

/Users/lorenzsaalman/PycharmProjects/ZeroB/TOF\_Spectra/tof\_spectrum\_plotter.py

```
1 from dataclasses import dataclass
2
3 import matplotlib.pyplot as plt
4 import numpy as np
5 from scipy.ndimage import gaussian_filter1d
6 from scipy.optimize import curve_fit
7 from scipy.signal import find_peaks
8
9 ion_products = {1: 'H', 2: 'H2', 10: 'Ar4', 12: 'C', 13: 'Ar3', 16: 'O', 17: 'OH', 18: 'H2O',
10                20: 'Ar2', 28: 'N2', 32: 'O2', 40: 'Ar', 43: 'CO2'}
11
12 colors = ['#bf212f', 'black', '#264b96', '#27b376', '#AA5486', '#FFEB3B']
13 line_styles = ['-', '-', '-', '-']
14 @dataclass
15 class PeakSettings:
16     match_peaks: bool = False
17     wlen: int = 300
18     width: float = 5
19     min_height_percent: float = 0.005
20     normalize: bool = False
21     integrate: bool = False
22
23
24 @dataclass
25 class Transformation:
26     function: callable = None
27     original_points: np.array = None
28     target_points: np.array = None
29     smoothing: float = 0.01
30
31 @dataclass
32 class ZoomInSettings:
33     enabled: bool = False
34     xlim: tuple = (0, 0)
35     position: tuple = (0.15, 0.35, 0.5, 0.4) # (x, y, width, height) in figure coordinates
36     linewidth: float = 1.5
37
38
39 def plot(file_names, transformation=Transformation(), interval=None, max_time=8,
40         peak_settings=PeakSettings(), zoom_settings=ZoomInSettings(), weights=None, product_labels=
41         ion_products):
42     if interval is None:
43         interval = [0, 0]
44
45     plt.figure(figsize=(10.5, 5))
46     main_axes = plt.gca() # Main plot axes
47     zoom_axes = None
48
49     if zoom_settings.enabled:
50         zoom_axes = plt.axes(zoom_settings.position) # Create inset
51
52     anchor = 0
53     x_values = []
54     count_values = []
55     peak_values = []
56
57     for i, file_name in enumerate(file_names):
58         x, count = np.loadtxt(file_name, unpack=True)
59         weight = (weights[i] if weights is not None else 1)
60
61         # Adjust interval
62         channels = len(x)
63         if interval == [0, 0]:
64             interval = [0, channels]
65
66         x = x[interval[0]:interval[1]]
67         count = count[interval[0]:interval[1]]
68
69         # Find peaks
70         peaks, peak_infos = find_peaks(count, height=max(count) * peak_settings.min_height_percent,
71                                       wlen=peak_settings.wlen, width=peak_settings.width)
72         peak_heights = peak_infos['peak_heights']
73
74         if peak_settings.match_peaks:
75             if anchor == 0:
76                 anchor = peaks[peak_heights.argmax()] + interval[0]
77             else:
78                 factor = (peaks[peak_heights.argmax()] + interval[0]) / anchor
79                 x = x / factor
80
81         # Apply transformation if given
82         if transformation.function is not None:
83             params, _ = curve_fit(transformation.function, transformation.original_points, transformation.
84             target_points)
85             x = transformation.function(x, *params)
86         else:
87             x = x / channels * max_time
88
89         largest = integrate_peaks(main_axes, x, count, peaks, peak_infos, colors[i], peak_settings.integrate
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87 , weight, product_labels)
88     if peak_settings.normalize:
89         count = count / largest * weight
90
91
92     x_values.append(x)
93     count_values.append(count)
94     peak_values.append(peaks)
95
96     count_smoothed = gaussian_filter1d(count, transformation.smoothing)
97
98     label = file_name.split('/')[-1].split('.')[0]
99
100 # Plot on main axes
101 main_axes.plot(x, count_smoothed, color=colors[i], linestyle=line_styles[i], lw=1.1, label=label,
102 alpha=0.7)
103
104 # Plot on zoomed-in inset if enabled
105 if zoom_settings.enabled:
106     zoom_axes.plot(x, count_smoothed, color=colors[i], linestyle=line_styles[i], lw=1.1, alpha=0.6)
107
108 # separate lists for inset and main
109 peaks_inset = []
110 for i, peaks in enumerate(peak_values):
111     peaks_inset.append([peak for peak in peaks if zoom_settings.xlim[0] <= x_values[i][peak] <=
112 zoom_settings.xlim[1]])
113 peaks_main = []
114 for i, peaks in enumerate(peak_values):
115     peaks_main.append([peak for peak in peaks if not zoom_settings.xlim[0] <= x_values[i][peak] <=
116 zoom_settings.xlim[1]])
117
118 if transformation.function is not None:
119     # Annotate peaks in main plot (excluding zoomed-in region)
120     annotate_peaks(main_axes, x_values, count_values, max(count), peaks_main, product_labels)
121
122     # Annotate peaks in inset (only zoomed-in region)
123     if zoom_settings.enabled:
124         max_height_inset = max(count[peak] for peaks in peaks_inset for peak in peaks)
125         annotate_peaks(zoom_axes, x_values, count_values, max_height_inset * 3, peaks_inset,
126 product_labels)
127
128 # Zoom settings
129 if zoom_settings.enabled:
130     zoom_axes.set_xlim(zoom_settings.xlim)
131
132     # Auto-scale inset y-axis
133     zoom_axes.set_ylim((0, max_height_inset))
134     yticks = np.arange(0, max_height_inset, 0.1)
135     zoom_axes.set_yticks(yticks)
136
137 # Draw a rectangle around the zoomed-in region in the main plot
138 x_rect = zoom_axes.get_xlim()
139 y_rect = zoom_axes.get_ylim()
140 main_axes.plot([x_rect[0], x_rect[0], x_rect[1], x_rect[1], x_rect[0]],
141 [y_rect[0], y_rect[1], y_rect[1], y_rect[0], y_rect[0]],
142 linestyle="--", color="gray", linewidth=zoom_settings.linewidth)
143 zoom_axes.spines['top'].set_visible(False)
144
145 # Formatting main plot
146 main_axes.spines['right'].set_visible(False)
147 main_axes.spines['top'].set_visible(False)
148 main_axes.set_xlabel('m/q [u/e] if transformation.function is not None else r't in $\\mu s$')
149 main_axes.set_ylabel('Normalisierte Counts if peak_settings.normalize else 'Counts')
150 legend = main_axes.legend(loc="upper left")
151 for line in legend.get_lines():
152     line.set_linewidth(4)
153 plt.tight_layout()
154 plt.show()
155
156 def integrate_peaks(axes, x, count, peaks, peak_infos, color, show_integration, weight, product_labels):
157     """ Returns the total counts of the largest peak """
158     largest_count = 0
159     total_counts = []
160     for j, peak in enumerate(peaks):
161         m_over_q = round(x[peak], 0)
162         lower_bound = peak_infos['left_bases'][j]
163         upper_bound = peak_infos['right_bases'][j]
164
165         integrated_count = np.trapz(count[lower_bound:upper_bound], x=x[lower_bound:upper_bound])
166         largest_count = max(largest_count, integrated_count)
167         if show_integration and m_over_q in product_labels:
168             total_counts.append((x[lower_bound], x[upper_bound], integrated_count))
169             axes.axvspan(x[lower_bound], x[upper_bound], hatch='////', facecolor=color, alpha=0.15,
170 edgecolor='grey')
171
172     print(f'{product_labels.get(m_over_q, m_over_q)}: {integrated_count:.0f}')
173
174 if show_integration:
175     total = 0
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171         for data in total_counts:
172             lower, higher, count = data
173             weighted = count/largest_count * weight
174             total += weighted
175             axes.text((lower + higher)/2, .5, f'{weighted:.2e}', rotation=90, ha='center', fontsize=9)
176
177     return largest_count
178
179
180 def annotate_peaks(axes, x_values, count_values, max_height, peak_values, product_labels):
181     """ Annotates peaks on the given axes (either main plot or zoomed-in inset). """
182     # create a dictionary with m/q as key where all height values for that peak are stored with their
    indices in the value lists
183     m_over_q_peaks = {}
184     for i, peaks in enumerate(peak_values):
185         for peak in peaks:
186             m_over_q = round(x_values[i][peak],0)
187             info = (i, count_values[i][peak], peak)
188             if m_over_q in m_over_q_peaks:
189                 m_over_q_peaks[m_over_q].append(info)
190             else:
191                 m_over_q_peaks[m_over_q] = [info]
192
193     plotted = []
194     for m_over_q, infos in m_over_q_peaks.items():
195         indices = [info[0] for info in infos]
196         heights = np.array([info[1] for info in infos])
197         peaks = [info[2] for info in infos]
198         peak_idx = heights.argmax()
199         list_idx = indices[peak_idx]
200
201         if m_over_q in product_labels and m_over_q not in plotted:
202             height = max(heights)
203             axes.text(x_values[list_idx][peaks[peak_idx]], height + max_height * .035, f'{m_over_q:.0f}',
    ha='center', fontsize=11)
204             txt = product_labels[m_over_q]
205             axes.text(x_values[list_idx][peaks[peak_idx]], height + max_height * .08, txt + '+', ha='center',
    ', fontsize=12 if 'Ar' in txt else 9)
206             plotted.append(m_over_q)
207
```