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Supporting information for article:

CatMass – Software for calculating optimal sample masses for X-ray absorption spectroscopy experiments involving complex sample compositions

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S1. Sample Building Examples

![Sample Building Examples](image)

**Figure S1** Examples of several complex catalysts when using the “Sample Builder” window; Left: 1 wt% Pt on Al₂O₃ (Aitbekova et al., 2022); Middle: 1 wt% Ir(CO)₂ on MgO where the wt% is percent metal (Hoffman et al., 2018); Right: 5 wt% Pt₂Sn nanoparticles on Al₂O₃ (Baraa Werghi et al., 2023). Clicking “Update Sample” will convert these inputs into a stoichiometric composition and pass the values to the main window.

S2. Ytterbium oxide (Yb₂O₃) details

S2.1. Experimental methods

Extended X-ray absorption fine structure (EXAFS) measurements were conducted at beamline 10-2 at the Stanford Synchrotron Radiation Lightsource (SSRL). Beamline 10-2 has a 33-pole, 1.72-Tesla wiggler source and a double-crystal, liquid-nitrogen-cooled Si(111) monochromator. Step-scan spectra were collected in transmission mode with nitrogen-filled ion chambers. A Cu foil was scanned simultaneously with the sample for energy calibration.

S2.2. Choosing a reference foil for the measurement

When measuring a material that a reference foil would be difficult to obtain, e.g. Yb₂O₃, *CatMass* can be used to visualize where standard metal foils would appear in k-space for reference foil selection. Using the “Sample and Dilution Definition” panel, potential elements to be used as a reference can be input as “diluents”. When the plot option is selected when calculating the results, the edges of the potential references are displayed in the k-space plot. In the example presented in Fig. S2, when scanning the Yb L₃-edge either the Cu or Zn reference foils could be used as a reference for internal energy calibration.
**Figure S2**  
*K*-space of ytterbium L$_{III}$ edge where the K edges of copper and zinc foils appear at $k = 3.0 \text{ Å}^{-1}$ and $k = 13.6 \text{ Å}^{-1}$, respectively. Data point density during the post-edge region near the metal foil edge would need to be modified to ensure a high enough resolution to use Cu or Zn as a reference for energy calibration.

**S2.3. CatMass calculations**

**Figure S3**  
Example of a Yb$_2$O$_3$ pellet diluted with cellulose at a 1:16 ratio. Calculation is optimized for a pellet to be placed 90° relative to beam path with a total mass of approx. 29 mg. The plotting limit is extended to display the other edges of interest (edges L$_{II}$ and L$_{I}$ of ytterbium as shown in the $k$-space plot). Transmission spectra should be recorded for L$_{III}$ and L$_{II}$ edges, and fluorescence for the L$_{I}$ edge based on the total absorption values in the photon energy plot.
S3. Example calculation of alternative solutions when using CatMass

S3.1. Smear on tape

Figure S4  Example of 1wt%CaO/CeO₂. Calculation could not be optimized with a diluent to prepare enough sample material into a 7 mm pellet. Based on the sample mass value, smearing the sample would make the most physical sense to prepare inside a glovebox.

S3.2. Stacked pellets

Figure S5  Example of 0.1wt%OsO₂/MgO. Calculation could not be optimized to satisfy the mass requirement range of one 7 mm pellet and keep a reasonable edge step for fluorescence. However, two pellets stacked on top of each other would add up to the estimated mass needed.
S3.3. Total absorption measurement

Figure S6  Example of 0.1 wt% OsO$_2$/CeO$_2$. Calculation could not be optimized to satisfy the mass requirement range of one 7 mm pellet and keep a reasonable edge step for fluorescence. Increasing the sample absorption to meet the minimum requirement of packing the sample in a 7 mm pellet would be ideal. Smear on tape could yield measurable data, however the edge step is an order magnitude smaller and would require a high number of scans. Regardless, the use of a solid-state detector would be needed for the measurement and a simultaneous off axis reference foil measurement.

References

Baraa Werghi, Amani Ebrahim, Simon Bare & Matteo Cargnello (2023). Small, 2207956.