The text files provide data for the XAS spectra in Figure 2 of the article 'Biomineral shell formation under ocean acidification: a shift from order to chaos'

Figure 2: The XAS spectra across the Ca L2,3-edge of Mytilus edulis shell grown under present day conditions for (a) the outer calcite, (b) the interface calcite, (c) the interface aragonite and (d) inner aragonite area. The colour of the present day (380 μ atm pCO2) solid line corresponds to the area with the same colour circle in Fig. 1. The spectra for each region of the shell grown under OA (1000 μ atm pCO2) conditions are shown as the solid black line in each panel. The spectra have been overlaid to highlight the increased ACC presence in shells grown under OA in the areas determined to be calcite and aragonite by XPEEM and EBSD. The six features in the XAS spectra are labelled 1–6. The solid vertical line in (a) indicates the position of the lower energy shoulder indicative of ACC. The dashed vertical line in (a) indicates the position of the peak that increases intensity from the outer calcite to the inner aragonite layer.

The text file 'outer calcite.txt' provides data for Figure 2(a), where the first column 'e\_80506' represents the energies of the spectra for shells grown under OA, the second column 'M\_80506\_s' represents the corresponding intensity, the third column 'e\_80473' represents the energies of the spectra for shells grown under present day conditions, the fourth column ‘M\_80473\_s’ represents the corresponding intensity.

The text file 'interface calcite.txt' provides data for Figure 2(b), where the first column 'e\_80508' represents the energies of the spectra for shells grown under OA, the second column 'M\_80508\_s' represents the corresponding intensity, the third column 'e\_80471' represents the energies of the spectra for shells grown under present day conditions, the fourth column ‘M\_80471\_s’ represents the corresponding intensity.

The text file 'interface aragonite.txt', provides data for Figure 2(c), where the first column 'e\_80477' represents the energies of the spectra for shells grown under OA, the second column 'M\_80477\_s' represents the corresponding intensity, the third column 'e\_80470' represents the energies of the spectra for shells grown under present day conditions, the fourth column ‘M\_80470\_s’ represents the corresponding intensity.

The text file 'inner aragonite.txt' provides data for Figure 2 (d), where the first column 'e\_80478' represents the energies of the spectra for shells grown under OA, the second column 'M\_80478\_s' represents the corresponding intensity, the third column 'e\_80448' represents the energies of the spectra for shells grown under present day conditions, the fourth column ‘M\_80448\_s’ represents the corresponding intensity.