In [2]:
```
import numpy as np
print(np.version.version)
from numpy import loadtxt
import matplotlib.pyplot as plt
from scipy.optimize import curve_fit
import glob
from numpy import diff
import pandas as pn
import math
import scipy.constants as sc
import pickle
import copy
from scipy import interpolate
from matplotlib import rcParams, cycler, cm, rc
plotall = True
overview_plot = True
from pylab import meshgrid,cm,imshow,contour,clabel,colorbar,axis,title,show,pcolor
import pandas as pd
import os
import matplotlib.ticker
from matplotlib.ticker import ScalarFormatter
from matplotlib.ticker import (MultipleLocator, AutoMinorLocator)
from numpy.polynomial import Polynomial
from scipy.interpolate import griddata
import matplotlib.cm as cm
import matplotlib as mpl
import numpy.ma as ma
```

```
1.24.3
```

In [3]:
```
%run XRD_Functions.ipynb
```

Closest Element

In [4]:
```
def closest_element(array,value):
    element = min(array, key=lambda x:abs(x-value))
    closest_element = np.where(array == element)[0][0]
    return closest_element
```

Closest Element Range

In [5]:
```
def closest_element_index(array,value):
    array1 = np.sort(array)
    closest_element = min(array1, key=lambda x:abs(x-value))
    closest_element_index = np.where(array1 == closest_element)[0][0]
    closest_index_range = array1[closest_element_index-1 : closest_element_index+1]
    mylist = []
    for i in closest_index_range:
        closest_index_actual = np.where(array == i)[0]
        mylist = np.sort(np.append(mylist,closest_index_actual))
```

```
    return mylist
```

In [6]:
```
"---Folder Paths---"

folder_STO_103_plus = r"C:\Users\pblah\Data\XRD\FM332\Exfoliated\RSM\hkl\Analysed\STO 103+"
pathlist_STO_103_plus = folderpath(folder_STO_103_plus)

folder_SRO_103_plus = r"C:\Users\pblah\Data\XRD\FM332\Exfoliated\RSM\hkl\Analysed\SRO 103+"
pathlist_SRO_103_plus = folderpath(folder_SRO_103_plus)


folder_STO_103_minus = r"C:\Users\pblah\Data\XRD\FM332\Exfoliated\RSM\hkl\Analysed\STO 103-"
pathlist_STO_103_minus = folderpath(folder_STO_103_minus)


folder_SRO_103_minus = r"C:\Users\pblah\Data\XRD\FM332\Exfoliated\RSM\hkl\Analysed\SRO 103-"
pathlist_SRO_103_minus = folderpath(folder_SRO_103_minus)


print(pathlist_STO_103_plus)
print(pathlist_SRO_103_plus)
print(pathlist_STO_103_minus)
print(pathlist_SRO_103_minus)
```

```
['C:\\Users\\pblah\\Data\\XRD\\FM332\\Exfoliated\\RSM\\hkl\\Analysed\\STO 103+\\Take_2_STO_103+_hkl.txt']
['C:\\Users\\pblah\\Data\\XRD\\FM332\\Exfoliated\\RSM\\hkl\\Analysed\\SRO 103+\\Take_2_SRO_103+_hkl.txt']
['C:\\Users\\pblah\\Data\\XRD\\FM332\\Exfoliated\\RSM\\hkl\\Analysed\\STO 103-\\Take_2_STO_103-_hkl.txt']
['C:\\Users\\pblah\\Data\\XRD\\FM332\\Exfoliated\\RSM\\hkl\\Analysed\\SRO 103-\\Take_2_SRO_103-_hkl.txt']
```

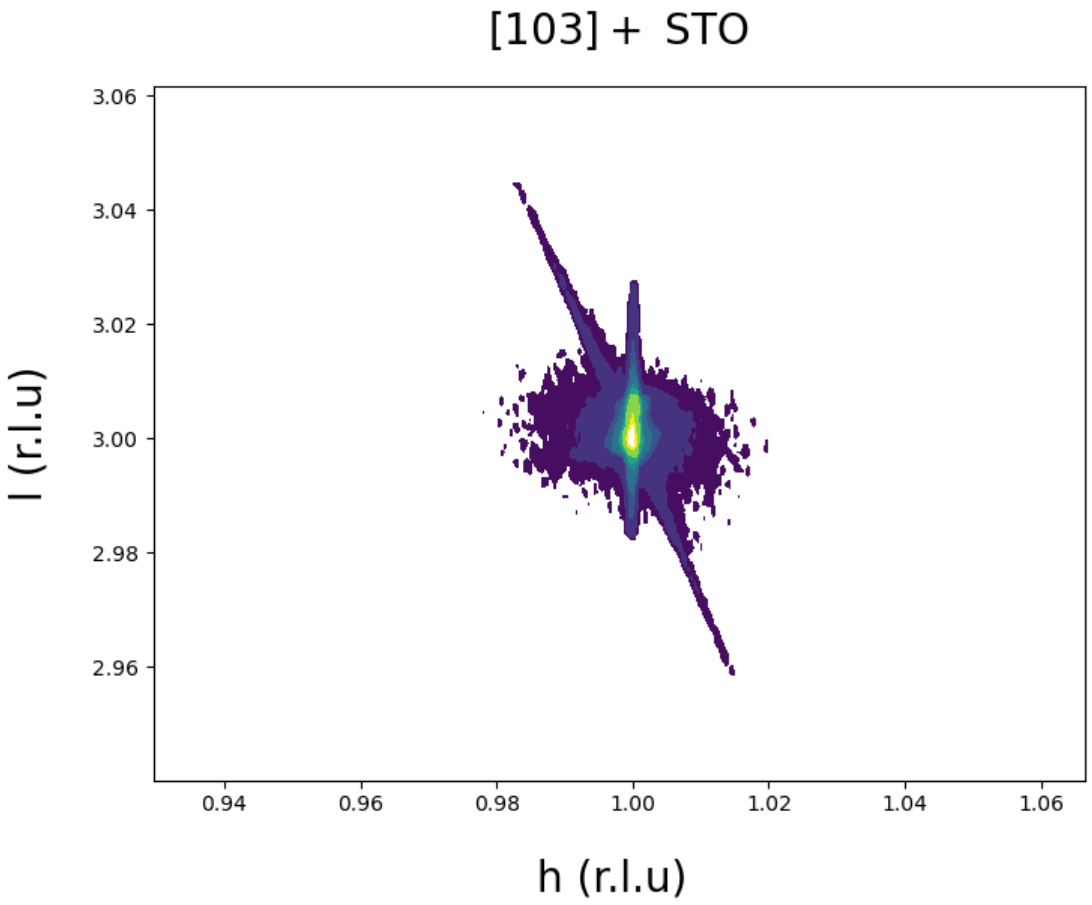
STO 103+

In [7]:
```
%%time

import sys
np.set_printoptions(threshold=1000) # can change to sys.maxsize, default is 1000

fig = plt.figure(figsize=(8,6))
ax = fig.add_subplot(111)
cm = plt.get_cmap('inferno', 30)



#npts = 200
ngridx = 300
ngridy = 300

for i,data in enumerate(pathlist_STO_103_plus):

    print("i",i)
    print("data",data)

    dataextracted = np.loadtxt(data,encoding="utf-8-sig", unpack = True)
```

```
l = dataextracted[0]
h = dataextracted[1]
counts = dataextracted[2]

l = np.ma.masked_invalid(l)
h = np.ma.masked_invalid(h)

print(len(h))



x = np.linspace(0.929580673,1.066431362, ngridx)
y = np.linspace(3.061808196,2.940177011, ngridy)
xi_STO, yi_STO = np.meshgrid(x, y)

zi_STO = griddata((h,l), counts, (xi_STO, yi_STO), method='linear')
zi_STO = np.ma.masked_invalid(zi_STO)
zi_array_STO = np.asarray(zi_STO)
zi_array_one_STO = np.ndarray.flatten(zi_array_STO)

print("max count value",np.nanmax(zi_STO))
print("max count value index",np.where(zi_STO == np.nanmax(zi_STO)))
z_max = np.where(zi_STO == np.nanmax(zi_STO))  # The linear interpolation of griddata is not perfect...Note: Say you get array[149],array[152]. This means it's the 152nd element of t
print("z_max",z_max)
y_max_index = z_max[0][0] # The yi_STO where we find the max count value, where yi-STO is kept contant and you sweep though a range of values for xi_STO. SO the xi_STO and yi_STO ind
print("y_max index",y_max_index)
print('y_max',yi_STO[z_max])
x_max_index = z_max
print("x_max index",x_max_index)
print('x_max',xi_STO[z_max])

y_correction = (3-yi_STO[y_max_index])[0]
x_correction = (1-xi_STO[x_max_index][0])
print('y_correction',y_correction)
print('x_correction',x_correction)


###### Showing what I explained in comment of z_max ######
#x_max_index = z_max[0][0]
#print("x_max index",x_max_index)
#print("zi_STO with x_max index", zi_STO[x_max_index])
#print("index of max value in 'zi_STO with x_max index'",np.where(zi_STO[x_max_index] == np.nanmax(zi_STO[x_max_index]))[0][0])
#print("x_max index actual",zi_STO[x_max_index][152])
##################################################




yi_STO = yi_STO + y_correction
xi_STO = xi_STO + x_correction
```

```
    #zi_min = np.nanmin(zi_array_one)
    #zi_max = np.nanmax(zi_array_one)


    #STO Max value at (8.0998, 0.002905), found via excel
    #STO Max value at (3.03326, 0.002905), found via excel after converting

    #qx_Peak_STO = 0.0029

    #NNO Max value at (8.3042,-0.0319), found via Excel

    #qx_Peak_NNO = -0.0319
    #NNO_a_parameter = 0.3905*(1+qx_Peak_NNO-qx_Peak_STO)
    #print('NNO_a_parameter',NNO_a_parameter)

    #plt.contour(xi,yi,zi, levels = np.arange(zi_min+4,100+zi_min,0.01),cmap = 'inferno',norm = matplotlib.colors.LogNorm(vmin=np.nanmin(counts)+1, vmax=np.nanmax(counts), clip=False),li
    plt.contourf(xi_STO,yi_STO,zi_STO, levels = [5,10,50,100,500,1000,5000,100000,120000,132000,140000,142000,143000,144500],norm = matplotlib.colors.LogNorm(vmin = 5, vmax =
    plt.title(r'$[103]+$ STO',fontsize = 20, pad = 20)
    plt.ylabel(r'l (r.l.u)',fontsize =20, labelpad = 20)
    plt.xlabel("h (r.l.u) ",fontsize =20,labelpad = 20)
    #plt.hlines(3,0.9525,1.05)
    #sm = plt.cm.ScalarMappable(cmap=cm,norm =  matplotlib.colors.LogNorm(vmin=np.nanmin(zi_min)+1, vmax=1000, clip=False))
    #cax = fig.add_axes([0.2, 0.65, 0.02, 0.20])
    #cbar = plt.colorbar(sm, cax=cax, shrink = 0.01, orientation='vertical', extend = 'max')
    #cbar_scale=np.arange(np.nanmin(counts),np.nanmax(counts),np.nanmax(counts)/4)



    #plt.savefig(r"C:\Users\pblah\Data\XRD\FM317\RSM\103 Plus\hkl\FM318 103 Plus RSM hkl.png", bbox_inches = "tight")







    #counts = np.ma.masked_invalid(counts)
    #print(l)
    #print(h)
    #print(counts)
    #print('xi',xi)
    #print('yi',yi)
    #print('zi',zi)
    #print('zi_array_one',zi_array_one)
    #print(zi_min)
    #print(np.nanmin(counts))
    #print(np.nanmax(counts))

xi_STO_plus = xi_STO
yi_STO_plus = yi_STO
zi_STO_plus = zi_STO

y_max_index_plus = yi_STO[z_max][0]
x_max_index_plus = xi_STO[z_max][0]
```

```
i 0
data C:\Users\pblah\Data\XRD\FM332\Exfoliated\RSM\hkl\Analysed\STO 103+\Take_2_STO_103+_hkl.txt
57589
max count value 540763.6157068422
max count value index (array([152], dtype=int64), array([154], dtype=int64))
z_max (array([152], dtype=int64), array([154], dtype=int64))
y_max index 152
y_max [2.99997562]
x_max index (array([152], dtype=int64), array([154], dtype=int64))
x_max [1.00006564]
y_correction 2.4379652173944777e-05
x_correction -6.56432541805696e-05
CPU times: total: 5.11 s
Wall time: 5.77 s
<timed exec>:92: UserWarning: Log scale: values of z <= 0 have been masked
<timed exec>:92: UserWarning: linewidths is ignored by contourf
```



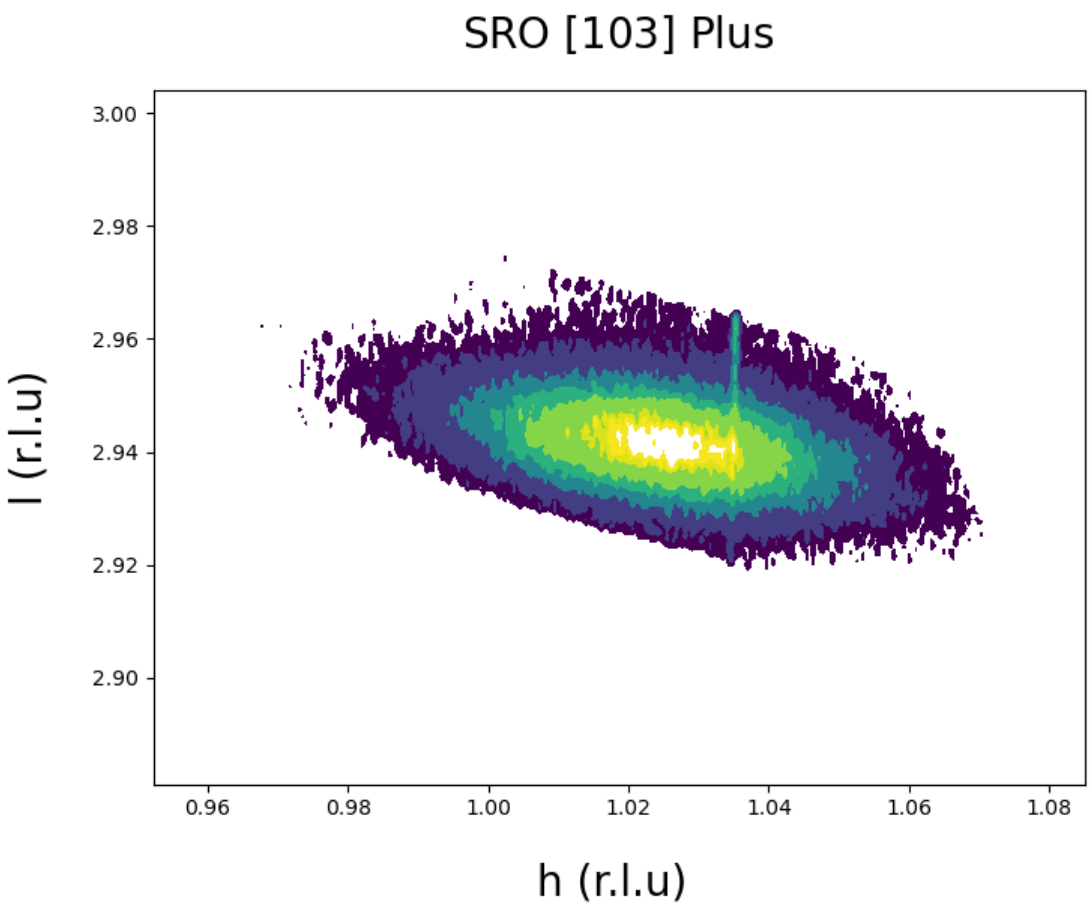
SRO 103+

In [8]:
```
%%time

import sys
np.set_printoptions(threshold=1000) # can change to sys.maxsize, default is 1000

fig = plt.figure(figsize=(8,6))
ax = fig.add_subplot(111)
cm = plt.get_cmap('inferno', 30)




npts = 200
ngridx = 300
ngridy = 300

for i,data in enumerate(pathlist_SRO_103_plus):

    print("i",i)
    print("data",data)

    dataextracted = np.loadtxt(data,encoding="utf-8-sig", unpack = True)
    l = (dataextracted[0])
    h = dataextracted[1]
    counts = dataextracted[2]

    l = np.ma.masked_invalid(l)
    h = np.ma.masked_invalid(h)

    x = np.linspace(0.952316359, 1.085023209 , ngridx)
    y = np.linspace(3.004203516,2.881096502 , ngridy)
    xi_NNO, yi_NNO = np.meshgrid(x, y)

    zi_NNO = griddata((h,l), counts, (xi_NNO, yi_NNO), method='linear')
    zi_NNO = np.ma.masked_invalid(zi_NNO)


    zi_array_NNO = np.asarray(zi_NNO)
    zi_array_one_NNO = np.ndarray.flatten(zi_array_NNO)
    #zi_min = np.nanmin(zi_array_one)
    #zi_max = np.nanmax(zi_array_one)


    #yi_NNO = yi_NNO - (STO_max-3)

    #NNO Max value at (3.0798,0.986455), found via Excel

    #print(np.nanmax(zi_STO))

    #y_max = np.where(zi_STO == np.nanmax(zi_STO))[1][0]
```

```
#print(y_max)
#print((3-yi_STO[y_max]))

#xi_NNO_max = 0.9681
#yi_NNO = yi_NNO + y_correction # Taking into account the fact that interpolation of STO data not perfect, using STO correction can't get correction for NNO
#xi_NNO = xi_NNO + x_correction # Taking into account the fact that interpolation of STO data not perfect, using STO correction can't get correction for NNO

z_max_NNO = np.where(zi_NNO == np.nanmax(zi_NNO))
print("z_max_NNO",z_max_NNO)
y_max_index_NNO = z_max_NNO[0][0] # The yi_STO where we find the max count value, where yi-STO is kept contant and you sweep though a range of values for xi_STO. SO the xi_STO and yi
print("y_max index_NNO",y_max_index_NNO)
print('y_max_NNO',yi_NNO[z_max_NNO])
x_max_index_NNO = z_max_NNO
print("x_max index_NNO",x_max_index_NNO)
print('x_max_NNO',xi_NNO[z_max_NNO])

yi_NNO = yi_NNO + y_correction
xi_NNO = xi_NNO + x_correction




#x_max_index = z_max
#x_max_NNO = np.where(zi_NNO == np.nanmax(zi_NNO))  # The linear interpolation of griddata is not perfect...
#print(x_max_NNO)
#y_max_NNO = np.where(zi_NNO == np.nanmax(zi_NNO))  # The linear interpolation of griddata is not perfect...
#print(y_max_NNO)
#xi_NNO_max = xi_NNO[x_max_NNO]
#yi_NNO_max = yi_NNO[y_max_NNO]



#print("yi_NNO",yi_NNO_max)

#qx_Peak_NNO = -0.0319
#NNO_a_parameter = 0.3905*(1+qx_Peak_NNO-qx_Peak_STO)
#print('NNO_a_parameter',NNO_a_parameter)


### For tricontour ###
#xi = np.ndarray.flatten(xi)
#yi = np.ndarray.flatten(yi)
############################




#plt.contourf(xi,yi,zi, levels = np.arange(zi_min+4,100+zi_min,0.1),cmap = 'inferno',norm = matplotlib.colors.LogNorm(vmin=np.nanmin(counts)+1, vmax=np.nanmax(counts), clip=False),li
plt.contourf(xi_NNO,yi_NNO,zi_NNO, levels = [3,5,10,15,20,30,33,35],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 5,vmax = 35),linewidths = 1, alpha = 1)
```

```
    #plt.tricontour(xi,yi,zi_array_one, levels = [3,5,10,15,20,35],cmap = 'binary',norm = matplotlib.colors.LogNorm(vmin = 5,vmax = 35),linewidths = 1, alpha = 1)
    plt.title(r'SRO $[103]$ Plus',fontsize = 20, pad = 20)
    plt.ylabel(r'l (r.l.u)',fontsize =20, labelpad = 20)
    plt.xlabel("h (r.l.u) ",fontsize =20,labelpad = 20)
    #sm = plt.cm.ScalarMappable(cmap=cm,norm =  matplotlib.colors.LogNorm(vmin=np.nanmin(zi_min)+1, vmax=1000, clip=False))
    #cax = fig.add_axes([0.2, 0.65, 0.02, 0.20])
    #cbar = plt.colorbar(sm, cax=cax, shrink = 0.01, orientation='vertical', extend = 'max')
    #cbar_scale=np.arange(np.nanmin(counts),np.nanmax(counts),np.nanmax(counts)/4)
    #norm = matplotlib.colors.LogNorm(vmin=1, vmax=35, clip=False)



    #plt.savefig(r"C:\Users\pblah\Data\XRD\FM317\RSM\103 Plus\hkl\FM318 103 Plus RSM hkl.png", bbox_inches = "tight")









    #counts = np.ma.masked_invalid(counts)
    #print(l)
    #print(h)
    #print(counts)
    #print('xi',xi)
    #print('yi',yi)
    #print('zi',zi)
    #print('zi_array_one',zi_array_one)
    #print(zi_min)
    #print(np.nanmin(counts))
    #print(np.nanmax(counts))

xi_NNO_plus = xi_NNO
yi_NNO_plus = yi_NNO
zi_NNO_plus = zi_NNO

x_max_index_NNO_plus = xi_NNO[z_max_NNO][0]
y_max_index_NNO_plus = yi_NNO[z_max_NNO][0]
```

```
i 0
data C:\Users\pblah\Data\XRD\FM332\Exfoliated\RSM\hkl\Analysed\SRO 103+\Take_2_SRO_103+_hkl.txt
z_max_NNO (array([151], dtype=int64), array([166], dtype=int64))
y_max index_NNO 151
y_max_NNO [2.94203242]
x_max index_NNO (array([151], dtype=int64), array([166], dtype=int64))
x_max_NNO [1.02599307]
CPU times: total: 1.91 s
Wall time: 1.9 s
<timed exec>:103: UserWarning: Log scale: values of z <= 0 have been masked
<timed exec>:103: UserWarning: linewidths is ignored by contourf
```

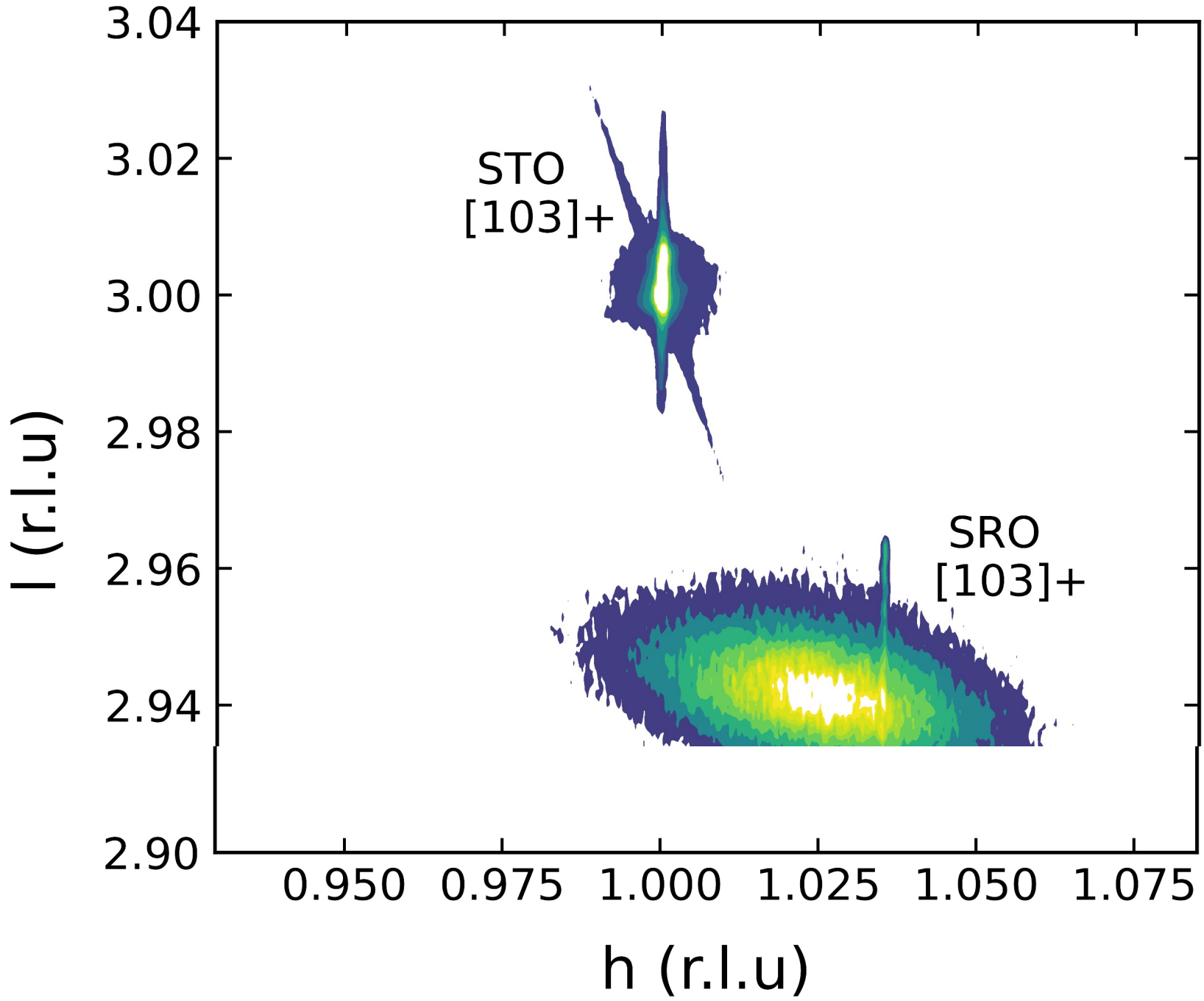


Both

In [9]:
```
#fig, ax_left = plt.subplots()
#ax_left.contourf(xi_NNO,yi_NNO,zi_NNO, levels = [3,5,10,15,20,35],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 5,vmax = 35),linewidths = 1, alpha = 1)
#plt.ylabel(r'l (r.l.u)',fontsize =20, labelpad = 20)
#plt.xlabel("h (r.l.u) ",fontsize =20,labelpad = 20)

#ax_right = ax_left.twinx()
#ax_right.contourf(xi_STO,yi_STO,zi_STO, levels = [5,10,50,100,500,1000,5000,10000,12000,13200,14000,14400],norm = matplotlib.colors.LogNorm(vmin = 5, vmax = 14400),cmap = 'viridis',line

fig, ax = plt.subplots(figsize=(12, 12), dpi = 500)

ax.contourf(xi_NNO,yi_NNO,zi_NNO, levels = [5,10,15,20,25,28,30,33,35],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 5,vmax = 35),linewidths = 1, alpha = 1)
ax.contourf(xi_STO,yi_STO,zi_STO, levels = [10,50,100,500,1000,5000,10000,12000,13200,14000,14200,14400],norm = matplotlib.colors.LogNorm(vmin = 5, vmax = 14400),cmap = 'viridis'
```

```
ax.tick_params(axis = 'x', which='major', labelsize=30, length = 10, width = 2, direction = 'in', pad = 10, top = True)
ax.tick_params(axis = 'y', which='major', labelsize=30, length = 10, width = 2, direction = 'in', pad = 10, right = False)
ax.tick_params(axis = 'y', which='major', labelsize=30, length = 10, width = 2, direction = 'in', pad = 10, right = True)

ax.spines["top"].set_linewidth(2.5)
ax.spines["bottom"].set_linewidth(2.5)
ax.spines["right"].set_linewidth(2.5)
ax.spines["left"].set_linewidth(2.5)

ax.set_ylim(2.9,3.04)

text = ax.text(0.25,0.78, ' STO\n[103]+', size=30, color = 'black',transform = ax.transAxes )
text = ax.text(0.73,0.4, ' SRO\n[103]+', size=30, color = 'black',transform = ax.transAxes )



#plt.vlines(xi_STO[z_max][0],2.9,3.04, color = "red", linestyle = 'dotted', lw = 1)
#plt.vlines(xi_NNO[z_max_NNO][0],2.9,3.04, color = "red",linestyle = 'dotted', lw = 1)

x_difference =  1 - xi_NNO[z_max_NNO]
y_difference = 3-yi_NNO[z_max_NNO]

print('x_difference',x_difference)
print('y_difference',y_difference)

NNO_a_parameter = (3.905 * (-1+x_difference))
NNO_c_parameter = 3.905 * ((3+y_difference)/3)

print('SRO_a_parameter',NNO_a_parameter[0])
print('SRO_c_parameter',NNO_c_parameter[0])




#plt.title(r'$[103]+$ STO and SRO',fontsize = 20, pad = 20)
ax.set_ylabel(r'l (r.l.u)',fontsize=40,labelpad = 25)
ax.set_xlabel(r'h (r.l.u)',fontsize=40,labelpad = 25)
plt.savefig(r"C:\Users\pblah\Data\XRD\FM332\Figures\FM332_103_Plus_RSM_hkl.png", bbox_inches = "tight")
plt.savefig(r"C:\Users\pblah\Data\XRD\FM332\Figures\FM332_103_Plus_RSM_hkl.pdf", bbox_inches = "tight", format = "pdf")
plt.show()
```

```
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\516850824.py:11: UserWarning: Log scale: values of z <= 0 have been masked
  ax.contourf(xi_NNO,yi_NNO,zi_NNO, levels = [5,10,15,20,25,28,30,33,35],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 5,vmax = 35),linewidths = 1, alpha = 1)
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\516850824.py:11: UserWarning: linewidths is ignored by contourf
  ax.contourf(xi_NNO,yi_NNO,zi_NNO, levels = [5,10,15,20,25,28,30,33,35],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 5,vmax = 35),linewidths = 1, alpha = 1)
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\516850824.py:12: UserWarning: Log scale: values of z <= 0 have been masked
  ax.contourf(xi_STO,yi_STO,zi_STO, levels = [10,50,100,500,1000,5000,10000,12000,13200,14000,14200,14400],norm = matplotlib.colors.LogNorm(vmin = 5, vmax = 14400),cmap = 'vir
idis',linewidths = 1, alpha = 1)
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\516850824.py:12: UserWarning: linewidths is ignored by contourf
  ax.contourf(xi_STO,yi_STO,zi_STO, levels = [10,50,100,500,1000,5000,10000,12000,13200,14000,14200,14400],norm = matplotlib.colors.LogNorm(vmin = 5, vmax = 14400),cmap = 'vir
idis',linewidths = 1, alpha = 1)
x_difference [-0.02592743]
y_difference [0.05794321]
SRO_a_parameter -4.006246608116188
SRO_c_parameter 3.980422738591048
```


3.04
3.02
3.00
2.98
2.96
2.94
2.90
l (r.l.u)
STO
[103]+
SRO
[103]+
0.950
0.975
1.000
1.025
1.050
1.075
h (r.l.u)

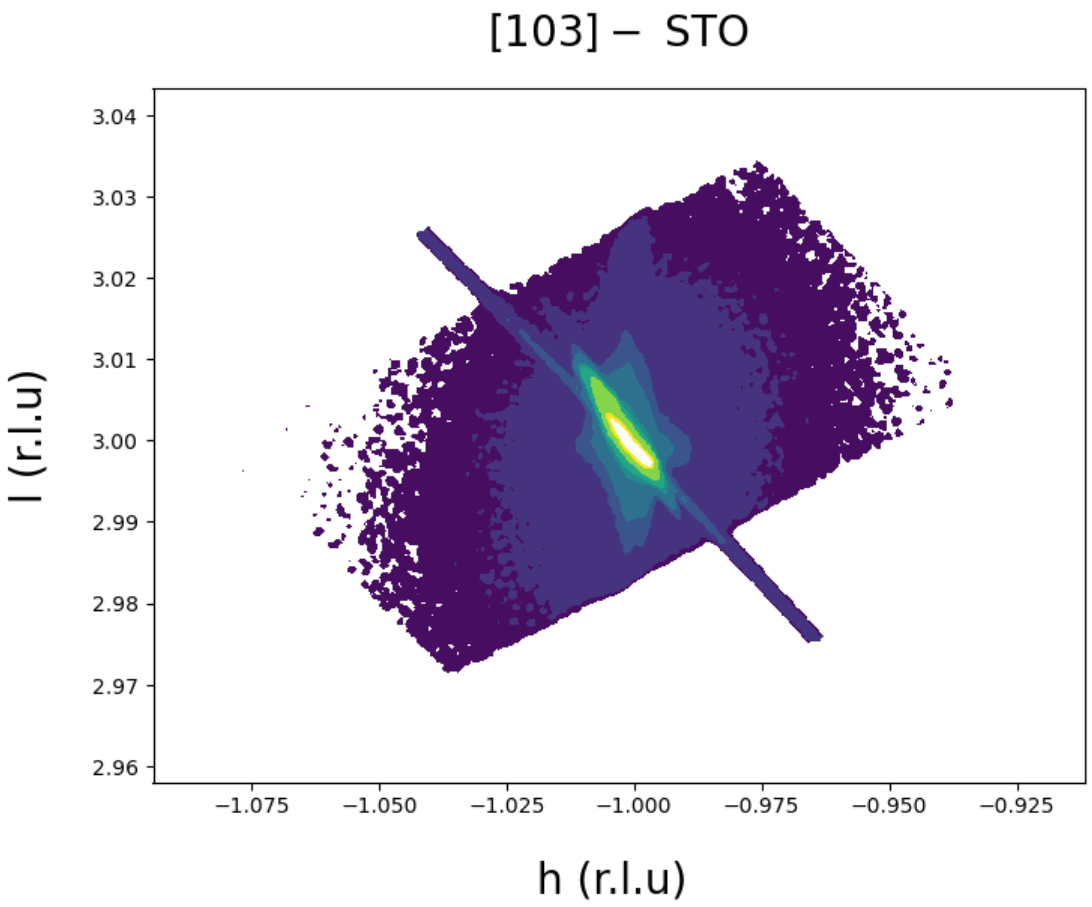
STO 103 Minus

In [10]:
```
%%time

import sys
np.set_printoptions(threshold=1000) # can change to sys.maxsize, default is 1000

fig = plt.figure(figsize=(8,6))
ax = fig.add_subplot(111)
cm = plt.get_cmap('inferno', 30)




#npts = 200
ngridx = 300
ngridy = 300

for i,data in enumerate(pathlist_STO_103_minus):

    print("i",i)
    print("data",data)

    dataextracted = np.loadtxt(data,encoding="utf-8-sig", unpack = True)
    l = dataextracted[0]
    h = dataextracted[1]
    counts = dataextracted[2]

    l = np.ma.masked_invalid(l)
    h = np.ma.masked_invalid(h)

    print(len(h))


    x = np.linspace(-1.09348, -0.911055 , ngridx)
```

```
y = np.linspace(3.04362,2.95828 , ngridy)
xi_STO, yi_STO = np.meshgrid(x, y)

zi_STO = griddata((h,l), counts, (xi_STO, yi_STO), method='linear')
zi_STO = np.ma.masked_invalid(zi_STO)
zi_array_STO = np.asarray(zi_STO)
zi_array_one_STO = np.ndarray.flatten(zi_array_STO)

print("max count value",np.nanmax(zi_STO))
print("max count value index",np.where(zi_STO == np.nanmax(zi_STO)))
z_max = np.where(zi_STO == np.nanmax(zi_STO))  # The linear interpolation of griddata is not perfect...Note: Say you get array[149],array[152]. This means it's the 152nd element of t
print("z_max",z_max)
y_max_index = z_max[0][0] # The yi_STO where we find the max count value, where yi-STO is kept contant and you sweep though a range of values for xi_STO. SO the xi_STO and yi_STO ind
print("y_max index",y_max_index)
print('y_max',yi_STO[z_max])
x_max_index = z_max
print("x_max index",x_max_index)
print('x_max',xi_STO[z_max])

y_correction = (3-yi_STO[y_max_index])[0]
x_correction = (-1-xi_STO[x_max_index][0])
print(y_correction)
print(x_correction)


###### Showing what I explained in comment of z_max ######
#x_max_index = z_max[0][0]
#print("x_max index",x_max_index)
#print("zi_STO with x_max index", zi_STO[x_max_index])
#print("index of max value in 'zi_STO with x_max index'",np.where(zi_STO[x_max_index] == np.nanmax(zi_STO[x_max_index]))[0][0])
#print("x_max index actual",zi_STO[x_max_index][152])
#####################################################




yi_STO = yi_STO + y_correction
xi_STO = xi_STO - x_correction



#zi_min = np.nanmin(zi_array_one)
#zi_max = np.nanmax(zi_array_one)


#STO Max value at (8.0998, 0.002905), found via excel
#STO Max value at (3.03326, 0.002905), found via excel after converting

#qx_Peak_STO = 0.0029

#NNO Max value at (8.3042,-0.0319), found via Excel
```

```
    #qx_Peak_NNO = -0.0319
    #NNO_a_parameter = 0.3905*(1+qx_Peak_NNO-qx_Peak_STO)
    #print('NNO_a_parameter',NNO_a_parameter)

    #plt.contour(xi,yi,zi, levels = np.arange(zi_min+4,100+zi_min,0.01),cmap = 'inferno',norm = matplotlib.colors.LogNorm(vmin=np.nanmin(counts)+1, vmax=np.nanmax(counts), clip=False),li
    plt.contourf(xi_STO,yi_STO,zi_STO, levels = [5,10,50,100,500,1000,5000,100000,120000,132000,140000,142000,143000,144500],norm = matplotlib.colors.LogNorm(vmin = 5, vmax =
    plt.title(r'$[103]-$ STO',fontsize = 20, pad = 20)
    plt.ylabel(r'l (r.l.u)',fontsize =20, labelpad = 20)
    plt.xlabel("h (r.l.u) ",fontsize =20,labelpad = 20)
    #plt.hlines(3,0.9525,1.05)
    #sm = plt.cm.ScalarMappable(cmap=cm,norm =  matplotlib.colors.LogNorm(vmin=np.nanmin(zi_min)+1, vmax=1000, clip=False))
    #cax = fig.add_axes([0.2, 0.65, 0.02, 0.20])
    #cbar = plt.colorbar(sm, cax=cax, shrink = 0.01, orientation='vertical', extend = 'max')
    #cbar_scale=np.arange(np.nanmin(counts),np.nanmax(counts),np.nanmax(counts)/4)



    #plt.savefig(r"C:\Users\pblah\Data\XRD\FM317\RSM\103 Plus\hkl\FM318 103 Plus RSM hkl.png", bbox_inches = "tight")









    #counts = np.ma.masked_invalid(counts)
    #print(l)
    #print(h)
    #print(counts)
    #print('xi',xi)
    #print('yi',yi)
    #print('zi',zi)
    #print('zi_array_one',zi_array_one)
    #print(zi_min)
    #print(np.nanmin(counts))
    #print(np.nanmax(counts))

xi_STO_minus = xi_STO
yi_STO_minus = yi_STO
zi_STO_minus = zi_STO

y_max_index_minus = yi_STO[z_max][0]
x_max_index_minus = xi_STO[z_max][0]
```

```
i 0
data C:\Users\pblah\Data\XRD\FM332\Exfoliated\RSM\hkl\Analysed\STO 103-\Take_2_STO_103-_hkl.txt
112200
max count value 978702.0958366791
max count value index (array([152], dtype=int64), array([152], dtype=int64))
z_max (array([152], dtype=int64), array([152], dtype=int64))
y_max index 152
y_max [3.00023645]
x_max index (array([152], dtype=int64), array([152], dtype=int64))
x_max [-1.00074221]
-0.00023645484949819107
0.00074220735785957
CPU times: total: 1.11 s
Wall time: 1.1 s
<timed exec>:91: UserWarning: Log scale: values of z <= 0 have been masked
<timed exec>:91: UserWarning: linewidths is ignored by contourf
```



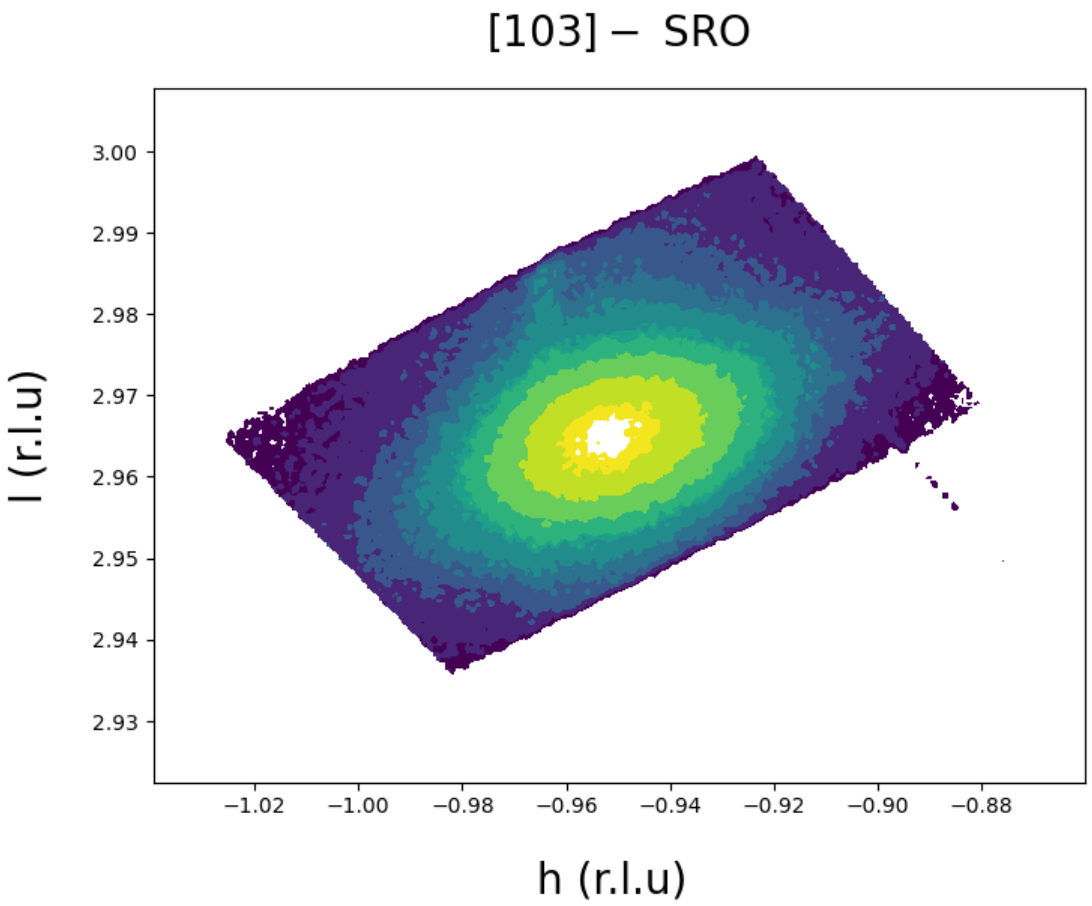
SRO 103 Minus

In [11]:
```
%%time

import sys
np.set_printoptions(threshold=1000) # can change to sys.maxsize, default is 1000

fig = plt.figure(figsize=(8,6))
ax = fig.add_subplot(111)
cm = plt.get_cmap('inferno', 30)



npts = 200
ngridx = 300
ngridy = 300

for i,data in enumerate(pathlist_SRO_103_minus):

    print("i",i)
    print("data",data)

    dataextracted = np.loadtxt(data,encoding="utf-8-sig", unpack = True)
    l = (dataextracted[0])
    h = dataextracted[1]
    counts = dataextracted[2]

    l = np.ma.masked_invalid(l)
    h = np.ma.masked_invalid(h)

    x = np.linspace(-1.03875, -0.859542 , ngridx)
    y = np.linspace(3.00812,2.9227 , ngridy)
    xi_NNO, yi_NNO = np.meshgrid(x, y)

    zi_NNO = griddata((h,l), counts, (xi_NNO, yi_NNO), method='linear')
    zi_NNO = np.ma.masked_invalid(zi_NNO)


    zi_array_NNO = np.asarray(zi_NNO)
    zi_array_one_NNO = np.ndarray.flatten(zi_array_NNO)
    #zi_min = np.nanmin(zi_array_one)
    #zi_max = np.nanmax(zi_array_one)


    #yi_NNO = yi_NNO - (STO_max-3)

    #NNO Max value at (3.0798,0.986455), found via Excel

    #print(np.nanmax(zi_STO))

    #y_max = np.where(zi_STO == np.nanmax(zi_STO))[1][0]
```

```
#print(y_max)
#print((3-yi_STO[y_max]))

#xi_NNO_max = 0.9681
#yi_NNO = yi_NNO + y_correction # Taking into account the fact that interpolation of STO data not perfect, using STO correction can't get correction for NNO
#xi_NNO = xi_NNO + x_correction # Taking into account the fact that interpolation of STO data not perfect, using STO correction can't get correction for NNO

z_max_NNO = np.where(zi_NNO == np.nanmax(zi_NNO))
print("z_max_NNO",z_max_NNO)
y_max_index_NNO = z_max_NNO[0][0] # The yi_STO where we find the max count value, where yi-STO is kept contant and you sweep though a range of values for xi_STO. SO the xi_STO and yi
print("y_max index_NNO",y_max_index_NNO)
print('y_max_NNO',yi_NNO[z_max_NNO])
x_max_index_NNO = z_max_NNO
print("x_max index_NNO",x_max_index_NNO)
print('x_max_NNO',xi_NNO[z_max_NNO])

yi_NNO = yi_NNO + y_correction
xi_NNO = xi_NNO - x_correction




#x_max_index = z_max
#x_max_NNO = np.where(zi_NNO == np.nanmax(zi_NNO))  # The linear interpolation of griddata is not perfect...
#print(x_max_NNO)
#y_max_NNO = np.where(zi_NNO == np.nanmax(zi_NNO))  # The linear interpolation of griddata is not perfect...
#print(y_max_NNO)
#xi_NNO_max = xi_NNO[x_max_NNO]
#yi_NNO_max = yi_NNO[y_max_NNO]



#print("yi_NNO",yi_NNO_max)

#qx_Peak_NNO = -0.0319
#NNO_a_parameter = 0.3905*(1+qx_Peak_NNO-qx_Peak_STO)
#print('NNO_a_parameter',NNO_a_parameter)


### For tricontour ###
#xi = np.ndarray.flatten(xi)
#yi = np.ndarray.flatten(yi)
############################




#plt.contourf(xi,yi,zi, levels = np.arange(zi_min+4,100+zi_min,0.1),cmap = 'inferno',norm = matplotlib.colors.LogNorm(vmin=np.nanmin(counts)+1, vmax=np.nanmax(counts), clip=False),li
plt.contourf(xi_NNO,yi_NNO,zi_NNO, levels = [3,5,10,15,20,30,33,35,50,80,120,135],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 5,vmax = 135),linewidths = 1, alpha
```

```
    #plt.tricontour(xi,yi,zi_array_one, levels = [3,5,10,15,20,35],cmap = 'binary',norm = matplotlib.colors.LogNorm(vmin = 5,vmax = 35),linewidths = 1, alpha = 1)
    plt.title(r'$[103]-$ SRO',fontsize = 20, pad = 20)
    plt.ylabel(r'l (r.l.u)',fontsize =20, labelpad = 20)
    plt.xlabel("h (r.l.u) ",fontsize =20,labelpad = 20)
    #sm = plt.cm.ScalarMappable(cmap=cm,norm =  matplotlib.colors.LogNorm(vmin=np.nanmin(zi_min)+1, vmax=1000, clip=False))
    #cax = fig.add_axes([0.2, 0.65, 0.02, 0.20])
    #cbar = plt.colorbar(sm, cax=cax, shrink = 0.01, orientation='vertical', extend = 'max')
    #cbar_scale=np.arange(np.nanmin(counts),np.nanmax(counts),np.nanmax(counts)/4)
    #norm = matplotlib.colors.LogNorm(vmin=1, vmax=35, clip=False)



    #plt.savefig(r"C:\Users\pblah\Data\XRD\FM317\RSM\103 Plus\hkl\FM318 103 Plus RSM hkl.png", bbox_inches = "tight")









    #counts = np.ma.masked_invalid(counts)
    #print(l)
    #print(h)
    #print(counts)
    #print('xi',xi)
    #print('yi',yi)
    #print('zi',zi)
    #print('zi_array_one',zi_array_one)
    #print(zi_min)
    #print(np.nanmin(counts))
    #print(np.nanmax(counts))

xi_NNO_minus = xi_NNO
yi_NNO_minus = yi_NNO
zi_NNO_minus = zi_NNO

y_max_index_NNO_minus = yi_NNO[z_max_NNO][0]
x_max_index_NNO_minus = xi_NNO[z_max_NNO][0]
```

```
i 0
data C:\Users\pblah\Data\XRD\FM332\Exfoliated\RSM\hkl\Analysed\SRO 103-\Take_2_SRO_103-_hkl.txt
z_max_NNO (array([150], dtype=int64), array([145], dtype=int64))
y_max index_NNO 150
y_max_NNO [2.96526716]
x_max index_NNO (array([150], dtype=int64), array([145], dtype=int64))
x_max_NNO [-0.95184311]
CPU times: total: 1.09 s
Wall time: 1.1 s
<timed exec>:103: UserWarning: Log scale: values of z <= 0 have been masked
<timed exec>:103: UserWarning: linewidths is ignored by contourf
```



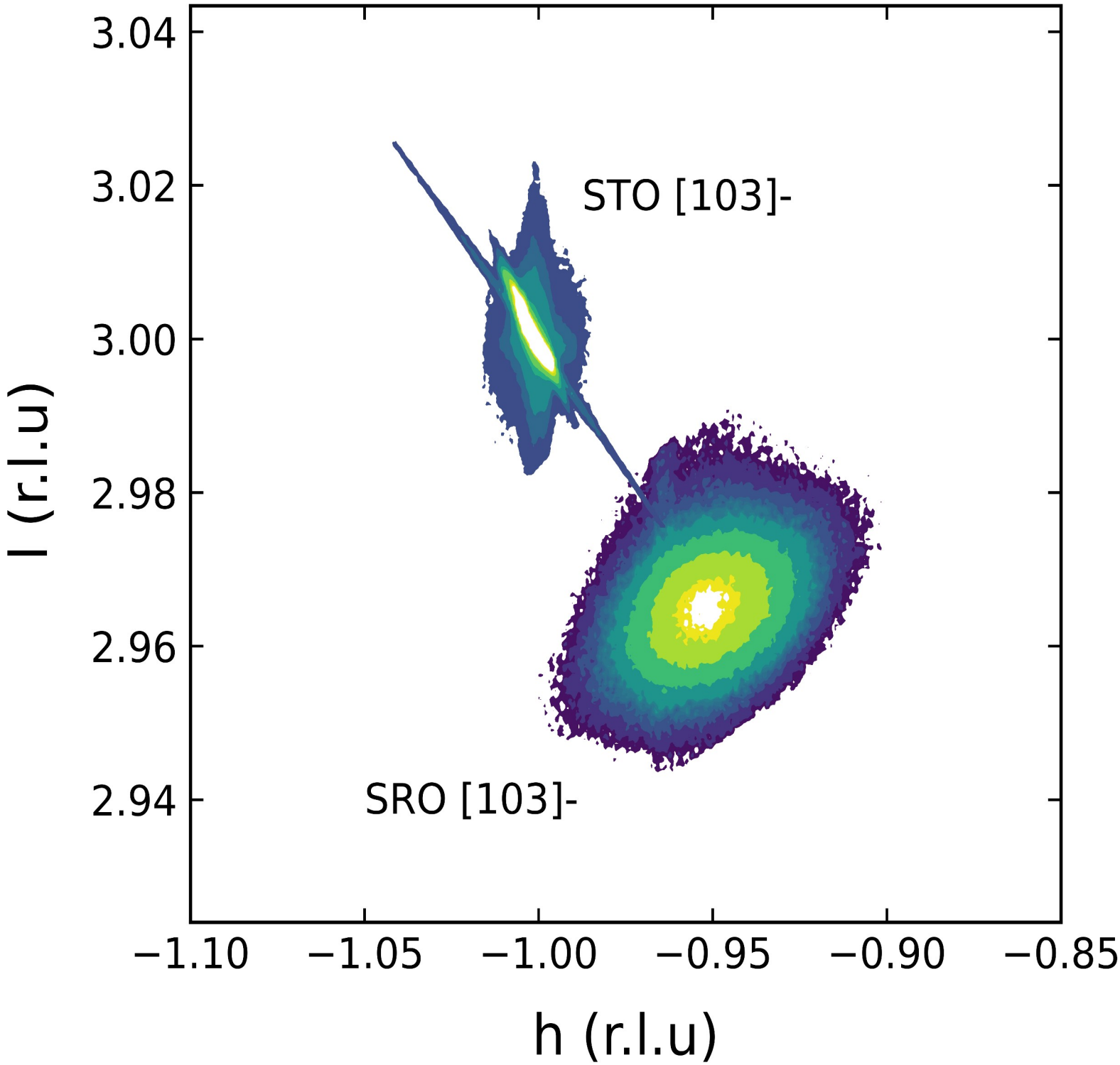
Both

In [12]:
```
#fig, ax_left = plt.subplots()
#ax_left.contourf(xi_NNO,yi_NNO,zi_NNO, levels = [3,5,10,15,20,35],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 5,vmax = 35),linewidths = 1, alpha = 1)
#plt.ylabel(r'l (r.l.u)',fontsize =20, labelpad = 20)
#plt.xlabel("h (r.l.u) ",fontsize =20,labelpad = 20)

#ax_right = ax_left.twinx()
#ax_right.contourf(xi_STO,yi_STO,zi_STO, levels = [5,10,50,100,500,1000,5000,10000,12000,13200,14000,14400],norm = matplotlib.colors.LogNorm(vmin = 5, vmax = 14400),cmap = 'viridis',line

fig, ax = plt.subplots(figsize=(12, 12), dpi = 500)


ax.contourf(xi_NNO,yi_NNO,zi_NNO, levels = [12,15,20,25,28,30,33,35,50,80,120,135],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 12,vmax = 135),linewidths = 1, alpha
ax.contourf(xi_STO,yi_STO,zi_STO, levels = [20,50,100,500,1000,5000,10000,12000,13200,14000,14200,14400],norm = matplotlib.colors.LogNorm(vmin = 5, vmax = 14400),cmap = 'viridis'
```

```
#plt.vlines(xi_STO_max,2.97,3.1, color = "red")
#plt.vlines(xi_NNO_max,2.97,3.1, color = "red")


ax.tick_params(axis = 'x', which='major', labelsize=30, length = 10, width = 2, direction = 'in', pad = 10, top = True)
ax.tick_params(axis = 'y', which='major', labelsize=30, length = 10, width = 2, direction = 'in', pad = 10, right = False)
ax.tick_params(axis = 'y', which='major', labelsize=30, length = 10, width = 2, direction = 'in', pad = 10, right = True)

ax.spines["top"].set_linewidth(2.5)
ax.spines["bottom"].set_linewidth(2.5)
ax.spines["right"].set_linewidth(2.5)
ax.spines["left"].set_linewidth(2.5)

ax.set_xlim(-1.1,-0.85)

text = ax.text(0.45,0.78, 'STO [103]-', size=30, color = 'black',transform = ax.transAxes )
text = ax.text(0.2,0.13, 'SRO [103]-', size=30, color = 'black',transform = ax.transAxes )

x_difference =  -1 - xi_NNO[z_max_NNO]
y_difference = 3-yi_NNO[z_max_NNO]

print('x_difference',x_difference)
print('y_difference',y_difference)

NNO_a_parameter = 3.905 * (1-x_difference)
NNO_c_parameter = 3.905 * ((3 + y_difference)/3)

print('SRO_a_parameter',NNO_a_parameter[0])
print('SRO_c_parameter',NNO_c_parameter[0])




#plt.title(r'$[103]-$ STO and SRO',fontsize = 20, pad = 20)
ax.set_ylabel(r'l (r.l.u)',fontsize=40,labelpad = 25)
ax.set_xlabel(r'h (r.l.u)',fontsize=40,labelpad = 25)
plt.savefig(r"C:\Users\pblah\Data\XRD\FM332\Figures\FM332_103_Minus_RSM_hkl.png", bbox_inches = "tight")
plt.savefig(r"C:\Users\pblah\Data\XRD\FM332\Figures\FM332_103_Minus_RSM_hkl.pdf", bbox_inches = "tight", format = "pdf")
plt.show()
```

```
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\2890475953.py:12: UserWarning: Log scale: values of z <= 0 have been masked
  ax.contourf(xi_NNO,yi_NNO,zi_NNO, levels = [12,15,20,25,28,30,33,35,50,80,120,135],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 12,vmax = 135),linewidths = 1, al
pha = 1)
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\2890475953.py:12: UserWarning: linewidths is ignored by contourf
  ax.contourf(xi_NNO,yi_NNO,zi_NNO, levels = [12,15,20,25,28,30,33,35,50,80,120,135],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 12,vmax = 135),linewidths = 1, al
pha = 1)
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\2890475953.py:13: UserWarning: Log scale: values of z <= 0 have been masked
  ax.contourf(xi_STO,yi_STO,zi_STO, levels = [20,50,100,500,1000,5000,10000,12000,13200,14000,14200,14400],norm = matplotlib.colors.LogNorm(vmin = 5, vmax = 14400),cmap = 'vir
idis',linewidths = 1, alpha = 1)
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\2890475953.py:13: UserWarning: linewidths is ignored by contourf
  ax.contourf(xi_STO,yi_STO,zi_STO, levels = [20,50,100,500,1000,5000,10000,12000,13200,14000,14200,14400],norm = matplotlib.colors.LogNorm(vmin = 5, vmax = 14400),cmap = 'vir
idis',linewidths = 1, alpha = 1)
```

```
x_difference [-0.04741468]
y_difference [0.0349693]
SRO_a_parameter 4.0901543342809354
SRO_c_parameter 3.950518369119286
```


3.04
3.02
3.00
2.98
2.96
2.94
l (r.l.u)
STO [103]-
SRO [103]-
−1.10
−1.05
−1.00
−0.95
−0.90
−0.85
h (r.l.u)

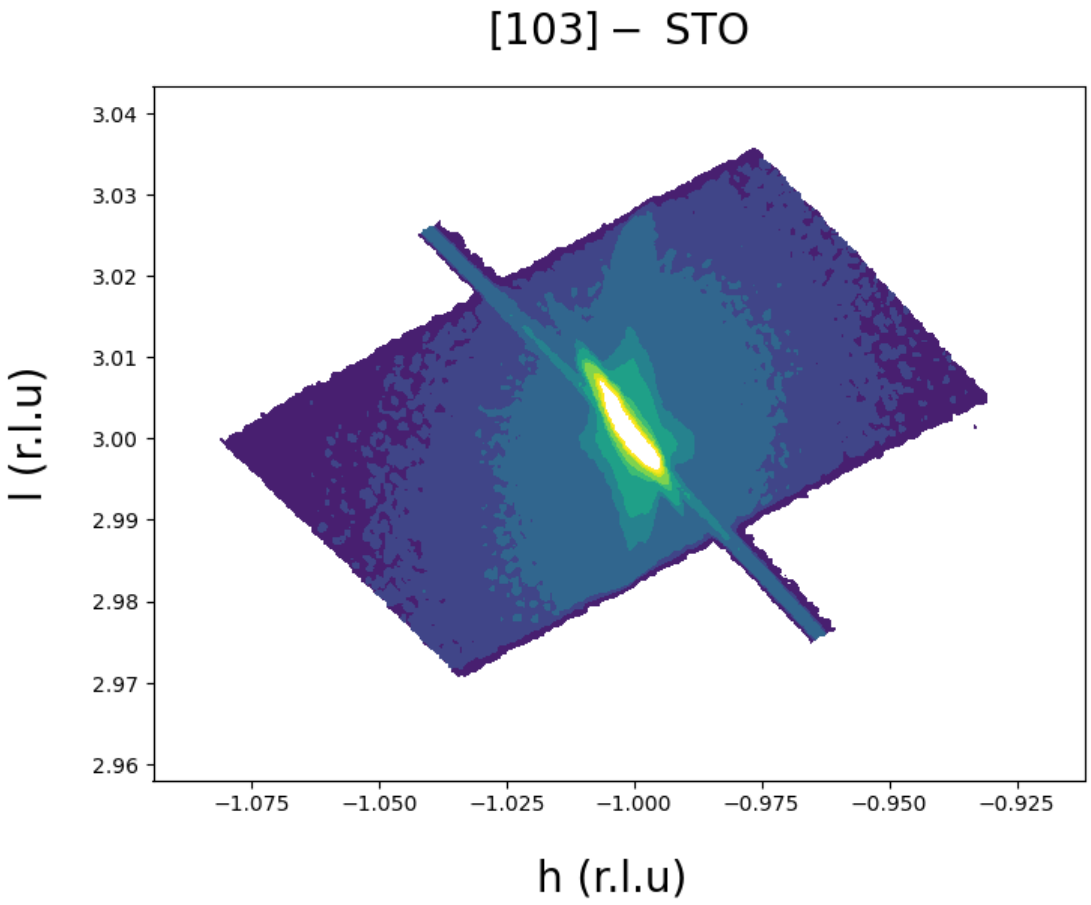
In [20]:
```
%%time

import sys
np.set_printoptions(threshold=1000) # can change to sys.maxsize, default is 1000

fig = plt.figure(figsize=(8,6))
ax = fig.add_subplot(111)
cm = plt.get_cmap('inferno', 30)




#npts = 200
ngridx = 300
ngridy = 300

for i,data in enumerate(pathlist_STO_103_minus):

    print("i",i)
    print("data",data)

    dataextracted = np.loadtxt(data,encoding="utf-8-sig", unpack = True)
    l = dataextracted[0]
    h = dataextracted[1]
    counts = dataextracted[2]

    l = np.ma.masked_invalid(l)
    h = np.ma.masked_invalid(h)

    print(len(h))



    x_minus = np.linspace(-1.09348, -0.911055 , ngridx)
    y_minus = np.linspace(3.04362,2.95828 , ngridy)
    xi_STO_minus, yi_STO_minus = np.meshgrid(x_minus, y_minus)

    zi_STO_minus = griddata((h,l), counts, (xi_STO_minus, yi_STO_minus), method='linear')
    #print(zi_STO_minus)
    zi_STO_minus = np.ma.masked_invalid(zi_STO_minus)
    zi_array_STO_minus = np.asarray(zi_STO_minus)
```

```
zi_array_one_STO_minus = np.ndarray.flatten(zi_array_STO_minus)



##############################################################################################
print("max count value",np.nanmax(zi_STO_minus))
print("max count value index",np.where(zi_STO_minus == np.nanmax(zi_STO_minus)))
z_max_minus = np.where(zi_STO_minus == np.nanmax(zi_STO_minus))  # The linear interpolation of griddata is not perfect...Note: Say you get array[149],array[152]. This means it's the
print("z_max",z_max_minus)
y_max_index_minus = z_max_minus[0][0] # The yi_STO where we find the max count value, where yi-STO is kept contant and you sweep though a range of values for xi_STO. SO the xi_STO an
print("y_max index",y_max_index_minus)
print('y_max',yi_STO_minus[z_max_minus])
x_max_index_minus = z_max_minus
print("x_max index",x_max_index_minus)
print('x_max',xi_STO_minus[z_max_minus])

y_correction_minus = (3-yi_STO_minus[y_max_index_minus])[0]
x_correction_minus = (1+xi_STO_minus[x_max_index_minus][0])
print('y_correction_minus',y_correction_minus)
print('x_correction_minus',x_correction_minus)


###### Showing what I explained in comment of z_max ######
#x_max_index = z_max[0][0]
#print("x_max index",x_max_index)
#print("zi_STO with x_max index", zi_STO[x_max_index])
#print("index of max value in 'zi_STO with x_max index'",np.where(zi_STO[x_max_index] == np.nanmax(zi_STO[x_max_index]))[0][0])
#print("x_max index actual",zi_STO[x_max_index][152])
##################################################

#############################################################
yi_STO_minus = yi_STO_minus + y_correction_minus
xi_STO_minus = xi_STO_minus + x_correction_minus

zi_STO_minus = griddata((h,l), counts, (xi_STO_minus, yi_STO_minus), method='linear')
#print(zi_STO_minus)
zi_STO_minus = np.ma.masked_invalid(zi_STO_minus)
zi_array_STO_minus = np.asarray(zi_STO_minus)
zi_array_one_STO_minus = np.ndarray.flatten(zi_array_STO_minus)



#zi_min = np.nanmin(zi_array_one)
#zi_max = np.nanmax(zi_array_one)


#STO Max value at (8.0998, 0.002905), found via excel
#STO Max value at (3.03326, 0.002905), found via excel after converting

#qx_Peak_STO = 0.0029
```

```
#NNO Max value at (8.3042,-0.0319), found via Excel

#qx_Peak_NNO = -0.0319
#NNO_a_parameter = 0.3905*(1+qx_Peak_NNO-qx_Peak_STO)
#print('NNO_a_parameter',NNO_a_parameter)

#print(xi_STO)

#plt.contour(xi,yi,zi, levels = np.arange(zi_min+4,100+zi_min,0.01),cmap = 'inferno',norm = matplotlib.colors.LogNorm(vmin=np.nanmin(counts)+1, vmax=np.nanmax(counts), clip=False),li
############################################################


plt.contourf(xi_STO_minus,yi_STO_minus,zi_STO_minus, levels = [1,5,10,50,100,500,1000,5000,10000,12000,13200,14000,14200,14400],norm = matplotlib.colors.LogNorm(vmin = 1,
plt.title(r'$[103]-$ STO',fontsize = 20, pad = 20)
plt.ylabel(r'l (r.l.u)',fontsize =20, labelpad = 20)
plt.xlabel("h (r.l.u) ",fontsize =20,labelpad = 20)




######################################################################
#plt.hlines(3,0.9525,1.05)
#sm = plt.cm.ScalarMappable(cmap=cm,norm =  matplotlib.colors.LogNorm(vmin=np.nanmin(zi_min)+1, vmax=1000, clip=False))
#cax = fig.add_axes([0.2, 0.65, 0.02, 0.20])
#cbar = plt.colorbar(sm, cax=cax, shrink = 0.01, orientation='vertical', extend = 'max')
#cbar_scale=np.arange(np.nanmin(counts),np.nanmax(counts),np.nanmax(counts)/4)



#plt.savefig(r"C:\Users\pblah\Data\XRD\FM317\RSM\113 minus\Figures\Take 2 Analysis\FM317_103_Minus_RSM_hkl.png", bbox_inches = "tight")
#plt.savefig(r"C:\Users\pblah\Data\XRD\FM317\RSM\113 minus\Figures\Take 2 Analysis\FM317_103_Minus_RSM_hkl.pdf", bbox_inches = "tight", format = "pdf")




#counts = np.ma.masked_invalid(counts)
#print(l)
#print(h)
#print(counts)
#print('xi',xi)
#print('yi',yi)
#print('zi',zi)
#print('zi_array_one',zi_array_one)
#print(zi_min)
#print(np.nanmin(counts))
#print(np.nanmax(counts))
```

```
i 0
data C:\Users\pblah\Data\XRD\FM332\Exfoliated\RSM\hkl\Analysed\STO 103-\Take_2_STO_103-_hkl.txt
112200
max count value 978702.0958366791
max count value index (array([152], dtype=int64), array([152], dtype=int64))
z_max (array([152], dtype=int64), array([152], dtype=int64))
y_max index 152
y_max [3.00023645]
x_max index (array([152], dtype=int64), array([152], dtype=int64))
x_max [-1.00074221]
y_correction_minus -0.00023645484949819107
x_correction_minus -0.00074220735785957
CPU times: total: 2.09 s
Wall time: 2.11 s
```

```
<timed exec>:106: UserWarning: Log scale: values of z <= 0 have been masked
<timed exec>:106: UserWarning: linewidths is ignored by contourf
```



In [ ]:
```
x = np.linspace(-1.09348, -0.911055 , ngridx)
```

```
    y = np.linspace(3.04362,2.95828 , ngridy)
```

In [ ]:

In [19]:
```
fig,ax = plt.subplots(figsize=(12, 12), dpi = 500)
#ax2 = ax1.twinx()

ax.tick_params(axis = 'x', which='major', labelsize=30, length = 10, width = 2, direction = 'in', pad = 10, top = True)
ax.tick_params(axis = 'y', which='major', labelsize=30, length = 10, width = 2, direction = 'in', pad = 10, right = False)
ax.tick_params(axis = 'y', which='major', labelsize=30, length = 10, width = 2, direction = 'in', pad = 10, right = False)

ax.spines["top"].set_linewidth(2.5)
ax.spines["bottom"].set_linewidth(2.5)
ax.spines["right"].set_linewidth(2.5)
ax.spines["left"].set_linewidth(2.5)




ax.contourf(xi_NNO_plus,yi_NNO_plus,zi_NNO_plus, levels = [5,10,15,20,25,28,30,33,35],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 5,vmax = 35),linewidths = 1, alpha
ax.contourf(xi_STO_plus,yi_STO_plus,zi_STO_plus, levels = [10,50,100,500,1000,5000,10000,12000,13200,14000,14200,14400],norm = matplotlib.colors.LogNorm(vmin = 5, vmax = 14400
ax.contourf(xi_NNO_minus,yi_NNO_minus,zi_NNO_minus, levels = [12,15,20,25,28,30,33,35,50,80,120,135],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 12,vmax = 135),linewidths
ax.contourf(xi_STO_minus,yi_STO_minus,zi_STO_minus, levels = [20,50,100,500,1000,5000,10000,12000,13200,14000,14200,14400],norm = matplotlib.colors.LogNorm(vmin = 5, vmax = 14400
ax.vlines(0,2.92,3.05, lw = 3)
ax.hlines(3,-1,1, lw = 3)
ax.hlines(2.9536,x_max_index_NNO_minus-0.3,x_max_index_NNO_plus-0.052+0.3, color = 'red',linestyle = 'dotted', lw = 3)

x_maxes_NNO = [x_max_index_NNO_minus,x_max_index_NNO_plus]
x_maxes_STO = [x_max_index_minus,x_max_index_minus]
y_maxes_NNO = [y_max_index_NNO_minus,y_max_index_NNO_plus]
y_maxes_STO = [y_max_index_minus,y_max_index_minus]

print(x_maxes_NNO,'x_maxes_NNO')
print(x_maxes_STO,'x_maxes_STO')
print(y_maxes_NNO,'y_maxes_NNO')
print(y_maxes_STO,'y_maxes_STO')


ax.plot(x_maxes_NNO,y_maxes_NNO, lw = 3)


a, b, = np.polynomial.polynomial.polyfit(x_maxes_NNO,y_maxes_NNO, 1)
print('a',a)
print('b',b)
fit = a + b*x_maxes_NNO[0] + b*x_maxes_NNO[1]
print('Polynomial Fit 1st Order', np.polynomial.polynomial.Polynomial([a,b]))


######## Left Triangle ##########

left_edge_length = y_max_index_NNO_minus - a
bottom_edge_length = -x_max_index_NNO_minus - 0
hypo = np.sqrt(bottom_edge_length**2 + left_edge_length**2)
```

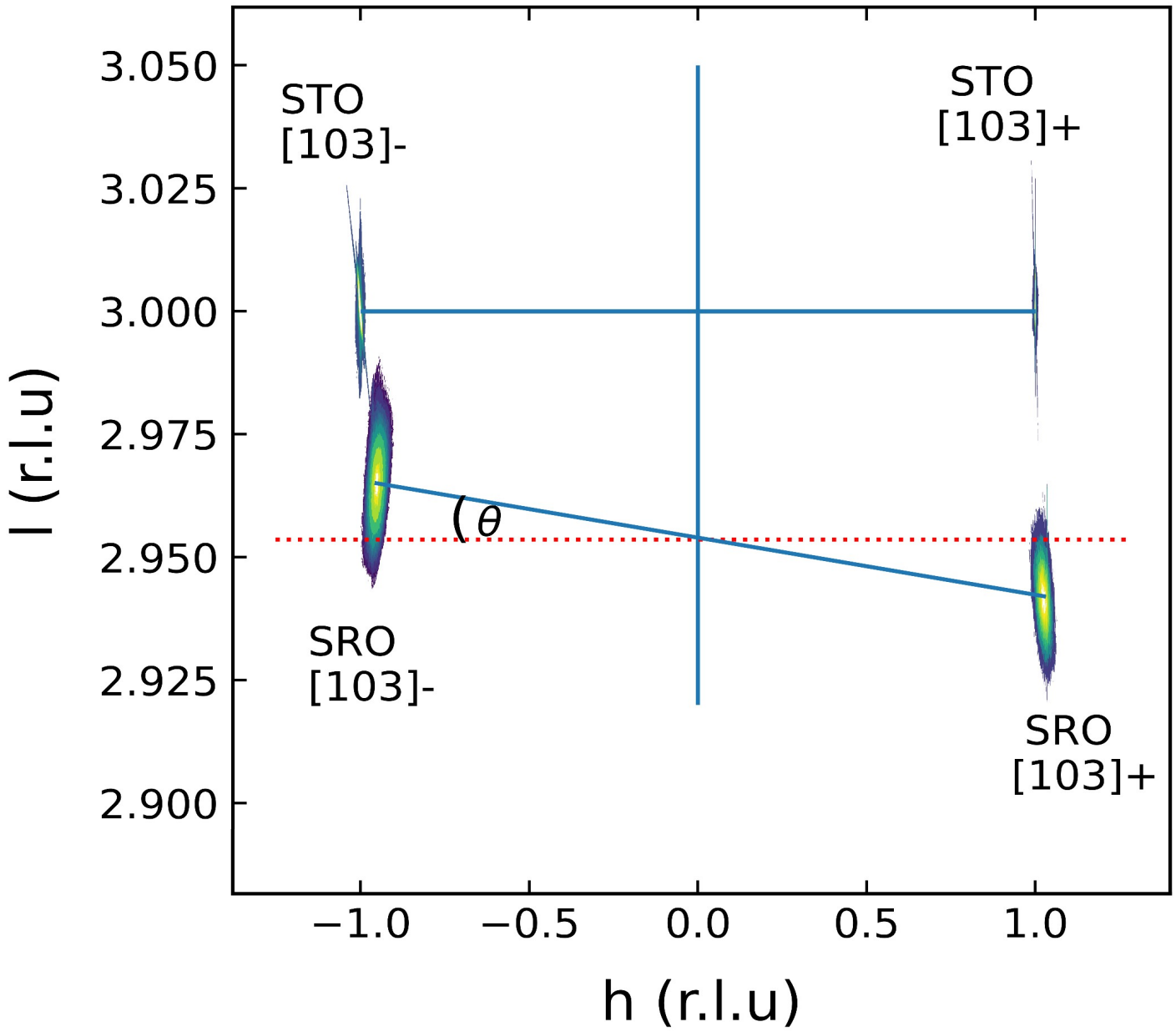
```
print('left_edge_length',left_edge_length)
print('bottom_edge_length',bottom_edge_length)

print('hypo',hypo)

ratios = left_edge_length/bottom_edge_length

print('ratios', ratios)

angle = np.arctan(ratios)#*(180/np.pi) (Python trig functions use rads! Will keep it as rads as the rotation formula does)

print('angle',angle)

rotation_matrix_minus = [[np.cos(angle),-np.sin(angle)],[np.sin(angle),np.cos(angle)]]


vector_minus = [[x_maxes_NNO[0]],[y_maxes_NNO[0]]]

print('rotation_matrix_minus',rotation_matrix_minus)
print('vector_minus',vector_minus)


#x_max_NNO_minus_rotated

#SRO_a_parameter_left = ((1+(1-hypo))*3.905)

#print('SRO_a_parameter_left',SRO_a_parameter_left)

#x_max_NNO_minus_rotated = np.cos(angle)*-hypo

vector_NNO_minus_rotated = np.matmul(rotation_matrix_minus,vector_minus)

print('vector_NNO_minus_rotated',vector_NNO_minus_rotated)

#SRO_a_parameter_left = ((1+(1+x_max_NNO_minus_rotated))*3.905)

#print('SRO_a_parameter_left',SRO_a_parameter_left)

######### Right Triangle #################

right_edge_length = y_max_index_NNO_plus - a
right_bottom_edge_length = x_max_index_NNO_plus - 0
hypo_right = np.sqrt(right_bottom_edge_length**2 + right_edge_length**2)

print('right_edge_length',left_edge_length)
print('right_bottom_edge_length',right_bottom_edge_length)

print('hypo_right',hypo_right)

ratios_right = left_edge_length/bottom_edge_length

print('ratios_right', ratios_right)
```

```
angle_right = np.tan(ratios_right)#*(180/np.pi)

print('angle_right',angle_right)


#SRO_a_parameter_left = ((1+(1-hypo))*3.905)

#print('SRO_a_parameter_left',SRO_a_parameter_left)

rotation_matrix_plus = [[np.cos(angle),-np.sin(angle)],[np.sin(angle),np.cos(angle)]]


vector_plus = [[x_maxes_NNO[1]],[y_maxes_NNO[1]]]

print('rotation_matrix_plus',rotation_matrix_plus)
print('vector_plus',vector_plus)

vector_NNO_plus_rotated = np.matmul(rotation_matrix_plus,vector_plus)

#x_max_NNO_plus_rotated = np.cos(angle_right)*hypo_right

print('vector_NNO_plus_rotated',vector_NNO_plus_rotated)

#SRO_a_parameter_right = ((1+(1+x_max_NNO_plus_rotated))*3.905)

#print('SRO_a_parameter_right',SRO_a_parameter_right)

#SRO_a_lattice_parameter =  (SRO_a_parameter_left + SRO_a_parameter_right)/2



############

total_length = -vector_NNO_minus_rotated[0] + vector_NNO_plus_rotated[0]

#print('total_length',total_length)

#oo2_SRO_x_position = total_length/2

#print('oo2_SRO_x_position',oo2_SRO_x_position)

#correction = 1-oo2_SRO_x_position

#print('correction',correction)

#SRO_a_lattice_parameter_left = (1+(x_max_NNO_minus_rotated  + oo2_SRO_x_position - correction))*3.905

#print('SRO_a_lattice_parameter_left',SRO_a_lattice_parameter_left)

#SRO_a_lattice_parameter_right = (1+(x_max_NNO_plus_rotated - correction - oo2_SRO_x_position - correction))*3.905

#print('SRO_a_lattice_parameter_right',SRO_a_lattice_parameter_right)

#SRO_a_lattice_parameter = (SRO_a_lattice_parameter_left + SRO_a_lattice_parameter_right)/2
```

```
#print('SRO_a_lattice_parameter',SRO_a_lattice_parameter)


##########



test = (1+(2-total_length)/2) * 3.905

print('test',test)

test2 = ((3+(3-2.953))/3)*3.905

print('test2',test2)

text = ax.text(0.05,0.83, 'STO\n[103]-', size=30, color = 'black',transform = ax.transAxes )
text = ax.text(0.08,0.22, 'SRO\n[103]-', size=30, color = 'black',transform = ax.transAxes )

text = ax.text(0.75,0.85, ' STO\n[103]+', size=30, color = 'black',transform = ax.transAxes )
text = ax.text(0.83,0.12, ' SRO\n[103]+', size=30, color = 'black',transform = ax.transAxes )

text = ax.text(0.26,0.405, r'$\theta$', size=30, color = 'black',transform = ax.transAxes )
text = ax.text(0.23,0.405, r'(', size=40, color = 'black',transform = ax.transAxes )

ax.set_ylabel(r'l (r.l.u)',fontsize=40,labelpad = 25)
ax.set_xlabel(r'h (r.l.u)',fontsize=40,labelpad = 25)

#plt.savefig(r"C:\Users\pblah\Data\XRD\FM332\Figures\Both_RSM_hkl.png", bbox_inches = "tight")
#plt.savefig(r"C:\Users\pblah\Data\XRD\FM332\Figures\Both_RSM_hkl.pdf", bbox_inches = "tight", format = "pdf")
```

```
[-0.9525853177257526, 1.0259274284548496] x_maxes_NNO
[-1.0014844147157191, -1.0014844147157191] x_maxes_STO
[2.9650307023411373, 2.942056794936455] y_maxes_NNO
[3.0, 3.0] y_maxes_STO
a 2.953969562135325
b -0.011611705534387786
Polynomial Fit 1st Order 2.95396956 - 0.01161171 x
left_edge_length 0.011061140205812503
bottom_edge_length 0.9525853177257526
hypo 0.9526495349126696
ratios 0.011611705534387612
angle 0.011611183701249419
rotation_matrix_minus [[0.9999325909638712, -0.011610922800509729], [0.011610922800509729, 0.9999325909638712]]
vector_minus [[-0.9525853177257526], [2.9650307023411373]]
vector_NNO_minus_rotated [[-0.98694785]
 [ 2.95377044]]
right_edge_length 0.011061140205812503
right_bottom_edge_length 1.0259274284548496
hypo_right 1.025996589896046
ratios_right 0.011611705534387612
angle_right 0.011612227437888862
rotation_matrix_plus [[0.9999325909638712, -0.011610922800509729], [0.011610922800509729, 0.9999325909638712]]
vector_plus [[1.0259274284548496], [2.942056794936455]]
vector_NNO_plus_rotated [[0.99169828]
 [2.95377044]]
test [3.94669344]
test2 3.966178333333333
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\4135251183.py:17: UserWarning: Log scale: values of z <= 0 have been masked
  ax.contourf(xi_NNO_plus,yi_NNO_plus,zi_NNO_plus, levels = [5,10,15,20,25,28,30,33,35],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 5,vmax = 35),linewidths = 1, a
lpha = 1)
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\4135251183.py:17: UserWarning: linewidths is ignored by contourf
  ax.contourf(xi_NNO_plus,yi_NNO_plus,zi_NNO_plus, levels = [5,10,15,20,25,28,30,33,35],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 5,vmax = 35),linewidths = 1, a
lpha = 1)
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\4135251183.py:18: UserWarning: Log scale: values of z <= 0 have been masked
  ax.contourf(xi_STO_plus,yi_STO_plus,zi_STO_plus, levels = [10,50,100,500,1000,5000,10000,12000,13200,14000,14200,14400],norm = matplotlib.colors.LogNorm(vmin = 5, vmax = 144
00),cmap = 'viridis',linewidths = 1, alpha = 1)
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\4135251183.py:18: UserWarning: linewidths is ignored by contourf
  ax.contourf(xi_STO_plus,yi_STO_plus,zi_STO_plus, levels = [10,50,100,500,1000,5000,10000,12000,13200,14000,14200,14400],norm = matplotlib.colors.LogNorm(vmin = 5, vmax = 144
00),cmap = 'viridis',linewidths = 1, alpha = 1)
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\4135251183.py:19: UserWarning: Log scale: values of z <= 0 have been masked
  ax.contourf(xi_NNO_minus,yi_NNO_minus,zi_NNO_minus, levels = [12,15,20,25,28,30,33,35,50,80,120,135],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 12,vmax = 13
5),linewidths = 1, alpha = 1)
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\4135251183.py:19: UserWarning: linewidths is ignored by contourf
  ax.contourf(xi_NNO_minus,yi_NNO_minus,zi_NNO_minus, levels = [12,15,20,25,28,30,33,35,50,80,120,135],cmap = 'viridis',norm = matplotlib.colors.LogNorm(vmin = 12,vmax = 13
5),linewidths = 1, alpha = 1)
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\4135251183.py:20: UserWarning: Log scale: values of z <= 0 have been masked
  ax.contourf(xi_STO_minus,yi_STO_minus,zi_STO_minus, levels = [20,50,100,500,1000,5000,10000,12000,13200,14000,14200,14400],norm = matplotlib.colors.LogNorm(vmin = 5, vmax =
14400),cmap = 'viridis',linewidths = 1, alpha = 1)
C:\Users\pblah\AppData\Local\Temp\ipykernel_14560\4135251183.py:20: UserWarning: linewidths is ignored by contourf
  ax.contourf(xi_STO_minus,yi_STO_minus,zi_STO_minus, levels = [20,50,100,500,1000,5000,10000,12000,13200,14000,14200,14400],norm = matplotlib.colors.LogNorm(vmin = 5, vmax =
14400),cmap = 'viridis',linewidths = 1, alpha = 1)
```

Out[19]: Text(0.5, 0, 'h (r.l.u)')


STO
[103]-
STO
[103]+
SRO
[103]-
SRO
[103]+
θ
3.050
3.025
3.000
2.975
2.950
2.925
2.900
l (r.l.u)
−1.0
−0.5
0.0
0.5
1.0
h (r.l.u)