   | 0.92836 | 5797.8   | 1.019973 | 5725.633 | 1.716681 |
| 5801.76  | 0.926718 | 5801.16  | 1.020782 | 5725.734 | 1.720521 |
| 5805.193 | 0.927131 | 5804.593 | 1.022527 | 5725.833 | 1.703287 |
| 5808.698 | 0.928651 | 5808.098 | 1.024518 | 5725.933 | 1.702634 |
| 5812.277 | 0.928813 | 5811.677 | 1.02795  | 5726.033 | 1.704493 |
| 5815.932 | 0.927582 | 5815.332 | 1.031231 | 5726.134 | 1.700124 |
| 5819.658 | 0.922692 | 5819.058 | 1.031555 | 5726.233 | 1.698964 |
| 5823.46  | 0.917394 | 5822.86  | 1.01417  | 5726.333 | 1.696187 |
| 5827.334 | 0.919198 | 5826.734 | 1.00715  | 5726.433 | 1.685768 |
| 5831.282 | 0.914171 | 5830.682 | 1.061846 | 5726.534 | 1.670239 |
| 5835.304 | 0.90783 | 5834.704 | 1.056891 | 5726.633 | 1.662587 |
| 5839.399 | 0.905004 | 5838.799 | 1.054824 | 5726.733 | 1.661234 |
| 5843.567 | 0.900143 | 5842.967 | 1.05538  | 5726.833 | 1.648236 |
| 5847.809 | 0.898856 | 5847.209 | 1.058034 | 5726.933 | 1.642114 |
| 5852.126 | 0.898478 | 5851.526 | 1.063342 | 5727.034 | 1.63179  |
|      |        |        |        |        |        |
|------|--------|--------|--------|--------|--------|
| 5856.514 | 0.889997 | 5855.914 | 1.06688 | 5727.133 | 1.616195 |
| 5860.978 | 0.876597 | 5860.378 | 1.062914 | 5727.233 | 1.616102 |
| 5865.515 | 0.860713 | 5864.915 | 1.052942 | 5727.333 | 1.618769 |
|         |        |        |        | 5727.433 | 1.610327 |
|         |        |        |        | 5727.534 | 1.599272 |
|         |        |        |        | 5727.633 | 1.597066 |
|         |        |        |        | 5727.733 | 1.587063 |
|         |        |        |        | 5727.833 | 1.578516 |
|         |        |        |        | 5727.933 | 1.573931 |
|         |        |        |        | 5728.034 | 1.570441 |
|         |        |        |        | 5728.134 | 1.56212 |
|         |        |        |        | 5728.233 | 1.560304 |
|         |        |        |        | 5728.333 | 1.552845 |
|         |        |        |        | 5728.433 | 1.539068 |
|         |        |        |        | 5728.533 | 1.541646 |
|         |        |        |        | 5728.633 | 1.547917 |
|         |        |        |        | 5728.734 | 1.543504 |
|         |        |        |        | 5728.834 | 1.540568 |
|         |        |        |        | 5728.933 | 1.531457 |
|         |        |        |        | 5729.033 | 1.525226 |
|         |        |        |        | 5729.133 | 1.528157 |
|         |        |        |        | 5729.233 | 1.527724 |
|         |        |        |        | 5729.333 | 1.523528 |
|         |        |        |        | 5729.433 | 1.520134 |
|         |        |        |        | 5729.534 | 1.517618 |
|         |        |        |        | 5729.634 | 1.518743 |
|         |        |        |        | 5729.734 | 1.520977 |
|         |        |        |        | 5729.833 | 1.519147 |
|         |        |        |        | 5729.933 | 1.525089 |
|         |        |        |        | 5730.033 | 1.518249 |
|         |        |        |        | 5730.133 | 1.515064 |
|         |        |        |        | 5730.233 | 1.522068 |
|         |        |        |        | 5730.333 | 1.516513 |
|         |        |        |        | 5730.433 | 1.514506 |
|         |        |        |        | 5730.533 | 1.52129 |
|         |        |        |        | 5730.633 | 1.516739 |
|         |        |        |        | 5730.733 | 1.508293 |
|         |        |        |        | 5730.833 | 1.507442 |
|         |        |        |        | 5730.934 | 1.50896 |
|         |        |        |        | 5731.034 | 1.503192 |
|         |        |        |        | 5731.134 | 1.502806 |
|         |        |        |        | 5731.234 | 1.508041 |
|         |        |        |        | 5731.334 | 1.497918 |
| Value 1   | Value 2   |
|----------|----------|
| 5731.434 | 1.503034 |
| 5731.534 | 1.504097 |
| 5731.634 | 1.498856 |
| 5731.734 | 1.49855  |
| 5731.867 | 1.501114 |
| 5732.067 | 1.498003 |
| 5732.267 | 1.504026 |
| 5732.467 | 1.499274 |
| 5732.667 | 1.496071 |
| 5732.867 | 1.491299 |
| 5733.066 | 1.494343 |
| 5733.266 | 1.500492 |
| 5733.467 | 1.48923  |
| 5733.667 | 1.491092 |
| 5733.867 | 1.500414 |
| 5734.067 | 1.49612  |
| 5734.267 | 1.502469 |
| 5734.467 | 1.508572 |
| 5734.667 | 1.507013 |
| 5734.867 | 1.51149  |
| 5735.067 | 1.524536 |
| 5735.266 | 1.531105 |
| 5735.467 | 1.5343   |
| 5735.667 | 1.535054 |
| 5735.866 | 1.533388 |
| 5736.067 | 1.529647 |
| 5736.267 | 1.529832 |
| 5736.467 | 1.527734 |
| 5736.666 | 1.513412 |
| 5736.866 | 1.506505 |
| 5737.067 | 1.499971 |
| 5737.267 | 1.474427 |
| 5737.467 | 1.460395 |
| 5737.667 | 1.43899  |
| 5737.867 | 1.415917 |
| 5738.067 | 1.401127 |
| 5738.267 | 1.388301 |
| 5738.467 | 1.368712 |
| 5738.666 | 1.346047 |
| 5738.866 | 1.328413 |
| 5739.067 | 1.315083 |
| 5739.267 | 1.297405 |
| 5739.467 | 1.28241  |

S42
|      |      |      |
|------|------|------|
| 5739.666 | 1.272414 |
| 5739.866 | 1.25755 |
| 5740.067 | 1.24978 |
| 5740.267 | 1.234044 |
| 5740.467 | 1.210051 |
| 5740.666 | 1.20606 |
| 5740.867 | 1.202762 |
| 5741.067 | 1.188903 |
| 5741.266 | 1.177373 |
| 5741.466 | 1.167809 |
| 5741.666 | 1.158174 |
| 5741.867 | 1.148856 |
| 5742.067 | 1.1559 |
| 5742.267 | 1.153764 |
| 5742.467 | 1.129145 |
| 5742.667 | 1.125158 |
| 5742.866 | 1.123984 |
| 5743.066 | 1.114546 |
| 5743.266 | 1.111874 |
| 5743.466 | 1.104287 |
| 5743.666 | 1.08864 |
| 5744.466 | 1.078265 |
| 5746.467 | 1.060916 |
| 5748.467 | 1.04529 |
| 5749.833 | 1.048733 |
| 5749.934 | 1.04869 |
| 5750.033 | 1.048658 |
| 5750.133 | 1.048639 |
| 5750.233 | 1.048637 |
| 5750.334 | 1.048643 |
| 5750.434 | 1.048666 |
| 5750.533 | 1.048699 |
| 5750.633 | 1.048741 |
| 5750.733 | 1.0488 |
| 5750.834 | 1.048868 |
| 5750.934 | 1.048953 |
| 5751.033 | 1.049044 |
| 5751.133 | 1.049145 |
| 5751.233 | 1.049261 |
| 5751.334 | 1.049386 |
| 5751.434 | 1.049527 |
| 5751.533 | 1.049673 |
| 5751.633 | 1.049827 |
|      |            |            |
|------|------------|------------|
| 5751.733 | 1.049998  |            |
| 5751.833 | 1.050176  |            |
| 5751.933 | 1.050368  |            |
| 5752.034 | 1.05057   |            |
| 5752.133 | 1.050771  |            |
| 5752.233 | 1.05099   |            |
| 5752.333 | 1.051219  |            |
| 5752.433 | 1.051459  |            |
| 5752.533 | 1.051703  |            |
| 5752.633 | 1.051956  |            |
| 5752.734 | 1.052222  |            |
| 5752.834 | 1.052496  |            |
| 5752.933 | 1.052775  |            |
| 5753.033 | 1.053066  |            |
| 5753.133 | 1.053358  |            |
| 5753.233 | 1.053665  |            |
| 5753.333 | 1.053977  |            |
| 5753.433 | 1.054297  |            |
| 5753.533 | 1.054626  |            |
| 5753.633 | 1.05496   |            |
| 5753.734 | 1.055305  |            |
| 5753.834 | 1.055655  |            |
| 5753.934 | 1.056013  |            |
| 5754.034 | 1.056417  |            |
| 5754.133 | 1.056867  |            |
| 5754.233 | 1.057262  |            |
| 5754.333 | 1.057651  |            |
| 5755.067 | 1.060051  |            |
| 5757.067 | 1.065727  |            |
| 5759.067 | 1.069218  |            |
| 5761.066 | 1.08209   |            |
| 5764.067 | 1.09813   |            |
| 5769.067 | 1.078563  |            |
| 5774.067 | 1.059375  |            |
| 5779.067 | 1.035758  |            |
| 5784.067 | 1.013829  |            |
| 5789.067 | 1.001376  |            |
| 5794.066 | 0.996816  |            |
| 5799.067 | 1.010769  |            |
| 5805.734 | 1.045539  |            |
| 5815.733 | 1.06009   |            |
| 5825.733 | 1.06314   |            |
| 5835.734 | 1.075152  |            |
Table S7. Anilide HERFD

| E(eV)    | Normalized HERFD |
|----------|------------------|
| 5680     | 7.28E-05         |
| 5681.334 | 2.81E-05         |
| 5682.333 | 1.46E-04         |
| 5683.333 | -2.96E-04        |
| 5684.334 | -2.95E-04        |
| 5685.334 | -1.65E-04        |
| 5686.333 | -1.17E-05        |
| 5687.333 | 1.07E-04         |
| 5688.334 | -4.35E-05        |
| 5689.334 | -1.71E-04        |
| 5690.334 | -9.89E-05        |
| 5691.333 | 6.74E-05         |
| 5692.333 | 1.99E-04         |
| 5693.333 | 2.82E-04         |
| 5694.333 | -3.35E-05        |
| 5695.334 | 3.10E-04         |
| 5696.334 | 1.74E-05         |
| 5697.333 | -1.70E-04        |
| 5698.334 | -3.85E-05        |
| 5699.334 | 1.64E-04         |
| 5700.334 | 2.36E-05         |
| 5701.334 | 8.38E-05         |
| 5702.334 | -4.01E-04        |
| 5703.334 | -2.70E-04        |
| 5704.334 | -2.45E-04        |
| 5705.334 | -1.94E-05        |
| 5706.334 | 2.42E-04         |
| 5707.334 | -3.08E-05        |
| 5708.334 | 2.78E-04         |
| 5709.334 | 4.07E-04         |
| 5710.334 | 2.52E-04         |
| 5711.334 | 1.68E-04         |
| Value     | Number   |
|-----------|----------|
| 5712.334  | 1.19E-04 |
| 5713.334  | 3.79E-04 |
| 5714.034  | 1.05E-03 |
| 5714.133  | 1.40E-03 |
| 5714.233  | 1.98E-03 |
| 5714.334  | 1.92E-03 |
| 5714.433  | 1.43E-03 |
| 5714.533  | 1.63E-03 |
| 5714.634  | 1.79E-03 |
| 5714.733  | 2.35E-03 |
| 5714.834  | 1.96E-03 |
| 5714.934  | 2.14E-03 |
| 5715.034  | 2.87E-03 |
| 5715.133  | 3.32E-03 |
| 5715.233  | 3.65E-03 |
| 5715.334  | 4.17E-03 |
| 5715.433  | 5.36E-03 |
| 5715.534  | 5.83E-03 |
| 5715.634  | 6.63E-03 |
| 5715.733  | 8.29E-03 |
| 5715.834  | 1.07E-02 |
| 5715.934  | 1.22E-02 |
| 5716.033  | 1.33E-02 |
| 5716.134  | 1.63E-02 |
| 5716.234  | 1.93E-02 |
| 5716.333  | 2.40E-02 |
| 5716.433  | 2.98E-02 |
| 5716.533  | 3.61E-02 |
| 5716.634  | 4.35E-02 |
| 5716.733  | 5.42E-02 |
| 5716.833  | 6.52E-02 |
| 5716.934  | 7.69E-02 |
| 5717.034  | 9.00E-02 |
| 5717.134  | 0.102022 |
| 5717.233  | 0.115622 |
| 5717.333  | 0.130704 |
| 5717.433  | 0.140945 |
| 5717.533  | 0.15054 |
| 5717.634  | 0.157275 |
| 5717.734  | 0.159842 |
| 5717.834  | 0.157776 |
| 5717.934  | 0.156474 |
| 5718.033  | 0.159187 |
|    |   |
|----|---|
| 5718.133 | 0.153938 |
| 5718.233 | 0.146258 |
| 5718.334 | 0.142568 |
| 5718.434 | 0.130082 |
| 5718.534 | 0.119740 |
| 5718.634 | 0.112325 |
| 5718.733 | 0.105138 |
| 5718.834 | 9.73E-02 |
| 5718.934 | 8.99E-02 |
| 5719.034 | 8.30E-02 |
| 5719.134 | 7.83E-02 |
| 5719.233 | 7.59E-02 |
| 5719.333 | 7.56E-02 |
| 5719.434 | 7.22E-02 |
| 5719.533 | 7.01E-02 |
| 5719.634 | 6.97E-02 |
| 5719.733 | 6.97E-02 |
| 5719.834 | 7.21E-02 |
| 5719.934 | 7.48E-02 |
| 5720.034 | 7.89E-02 |
| 5720.134 | 8.31E-02 |
| 5720.234 | 8.85E-02 |
| 5720.333 | 9.38E-02 |
| 5720.433 | 1.01629  |
| 5720.533 | 0.110645 |
| 5720.633 | 0.117395 |
| 5720.733 | 0.132165 |
| 5720.833 | 0.142669 |
| 5720.934 | 0.158909 |
| 5721.034 | 0.177477 |
| 5721.134 | 0.197695 |
| 5721.233 | 0.221093 |
| 5721.333 | 0.246642 |
| 5721.433 | 0.276916 |
| 5721.533 | 0.312625 |
| 5721.634 | 0.352984 |
| 5721.733 | 0.399332 |
| 5721.833 | 0.447363 |
| 5721.933 | 0.507087 |
| 5722.033 | 0.570816 |
| 5722.134 | 0.646345 |
| 5722.233 | 0.717874 |
| 5722.333 | 0.78806  |
| 5722.434 | 0.863923 |
| 5722.533 | 0.944593 |
| 5722.633 | 1.015084 |
| 5722.733 | 1.097348 |
| 5722.834 | 1.159422 |
| 5722.934 | 1.218470 |
| 5723.033 | 1.276800 |
| 5723.133 | 1.328766 |
| 5723.233 | 1.375749 |
| 5723.333 | 1.423115 |
| 5723.433 | 1.461281 |
| 5723.534 | 1.508267 |
| 5723.633 | 1.548771 |
| 5723.733 | 1.585034 |
| 5723.834 | 1.626981 |
| 5723.933 | 1.670224 |
| 5724.033 | 1.712996 |
| 5724.133 | 1.762062 |
| 5724.234 | 1.819186 |
| 5724.333 | 1.875766 |
| 5724.433 | 1.920633 |
| 5724.534 | 1.960664 |
| 5724.633 | 2.004492 |
| 5724.733 | 2.040640 |
| 5724.833 | 2.084447 |
| 5724.934 | 2.111756 |
| 5725.033 | 2.140803 |
| 5725.133 | 2.159092 |
| 5725.233 | 2.172897 |
| 5725.334 | 2.188952 |
| 5725.433 | 2.184391 |
| 5725.533 | 2.179174 |
| 5725.633 | 2.182233 |
| 5725.734 | 2.156125 |
| 5725.833 | 2.145373 |
| 5725.933 | 2.142239 |
| 5726.033 | 2.119534 |
| 5726.133 | 2.098460 |
| 5726.234 | 2.081596 |
| 5726.333 | 2.056989 |
| 5726.433 | 2.032575 |
| 5726.533 | 2.018249 |
| 5726.633 | 1.993377 |
|      |          |
|------|----------|
| 5726.734 | 1.962407  |
| 5726.833 | 1.953711  |
| 5726.933 | 1.935093  |
| 5727.033 | 1.910469  |
| 5727.133 | 1.903261  |
| 5727.234 | 1.885113  |
| 5727.334 | 1.865506  |
| 5727.433 | 1.853382  |
| 5727.533 | 1.829172  |
| 5727.633 | 1.825792  |
| 5727.733 | 1.814546  |
| 5727.833 | 1.800968  |
| 5727.934 | 1.798923  |
| 5728.034 | 1.791247  |
| 5728.133 | 1.779584  |
| 5728.233 | 1.777978  |
| 5728.333 | 1.761229  |
| 5728.433 | 1.748837  |
| 5728.533 | 1.749079  |
| 5728.633 | 1.748516  |
| 5728.734 | 1.749517  |
| 5728.834 | 1.740626  |
| 5728.934 | 1.72621   |
| 5729.033 | 1.713507  |
| 5729.133 | 1.70146   |
| 5729.233 | 1.700055  |
| 5729.333 | 1.706289  |
| 5729.433 | 1.686083  |
| 5729.533 | 1.66375   |
| 5729.633 | 1.667309  |
| 5729.733 | 1.657463  |
| 5729.833 | 1.64698   |
| 5729.933 | 1.64854   |
| 5730.033 | 1.646244  |
| 5730.134 | 1.624619  |
| 5730.234 | 1.612739  |
| 5730.334 | 1.590956  |
| 5730.434 | 1.587517  |
| 5730.534 | 1.59011   |
| 5730.634 | 1.579417  |
| 5730.734 | 1.569637  |
| 5730.834 | 1.561753  |
| 5730.934 | 1.554089  |
|      |      |
|------|------|
| 5731.067 | 1.535802 |
| 5731.267 | 1.523669 |
| 5731.467 | 1.511441 |
| 5731.667 | 1.493118 |
| 5731.867 | 1.475056 |
| 5732.067 | 1.468055 |
| 5732.266 | 1.459805 |
| 5732.466 | 1.458733 |
| 5732.667 | 1.448264 |
| 5732.867 | 1.447546 |
| 5733.067 | 1.450201 |
| 5733.267 | 1.460603 |
| 5733.467 | 1.458588 |
| 5733.667 | 1.464659 |
| 5733.867 | 1.488579 |
| 5734.067 | 1.499722 |
| 5734.267 | 1.510048 |
| 5734.466 | 1.530127 |
| 5734.667 | 1.551457 |
| 5734.867 | 1.573941 |
| 5735.066 | 1.599171 |
| 5735.267 | 1.629361 |
| 5735.467 | 1.666283 |
| 5735.667 | 1.713218 |
| 5735.866 | 1.744255 |
| 5736.066 | 1.783895 |
| 5736.267 | 1.832251 |
| 5736.467 | 1.84071 |
| 5736.667 | 1.851682 |
| 5736.867 | 1.849597 |
| 5737.067 | 1.839702 |
| 5737.267 | 1.822536 |
| 5737.467 | 1.810525 |
| 5737.667 | 1.784162 |
| 5737.866 | 1.751368 |
| 5738.066 | 1.71324 |
| 5738.267 | 1.688816 |
| 5738.467 | 1.640032 |
| 5738.667 | 1.581497 |
| 5738.866 | 1.514639 |
| 5739.066 | 1.443954 |
| 5739.267 | 1.376057 |
| 5739.467 | 1.301672 |
### Table S8. Imido HERFD

|       | 1-K                  |       | 1-Rb                  |       | 1-Cs                  |
|-------|----------------------|-------|----------------------|-------|----------------------|
| E(eV) | Normalized HERFD    | E(eV) | Normalized HERFD    | E(eV) | Normalized HERFD    |
| 5680  | 4.99E-04             | 5680  | 1.27E-04             | 5680  | 2.59E-04             |
| 5681.334 | -2.30E-04         | 5681.334 | -3.26E-05         | 5681.334 | 7.01E-05         |
| 5682.333 | 2.92E-05           | 5682.333 | -3.57E-05         | 5682.333 | 1.58E-04         |
| 5683.333 | 8.92E-05           | 5683.333 | -1.43E-04         | 5683.333 | -1.61E-04         |
| 5684.334 | -5.99E-04          | 5684.334 | 4.25E-05           | 5684.334 | 2.07E-04           |
| 5685.334 | -1.10E-04          | 5685.334 | -2.55E-05         | 5685.334 | 3.38E-04           |
| 5686.333 | 4.33E-04           | 5686.333 | 3.06E-05           | 5686.333 | -4.96E-04         |
| 5687.333 | 3.83E-04           | 5687.333 | -6.22E-05         | 5687.333 | -3.86E-04         |
| 5688.334 | 4.14E-04           | 5688.334 | -8.98E-05         | 5688.334 | -6.84E-04         |
| Value | Value | Value | Value | Value | Value |
|-------|-------|-------|-------|-------|-------|
| 5689.334 | -1.09E-05 | 5689.334 | 1.92E-04 | 5689.334 | -2.08E-04 |
| 5690.334 | -8.41E-04 | 5690.334 | 7.12E-05 | 5690.334 | -1.62E-04 |
| 5691.333 | -3.25E-04 | 5691.333 | 7.78E-05 | 5691.333 | 7.76E-05 |
| 5692.333 | 1.10E-04 | 5692.333 | 2.18E-04 | 5692.333 | 5.92E-05 |
| 5693.333 | 4.41E-04 | 5693.333 | 1.27E-04 | 5693.333 | -2.62E-06 |
| 5694.334 | 4.95E-04 | 5694.333 | 1.95E-05 | 5694.333 | 6.57E-05 |
| 5695.334 | 2.67E-04 | 5695.334 | -3.68E-04 | 5695.334 | 6.53E-04 |
| 5696.334 | 6.44E-04 | 5696.334 | -1.40E-04 | 5696.334 | 6.13E-04 |
| 5697.333 | -2.41E-04 | 5697.333 | 1.59E-04 | 5697.333 | 1.40E-04 |
| 5698.334 | -5.84E-04 | 5698.334 | 5.63E-05 | 5698.334 | -2.69E-04 |
| 5699.334 | -5.31E-04 | 5699.334 | -1.34E-04 | 5699.334 | -1.14E-04 |
| 5700.334 | -4.13E-05 | 5700.334 | -1.45E-04 | 5700.334 | -3.94E-04 |
| 5701.334 | -3.23E-04 | 5701.334 | 4.34E-05 | 5701.334 | 2.60E-04 |
| 5702.334 | -4.80E-04 | 5702.334 | -1.68E-04 | 5702.334 | 5.44E-04 |
| 5703.334 | -2.64E-04 | 5703.334 | -1.16E-04 | 5703.334 | 4.57E-05 |
| 5704.334 | -2.42E-04 | 5704.334 | -1.83E-04 | 5704.334 | 2.58E-05 |
| 5705.334 | -2.16E-04 | 5705.334 | -3.58E-05 | 5705.334 | 1.79E-04 |
| 5706.334 | 9.24E-05 | 5706.334 | 1.92E-04 | 5706.334 | 4.84E-04 |
| 5707.334 | 2.56E-04 | 5707.334 | 5.65E-05 | 5707.334 | 5.28E-04 |
| 5708.334 | -2.70E-04 | 5708.334 | 4.36E-04 | 5708.334 | 6.98E-05 |
| 5709.334 | -5.09E-05 | 5709.334 | 6.17E-04 | 5709.334 | -1.27E-04 |
| 5710.334 | -1.28E-04 | 5710.334 | 3.74E-04 | 5710.334 | 5.04E-04 |
| 5711.334 | 2.80E-04 | 5711.334 | 9.43E-04 | 5711.334 | 7.63E-04 |
| 5712.334 | 5.14E-04 | 5712.334 | 1.05E-03 | 5712.334 | 3.25E-04 |
| 5713.334 | 8.09E-04 | 5713.334 | 1.30E-03 | 5713.334 | 9.53E-04 |
| 5714.034 | 1.60E-03 | 5714.034 | 2.78E-03 | 5714.034 | 1.88E-03 |
| 5714.133 | 1.81E-03 | 5714.133 | 3.56E-03 | 5714.133 | 1.80E-03 |
| 5714.233 | 1.22E-03 | 5714.233 | 3.26E-03 | 5714.233 | 2.86E-03 |
| 5714.334 | 1.93E-03 | 5714.334 | 3.96E-03 | 5714.334 | 2.71E-03 |
| 5714.433 | 2.07E-03 | 5714.433 | 4.61E-03 | 5714.433 | 3.14E-03 |
| 5714.533 | 2.75E-03 | 5714.533 | 4.83E-03 | 5714.533 | 3.88E-03 |
| 5714.634 | 4.42E-03 | 5714.634 | 6.11E-03 | 5714.634 | 3.38E-03 |
| 5714.733 | 4.34E-03 | 5714.733 | 7.95E-03 | 5714.733 | 4.16E-03 |
| 5714.833 | 5.80E-03 | 5714.833 | 8.96E-03 | 5714.833 | 6.35E-03 |
| 5714.934 | 7.34E-03 | 5714.934 | 1.09E-02 | 5714.934 | 7.18E-03 |
| 5715.034 | 7.59E-03 | 5715.034 | 1.40E-02 | 5715.034 | 8.11E-03 |
| 5715.133 | 8.33E-03 | 5715.133 | 1.83E-02 | 5715.133 | 1.04E-02 |
| 5715.233 | 1.06E-02 | 5715.233 | 2.00E-02 | 5715.233 | 1.27E-02 |
| 5715.334 | 1.26E-02 | 5715.334 | 2.19E-02 | 5715.334 | 1.48E-02 |
| 5715.433 | 1.36E-02 | 5715.433 | 2.58E-02 | 5715.433 | 1.77E-02 |
| 5715.534 | 1.72E-02 | 5715.534 | 3.02E-02 | 5715.534 | 2.17E-02 |
| 5715.634 | 2.10E-02 | 5715.634 | 3.33E-02 | 5715.634 | 2.47E-02 |
| 5715.733 | 2.39E-02 | 5715.733 | 3.59E-02 | 5715.733 | 2.63E-02 |
|          |          |          |          |          |
|----------|----------|----------|----------|----------|
| 5715.834 | 2.72E-02 | 5715.834 | 3.76E-02 | 5715.834 | 2.92E-02 |
| 5715.934 | 3.14E-02 | 5715.934 | 4.09E-02 | 5715.934 | 3.20E-02 |
| 5716.033 | 3.40E-02 | 5716.033 | 4.48E-02 | 5716.033 | 3.45E-02 |
| 5716.134 | 3.31E-02 | 5716.134 | 4.40E-02 | 5716.134 | 3.96E-02 |
| 5716.234 | 3.70E-02 | 5716.234 | 4.91E-02 | 5716.234 | 4.17E-02 |
| 5716.333 | 4.41E-02 | 5716.333 | 5.78E-02 | 5716.333 | 4.08E-02 |
| 5716.433 | 5.28E-02 | 5716.433 | 6.61E-02 | 5716.433 | 4.25E-02 |
| 5716.533 | 6.13E-02 | 5716.533 | 7.51E-02 | 5716.533 | 4.72E-02 |
| 5716.634 | 7.00E-02 | 5716.634 | 8.52E-02 | 5716.634 | 5.31E-02 |
| 5716.733 | 8.29E-02 | 5716.733 | 9.60E-02 | 5716.733 | 5.72E-02 |
| 5716.833 | 9.67E-02 | 5716.833 | 1.07778  | 5716.833 | 6.37E-02 |
| 5716.934 | 0.108368 | 5716.934 | 0.119479 | 5716.934 | 7.03E-02 |
| 5717.034 | 0.120095 | 5717.034 | 0.12876  | 5717.034 | 8.03E-02 |
| 5717.134 | 0.128785 | 5717.134 | 0.137812 | 5717.134 | 8.85E-02 |
| 5717.233 | 0.13461  | 5717.233 | 0.145903 | 5717.233 | 9.74E-02 |
| 5717.333 | 0.141905 | 5717.333 | 0.152286 | 5717.333 | 1.02625 |
| 5717.433 | 0.156514 | 5717.433 | 0.155881 | 5717.433 | 0.111304 |
| 5717.533 | 0.159399 | 5717.533 | 0.155066 | 5717.533 | 0.122477 |
| 5717.634 | 0.154851 | 5717.634 | 0.159219 | 5717.634 | 0.127972 |
| 5717.734 | 0.157986 | 5717.734 | 0.161042 | 5717.734 | 0.134119 |
| 5717.834 | 0.166178 | 5717.834 | 0.157046 | 5717.834 | 0.140786 |
| 5717.934 | 0.156232 | 5717.934 | 0.153597 | 5717.934 | 0.144714 |
| 5718.033 | 0.152114 | 5718.033 | 0.153055 | 5718.033 | 0.14298 |
| 5718.133 | 0.148163 | 5718.133 | 0.150053 | 5718.133 | 0.141736 |
| 5718.233 | 0.144819 | 5718.233 | 0.141973 | 5718.233 | 0.141992 |
| 5718.334 | 0.144391 | 5718.334 | 0.141097 | 5718.334 | 0.1405 |
| 5718.434 | 0.137264 | 5718.434 | 0.136399 | 5718.434 | 0.140159 |
| 5718.534 | 0.130661 | 5718.534 | 0.131639 | 5718.534 | 0.136651 |
| 5718.634 | 0.120607 | 5718.634 | 0.129994 | 5718.634 | 0.131473 |
| 5718.733 | 0.116515 | 5718.733 | 0.128011 | 5718.733 | 0.125851 |
| 5718.834 | 0.114146 | 5718.834 | 0.127658 | 5718.834 | 0.127907 |
| 5718.934 | 0.117086 | 5718.934 | 0.126237 | 5718.934 | 0.123132 |
| 5719.034 | 0.111081 | 5719.034 | 0.127926 | 5719.034 | 0.117387 |
| 5719.134 | 0.104731 | 5719.134 | 0.128664 | 5719.134 | 0.116068 |
| 5719.233 | 0.106023 | 5719.233 | 0.131529 | 5719.233 | 0.117756 |
| 5719.333 | 0.111178 | 5719.333 | 0.139107 | 5719.333 | 0.118545 |
| 5719.434 | 0.114953 | 5719.434 | 0.154284 | 5719.434 | 0.120143 |
| 5719.533 | 0.115493 | 5719.533 | 0.163552 | 5719.533 | 0.127167 |
| 5719.634 | 0.118523 | 5719.634 | 0.177822 | 5719.634 | 0.136114 |
| 5719.733 | 0.129417 | 5719.733 | 0.194206 | 5719.733 | 0.142308 |
| 5719.834 | 0.145966 | 5719.834 | 0.213406 | 5719.834 | 0.153574 |
| 5719.934 | 0.156866 | 5719.934 | 0.235874 | 5719.934 | 0.169254 |
| 5720.034 | 0.160032 | 5720.034 | 0.262282 | 5720.034 | 0.188961 |
|      | 5720.134  | 0.175336  | 5720.134  | 0.296939  | 5720.134  | 0.210657  |
|-----|-----------|-----------|-----------|-----------|-----------|-----------|
| 5720.234 | 0.196547  | 5720.234  | 0.325982  | 5720.234  | 0.231941  |
| 5720.333 | 0.208548  | 5720.333  | 0.357288  | 5720.333  | 0.258358  |
| 5720.433 | 0.233204  | 5720.433  | 0.394848  | 5720.433  | 0.284193  |
| 5720.533 | 0.258822  | 5720.533  | 0.434584  | 5720.533  | 0.319587  |
| 5720.633 | 0.286159  | 5720.633  | 0.46832   | 5720.633  | 0.357096  |
| 5720.733 | 0.319836  | 5720.733  | 0.507721  | 5720.733  | 0.396417  |
| 5720.833 | 0.344068  | 5720.833  | 0.553486  | 5720.833  | 0.438248  |
| 5720.934 | 0.374704  | 5720.934  | 0.59381   | 5720.934  | 0.476327  |
| 5721.034 | 0.407869  | 5721.034  | 0.630541  | 5721.034  | 0.513676  |
| 5721.134 | 0.441976  | 5721.134  | 0.671175  | 5721.134  | 0.548742  |
| 5721.233 | 0.481135  | 5721.233  | 0.711539  | 5721.233  | 0.596123  |
| 5721.333 | 0.535395  | 5721.333  | 0.766212  | 5721.333  | 0.647719  |
| 5721.433 | 0.580569  | 5721.433  | 0.824686  | 5721.433  | 0.694213  |
| 5721.533 | 0.630901  | 5721.533  | 0.881849  | 5721.533  | 0.736046  |
| 5721.634 | 0.688201  | 5721.634  | 0.948312  | 5721.634  | 0.787369  |
| 5721.733 | 0.748866  | 5721.733  | 1.029386  | 5721.733  | 0.834201  |
| 5721.833 | 0.833006  | 5721.833  | 1.106854  | 5721.833  | 0.897925  |
| 5721.933 | 0.907739  | 5721.933  | 1.190985  | 5721.933  | 0.957135  |
| 5722.033 | 0.993292  | 5722.033  | 1.269061  | 5722.033  | 1.024792  |
| 5722.134 | 1.081441  | 5722.134  | 1.346184  | 5722.134  | 1.091829  |
| 5722.233 | 1.152763  | 5722.233  | 1.430021  | 5722.233  | 1.159879  |
| 5722.333 | 1.244423  | 5722.333  | 1.501577  | 5722.333  | 1.236863  |
| 5722.434 | 1.319386  | 5722.434  | 1.580738  | 5722.434  | 1.307266  |
| 5722.533 | 1.396087  | 5722.533  | 1.661953  | 5722.533  | 1.388379  |
| 5722.633 | 1.480141  | 5722.633  | 1.725034  | 5722.633  | 1.471015  |
| 5722.733 | 1.552856  | 5722.733  | 1.779091  | 5722.733  | 1.549178  |
| 5722.834 | 1.605394  | 5722.834  | 1.846757  | 5722.834  | 1.645883  |
| 5722.934 | 1.665249  | 5722.934  | 1.91026   | 5722.934  | 1.731344  |
| 5723.034 | 1.750114  | 5723.034  | 1.963505  | 5723.034  | 1.797097  |
| 5723.133 | 1.818717  | 5723.133  | 2.019095  | 5723.133  | 1.870279  |
| 5723.234 | 1.857579  | 5723.234  | 2.064177  | 5723.234  | 1.949304  |
| 5723.333 | 1.948372  | 5723.333  | 2.104659  | 5723.333  | 2.008783  |
| 5723.433 | 2.003052  | 5723.433  | 2.135865  | 5723.433  | 2.080534  |
| 5723.534 | 2.045397  | 5723.534  | 2.196232  | 5723.534  | 2.13867   |
| 5723.633 | 2.099893  | 5723.633  | 2.240903  | 5723.633  | 2.186842  |
| 5723.733 | 2.153872  | 5723.733  | 2.271075  | 5723.733  | 2.240596  |
| 5723.834 | 2.206115  | 5723.834  | 2.290284  | 5723.834  | 2.294358  |
| 5723.933 | 2.224132  | 5723.933  | 2.318048  | 5723.933  | 2.333565  |
| 5724.033 | 2.225865  | 5724.033  | 2.33429   | 5724.033  | 2.358129  |
| 5724.133 | 2.275543  | 5724.133  | 2.352603  | 5724.133  | 2.399118  |
| 5724.234 | 2.314314  | 5724.234  | 2.336913  | 5724.234  | 2.44887   |
| 5724.333 | 2.323911  | 5724.333  | 2.343621  | 5724.333  | 2.456654  |
|      |       |       |       |       |
|------|-------|-------|-------|-------|
| 5724.433 | 2.327334 | 5724.433 | 2.346381 | 5724.433 | 2.460103 |
| 5724.534 | 2.324753 | 5724.534 | 2.333947 | 5724.534 | 2.450459 |
| 5724.633 | 2.314721 | 5724.633 | 2.324311 | 5724.633 | 2.479341 |
| 5724.733 | 2.300366 | 5724.733 | 2.317134 | 5724.733 | 2.480631 |
| 5724.833 | 2.299444 | 5724.833 | 2.307406 | 5724.833 | 2.478676 |
| 5724.934 | 2.290503 | 5724.934 | 2.288078 | 5724.934 | 2.454802 |
| 5725.033 | 2.267578 | 5725.033 | 2.266402 | 5725.033 | 2.452832 |
| 5725.133 | 2.239794 | 5725.133 | 2.244537 | 5725.133 | 2.449239 |
| 5725.233 | 2.223054 | 5725.233 | 2.239268 | 5725.233 | 2.431843 |
| 5725.334 | 2.215745 | 5725.334 | 2.194377 | 5725.334 | 2.411477 |
| 5725.433 | 2.202411 | 5725.433 | 2.165802 | 5725.433 | 2.386608 |
| 5725.533 | 2.125912 | 5725.533 | 2.149791 | 5725.533 | 2.381602 |
| 5725.633 | 2.09873 | 5725.633 | 2.126174 | 5725.633 | 2.345603 |
| 5725.734 | 2.095603 | 5725.734 | 2.110465 | 5725.734 | 2.29795 |
| 5725.833 | 2.050547 | 5725.833 | 2.091822 | 5725.833 | 2.280163 |
| 5725.933 | 2.048507 | 5725.933 | 2.046298 | 5725.933 | 2.243554 |
| 5726.033 | 2.030815 | 5726.033 | 2.005855 | 5726.033 | 2.226494 |
| 5726.133 | 2.001097 | 5726.133 | 1.995419 | 5726.133 | 2.214674 |
| 5726.234 | 1.995692 | 5726.234 | 1.982798 | 5726.234 | 2.186836 |
| 5726.333 | 1.960745 | 5726.333 | 1.948379 | 5726.333 | 2.137725 |
| 5726.433 | 1.906068 | 5726.433 | 1.926515 | 5726.433 | 2.104957 |
| 5726.533 | 1.891904 | 5726.533 | 1.912414 | 5726.533 | 2.058111 |
| 5726.633 | 1.891893 | 5726.633 | 1.883567 | 5726.633 | 2.047446 |
| 5726.734 | 1.855933 | 5726.734 | 1.871516 | 5726.734 | 2.042388 |
| 5726.833 | 1.831758 | 5726.833 | 1.847002 | 5726.833 | 2.010362 |
| 5726.933 | 1.84388 | 5726.933 | 1.824339 | 5726.933 | 1.97545 |
| 5727.033 | 1.83605 | 5727.033 | 1.806473 | 5727.033 | 1.939202 |
| 5727.133 | 1.806746 | 5727.133 | 1.800072 | 5727.133 | 1.918869 |
| 5727.234 | 1.788581 | 5727.234 | 1.792582 | 5727.234 | 1.896302 |
| 5727.334 | 1.781501 | 5727.334 | 1.775828 | 5727.334 | 1.874281 |
| 5727.433 | 1.755052 | 5727.433 | 1.74806 | 5727.433 | 1.86733 |
| 5727.533 | 1.742232 | 5727.533 | 1.74382 | 5727.533 | 1.847525 |
| 5727.633 | 1.744148 | 5727.633 | 1.724643 | 5727.633 | 1.822693 |
| 5727.733 | 1.751835 | 5727.733 | 1.701196 | 5727.733 | 1.810089 |
| 5727.833 | 1.748073 | 5727.833 | 1.71253 | 5727.833 | 1.795985 |
| 5727.934 | 1.735921 | 5727.934 | 1.721567 | 5727.934 | 1.786247 |
| 5728.034 | 1.716506 | 5728.034 | 1.698029 | 5728.034 | 1.761349 |
| 5728.133 | 1.716976 | 5728.133 | 1.680949 | 5728.133 | 1.739604 |
| 5728.233 | 1.684712 | 5728.233 | 1.668899 | 5728.233 | 1.732636 |
| 5728.333 | 1.681855 | 5728.333 | 1.661182 | 5728.333 | 1.718161 |
| 5728.433 | 1.690009 | 5728.433 | 1.667081 | 5728.433 | 1.689084 |
| 5728.533 | 1.711446 | 5728.533 | 1.645872 | 5728.533 | 1.697637 |
| 5728.633 | 1.689858 | 5728.633 | 1.628788 | 5728.633 | 1.697613 |
|      |               |               |               |               |              |              |
|------|---------------|---------------|---------------|---------------|--------------|--------------|
| 5728.734 | 1.676063     | 5728.734     | 1.623442     | 5728.734     | 1.686557     |
| 5728.834 | 1.648042     | 5728.834     | 1.616061     | 5728.834     | 1.668642     |
| 5728.934 | 1.630141     | 5728.934     | 1.610178     | 5728.934     | 1.664796     |
| 5729.033 | 1.642995     | 5729.033     | 1.596594     | 5729.033     | 1.651273     |
| 5729.133 | 1.642598     | 5729.133     | 1.587365     | 5729.133     | 1.654898     |
| 5729.233 | 1.630145     | 5729.233     | 1.577438     | 5729.233     | 1.634233     |
| 5729.333 | 1.61782      | 5729.333     | 1.555628     | 5729.333     | 1.614096     |
| 5729.433 | 1.623396     | 5729.433     | 1.551729     | 5729.433     | 1.618086     |
| 5729.533 | 1.629685     | 5729.533     | 1.545467     | 5729.533     | 1.608477     |
| 5729.633 | 1.603552     | 5729.633     | 1.546701     | 5729.633     | 1.606992     |
| 5729.733 | 1.584949     | 5729.733     | 1.543404     | 5729.733     | 1.60248      |
| 5729.833 | 1.572405     | 5729.833     | 1.535904     | 5729.833     | 1.599422     |
| 5729.933 | 1.57209      | 5729.933     | 1.524863     | 5729.933     | 1.584558     |
| 5730.033 | 1.554791     | 5730.033     | 1.522305     | 5730.033     | 1.565477     |
| 5730.134 | 1.567582     | 5730.134     | 1.51468      | 5730.134     | 1.564008     |
| 5730.234 | 1.558673     | 5730.234     | 1.499821     | 5730.234     | 1.567857     |
| 5730.334 | 1.539505     | 5730.334     | 1.49763      | 5730.334     | 1.554084     |
| 5730.434 | 1.529545     | 5730.434     | 1.495195     | 5730.434     | 1.523958     |
| 5730.534 | 1.537564     | 5730.534     | 1.484019     | 5730.534     | 1.52494      |
| 5730.634 | 1.512084     | 5730.634     | 1.469692     | 5730.634     | 1.52127      |
| 5730.734 | 1.493798     | 5730.734     | 1.46746      | 5730.734     | 1.505928     |
| 5730.834 | 1.489896     | 5730.834     | 1.459697     | 5730.834     | 1.509345     |
| 5730.934 | 1.507663     | 5730.934     | 1.450102     | 5730.934     | 1.503567     |
| 5731.067 | 1.485729     | 5731.067     | 1.443281     | 5731.067     | 1.504822     |
| 5731.267 | 1.464088     | 5731.267     | 1.437407     | 5731.267     | 1.498632     |
| 5731.467 | 1.463381     | 5731.467     | 1.424542     | 5731.467     | 1.469509     |
| 5731.667 | 1.447526     | 5731.667     | 1.415361     | 5731.667     | 1.450015     |
| 5731.867 | 1.460096     | 5731.867     | 1.405655     | 5731.867     | 1.451316     |
| 5732.067 | 1.444843     | 5732.067     | 1.393199     | 5732.067     | 1.449852     |
| 5732.266 | 1.425941     | 5732.266     | 1.396249     | 5732.266     | 1.446159     |
| 5732.466 | 1.420983     | 5732.466     | 1.401864     | 5732.466     | 1.445888     |
| 5732.667 | 1.437828     | 5732.667     | 1.393147     | 5732.667     | 1.420615     |
| 5732.867 | 1.407201     | 5732.867     | 1.37969      | 5732.867     | 1.413132     |
| 5733.067 | 1.390714     | 5733.067     | 1.380908     | 5733.067     | 1.416696     |
| 5733.267 | 1.404243     | 5733.267     | 1.393268     | 5733.267     | 1.417195     |
| 5733.467 | 1.433662     | 5733.467     | 1.388628     | 5733.467     | 1.41216      |
| 5733.667 | 1.422591     | 5733.667     | 1.393094     | 5733.667     | 1.401748     |
| 5733.867 | 1.435746     | 5733.867     | 1.404324     | 5733.867     | 1.403631     |
| 5734.067 | 1.431296     | 5734.067     | 1.399113     | 5734.067     | 1.403843     |
| 5734.267 | 1.44495      | 5734.267     | 1.414549     | 5734.267     | 1.41274      |
| 5734.466 | 1.439966     | 5734.466     | 1.427857     | 5734.466     | 1.416946     |
| 5734.667 | 1.469445     | 5734.667     | 1.436223     | 5734.667     | 1.420339     |
| 5734.867 | 1.481291     | 5734.867     | 1.456862     | 5734.867     | 1.434379     |
| 5735.066 | 1.504403 | 5735.066 | 1.481628 | 5735.066 | 1.439404 |
| 5735.267 | 1.514012 | 5735.267 | 1.49707  | 5735.267 | 1.451353 |
| 5735.467 | 1.53427  | 5735.467 | 1.527198 | 5735.467 | 1.461496 |
| 5735.667 | 1.573051 | 5735.667 | 1.542132 | 5735.667 | 1.477328 |
| 5735.866 | 1.609733 | 5735.866 | 1.577531 | 5735.866 | 1.489504 |
| 5736.066 | 1.635532 | 5736.066 | 1.597861 | 5736.066 | 1.509464 |
| 5736.267 | 1.665668 | 5736.267 | 1.633678 | 5736.267 | 1.518246 |
| 5736.467 | 1.674368 | 5736.467 | 1.651989 | 5736.467 | 1.541563 |
| 5736.667 | 1.673519 | 5736.667 | 1.650554 | 5736.667 | 1.561175 |
| 5736.867 | 1.687158 | 5736.867 | 1.644976 | 5736.867 | 1.574723 |
| 5737.067 | 1.656801 | 5737.067 | 1.648333 | 5737.067 | 1.581612 |
| 5737.267 | 1.631543 | 5737.267 | 1.630172 | 5737.267 | 1.565953 |
| 5737.467 | 1.640175 | 5737.467 | 1.607476 | 5737.467 | 1.558047 |
| 5737.667 | 1.579039 | 5737.667 | 1.572711 | 5737.667 | 1.544362 |
| 5737.867 | 1.544648 | 5737.867 | 1.532678 | 5737.867 | 1.51289 |
| 5738.066 | 1.511147 | 5738.066 | 1.501799 | 5738.066 | 1.474336 |
| 5738.267 | 1.455046 | 5738.267 | 1.465963 | 5738.267 | 1.450393 |
| 5738.467 | 1.410767 | 5738.467 | 1.414895 | 5738.467 | 1.419946 |
| 5738.667 | 1.360701 | 5738.667 | 1.360159 | 5738.667 | 1.379286 |
| 5738.867 | 1.308827 | 5738.867 | 1.311669 | 5738.867 | 1.328974 |
| 5739.066 | 1.278142 | 5739.066 | 1.27099  | 5739.066 | 1.285321 |
| 5739.267 | 1.227225 | 5739.267 | 1.239504 | 5739.267 | 1.243732 |
| 5739.467 | 1.189092 | 5739.467 | 1.196153 | 5739.467 | 1.220922 |
| 5739.667 | 1.146883 | 5739.667 | 1.156736 | 5739.667 | 1.17903 |
| 5739.867 | 1.1055  | 5739.867 | 1.12356  | 5739.867 | 1.154912 |
| 5740.067 | 1.081079 | 5740.067 | 1.094273 | 5740.067 | 1.120674 |
| 5740.267 | 1.078528 | 5740.267 | 1.072423 | 5740.267 | 1.092283 |
| 5740.466 | 1.062976 | 5740.466 | 1.074734 | 5740.466 | 1.064816 |
| 5740.666 | 1.050826 | 5740.666 | 1.054197 | 5740.666 | 1.04931 |
| 5740.866 | 1.029386 | 5740.866 | 1.041992 | 5740.866 | 1.043556 |
| 5741.067 | 1.027976 | 5741.067 | 1.023663 | 5741.067 | 1.016264 |
| 5741.267 | 1.009684 | 5741.267 | 1.030843 | 5741.267 | 1.008097 |
| 5741.467 | 0.98014  | 5741.467 | 1.025581 | 5741.467 | 1.002799 |
| 5741.667 | 0.992159 | 5741.667 | 1.010304 | 5741.667 | 0.993497 |
| 5741.867 | 0.985707 | 5741.867 | 1.01648  | 5741.867 | 0.986546 |
| 5742.066 | 0.979977 | 5742.066 | 1.012296 | 5742.066 | 0.982667 |
| 5742.266 | 0.999912 | 5742.266 | 1.015224 | 5742.266 | 0.981442 |
| 5742.466 | 0.992392 | 5742.466 | 1.015821 | 5742.466 | 0.982353 |
| 5742.666 | 0.993816 | 5742.666 | 1.008703 | 5742.666 | 0.976056 |
| 5742.866 | 1.005895 | 5742.866 | 1.008584 | 5742.866 | 0.976337 |
| 5743.666 | 0.998657 | 5743.666 | 1.013293 | 5743.666 | 0.974343 |
| 5745.667 | 0.972681 | 5745.667 | 1.009797 | 5745.667 | 0.959318 |
| 5747.667 | 0.979779 | 5747.667 | 1.009851 | 5747.667 | 0.964442 |
| 5749.033 | 0.95347 | 5749.033 | 1.020622 | 5749.033 | 0.975735 |
| 5749.134 | 0.955658 | 5749.134 | 1.017867 | 5749.134 | 0.967079 |
| 5749.233 | 0.96586 | 5749.233 | 1.013228 | 5749.233 | 0.97841 |
| 5749.333 | 0.976284 | 5749.333 | 1.010499 | 5749.333 | 0.975577 |
| 5749.433 | 0.97737 | 5749.433 | 1.016418 | 5749.433 | 0.972456 |
| 5749.534 | 0.972746 | 5749.534 | 1.014353 | 5749.534 | 0.96726 |
| 5749.634 | 0.974048 | 5749.634 | 1.016743 | 5749.634 | 0.980481 |
| 5749.733 | 0.951713 | 5749.733 | 1.020972 | 5749.733 | 0.990051 |
| 5749.833 | 0.967322 | 5749.833 | 1.027143 | 5749.833 | 0.980776 |
| 5749.933 | 0.969594 | 5749.933 | 1.026298 | 5749.933 | 0.966185 |
| 5750.034 | 0.95525 | 5750.034 | 1.023665 | 5750.034 | 0.976012 |
| 5750.134 | 0.960027 | 5750.134 | 1.029473 | 5750.134 | 0.97056 |
| 5750.234 | 0.976767 | 5750.233 | 1.035913 | 5750.233 | 0.96649 |
| 5750.333 | 0.973327 | 5750.333 | 1.039532 | 5750.333 | 0.979514 |
| 5750.433 | 0.989109 | 5750.433 | 1.018296 | 5750.433 | 0.981187 |
| 5750.534 | 0.983708 | 5750.534 | 1.024145 | 5750.534 | 0.965611 |
| 5750.634 | 0.974674 | 5750.634 | 1.030404 | 5750.634 | 0.978098 |
| 5750.733 | 0.969174 | 5750.733 | 1.031185 | 5750.733 | 0.993613 |
| 5750.833 | 0.956196 | 5750.833 | 1.034756 | 5750.833 | 0.99675 |
| 5750.933 | 0.976855 | 5750.933 | 1.031869 | 5750.933 | 0.999647 |
| 5751.033 | 0.985064 | 5751.033 | 1.028481 | 5751.033 | 0.988473 |
| 5751.133 | 0.976287 | 5751.133 | 1.022547 | 5751.133 | 0.985516 |
| 5751.234 | 0.986078 | 5751.234 | 1.023432 | 5751.234 | 0.99199 |
| 5751.333 | 0.988615 | 5751.333 | 1.033846 | 5751.333 | 0.993036 |
| 5751.433 | 0.980908 | 5751.433 | 1.033522 | 5751.433 | 0.989596 |
| 5751.533 | 0.980654 | 5751.533 | 1.037108 | 5751.533 | 0.995647 |
| 5751.633 | 0.990503 | 5751.633 | 1.037753 | 5751.633 | 0.993576 |
| 5751.733 | 0.983098 | 5751.733 | 1.042436 | 5751.733 | 0.99288 |
| 5751.833 | 0.973904 | 5751.833 | 1.03854 | 5751.833 | 0.999074 |
| 5751.934 | 0.991081 | 5751.934 | 1.037277 | 5751.934 | 0.99296 |
| 5752.034 | 0.99875 | 5752.034 | 1.04551 | 5752.034 | 0.997341 |
| 5752.133 | 0.987277 | 5752.133 | 1.048347 | 5752.133 | 0.996292 |
| 5752.233 | 0.970644 | 5752.233 | 1.040505 | 5752.233 | 0.990164 |
| 5752.333 | 0.988785 | 5752.333 | 1.046124 | 5752.966 | 1.007254 |
| 5752.433 | 0.976106 | 5752.433 | 1.050533 | 5754.966 | 1.022043 |
| 5752.533 | 0.971318 | 5752.533 | 1.051267 | 5756.967 | 1.042348 |
| 5752.633 | 0.987521 | 5752.633 | 1.048567 | 5758.967 | 1.058243 |
| 5752.733 | 1.001996 | 5752.733 | 1.053199 | 5761.966 | 1.066126 |
| 5752.833 | 0.990001 | 5752.833 | 1.043525 | 5766.966 | 1.063166 |
| 5752.934 | 0.996856 | 5752.934 | 1.035409 | 5771.967 | 1.074787 |
| 5753.034 | 0.999537 | 5753.034 | 1.039785 | 5776.967 | 1.062527 |
| 5753.134 | 0.982594 | 5753.134 | 1.042761 | 5781.966 | 1.059871 |
| 5753.234 | 0.975726 | 5753.234 | 1.043046 | 5786.967 | 1.0613 |
| E(eV) | [2-K]$_4$ | [2-Rb]$_4$ | [2-Cs]$_4$ |
|------|-----------|-----------|-----------|
|      | Normalized HERFD | Normalized HERFD | Normalized HERFD |
| 5680 | -7.83E-05 | 1.69E-04 | 4.17E-04 |
| 5681.334 | 8.2E-05 | 2.07E-04 | -4.62E-04 |
| 5682.333 | 0.00027 | 4.65E-05 | -5.80E-05 |
| 5683.333 | -5.61E-05 | -1.78E-04 | -1.99E-04 |
| 5684.334 | -9.66E-05 | -1.73E-04 | -8.78E-05 |
| 5685.334 | -2.05E-05 | -1.50E-05 | -7.14E-06 |
| 5686.333 | 0.000117 | -5.06E-05 | -1.12E-04 |
| 5687.333 | -6.04E-05 | -2.83E-05 | 1.13E-05 |
| 5688.334 | -5.94E-05 | -8.87E-06 | -2.40E-04 |
| 5689.334 | -8.14E-05 | -2.94E-04 | -1.73E-05 |
| 5690.334 | 0.000147 | -5.22E-05 | -3.25E-04 |
| 5691.333 | 5.85E-05 | 5.37E-05 | 1.76E-04 |
| 5692.333 | -3.87E-05 | -9.36E-06 | 4.29E-04 |
|                |        |        |        |        |
|----------------|--------|--------|--------|--------|
| 5693.333       | -7.02E-05 | 5693.333 | -8.45E-05 | 5693.333 | 1.06E-04 |
| 5694.333       | 6.34E-05  | 5694.333 | 4.35E-05  | 5694.333 | 1.12E-04 |
| 5695.334       | 0.000117  | 5695.334 | 1.09E-04  | 5695.334 | 1.91E-05 |
| 5696.334       | -3.72E-05 | 5696.334 | 1.79E-05  | 5696.334 | 3.64E-04 |
| 5697.333       | -4.08E-05 | 5697.333 | -8.17E-05 | 5697.333 | 9.07E-05 |
| 5698.334       | -0.000115 | 5698.334 | 1.90E-04  | 5698.334 | 5.99E-05 |
| 5699.334       | -0.000124 | 5699.334 | 1.80E-04  | 5699.334 | 1.19E-04 |
| 5700.334       | 3.94E-05  | 5700.334 | 1.46E-04  | 5700.334 | 2.50E-04 |
| 5701.334       | -4.94E-05 | 5701.334 | -2.08E-05 | 5701.334 | 8.38E-05 |
| 5702.334       | -0.000124 | 5702.334 | 2.40E-06  | 5702.334 | 2.89E-04 |
| 5703.334       | -4.75E-05 | 5703.334 | 2.33E-05  | 5703.334 | -5.45E-05 |
| 5704.334       | -0.000143 | 5704.334 | 1.15E-04  | 5704.334 | 1.18E-04 |
| 5705.334       | -6.64E-05 | 5705.334 | 1.04E-04  | 5705.334 | 3.52E-04 |
| 5706.334       | 4.36E-05  | 5706.334 | 9.21E-05  | 5706.334 | 1.65E-04 |
| 5707.334       | 0.000129  | 5707.334 | -7.76E-05 | 5707.334 | 4.81E-04 |
| 5708.334       | 8.68E-05  | 5708.334 | 8.82E-05  | 5708.334 | -1.03E-05 |
| 5709.334       | 9.63E-05  | 5709.334 | 1.56E-04  | 5709.334 | -6.47E-05 |
| 5710.334       | 0.000418  | 5710.334 | 1.52E-05  | 5710.334 | 5.97E-04 |
| 5711.334       | 0.000389  | 5711.334 | 1.82E-04  | 5711.334 | 5.85E-05 |
| 5712.334       | 0.000411  | 5712.334 | 5.98E-04  | 5712.334 | -4.53E-05 |
| 5713.334       | 0.00068   | 5713.334 | 7.11E-04  | 5713.334 | 8.59E-04 |
| 5714.034       | 0.001263  | 5714.034 | 1.11E-03  | 5714.034 | 1.42E-03 |
| 5714.133       | 0.001452  | 5714.133 | 1.07E-03  | 5714.133 | 1.13E-03 |
| 5714.233       | 0.001637  | 5714.233 | 1.35E-03  | 5714.233 | 1.33E-03 |
| 5714.334       | 0.00192   | 5714.334 | 1.87E-03  | 5714.334 | 1.81E-03 |
| 5714.433       | 0.002271  | 5714.433 | 1.43E-03  | 5714.433 | 1.95E-03 |
| 5714.533       | 0.002598  | 5714.533 | 1.46E-03  | 5714.533 | 1.83E-03 |
| 5714.634       | 0.003436  | 5714.634 | 2.18E-03  | 5714.634 | 2.34E-03 |
| 5714.733       | 0.003919  | 5714.733 | 2.79E-03  | 5714.733 | 4.02E-03 |
| 5714.833       | 0.004586  | 5714.833 | 2.68E-03  | 5714.833 | 4.55E-03 |
| 5714.934       | 0.00558   | 5714.934 | 2.99E-03  | 5714.934 | 5.10E-03 |
| 5715.034       | 0.006769  | 5715.034 | 4.07E-03  | 5715.034 | 5.39E-03 |
| 5715.133       | 0.00784   | 5715.133 | 5.00E-03  | 5715.133 | 5.22E-03 |
| 5715.233       | 0.009122  | 5715.233 | 5.57E-03  | 5715.233 | 6.85E-03 |
| 5715.334       | 0.010713  | 5715.334 | 6.45E-03  | 5715.334 | 8.47E-03 |
| 5715.433       | 0.012554  | 5715.433 | 7.56E-03  | 5715.433 | 1.03E-02 |
| 5715.534       | 0.015022  | 5715.534 | 7.84E-03  | 5715.534 | 1.08E-02 |
| 5715.634       | 0.017422  | 5715.634 | 9.45E-03  | 5715.634 | 1.28E-02 |
| 5715.733       | 0.020967  | 5715.733 | 1.09E-02  | 5715.733 | 1.50E-02 |
| 5715.834       | 0.024137  | 5715.834 | 1.21E-02  | 5715.834 | 1.58E-02 |
| 5715.934       | 0.025903  | 5715.934 | 1.35E-02  | 5715.934 | 1.73E-02 |
| 5716.033       | 0.028552  | 5716.033 | 1.54E-02  | 5716.033 | 2.03E-02 |
| 5716.134       | 0.031863  | 5716.134 | 1.71E-02  | 5716.134 | 2.18E-02 |
|   |      |      |      |      |      |      |      |
|---|------|------|------|------|------|------|------|
|   | 5716.234 | 0.034197 | 5716.234 | 1.92E-02 | 5716.234 | 2.45E-02 |
|   | 5716.333 | 0.036217 | 5716.333 | 2.16E-02 | 5716.333 | 2.34E-02 |
|   | 5716.433 | 0.038576 | 5716.433 | 2.47E-02 | 5716.433 | 2.73E-02 |
|   | 5716.533 | 0.040098 | 5716.533 | 2.91E-02 | 5716.533 | 3.09E-02 |
|   | 5716.634 | 0.040824 | 5716.634 | 3.37E-02 | 5716.634 | 3.14E-02 |
|   | 5716.733 | 0.043297 | 5716.733 | 3.89E-02 | 5716.733 | 3.66E-02 |
|   | 5716.833 | 0.045267 | 5716.833 | 4.81E-02 | 5716.833 | 4.48E-02 |
|   | 5716.934 | 0.050073 | 5716.934 | 5.84E-02 | 5716.934 | 5.12E-02 |
|   | 5717.034 | 0.055943 | 5717.034 | 7.22E-02 | 5717.034 | 5.95E-02 |
|   | 5717.134 | 0.062752 | 5717.134 | 8.65E-02 | 5717.134 | 6.82E-02 |
|   | 5717.233 | 0.073818 | 5717.233 | 0.103055 | 5717.233 | 7.99E-02 |
|   | 5717.333 | 0.086181 | 5717.333 | 0.121111 | 5717.333 | 9.55E-02 |
|   | 5717.433 | 0.097419 | 5717.433 | 0.143541 | 5717.433 | 0.114968 |
|   | 5717.533 | 0.111861 | 5717.533 | 0.166232 | 5717.533 | 0.133718 |
|   | 5717.634 | 0.126053 | 5717.634 | 0.185237 | 5717.634 | 0.148032 |
|   | 5717.734 | 0.142265 | 5717.734 | 0.202743 | 5717.734 | 0.160296 |
|   | 5717.834 | 0.156936 | 5717.834 | 0.222009 | 5717.834 | 0.180097 |
|   | 5717.934 | 0.172726 | 5717.934 | 0.236061 | 5717.934 | 0.189792 |
|   | 5718.033 | 0.183451 | 5718.033 | 0.241061 | 5718.033 | 0.193241 |
|   | 5718.133 | 0.191507 | 5718.133 | 0.240581 | 5718.133 | 0.199034 |
|   | 5718.233 | 0.198127 | 5718.233 | 0.2365 | 5718.233 | 0.199394 |
|   | 5718.334 | 0.200467 | 5718.334 | 0.229103 | 5718.334 | 0.194802 |
|   | 5718.434 | 0.198427 | 5718.434 | 0.21923 | 5718.434 | 0.18957 |
|   | 5718.534 | 0.192488 | 5718.534 | 0.209686 | 5718.534 | 0.179033 |
|   | 5718.634 | 0.186766 | 5718.634 | 0.195437 | 5718.634 | 0.167785 |
|   | 5718.733 | 0.180671 | 5718.733 | 0.181673 | 5718.733 | 0.15642 |
|   | 5718.834 | 0.170565 | 5718.834 | 0.16795 | 5718.834 | 0.150546 |
|   | 5718.934 | 0.161981 | 5718.934 | 0.152111 | 5718.934 | 0.144173 |
|   | 5719.034 | 0.153771 | 5719.034 | 0.142241 | 5719.034 | 0.138684 |
|   | 5719.134 | 0.144504 | 5719.134 | 0.128026 | 5719.134 | 0.123541 |
|   | 5719.233 | 0.1355 | 5719.233 | 0.115206 | 5719.233 | 0.109434 |
|   | 5719.333 | 0.128245 | 5719.333 | 0.107411 | 5719.333 | 0.103502 |
|   | 5719.434 | 0.120837 | 5719.434 | 0.100365 | 5719.434 | 0.103622 |
|   | 5719.533 | 0.117586 | 5719.533 | 9.52E-02 | 5719.533 | 9.91E-02 |
|   | 5719.634 | 0.115187 | 5719.634 | 9.17E-02 | 5719.634 | 9.47E-02 |
|   | 5719.733 | 0.114228 | 5719.733 | 9.07E-02 | 5719.733 | 9.36E-02 |
|   | 5719.834 | 0.116804 | 5719.834 | 8.91E-02 | 5719.834 | 9.52E-02 |
|   | 5719.934 | 0.11941 | 5719.934 | 9.21E-02 | 5719.934 | 9.76E-02 |
|   | 5720.034 | 0.123304 | 5720.034 | 9.40E-02 | 5720.034 | 9.66E-02 |
|   | 5720.134 | 0.131886 | 5720.134 | 9.66E-02 | 5720.134 | 1.06728 |
|   | 5720.234 | 0.142917 | 5720.234 | 0.100595 | 5720.234 | 0.118912 |
|   | 5720.333 | 0.155441 | 5720.333 | 0.107825 | 5720.333 | 0.126437 |
|   | 5720.433 | 0.171574 | 5720.433 | 0.115498 | 5720.433 | 0.136015 |
|     |       |       |       |       |       |
|-----|-------|-------|-------|-------|-------|
| 5720.533 | 0.195832 | 5720.533 | 0.127099 | 5720.533 | 0.151017 |
| 5720.633 | 0.219212 | 5720.633 | 0.137458 | 5720.633 | 0.17326 |
| 5720.733 | 0.2455 | 5720.733 | 0.150665 | 5720.733 | 0.196201 |
| 5720.833 | 0.274996 | 5720.833 | 0.165486 | 5720.833 | 0.212259 |
| 5720.934 | 0.305858 | 5720.934 | 0.176476 | 5720.934 | 0.225304 |
| 5721.034 | 0.341592 | 5721.034 | 0.189283 | 5721.034 | 0.248469 |
| 5721.134 | 0.37954 | 5721.134 | 0.208017 | 5721.134 | 0.283561 |
| 5721.233 | 0.418958 | 5721.233 | 0.225417 | 5721.233 | 0.307953 |
| 5721.333 | 0.465406 | 5721.333 | 0.242999 | 5721.333 | 0.324916 |
| 5721.433 | 0.508921 | 5721.433 | 0.259158 | 5721.433 | 0.352148 |
| 5721.533 | 0.549536 | 5721.533 | 0.274171 | 5721.533 | 0.387496 |
| 5721.634 | 0.586687 | 5721.634 | 0.293144 | 5721.634 | 0.415255 |
| 5721.733 | 0.62861 | 5721.733 | 0.319195 | 5721.733 | 0.441759 |
| 5721.833 | 0.667527 | 5721.833 | 0.34326 | 5721.833 | 0.474312 |
| 5721.933 | 0.706408 | 5721.933 | 0.36964 | 5721.933 | 0.50985 |
| 5722.033 | 0.748384 | 5722.033 | 0.404437 | 5722.033 | 0.546996 |
| 5722.134 | 0.789966 | 5722.134 | 0.441219 | 5722.134 | 0.602186 |
| 5722.233 | 0.832312 | 5722.233 | 0.483449 | 5722.233 | 0.657056 |
| 5722.333 | 0.876237 | 5722.333 | 0.534301 | 5722.333 | 0.690199 |
| 5722.434 | 0.92814 | 5722.434 | 0.594553 | 5722.434 | 0.73203 |
| 5722.533 | 0.985593 | 5722.533 | 0.657062 | 5722.533 | 0.802228 |
| 5722.633 | 1.047997 | 5722.633 | 0.731426 | 5722.633 | 0.882735 |
| 5722.733 | 1.115569 | 5722.733 | 0.810629 | 5722.733 | 0.966657 |
| 5722.834 | 1.190181 | 5722.834 | 0.898035 | 5722.834 | 1.062366 |
| 5722.934 | 1.270306 | 5722.934 | 1.000318 | 5722.934 | 1.152057 |
| 5723.033 | 1.351698 | 5723.033 | 1.102507 | 5723.033 | 1.24099 |
| 5723.133 | 1.443081 | 5723.133 | 1.207454 | 5723.133 | 1.350488 |
| 5723.234 | 1.534745 | 5723.234 | 1.3162 | 5723.234 | 1.450643 |
| 5723.333 | 1.625287 | 5723.333 | 1.418477 | 5723.333 | 1.552819 |
| 5723.433 | 1.716839 | 5723.433 | 1.518055 | 5723.433 | 1.652558 |
| 5723.534 | 1.80936 | 5723.534 | 1.618617 | 5723.534 | 1.748161 |
| 5723.633 | 1.898487 | 5723.633 | 1.702422 | 5723.633 | 1.84359 |
| 5723.733 | 1.979726 | 5723.733 | 1.785289 | 5723.733 | 1.945627 |
| 5723.834 | 2.048657 | 5723.834 | 1.854367 | 5723.834 | 2.046075 |
| 5723.933 | 2.121745 | 5723.933 | 1.92756 | 5723.933 | 2.119167 |
| 5724.033 | 2.188074 | 5724.033 | 1.998552 | 5724.033 | 2.186863 |
| 5724.133 | 2.245525 | 5724.133 | 2.048423 | 5724.133 | 2.261099 |
| 5724.234 | 2.286807 | 5724.234 | 2.096754 | 5724.234 | 2.30203 |
| 5724.333 | 2.333307 | 5724.333 | 2.144606 | 5724.333 | 2.325877 |
| 5724.433 | 2.370751 | 5724.433 | 2.172969 | 5724.433 | 2.376807 |
| 5724.534 | 2.400095 | 5724.534 | 2.192943 | 5724.534 | 2.400536 |
| 5724.633 | 2.416801 | 5724.633 | 2.20182 | 5724.633 | 2.418454 |
| 5724.733 | 2.432196 | 5724.733 | 2.209096 | 5724.733 | 2.430029 |
| 5724.833 | 2.430977 | 5724.833 | 2.196509 | 5724.833 | 2.417825 |
| 5724.934 | 2.425363 | 5724.934 | 2.178859 | 5724.934 | 2.397697 |
| 5725.033 | 2.413702 | 5725.033 | 2.160752 | 5725.033 | 2.361923 |
| 5725.133 | 2.393716 | 5725.133 | 2.137129 | 5725.133 | 2.332598 |
| 5725.233 | 2.374926 | 5725.233 | 2.103657 | 5725.233 | 2.319668 |
| 5725.334 | 2.350233 | 5725.334 | 2.081085 | 5725.334 | 2.300872 |
| 5725.433 | 2.319214 | 5725.433 | 2.060451 | 5725.433 | 2.245042 |
| 5725.533 | 2.274731 | 5725.533 | 2.019226 | 5725.533 | 2.220206 |
| 5725.633 | 2.247448 | 5725.633 | 1.986192 | 5725.633 | 2.210704 |
| 5725.734 | 2.221276 | 5725.734 | 1.959954 | 5725.734 | 2.156557 |
| 5725.833 | 2.184051 | 5725.833 | 1.931308 | 5725.833 | 2.126081 |
| 5725.933 | 2.149735 | 5725.933 | 1.896939 | 5725.933 | 2.088646 |
| 5726.033 | 2.11802 | 5726.033 | 1.85966 | 5726.033 | 2.058235 |
| 5726.133 | 2.085558 | 5726.133 | 1.842043 | 5726.133 | 2.03794 |
| 5726.234 | 2.05387 | 5726.234 | 1.815949 | 5726.234 | 1.98741 |
| 5726.333 | 2.017907 | 5726.333 | 1.788891 | 5726.333 | 1.946084 |
| 5726.433 | 1.982859 | 5726.433 | 1.756806 | 5726.433 | 1.89903 |
| 5726.533 | 1.949397 | 5726.533 | 1.731012 | 5726.533 | 1.891292 |
| 5726.633 | 1.913217 | 5726.633 | 1.710081 | 5726.633 | 1.847943 |
| 5726.734 | 1.874442 | 5726.734 | 1.688309 | 5726.734 | 1.806573 |
| 5726.833 | 1.842247 | 5726.833 | 1.658396 | 5726.833 | 1.792974 |
| 5726.933 | 1.816776 | 5726.933 | 1.64299 | 5726.933 | 1.786141 |
| 5727.033 | 1.788837 | 5727.033 | 1.626353 | 5727.033 | 1.754647 |
| 5727.133 | 1.759233 | 5727.133 | 1.624715 | 5727.133 | 1.735003 |
| 5727.234 | 1.732483 | 5727.234 | 1.610602 | 5727.234 | 1.723793 |
| 5727.334 | 1.7004 | 5727.334 | 1.595836 | 5727.334 | 1.703667 |
| 5727.433 | 1.674785 | 5727.433 | 1.58375 | 5727.433 | 1.693359 |
| 5727.533 | 1.65727 | 5727.533 | 1.57054 | 5727.533 | 1.675556 |
| 5727.633 | 1.635017 | 5727.633 | 1.56576 | 5727.633 | 1.675318 |
| 5727.733 | 1.616595 | 5727.733 | 1.563042 | 5727.733 | 1.660105 |
| 5727.833 | 1.597963 | 5727.833 | 1.54856 | 5727.833 | 1.649879 |
| 5727.934 | 1.579799 | 5727.934 | 1.545948 | 5727.934 | 1.640335 |
| 5728.034 | 1.56558 | 5728.034 | 1.543391 | 5728.034 | 1.646746 |
| 5728.133 | 1.562172 | 5728.133 | 1.541088 | 5728.133 | 1.633756 |
| 5728.233 | 1.549498 | 5728.233 | 1.543629 | 5728.233 | 1.630647 |
| 5728.333 | 1.540896 | 5728.333 | 1.537819 | 5728.333 | 1.637093 |
| 5728.433 | 1.533139 | 5728.433 | 1.542899 | 5728.433 | 1.629638 |
| 5728.533 | 1.52954 | 5728.533 | 1.542199 | 5728.533 | 1.631593 |
| 5728.633 | 1.524595 | 5728.633 | 1.546031 | 5728.633 | 1.623987 |
| 5728.734 | 1.519603 | 5728.734 | 1.538812 | 5728.734 | 1.619239 |
| 5728.834 | 1.512554 | 5728.834 | 1.545859 | 5728.834 | 1.626531 |
| 5728.934 | 1.504049 | 5728.934 | 1.547811 | 5728.934 | 1.612796 |
| 5729.033 | 1.504506 | 5729.033 | 1.53494 | 5729.033 | 1.619416 |
| 5729.133 | 1.500911 | 5729.133 | 1.540082 | 5729.133 | 1.612609 |
| 5729.233 | 1.501727 | 5729.233 | 1.548273 | 5729.233 | 1.609607 |
| 5729.333 | 1.495069 | 5729.333 | 1.546501 | 5729.333 | 1.619954 |
| 5729.433 | 1.489105 | 5729.433 | 1.539108 | 5729.433 | 1.635474 |
| 5729.533 | 1.482224 | 5729.533 | 1.542818 | 5729.533 | 1.614979 |
| 5729.633 | 1.481069 | 5729.633 | 1.552068 | 5729.633 | 1.623977 |
| 5729.733 | 1.479906 | 5729.733 | 1.542437 | 5729.733 | 1.619951 |
| 5729.833 | 1.480971 | 5729.833 | 1.536641 | 5729.833 | 1.595092 |
| 5729.933 | 1.470507 | 5729.933 | 1.528335 | 5729.933 | 1.599044 |
| 5730.033 | 1.469074 | 5730.033 | 1.527978 | 5730.033 | 1.587026 |
| 5730.134 | 1.467868 | 5730.134 | 1.527768 | 5730.134 | 1.579141 |
| 5730.234 | 1.461425 | 5730.234 | 1.534446 | 5730.234 | 1.592529 |
| 5730.334 | 1.453874 | 5730.334 | 1.530735 | 5730.334 | 1.588406 |
| 5730.434 | 1.453334 | 5730.434 | 1.524089 | 5730.434 | 1.594239 |
| 5730.534 | 1.451069 | 5730.534 | 1.515574 | 5730.534 | 1.584653 |
| 5730.634 | 1.446692 | 5730.634 | 1.512541 | 5730.634 | 1.567023 |
| 5730.734 | 1.439207 | 5730.734 | 1.511266 | 5730.734 | 1.562881 |
| 5730.834 | 1.436619 | 5730.834 | 1.509585 | 5730.834 | 1.537816 |
| 5730.934 | 1.430649 | 5730.934 | 1.50157 | 5730.934 | 1.559899 |
| 5731.134 | 1.425398 | 5731.067 | 1.500399 | 5731.067 | 1.550292 |
| 5731.234 | 1.407369 | 5731.267 | 1.491571 | 5731.267 | 1.54104 |
| 5731.334 | 1.395373 | 5731.467 | 1.480645 | 5731.467 | 1.517188 |
| 5732.333 | 1.378749 | 5731.667 | 1.473128 | 5731.667 | 1.499145 |
| 5732.733 | 1.367115 | 5731.867 | 1.46961 | 5731.867 | 1.493902 |
| 5733.133 | 1.347039 | 5732.067 | 1.456631 | 5732.067 | 1.486257 |
| 5733.534 | 1.334082 | 5732.266 | 1.442168 | 5732.266 | 1.482532 |
| 5733.934 | 1.321657 | 5732.466 | 1.439607 | 5732.466 | 1.480317 |
| 5734.334 | 1.305025 | 5732.667 | 1.430629 | 5732.667 | 1.464633 |
| 5734.733 | 1.297529 | 5732.867 | 1.426263 | 5732.867 | 1.442465 |
| 5735.133 | 1.286058 | 5733.067 | 1.417425 | 5733.067 | 1.447091 |
| 5735.534 | 1.283166 | 5733.267 | 1.410392 | 5733.267 | 1.440277 |
| 5735.933 | 1.297726 | 5733.467 | 1.400252 | 5733.467 | 1.437174 |
| 5736.334 | 1.325724 | 5733.667 | 1.397227 | 5733.667 | 1.423821 |
| 5736.733 | 1.339407 | 5733.867 | 1.386939 | 5733.867 | 1.408215 |
| 5737.133 | 1.359206 | 5734.067 | 1.380466 | 5734.067 | 1.407793 |
| 5737.533 | 1.367234 | 5734.267 | 1.378752 | 5734.267 | 1.414789 |
| 5737.933 | 1.347796 | 5734.466 | 1.377919 | 5734.466 | 1.404868 |
| 5738.334 | 1.304101 | 5734.667 | 1.37429 | 5734.667 | 1.411031 |
| 5738.733 | 1.250329 | 5734.867 | 1.373066 | 5734.867 | 1.415833 |
| 5739.133 | 1.178568 | 5735.066 | 1.379828 | 5735.066 | 1.421776 |
| 5739.533 | 1.112475 | 5735.267 | 1.384459 | 5735.267 | 1.417833 |
| 5739.933 | 1.06525 | 5735.467 | 1.38244 | 5735.467 | 1.409894 |
| 5740.334 | 1.0346 | 5735.667 | 1.397042 | 5735.667 | 1.413177 |
|      |         |         |         |         |         |
|------|---------|---------|---------|---------|---------|
| 5740.733 | 1.007871 | 5735.866 | 1.416205 | 5735.866 | 1.420711 |
| 5741.134 | 0.986312 | 5736.066 | 1.413517 | 5736.066 | 1.436972 |
| 5741.533 | 0.974753 | 5736.267 | 1.431157 | 5736.267 | 1.461224 |
| 5741.933 | 0.957858 | 5736.467 | 1.45469  | 5736.467 | 1.483896 |
| 5742.333 | 0.946274 | 5736.666 | 1.475554 | 5736.666 | 1.497349 |
| 5743.666 | 0.939641 | 5737.066 | 1.493966 | 5737.066 | 1.517835 |
| 5744.933 | 0.935404 | 5737.267 | 1.50595  | 5737.267 | 1.504339 |
| 5746.233 | 0.934597 | 5737.467 | 1.510407 | 5737.467 | 1.528604 |
| 5747.533 | 0.932078 | 5737.667 | 1.51495  | 5737.667 | 1.543728 |
| 5748.933 | 0.930507 | 5738.066 | 1.51815  | 5738.066 | 1.546504 |
| 5750.233 | 0.930705 | 5738.267 | 1.52085  | 5738.267 | 1.548204 |
| 5751.533 | 0.93013 | 5738.466 | 1.52275  | 5738.466 | 1.549604 |
| 5752.833 | 0.929557 | 5738.666 | 1.52405  | 5738.666 | 1.549804 |
| 5754.133 | 0.928988 | 5738.866 | 1.52535  | 5738.866 | 1.549904 |
| 5755.433 | 0.928423 | 5739.066 | 1.52615  | 5739.066 | 1.549904 |
| 5756.733 | 0.927868 | 5739.267 | 1.52705  | 5739.267 | 1.549904 |
| 5758.033 | 0.927323 | 5739.467 | 1.52795  | 5739.467 | 1.549904 |
| 5760.333 | 0.926793 | 5739.666 | 1.52885  | 5739.666 | 1.549904 |
| 5761.633 | 0.926263 | 5739.866 | 1.52975  | 5739.866 | 1.549904 |
| 5763.933 | 0.925743 | 5740.066 | 1.53065  | 5740.066 | 1.549904 |
| 5765.233 | 0.925233 | 5740.267 | 1.53155  | 5740.267 | 1.549904 |
| 5766.533 | 0.924723 | 5740.467 | 1.53245  | 5740.467 | 1.549904 |

S66
| 5754.966 | 0.983469 | 5749.433 | 0.925883 | 5749.433 | 0.932974 |
| 5756.967 | 0.999296 | 5749.534 | 0.929799 | 5749.534 | 0.93388 |
| 5758.967 | 1.005198 | 5749.634 | 0.93032 | 5749.634 | 0.911291 |
| 5761.966 | 1.003551 | 5749.733 | 0.93057 | 5749.733 | 0.932646 |
| 5766.966 | 1.003472 | 5749.833 | 0.93242 | 5749.833 | 0.928811 |
| 5771.967 | 1.009996 | 5749.933 | 0.933311 | 5749.933 | 0.916545 |
| 5776.967 | 1.009537 | 5750.034 | 0.935545 | 5750.034 | 0.909027 |
| 5781.966 | 1.007535 | 5750.134 | 0.937723 | 5750.134 | 0.940376 |
| 5786.967 | 1.00499 | 5750.233 | 0.938969 | 5750.233 | 0.932483 |
| 5791.967 | 1.003294 | 5750.333 | 0.940303 | 5750.333 | 0.923241 |
| 5796.966 | 1.002303 | 5750.433 | 0.946608 | 5750.433 | 0.923716 |
| 5803.633 | 1.01516 | 5750.534 | 0.935545 | 5750.534 | 0.927081 |
| 5813.633 | 1.047518 | 5750.634 | 0.937723 | 5750.634 | 0.940376 |
| 5823.633 | 1.067334 | 5750.733 | 0.938969 | 5750.733 | 0.932483 |
| 5833.633 | 1.075684 | 5750.833 | 0.94303 | 5750.833 | 0.923241 |
| 5750.933 | 0.946608 | 5750.933 | 0.923716 | 5750.933 | 0.923716 |
| 5751.033 | 0.94562 | 5751.033 | 0.920971 | 5751.033 | 0.920971 |
| 5751.133 | 0.938252 | 5751.133 | 0.922495 | 5751.133 | 0.922495 |
| 5751.234 | 0.932543 | 5751.234 | 0.922703 | 5751.234 | 0.922703 |
| 5751.333 | 0.939498 | 5751.333 | 0.931715 | 5751.333 | 0.931715 |
| 5751.433 | 0.939022 | 5751.433 | 0.927016 | 5751.433 | 0.927016 |
| 5751.533 | 0.938236 | 5751.533 | 0.927792 | 5751.533 | 0.927792 |
| 5751.633 | 0.943346 | 5751.633 | 0.925826 | 5751.633 | 0.925826 |
| 5751.733 | 0.935429 | 5751.733 | 0.920386 | 5751.733 | 0.920386 |
| 5751.833 | 0.934903 | 5751.833 | 0.921883 | 5751.833 | 0.921883 |
| 5751.934 | 0.937732 | 5751.934 | 0.916605 | 5751.934 | 0.916605 |
| 5752.034 | 0.936149 | 5752.034 | 0.929028 | 5752.034 | 0.929028 |
| 5752.133 | 0.934446 | 5752.133 | 0.930031 | 5752.133 | 0.930031 |
| 5752.233 | 0.943934 | 5752.233 | 0.931024 | 5752.233 | 0.931024 |
| 5752.333 | 0.943384 | 5752.333 | 0.925956 | 5752.333 | 0.925956 |
| 5752.433 | 0.948278 | 5752.433 | 0.934635 | 5752.433 | 0.934635 |
| 5752.533 | 0.951883 | 5752.533 | 0.930169 | 5752.533 | 0.930169 |
| 5752.633 | 0.951526 | 5752.633 | 0.924405 | 5752.633 | 0.924405 |
| 5752.733 | 0.945836 | 5752.733 | 0.940366 | 5752.733 | 0.940366 |
| 5752.833 | 0.941216 | 5752.833 | 0.930106 | 5752.833 | 0.930106 |
| 5752.934 | 0.944962 | 5752.934 | 0.946357 | 5752.934 | 0.946357 |
| 5753.034 | 0.950692 | 5753.034 | 0.949904 | 5753.034 | 0.949904 |
| 5753.134 | 0.946656 | 5753.134 | 0.936351 | 5753.134 | 0.936351 |
| 5753.234 | 0.940079 | 5753.234 | 0.929001 | 5753.234 | 0.929001 |
| 5753.333 | 0.948206 | 5753.333 | 0.953087 | 5753.333 | 0.953087 |
| 5753.433 | 0.955156 | 5753.433 | 0.962826 | 5753.433 | 0.962826 |
| 5753.533 | 0.948252 | 5753.533 | 0.950817 | 5753.533 | 0.950817 |
| 5754.267 | 0.949466 | 5754.267 | 0.947102 | 5754.267 | 0.947102 |
| Value 1     | Value 2     | Value 3     | Value 4     |
|------------|------------|------------|------------|
| 5756.267   | 0.968843   | 5756.267   | 0.966629   |
| 5758.267   | 0.97914    | 5758.267   | 0.989946   |
| 5760.266   | 0.996083   | 5760.266   | 1.002162   |
| 5763.267   | 0.999391   | 5763.267   | 0.994604   |
| 5768.267   | 0.993026   | 5768.267   | 0.992082   |
| 5773.267   | 0.997287   | 5773.267   | 1.008256   |
| 5778.267   | 0.995749   | 5778.267   | 1.002355   |
| 5783.267   | 0.993235   | 5783.267   | 1.006403   |
| 5788.267   | 0.993585   | 5788.267   | 1.009677   |
| 5793.266   | 0.997794   | 5793.266   | 0.988176   |
| 5798.267   | 1.00158    | 5798.267   | 1.002879   |
| 5804.934   | 1.015628   | 5804.934   | 1.017424   |
| 5814.933   | 1.031823   | 5814.933   | 1.03287    |
| 5824.933   | 1.04495    | 5824.933   | 1.044159   |
| 5834.934   | 1.057768   | 5834.934   | 1.067354   |
| 5844.933   | 1.067344   | 5844.933   | 1.071473   |
| 5854.933   | 1.072859   | 5854.933   | 1.079334   |
| 5864.934   | 1.060723   | 5864.934   | 1.075851   |
| 5874.933   | 1.069641   | 5874.933   | 1.072626   |
| 5884.933   | 1.092297   | 5884.933   | 1.084406   |
Additional HERFD and FDMNES results

Figure S17. 1-H HERFD spectrum.

Figure S18. 1-H FDMNES simulation and local density of state (LDOS).
Figure S19. $^{1-}$ HERFD spectrum.

Figure S20. $^{1-}$ FDMNES simulation and local density of state (LDOS).
Further details of magnetism results

*Magnetic susceptibility curves*

Magnetic susceptibility curves for all samples are shown. In cases where more than one data set was collected, average $\chi_0$ values have been reported in Table 1 of the manuscript, with error bars included to represent variation in results. Here, only one representative data set per sample has been shown, with the exception of 1, given the especially wide variation compared with the other samples, whose results varied minimally between data sets.
Figure S21a. Magnetic susceptibility curves and fitting for 1-H.
Figure S21b. Magnetic susceptibility curves and fitting for 1-Li.
Figure S21c. Magnetic susceptibility curves and fitting for 1-K.
Figure S21d. Magnetic susceptibility curves and fitting for 1-Rb.
Figure S21e. Magnetic susceptibility curves and fitting for 1-Cs.
Figure S21f. Magnetic susceptibility curves and fitting for 1. Here, two different data sets were included from samples synthesized at different times, to represent the wider variation observed in the results for this sample.
Figure S21g. Magnetic susceptibility curves and fitting for (2-K)$_4$. 

\[ C_I = 2.92 \times 10^{-2} \pm 4.0 \times 10^{-4} \text{ emu K/mol} \]
\[ \Theta_CW = -2.0 \pm 0.1 \text{ K} \]
\[ \chi_0 = 4.66 \times 10^{-04} \pm 1 \times 10^{-05} \text{ emu/mol} \]
Figure S21h. Magnetic susceptibility curves and fitting for (2-Rb)_4.
Figure S21i. Magnetic susceptibility curves and fitting for $(2$-$Cs)_4$. 

\begin{align*}
\chi & = 6.59e^{-02} \pm 9e^{-04} \text{ emu\cdotK/mol} \\
\theta_{CW} & = 1.8 \pm 0.1 \text{ K} \\
x_0 & = 3.87e^{-04} \pm 3e^{-05} \text{ emu/mol}
\end{align*}
**Evans Method Analysis**

**Evans measurement of (2-K)$_4$ susceptibility:** 1.9 mM solution of (2-K)$_4$ in THF-$d_8$ was used. $\Delta_{ppm} = 0.025$ ppm was observed. $\chi_m = 0.0033$ emu/mol.

**Evans measurement of (2-Cs)$_4$ susceptibility:** 2.85 mM solution of (2-Cs)$_4$ in THF-$d_8$ was used. Peak splitting was not observable by $^1$H NMR.

**Further details of computational results**

**Figure S22.** Restricted Open-Shell Hartree-Fock molecular orbitals used to build the Complete Active Space (CAS) for each Ce imido and oxo complex. Spin-multiplicity values are shown in brackets.

1-K: [Triplet]

1-Rb: [Singlet]

1-Cs: [Singlet]
HOMO-2  HOMO-1  HOMO  LUMO+

LUMO+18

(2-K)$_4$:  [Quintet]

(2-KD)$_4$:  [Singlet]

(2-Cs)$_4$:  [Singlet]
**Cartesian coordinates of all optimized structures**

**1-K**

| Atom | X    | Y    | Z    |
|------|------|------|------|
| C    | 14.302878 | 7.008390 | 23.715996 |
| C    | 14.949615  | 8.200888  | 24.057827  |
| C    | 16.282971  | 8.444600  | 23.618198  |
| C    | 16.901219  | 7.417483  | 22.863749  |
| C    | 16.246860  | 6.232327  | 22.552165  |
| C    | 14.932151  | 6.019567  | 22.966817  |
| C    | 14.280901  | 9.171490  | 24.993263  |
| N    | 13.767685  | 10.397101 | 24.348188  |
| C    | 13.379911  | 11.394805 | 25.365521  |
| C    | 14.514690  | 11.934760 | 26.196521  |
| C    | 14.626810  | 11.546597 | 27.535603  |
| C    | 15.553451  | 12.125232 | 28.397533  |
| C    | 16.380186  | 13.133586 | 27.902481  |
| C    | 16.299345  | 13.519290 | 26.569991  |
| C    | 15.385417  | 12.928549 | 25.662166  |
| N    | 15.309174  | 13.245967 | 24.306881  |
| C    | 15.266962  | 14.667851 | 23.890156  |
| C    | 14.501706  | 14.707432 | 22.558722  |
| N    | 16.880296  | 9.669119  | 23.919962  |
| C    | 18.257500  | 9.700939  | 24.449954  |
| C    | 18.354307  | 10.987608 | 25.287136  |
| C    | 12.625233  | 10.077946 | 23.467184  |
| C    | 12.167195  | 11.218575 | 22.596714  |
| C    | 12.918661  | 11.592084 | 21.447766  |
| C    | 12.373027  | 12.607149 | 20.628086  |
| C    | 11.154576  | 13.210547 | 20.913946  |
| C    | 10.432090  | 12.841289 | 22.048363  |
| C    | 10.951723  | 11.852620 | 22.877325  |
| N    | 14.161212  | 10.989223 | 21.212213  |
| Ce   | 15.715507  | 11.435927 | 22.834691  |
| N    | 17.230086  | 12.313722 | 21.690379  |
| K    | 19.544858  | 13.228678 | 22.978052  |
| C    | 14.437777  | 10.336617 | 19.909670  |
| C    | 15.708765  | 9.500915  | 20.112881  |
| C    | 14.702086  | 11.320185 | 18.750267  |
| C    | 13.286715  | 9.394726  | 19.521552  |
| C    | 19.333672  | 9.755788  | 23.341532  |
| C    | 18.560519  | 8.526030  | 25.395102  |
| C    | 16.668006  | 15.269291 | 23.629360  |
| C    | 14.504222  | 15.551813 | 24.890612  |
| H    | 11.779833  | 9.723986  | 24.083463  |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | 12.945055 | 9.248850  | 22.828819 |
| H    | 10.392505 | 11.539787 | 23.757262 |
| H    | 9.481592  | 13.312484 | 22.283166 |
| H    | 10.776164 | 11.987643 | 20.254191 |
| H    | 12.939232 | 12.974128 | 19.769989 |
| H    | 16.558063 | 10.139307 | 20.393166 |
| H    | 15.989154 | 8.988497  | 19.186643 |
| H    | 15.559815 | 8.740186  | 20.884512 |
| H    | 13.787857 | 11.807762 | 18.402680 |
| H    | 15.120627 | 10.782732 | 17.891257 |
| H    | 15.419965 | 12.088374 | 19.051997 |
| H    | 13.136748 | 8.630373  | 20.291058 |
| H    | 13.508170 | 8.886910  | 18.575960 |
| H    | 12.349241 | 9.945724  | 19.396414 |
| H    | 12.618243 | 10.953418 | 26.032663 |
| H    | 12.914200 | 12.226585 | 24.827684 |
| H    | 13.941295 | 10.791074 | 27.915311 |
| H    | 15.614102 | 11.812864 | 29.435754 |
| H    | 17.100343 | 13.619591 | 28.557102 |
| H    | 16.968766 | 14.294047 | 26.211444 |
| H    | 14.980685 | 10.063312 | 21.810064 |
| H    | 14.477768 | 15.722456 | 22.145319 |
| H    | 13.472339 | 14.366151 | 22.692564 |
| H    | 17.285858 | 15.286030 | 24.534117 |
| H    | 16.592096 | 16.301137 | 23.266544 |
| H    | 17.155357 | 14.670210 | 22.851719 |
| H    | 13.506219 | 15.140525 | 25.072721 |
| H    | 14.386343 | 16.561958 | 24.483471 |
| H    | 15.012810 | 15.634227 | 25.854445 |
| H    | 13.453460 | 8.666553  | 25.522358 |
| H    | 15.013007 | 9.497026  | 25.738263 |
| H    | 13.289178 | 6.844818  | 24.077360 |
| H    | 14.412729 | 5.098379  | 22.720234 |
| H    | 16.763736 | 5.476042  | 21.966175 |
| H    | 17.908178 | 7.570835  | 22.492417 |
| H    | 18.010729 | 11.861649 | 24.716527 |
| H    | 19.380009 | 11.165222 | 25.639318 |
| H    | 17.700130 | 10.935197 | 26.160146 |
| H    | 19.456807 | 8.796075  | 22.833738 |
| H    | 20.319340 | 10.020948 | 23.751701 |
| H    | 19.025701 | 10.482179 | 22.581009 |
| H    | 17.824395 | 8.488484  | 26.204221 |
| H    | 19.554386 | 8.644236  | 25.842290 |
| H    | 18.538724 | 7.565114  | 24.875548 |
| C    | 17.904212 | 12.795834 | 20.622443 |
| C    | 19.044704 | 12.130167 | 20.075416 |
|    |        |        |        |
|----|--------|--------|--------|
| C  | 19.821887 | 12.697960 | 19.067522 |
| C  | 19.510998  | 13.938583 | 18.516729 |
| C  | 18.375081  | 14.595970 | 19.003791 |
| C  | 17.594895  | 14.055595 | 20.015603 |
| H  | 19.289929  | 11.138707 | 20.447501 |
| C  | 20.115382  | 14.370357 | 17.729330 |
| C  | 18.050344  | 15.967359 | 18.478400 |
| H  | 16.720251  | 14.592627 | 20.366284 |
| F  | 16.742936  | 16.264567 | 18.588250 |
| F  | 18.725568  | 16.922156 | 19.163785 |
| F  | 18.391328  | 16.108431 | 17.183843 |
| F  | 21.600415  | 12.466182 | 17.513795 |
| F  | 22.026414  | 12.068231 | 19.604431 |
| F  | 20.854607  | 10.657397 | 18.453914 |

| 1-Rb |
|------|
| C    | 14.299032 | 7.032337 | 23.765430 |
| C    | 14.949165 | 8.227576 | 24.090374 |
| C    | 16.275490 | 8.470379 | 23.629828 |
| C    | 16.884124 | 7.439875 | 22.872410 |
| C    | 16.226723 | 6.252143 | 22.577287 |
| C    | 14.918659 | 6.039955 | 23.012806 |
| C    | 14.292875 | 9.204073 | 25.028414 |
| N    | 13.771555 | 10.425272 | 24.381998 |
| C    | 13.393689 | 11.428288 | 25.397600 |
| C    | 14.536840 | 11.979857 | 26.209008 |
| C    | 14.670677 | 11.600372 | 27.548466 |
| C    | 15.603828 | 12.191887 | 28.394602 |
| C    | 16.413920 | 13.205112 | 27.882494 |
| C    | 16.311835 | 13.582564 | 26.549096 |
| C    | 15.392000 | 12.977714 | 25.656077 |
| N    | 15.293962 | 13.283332 | 24.300397 |
| C    | 15.249227 | 14.700036 | 23.868752 |
| C    | 14.498044 | 14.722456 | 22.528717 |
| N    | 16.875155 | 9.697103  | 23.916963 |
| C    | 18.257004 | 9.734402  | 24.434331 |
| C    | 18.362490 | 11.032753 | 25.251345 |
| C    | 12.619559 | 10.099967 | 23.516159 |
| C    | 12.145261 | 11.235634 | 22.648003 |
| C    | 12.879155 | 11.606120 | 21.486492 |
| C    | 12.312293 | 12.608223 | 20.664813 |
| C    | 11.093957 | 13.205533 | 20.963525 |
| C    | 10.391176 | 12.842336 | 22.112222 |
H  14.396857  5.116733  22.779079
H  16.735775  5.493178  21.987876
H  17.885363  7.592552  22.485709
H  18.042909 11.900616  24.658155
H  19.387623 11.201011  25.609744
H  17.699598 11.003474  26.118884
H  19.435418  8.812724  22.812149
H  20.315134 10.031768  23.721311
H  19.019310 10.505473  22.559511
H  17.837188  8.546434  26.208631
H  19.563856  8.688090  25.825672
H  18.531460  7.603071  24.883228
C  17.903636 12.728992  20.594635
C  18.925345 11.944036  19.972609
C  19.731600 12.450010  18.957158
C  19.572503 13.748511  18.472364
C  18.553607 14.525722  19.032222
C  17.740925 14.043522  20.050110
H  19.059414 10.919014  20.305999
H  19.200058 11.032266  20.352179
H  20.859448 11.596241  18.450376
H  20.200058 14.326212  17.678496
C  18.400471 15.955361  18.593216
H  16.952921 14.670586  20.453867
F  17.134619 16.396024  18.702366
F  19.163522 16.778609  19.358327
F  18.789258 16.145312  17.319505
F  21.349897 12.025971  17.275406
F  21.896915 11.602129  19.331330
F  20.501577 10.308825  18.296880

1-Cs

C  14.431524  6.926392  23.860361
C  15.060192  8.157941  24.075285
C  16.266482  8.471575  23.393998
C  16.761092  7.506265  22.487876
C  16.131478  6.281510  22.297102
C  14.958852  5.979495  22.988603
C  14.472374  9.134057  25.058623
N  13.861505 10.322266  24.430434
C  13.530340 11.330007  25.457738
C  14.719174 11.940957  26.151169
C  14.990735 11.597526  27.478907
C  15.984016  9.134057  28.220284
C  16.715837 13.249335  27.610233
| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| C       | 16.473653| 13.596384| 26.286203|
| C       | 15.482695| 12.955049| 25.498545|
| N       | 16.871503| 9.731074 | 23.571561|
| C       | 12.657132| 9.938681 | 23.662692|
| C       | 10.831935| 10.907779| 21.222212|
| Ce      | 15.575607| 11.427610| 22.666720|
| Cs      | 20.103109| 14.355764| 22.524963|
| C       | 14.057752| 10.439351| 19.831382|
| C       | 12.856487| 9.631407 | 19.316039|
| N       | 18.200371| 9.789361 | 24.211826|
| Cs      | 20.869249| 14.355764| 22.524963|
| H       | 11.903480| 9.526463 | 24.357284|
| H       | 12.962995| 9.137285 | 22.982803|
| H       | 10.419516| 11.285031| 24.242522|
| H       | 9.196021 | 12.957648| 22.879272|
| H       | 10.135199| 13.627388| 20.661297|
| H       | 12.260130| 12.702973| 19.890497|
| H       | 16.170509| 10.041700| 20.229749|
| H       | 15.501954| 9.089619 | 18.908727|
| H       | 15.085740| 8.668581 | 20.581985|
| H       | 13.541313| 12.186171| 18.575814|
| H       | 14.773577| 11.133563| 17.894319|
| H       | 15.186042| 12.205236| 19.248209|
| H       | 12.646908| 8.790144 | 19.984925|
| H       | 13.068066| 9.231487 | 18.317992|
| H       | 11.952625| 10.243486| 19.248199|
| H       | 12.862713| 10.875229| 26.211297|
| H       | 12.974072| 12.124179| 24.950590|
| H       | 14.378958| 10.830455| 27.950583|
| H       | 16.168480| 11.952593| 29.253146|
(2-K)$_4$

\begin{tabular}{cccc}
C & 15.918138 & 8.233170 & 23.816977 \\
C & 14.534249 & 8.218580 & 24.191826 \\
C & 13.726931 & 7.122176 & 23.869694 \\
C & 14.215143 & 6.008370 & 23.193896 \\
C & 15.564919 & 5.995555 & 22.843181 \\
C & 16.388474 & 7.072233 & 23.142509 \\
C & 13.959344 & 9.300000 & 25.068067 \\
N & 13.607054 & 10.564046 & 24.378857 \\
C & 13.205113 & 11.596915 & 25.356879 \\
C & 14.304912 & 11.996089 & 26.301982 \\
C & 14.252789 & 11.582361 & 27.637338 \\
C & 15.230775 & 11.949595 & 28.555243 \\
C & 16.300382 & 12.728615 & 28.115177 \\
C & 16.373487 & 13.139274 & 26.789150 \\
C & 15.372242 & 12.815526 & 25.842006 \\
N & 15.426226 & 13.19207 & 24.492546 \\
C & 15.405900 & 14.640552 & 24.177801 \\
C & 14.103697 & 15.281483 & 24.694904 \\
N & 16.681975 & 9.348629 & 24.104096 \\
C & 18.122896 & 9.244584 & 24.434055 \\
C & 18.392614 & 8.107179 & 25.433138 \\
Ce & 15.840951 & 11.327945 & 23.112880 \\
N & 14.354873 & 11.042080 & 21.164666 \\
C & 14.405789 & 10.029902 & 20.081972 \\
C & 13.378129 & 8.901057 & 20.305322 \\
O & 17.243681 & 11.975107 & 22.060538 \\
C & 13.148246 & 11.746360 & 21.341365 \\
C & 12.288271 & 11.498809 & 22.451056 \\
C & 11.150334 & 12.290805 & 22.648603 \\
C & 10.805241 & 13.323860 & 21.783034 \\
C & 11.621573 & 13.572816 & 20.682406 \\
C & 12.762401 & 12.803017 & 20.479633 \\
C & 12.537851 & 10.342602 & 23.388986 \\
C & 15.804327 & 9.398198 & 20.091485 \\
C & 14.132985 & 10.586518 & 18.662956 \\
C & 15.438195 & 14.769564 & 22.647327 \\
C & 16.601341 & 15.455149 & 24.717875 \\
C & 18.490822 & 10.569210 & 25.126489 \\
C & 19.046079 & 9.113624 & 23.201347 \\
K & 16.304144 & 12.972067 & 19.919808 \\
H & 11.597999 & 10.098369 & 23.916034 \\
H & 12.824805 & 9.463775 & 22.810350 \\
H & 10.510225 & 12.074239 & 23.501744 \\
H & 9.914351 & 13.918747 & 21.961357
\end{tabular}
H  11.375702  14.370252  19.984974
H  13.380924  13.014646  19.609390
H  16.601393  10.140621  19.967280
H  15.902504  8.661236  19.287079
H  15.991544  8.873560  21.033804
H  13.132286  11.018846  18.582043
H  14.208895  9.784901  17.920189
H  14.856430  11.356865  18.35983
H  13.606999  8.347174  21.219883
H  13.387867  8.185965  19.474105
H  12.364233  9.308794  20.381811
H  12.335986  11.230796  25.932537
H  12.88444  12.470502  24.780755
H  13.41594  10.965968  27.960049
H  15.167456  11.623331  29.589338
H  17.095296  13.003845  28.804448
H  17.241094  13.697453  26.459206
H  16.396917  14.379913  22.285779
H  15.344406  15.818814  22.345559
H  14.604628  14.212767  22.199559
H  16.556655  15.575094  25.802850
H  16.599659  16.462280  24.283006
H  17.547826  14.970233  24.455715
H  13.232155  14.819774  24.219488
H  14.078507  16.357811  24.485177
H  14.014747  15.148534  25.777996
H  13.059775  8.912155  25.578192
H  14.695405  9.559931  25.835005
H  12.687036  7.137694  24.192648
H  13.566562  5.168342  22.964510
H  15.985511  5.137346  22.323339
H  17.426369  7.025388  22.838835
H  18.390235  11.420429  24.439943
H  19.536175  10.556733  25.455262
H  17.854246  10.741261  25.998879
H  18.945960  8.153867  22.688751
H  20.096000  9.208307  23.504079
H  18.823960  9.912376  22.486102
H  17.783994  8.245552  26.332744
H  19.447609  8.104381  25.729440
H  18.158662  7.123588  25.018108
(2-Rb)$_4$

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| C    | 15.914915 | 8.234859 | 23.810939 |
| C    | 14.533104  | 8.216645 | 24.192779 |
| C    | 13.726606  | 7.118663 | 23.874946 |
| C    | 14.213860  | 6.005810 | 23.196463 |
| C    | 15.561707  | 5.996294 | 22.838566 |
| C    | 16.384328  | 7.075047 | 23.133744 |
| C    | 13.961740  | 9.297618 | 25.071394 |
| N    | 13.608220  | 10.561743 | 24.384135 |
| C    | 13.208992  | 11.593053 | 25.364682 |
| C    | 14.311457  | 11.994414 | 26.305470 |
| C    | 14.266606  | 11.579537 | 27.640683 |
| C    | 15.247329  | 11.949455 | 28.554691 |
| C    | 16.312150  | 12.732605 | 28.110363 |
| C    | 16.377931  | 13.144309 | 26.784266 |
| C    | 15.373841  | 12.817748 | 25.840916 |
| N    | 15.421698  | 13.200741 | 24.491651 |
| C    | 15.389258  | 14.640412 | 24.174497 |
| C    | 14.069931  | 15.265997 | 24.667135 |
| N    | 16.677725  | 9.351637  | 24.095394 |
| C    | 18.117688  | 9.244802  | 24.429229 |
| C    | 18.383867  | 8.103187  | 25.424723 |
| Ce   | 15.838686  | 11.334345 | 23.096565 |
| N    | 14.348997  | 11.021277 | 21.178303 |
| C    | 14.394746  | 10.019112 | 20.089578 |
| C    | 13.367623  | 8.888845  | 20.312305 |
| O    | 17.271554  | 11.965325 | 22.077046 |
| C    | 13.153102  | 11.740772 | 21.354236 |
| C    | 12.288517  | 11.498414 | 22.461234 |
| C    | 11.155422  | 12.297910 | 22.656092 |
| C    | 10.821630  | 13.334616 | 21.790353 |
| C    | 11.646518  | 13.581919 | 20.695229 |
| C    | 12.782656  | 12.804909 | 20.495518 |
| C    | 12.533723  | 10.341973 | 23.399494 |
| C    | 15.792798  | 9.386832  | 20.090143 |
| C    | 14.113218  | 10.583918 | 18.676397 |
| C    | 15.448608  | 14.765053 | 22.644973 |
| C    | 16.563339  | 15.472250 | 24.734808 |
| C    | 18.485999  | 10.565678 | 25.128530 |
| C    | 19.044551  | 9.116703  | 23.198889 |
| Rb   | 16.563309  | 13.081572 | 19.751203 |
| H    | 11.594736  | 10.103037 | 23.930673 |
| H    | 12.815453  | 9.461301  | 22.820956 |
| H    | 10.510568  | 12.084749 | 23.506561 |
| H    | 9.933938   | 13.935318 | 21.965472 |
| X   | Y   | Z    |
|-----|-----|------|
| H   | 11.410793 | 14.385182 | 20.000832 |
| H   | 13.415775  | 13.016770  | 19.636653  |
| H   | 16.586557  | 10.134496  | 19.979258  |
| H   | 15.892811  | 8.661295   | 19.275489  |
| H   | 15.979818  | 8.849858   | 21.025540  |
| H   | 13.108916  | 11.009283  | 18.602871  |
| H   | 14.193006  | 9.788761   | 17.926876  |
| H   | 14.827680  | 11.365133  | 18.379865  |
| H   | 13.599327  | 8.332443   | 21.224617  |
| H   | 13.374005  | 8.176465   | 19.478547  |
| H   | 12.354234  | 9.297017   | 20.393682  |
| H   | 12.342913  | 11.224924  | 25.943918  |
| H   | 12.888006  | 12.466404  | 24.790695  |
| H   | 13.433008  | 10.959813  | 27.966423  |
| H   | 15.189920  | 11.621890  | 29.588754  |
| H   | 17.109395  | 13.009837  | 28.796215  |
| H   | 17.242560  | 13.705024  | 26.450682  |
| H   | 16.416069  | 14.380029  | 22.303285  |
| H   | 15.351133  | 15.812644  | 22.336682  |
| H   | 14.631446  | 14.198072  | 22.180666  |
| H   | 16.501832  | 15.586078  | 25.819676  |
| H   | 16.550967  | 16.481182  | 24.304030  |
| H   | 17.521527  | 15.004221  | 24.484260  |
| H   | 13.213327  | 14.792154  | 24.176969  |
| H   | 14.034012  | 16.341869  | 24.455918  |
| H   | 13.963969  | 15.132770  | 25.748757  |
| H   | 13.063803  | 8.909690   | 25.584665  |
| H   | 14.700992  | 9.556755   | 25.835522  |
| H   | 12.688315  | 7.132007   | 24.203207  |
| H   | 13.565992  | 5.164312   | 22.970305  |
| H   | 15.981506  | 5.139206   | 22.316111  |
| H   | 17.420723  | 7.031033   | 22.824240  |
| H   | 18.386816  | 11.419459  | 24.445385  |
| H   | 19.530587  | 10.549906  | 25.460039  |
| H   | 17.847432  | 10.734251  | 26.000096  |
| H   | 18.943170  | 8.159176   | 22.682179  |
| H   | 20.093955  | 9.207435   | 23.505041  |
| H   | 18.825104  | 9.919383   | 22.487338  |
| H   | 17.772117  | 8.238128   | 26.322733  |
| H   | 19.437842  | 8.099460   | 25.724801  |
| H   | 18.151514  | 7.121062   | 25.005346  |
(2-Cs)$_4$

C 15.900723  8.154889  23.906656
C 14.544432  8.062806  24.352885
C 13.788780  6.917238  24.085565
C 14.314583  5.823575  23.405121
C 15.644393  5.884733  22.989242
C 16.412349  7.016691  23.229085
C 13.955066  9.135855  25.231117
N 13.528964  10.363062  24.525719
C 13.169290  11.429636  25.483200
C 14.305855  11.940856  26.328306
C 14.360933  11.587304  27.679338
C 15.299974  12.130678  28.550634
C 16.204367  13.063303  28.044554
C 16.179185  13.420715  26.702324
C 15.243684  12.873898  25.785451
N 15.197444  13.153974  24.427670
C 15.438652  14.519289  23.927429
C 14.702796  15.577429  24.766974
N 16.600725  9.329575  24.132758
C 18.038644  9.312737  24.477026
C 18.366528  8.210913  25.498816
Ce 15.575229  11.197827  23.090078
N 14.012688  10.782278  21.328979
C 14.436269  10.307796  19.997256
C 13.269707  9.683537  19.212837
O 17.017121  11.848238  22.065196
C 12.820529  11.466962  21.502219
C 12.045585  11.216535  22.678303
C 10.871528  11.936188  22.917441
C 10.395738  12.897157  22.030355
C 11.120628  13.130211  20.862248
C 12.298170  12.438322  20.608023
C 12.410716  10.083904  23.601058
C 15.477633  9.203655  20.250663
C 15.131638  11.389189  19.133818
C 14.852280  14.562025  22.505125
C 16.938452  14.896471  23.813143
C 18.329263  10.668681  25.144107
C 18.978557  9.199388  23.253712
Cs 18.597356  13.471366  20.486077
H 11.523676  9.793023  24.191796
H 12.712433  9.222188  22.997202
H 10.300871  11.707888  23.816210
H 9.476263  13.436850  22.236775
| H  | 10.771329 | 13.866303 | 20.140979 |
|----|-----------|-----------|-----------|
| H  | 12.843276 | 12.663220 | 19.699389 |
| H  | 16.369250 | 9.610574  | 20.744481 |
| H  | 15.807245 | 8.750493  | 19.308005 |
| H  | 15.060166 | 8.417874  | 20.885800 |
| H  | 14.443346 | 12.159428 | 18.776115 |
| H  | 15.602624 | 10.935150 | 18.252074 |
| H  | 15.904982 | 11.866492 | 19.745340 |
| H  | 12.826065 | 8.867420  | 19.791859 |
| H  | 13.623222 | 9.273819  | 18.259421 |
| H  | 12.480978 | 10.409206 | 18.997194 |
| H  | 12.360992 | 11.062051 | 26.140386 |
| H  | 12.772912 | 12.259475 | 24.889426 |
| H  | 13.621396 | 10.883994 | 28.058743 |
| H  | 15.317023 | 11.844412 | 29.598024 |
| H  | 16.948683 | 13.512456 | 28.698855 |
| H  | 16.918631 | 14.126458 | 26.344233 |
| H  | 15.381524 | 13.862519 | 21.844789 |
| H  | 14.939400 | 15.566864 | 22.072595 |
| H  | 13.796135 | 14.280632 | 22.513140 |
| H  | 17.397626 | 15.119348 | 24.779091 |
| H  | 17.066528 | 15.791037 | 23.186384 |
| H  | 17.476486 | 14.051933 | 23.369004 |
| H  | 13.629587 | 15.363084 | 24.780494 |
| H  | 14.847906 | 16.578033 | 24.342375 |
| H  | 15.055542 | 15.594342 | 25.801465 |
| H  | 13.090407 | 8.722748  | 25.780592 |
| H  | 14.707834 | 9.442557  | 25.964478 |
| H  | 12.764722 | 6.878094  | 24.453503 |
| H  | 13.708454 | 4.942168  | 23.217791 |
| H  | 16.089937 | 5.044159  | 22.461254 |
| H  | 17.432966 | 7.034194  | 22.867338 |
| H  | 18.166103 | 11.493622 | 24.439000 |
| H  | 19.373157 | 10.726123 | 25.475193 |
| H  | 17.680986 | 10.821149 | 26.011263 |
| H  | 18.934028 | 8.219463  | 22.772161 |
| H  | 20.020944 | 9.363991  | 23.556460 |
| H  | 18.701385 | 9.959350  | 22.515355 |
| H  | 17.746443 | 8.332243  | 26.392886 |
| H  | 19.418643 | 8.270531  | 25.800591 |
| H  | 18.186959 | 7.209433  | 25.099377 |
References

1. C. H. Booth, D. Kazhdan, E. L. Werkema, M. D. Walter, W. W. Lukens, E. D. Bauer, Y.-J. Hu, L. Maron, O. Eisenstein, M. Head-Gordon and R. A. Andersen, *J. Am. Chem. Soc.*, 2010, **132**, 17537-17549.

2. C. H. Booth, M. D. Walter, D. Kazhdan, Y.-J. Hu, W. W. Lukens, E. D. Bauer, L. Maron, O. Eisenstein and R. A. Andersen, *J. Am. Chem. Soc.*, 2009, **131**, 6480-6491.

3. R. L. Halbach, G. Nocton, C. H. Booth, L. Maron and R. A. Andersen, *Inorg. Chem.*, 2018, **57**, 7290-7298.

4. C. H. Booth, M. D. Walter, M. Daniel, W. W. Lukens and R. A. Andersen, *Phys. Rev. Lett.*, 2005, **95**, 267202.

5. K. O. Kvashnina, S. M. Butorin and P. Glatzel, *J. Anal. At. Spectrom.*, 2011, **26**, 1265-1272.

6. O. Hirsch, K. O. Kvashnina, L. Luo, M. J. Süess, P. Glatzel and D. Koziej, *Proc. Natl. Acad. Sci.*, 2015, **112**, 15803.