

# 1 Different Greedy Methods- I Named them results based on folder

(Note: 2 exponents are redundant if they're similar to the third decimal place, default factor is 2.)

**results** - exits if number of functions is 30 or KL-Divergence is less than  $1e-6$  or redundancies are found or the next set of choices for  $n+1$  basis functions is not better than current  $n$  basis functions.

**results\_original** - same as results except completely Ignores if redundancies occurred but it does record that it did find them.

The point of this method was to see if "one can get out of being redundant if we ignore their presence". Answer is no.

**results\_redundancies** - same as results except if redundancies are found and they have better error (KL diverg.) then it reverts back to the smaller/condensed parameters. If not, it goes back to  $n$  basis function and tries again with a new factor. If redundancies are found 5 times in a row, it exits.

The point of this method was to see if "changing the factor gives different answer" and "use redundancies to refine our parameters and continue greedy from that "condensed" parameters".

## 2 How each Element Exited Based on Method

No method exited because it reached 30 basis functions or because it found five redundancies in a row.

**results** - Format: element name (number of basis functions)-

Exited because Redundancies Were Found: he(8), li(8), b(13), be(11), c(10).

Exited because objective function was small: n(10), o(8), f(8), ne(8).

**results\_original** -

Exited because next  $n+1$  basis func was not better: he(13), li(10), be(12), b(14), c(21)

Exited because objective function was small: n(10), o(8), f(8), ne(8).

**results\_redundancies** -

Exited because next  $n+1$  basis func was not better: he(7), li(8), be(9), b(10), c(20)

Exited because objective function was small: n(10), o(8), f(8), ne(8).

Exited because 5 redundancies were found in a row : None  $\Rightarrow$  having an adaptive factor here is useless

General Conclusion is small elements tend to exit by not finding better choices and converges mostly around 8 functions.

## 3 Redundancies Information Format: Element(Numb.of Basis Functions, Numb. after removing redundancy)

**results**- Note: exits if redun. He(8, 7), Li(8, 7), Be(11, 8), B(13, 8), C(10, 9). Rest of elements no redundancies were found.

**result\_original** Note: this method only records that redundancies occurred

- He[[8, 7], [9, 7], [10, 7], [11, 7], [12, 7], [13, 7]]. Here the number of redundant exponents in each iteration is inc. by one.

Below we see that the number of redundancies is constant throughout

Li [[8, 7], [9, 8], [10, 9]].

Be[[11, 8], [12, 9]]

B [[13, 8], [14, 9]]

C[[10, 9], [11, 10], [12, 11], [13, 12], [14, 13], [15, 14], [16, 15], [17, 16], [18, 17], [19, 18], [20, 19], [21, 20]].

**result\_redundancies** He[[8, 7, 'Gave Better Answer']], Note: Finished right after removing redund. i.e. 7 basis func

Li[[8, 7, 'Gave Better Answer']] Note: finished at 8 basis func.

Be[[11, 8, 'Gave Better Answer']] Note: finished at 9 basis func.

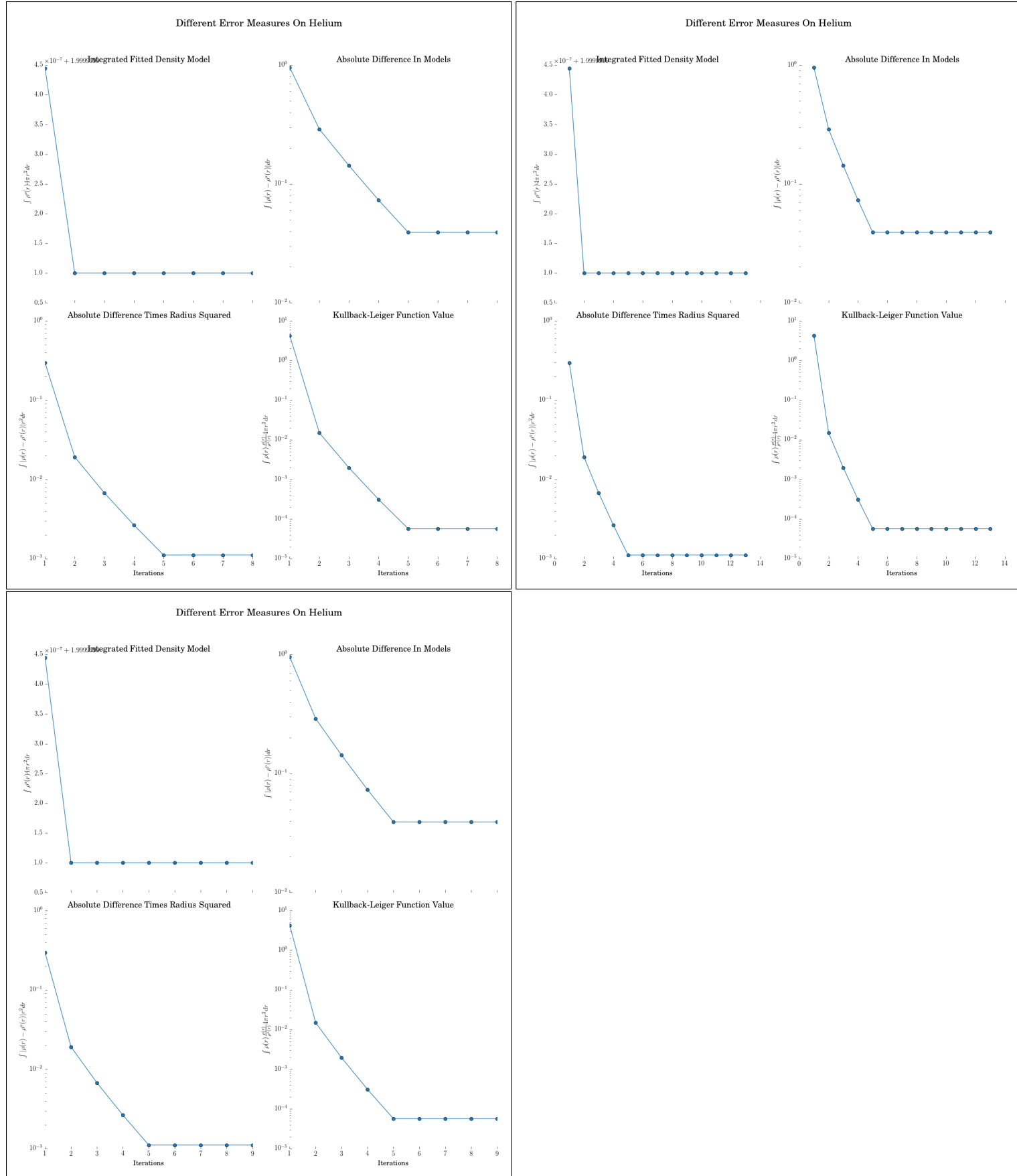
B[[13, 8, 'Gave Better Answer']] Note: finished at 10

C[[10, 9, 'Gave Better Answer']] Note: Carbon finished with 20 basis func.

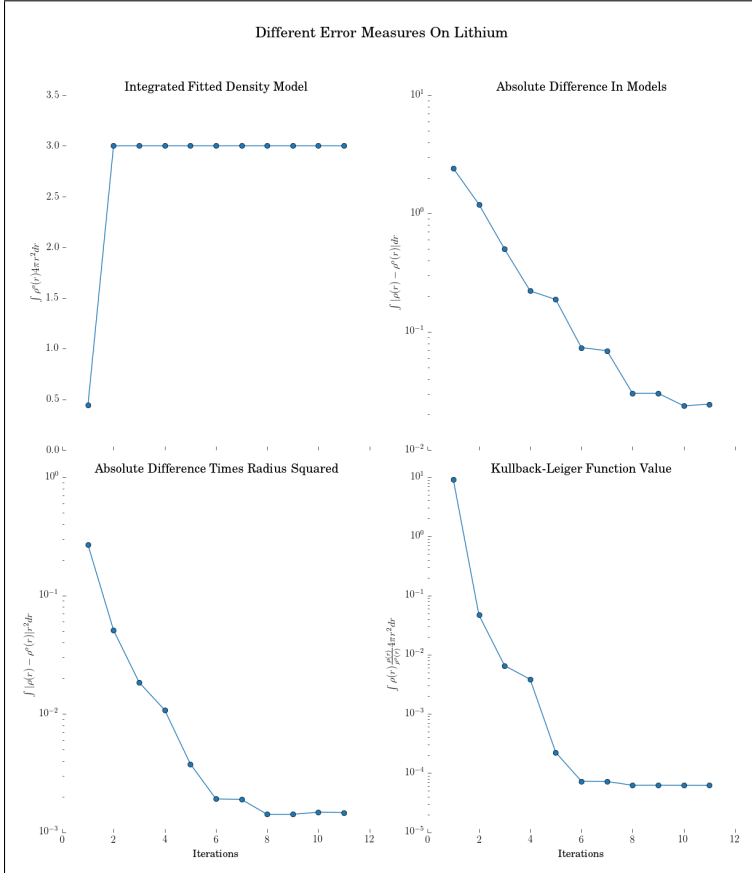
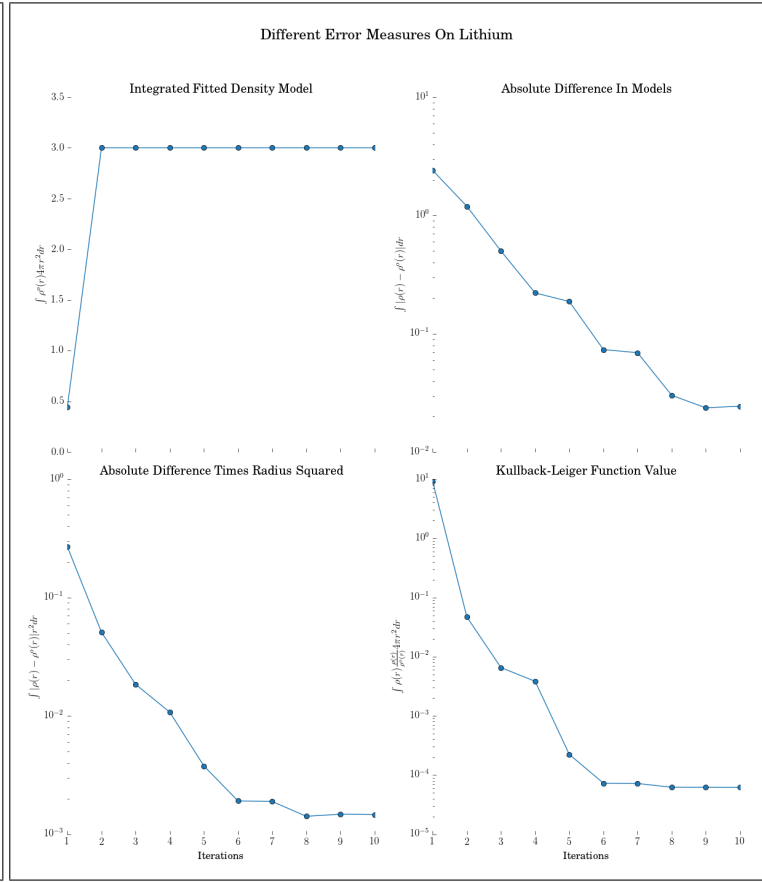
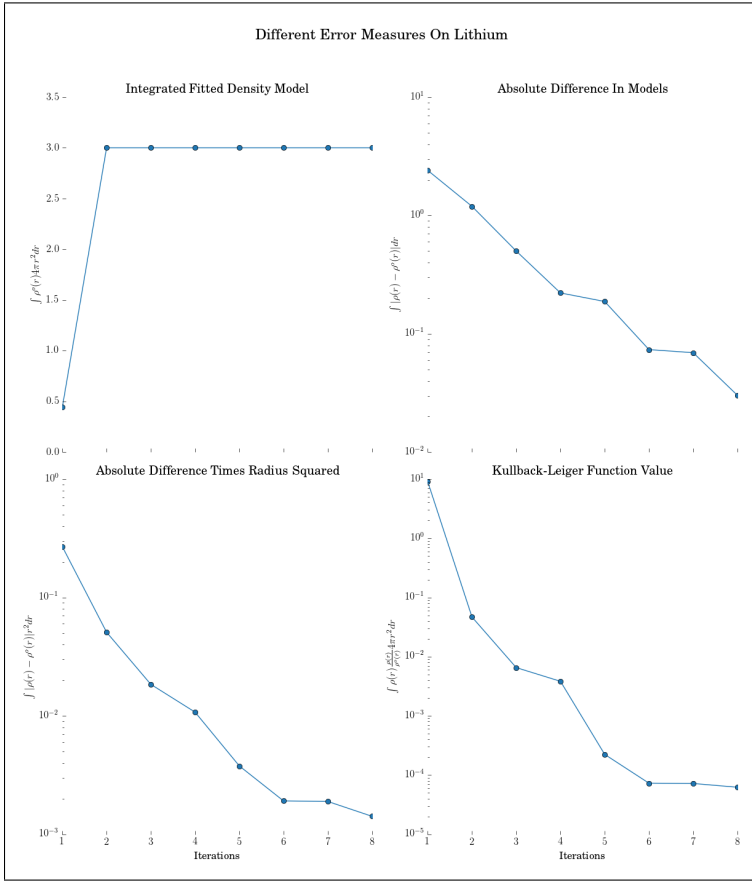
Conclusion: Even though result\_redundancies found/removed redundant exponents it still gave a lower error overall, hence my adaptive factor idea is useless here. It appears that removing redundancy is a better choice than ignoring them, as once they're removed they never show up again, however exiting when redundancy were found seems to be the best choice as error does not dec. greatly (look at plots below), or even exiting when the change in obj function is small (Counter example is Nit. as it had a slightly dec. in error). Ultimately, this shows that global optimum at each iteration is not guaranteed and caring about redundancy is pretty much pointless, as seen by comparing the change in error from plots.

## 4 Plotting Elements Side by Side, (Results, Results-O, Results-R)

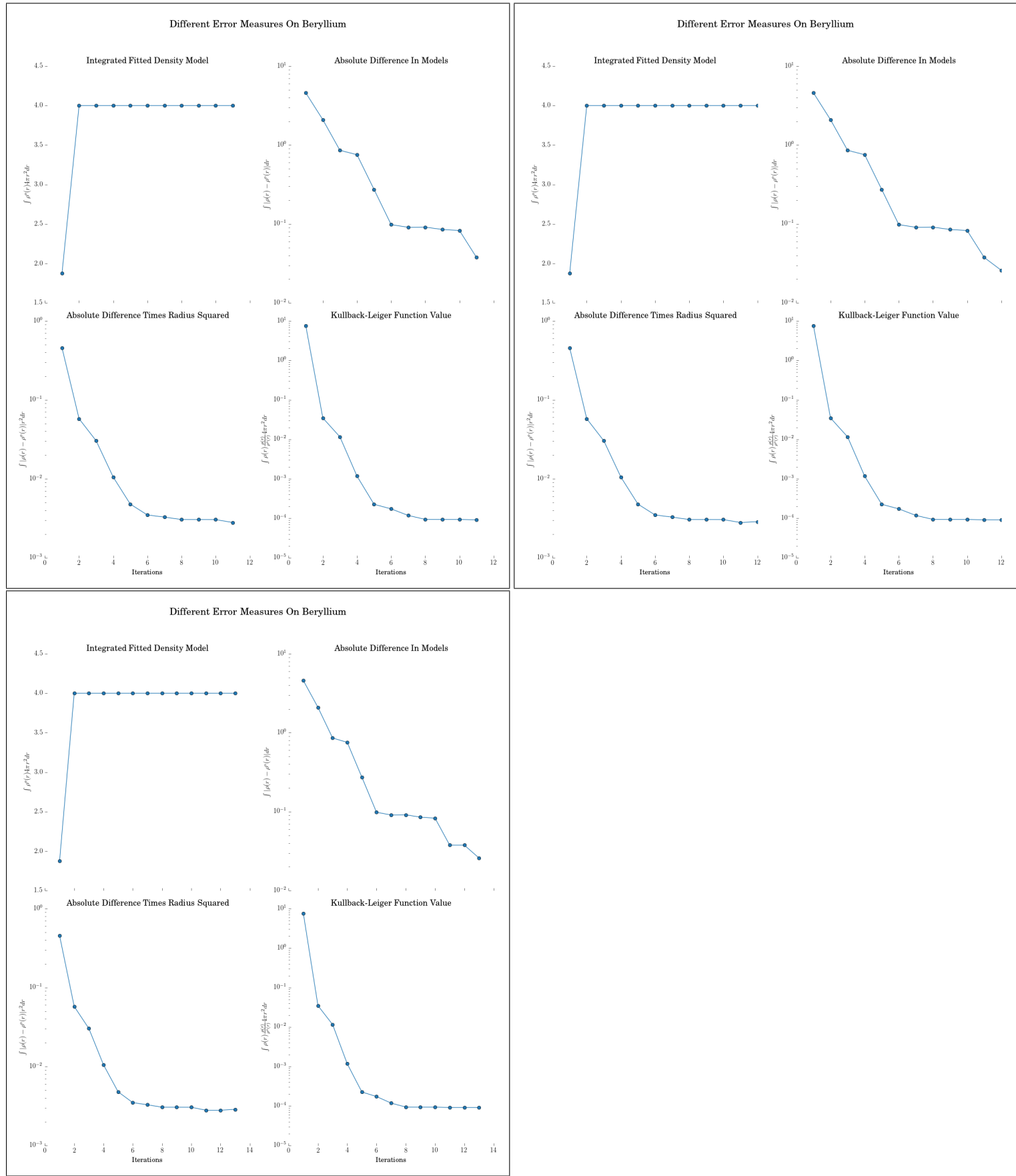
### 4.1 HE



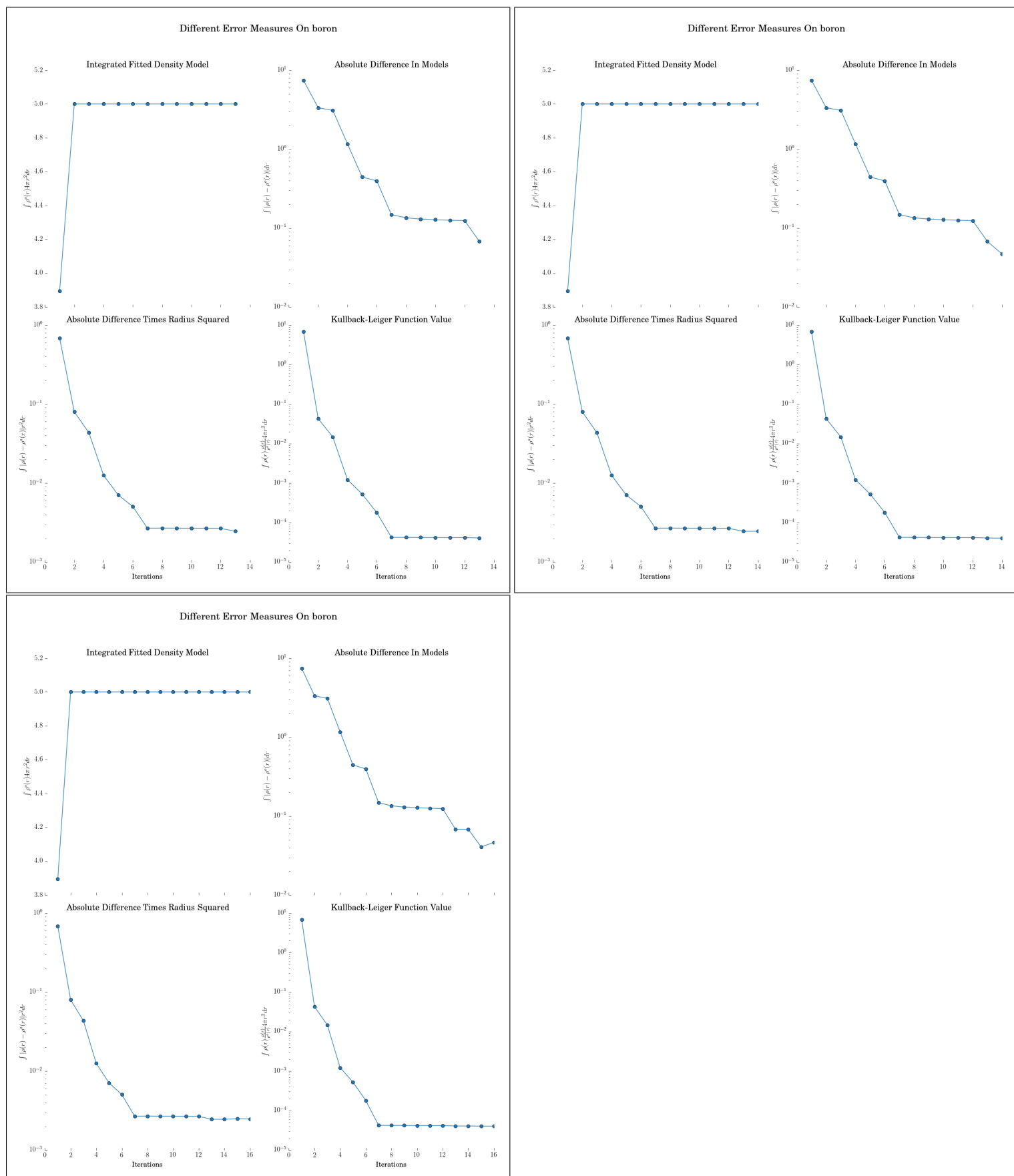
## 4.2 Li



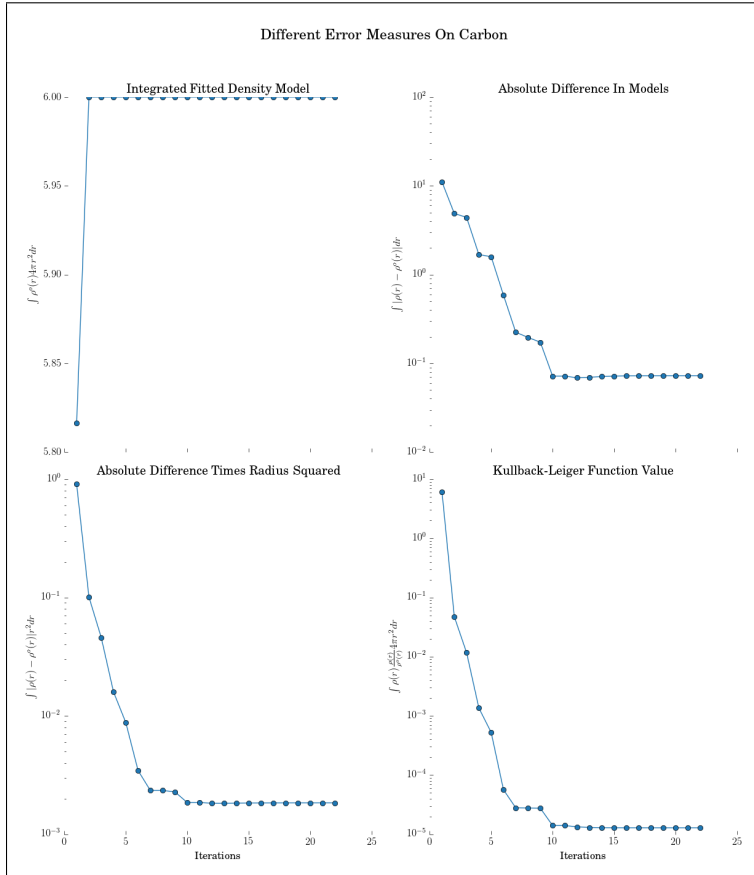
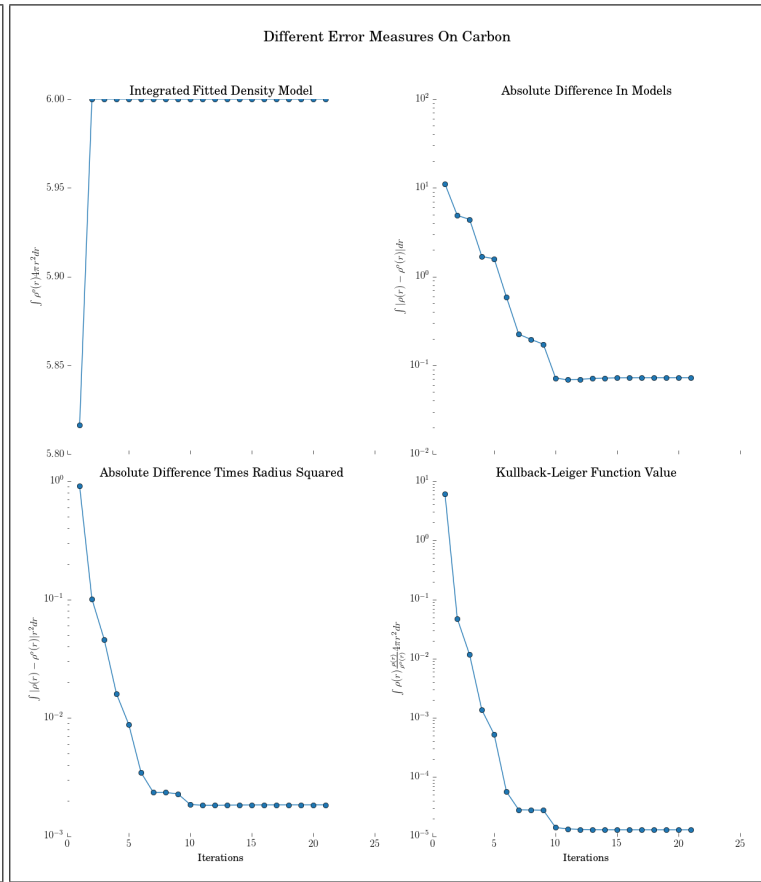
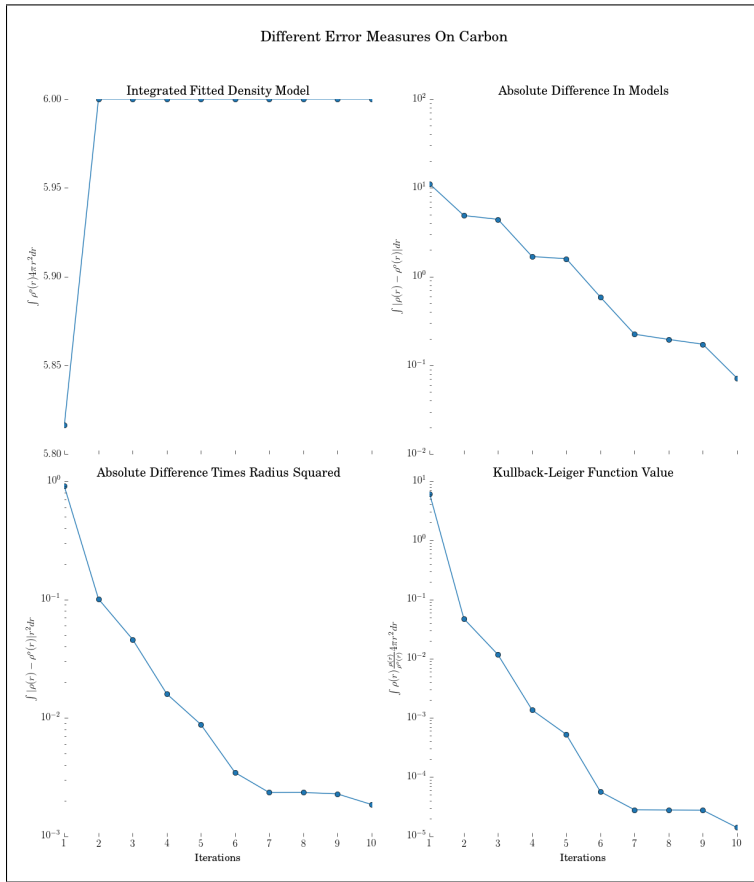
### 4.3 Be



## 4.4 b



## 4.5 c



The figure displays four plots related to the error measures on nitrogen data, showing the results of the Integrated Fitted Density Model over 10 iterations.

**Top Left Plot: Integrated Fitted Density Model**

The y-axis represents the integrated fitted density model, ranging from 0.000 to 0.008. The x-axis represents the iterations (1 to 10). The error starts at approximately 0.0003 and rapidly increases to about 0.007 by iteration 2, remaining stable thereafter.

**Top Right Plot: Absolute Difference In Models**

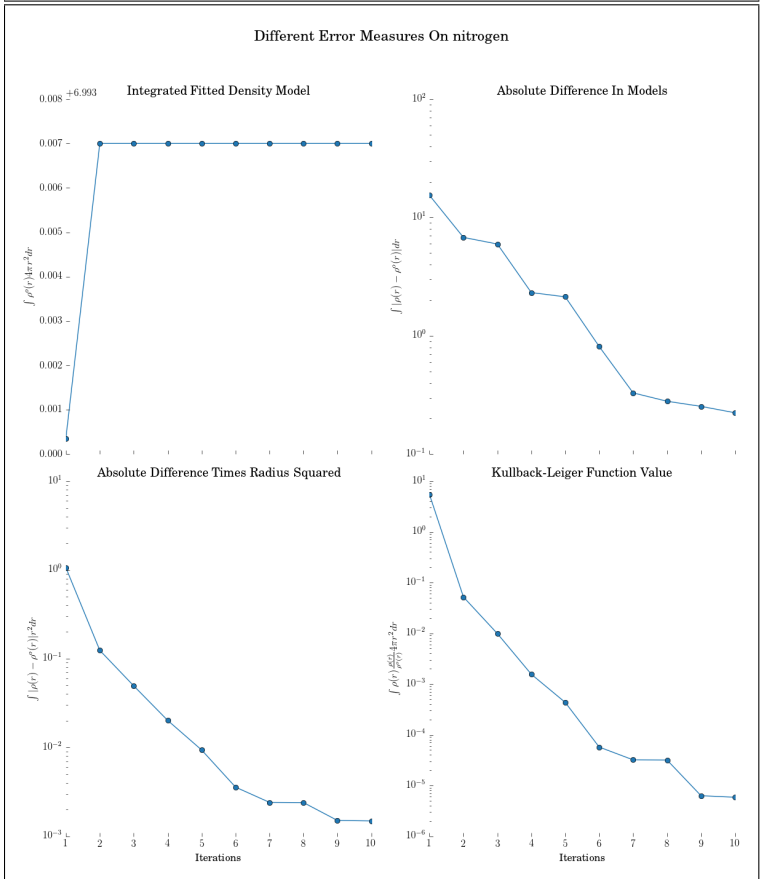
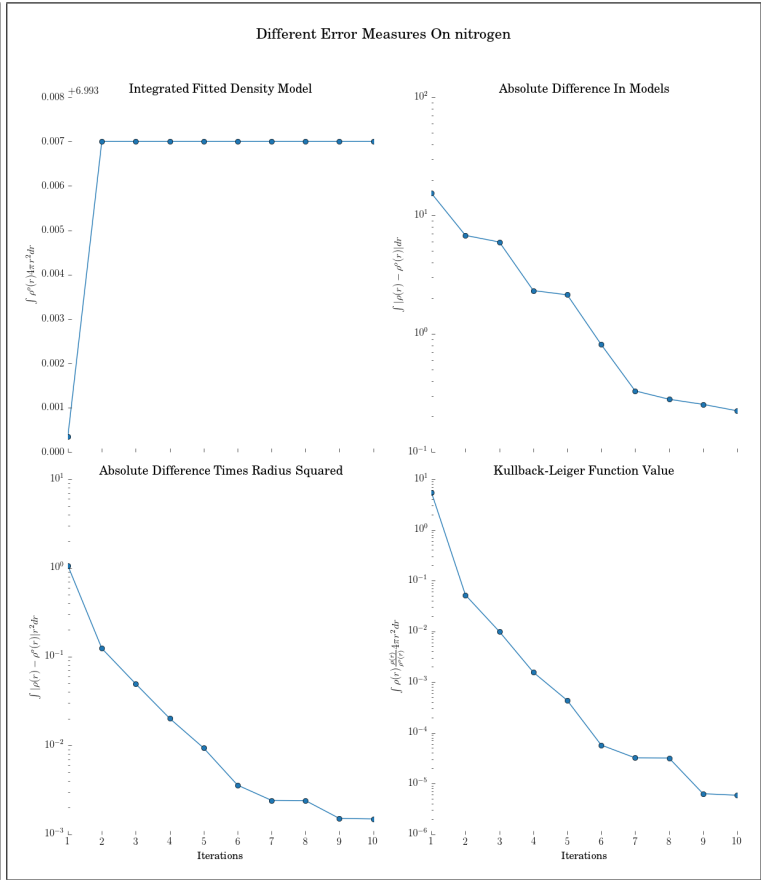
The y-axis represents the absolute difference in models, plotted on a logarithmic scale from  $10^0$  to  $10^2$ . The x-axis represents the iterations (1 to 10). The error starts at approximately 100 and decreases steadily to about 0.1 by iteration 10.

**Bottom Left Plot: Absolute Difference Times Radius Squared**

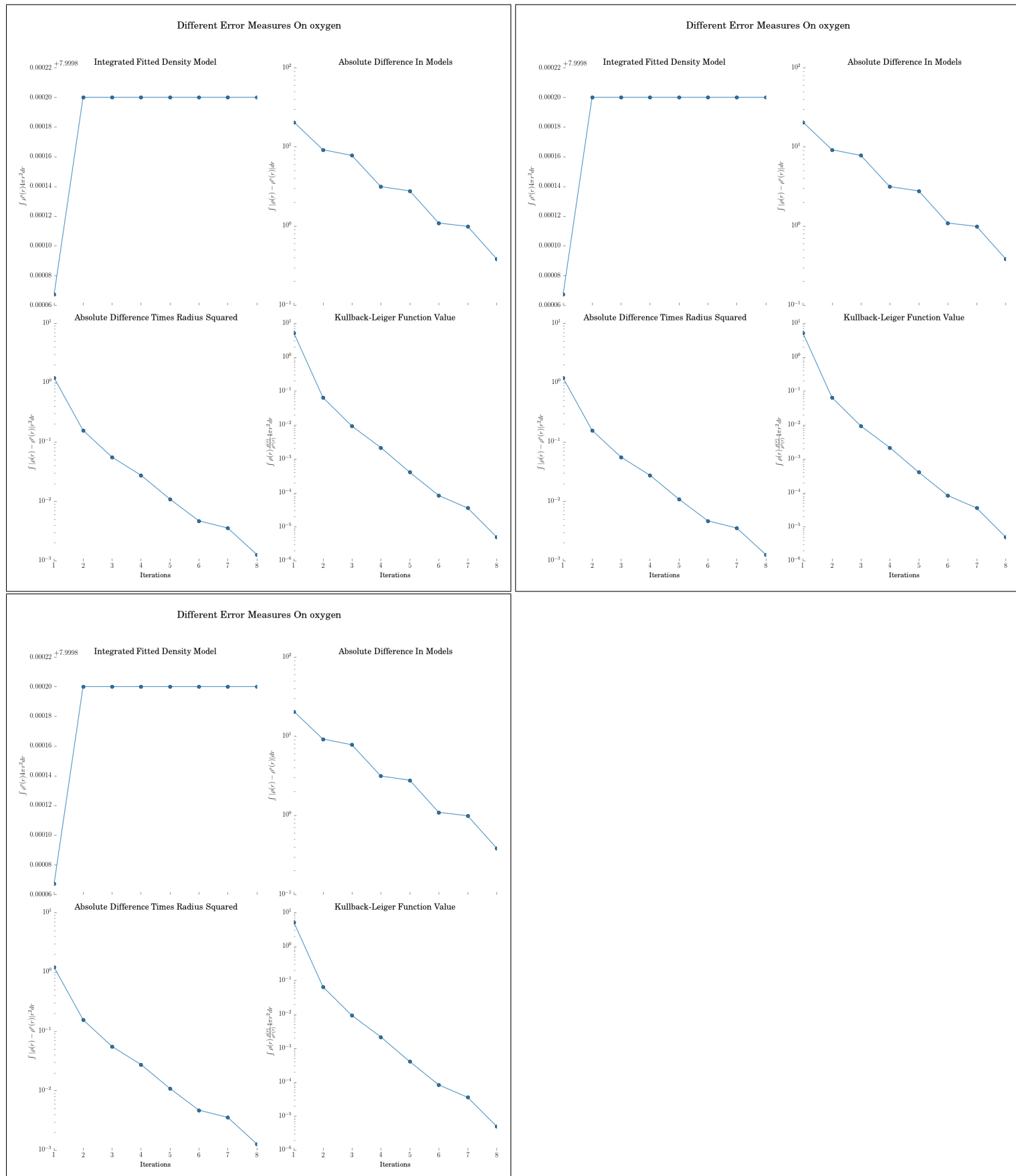
The y-axis represents the absolute difference times radius squared, plotted on a logarithmic scale from  $10^{-3}$  to  $10^0$ . The x-axis represents the iterations (1 to 10). The error starts at approximately 1.0 and decreases steadily to about  $10^{-3}$  by iteration 10.

**Bottom Right Plot: Kullback-Leiger Function Value**

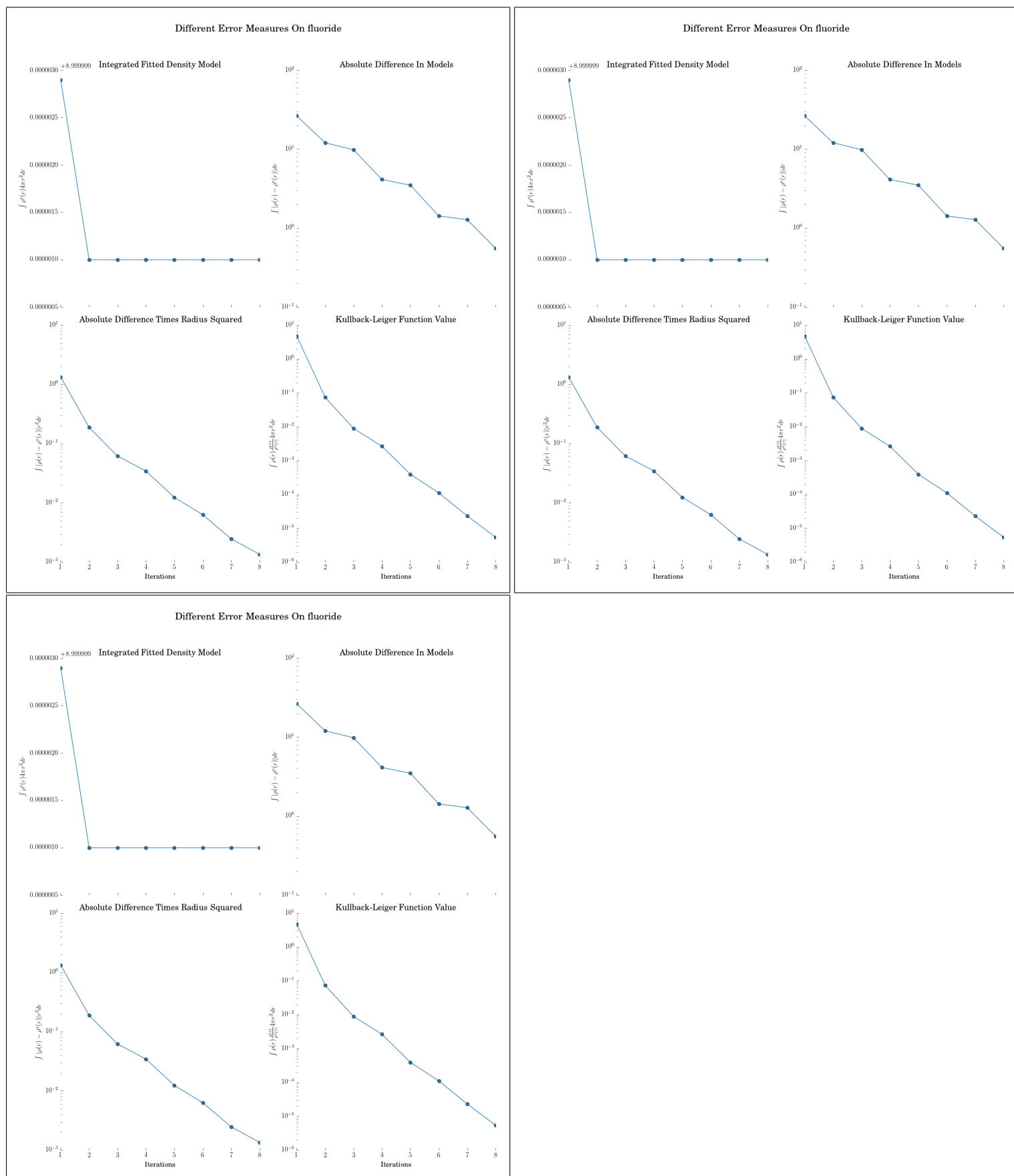
The y-axis represents the Kullback-Leiger function value, plotted on a logarithmic scale from  $10^{-6}$  to  $10^1$ . The x-axis represents the iterations (1 to 10). The error starts at approximately 10 and decreases steadily to about  $10^{-5}$  by iteration 10.

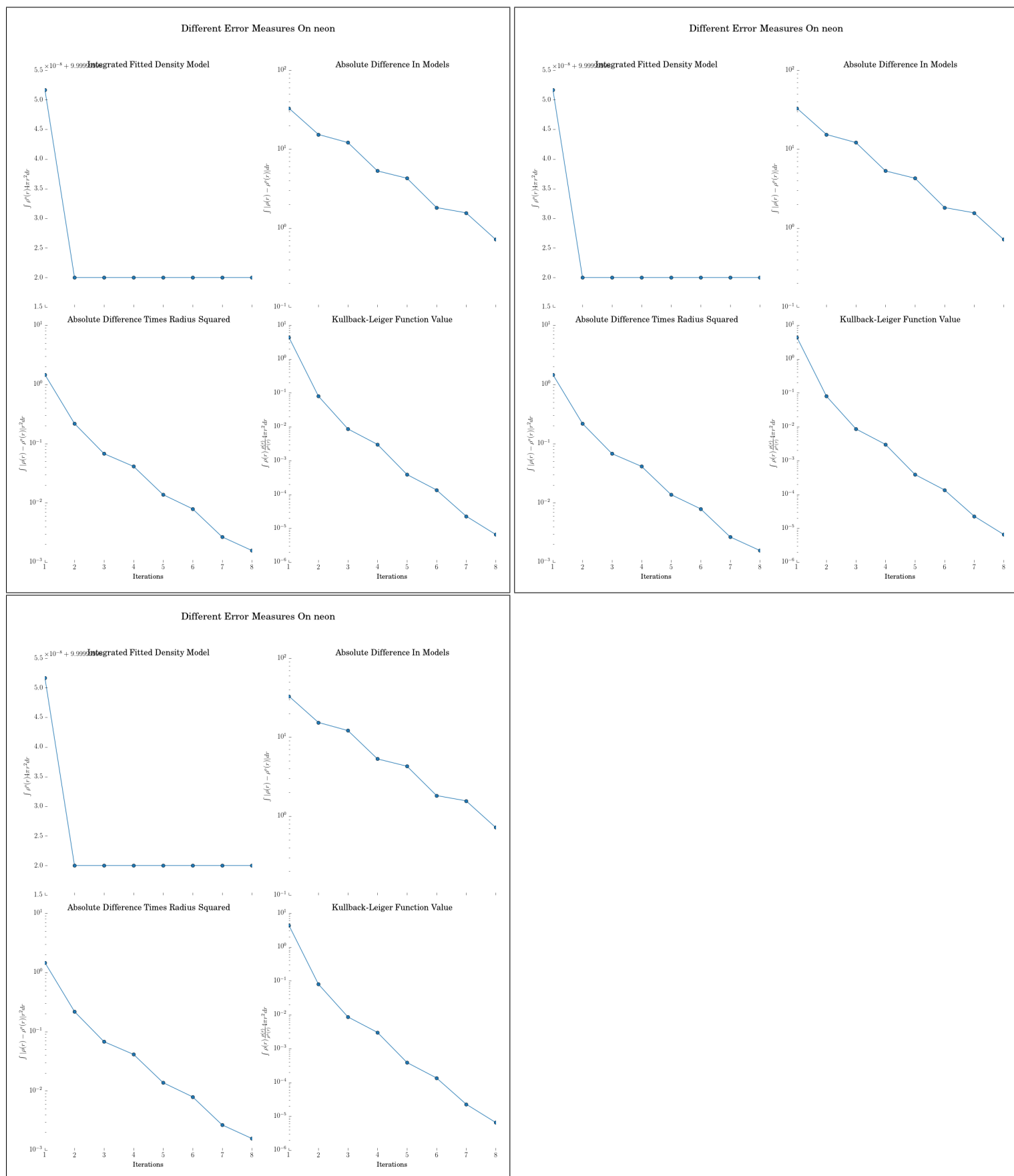


## 4.7 o



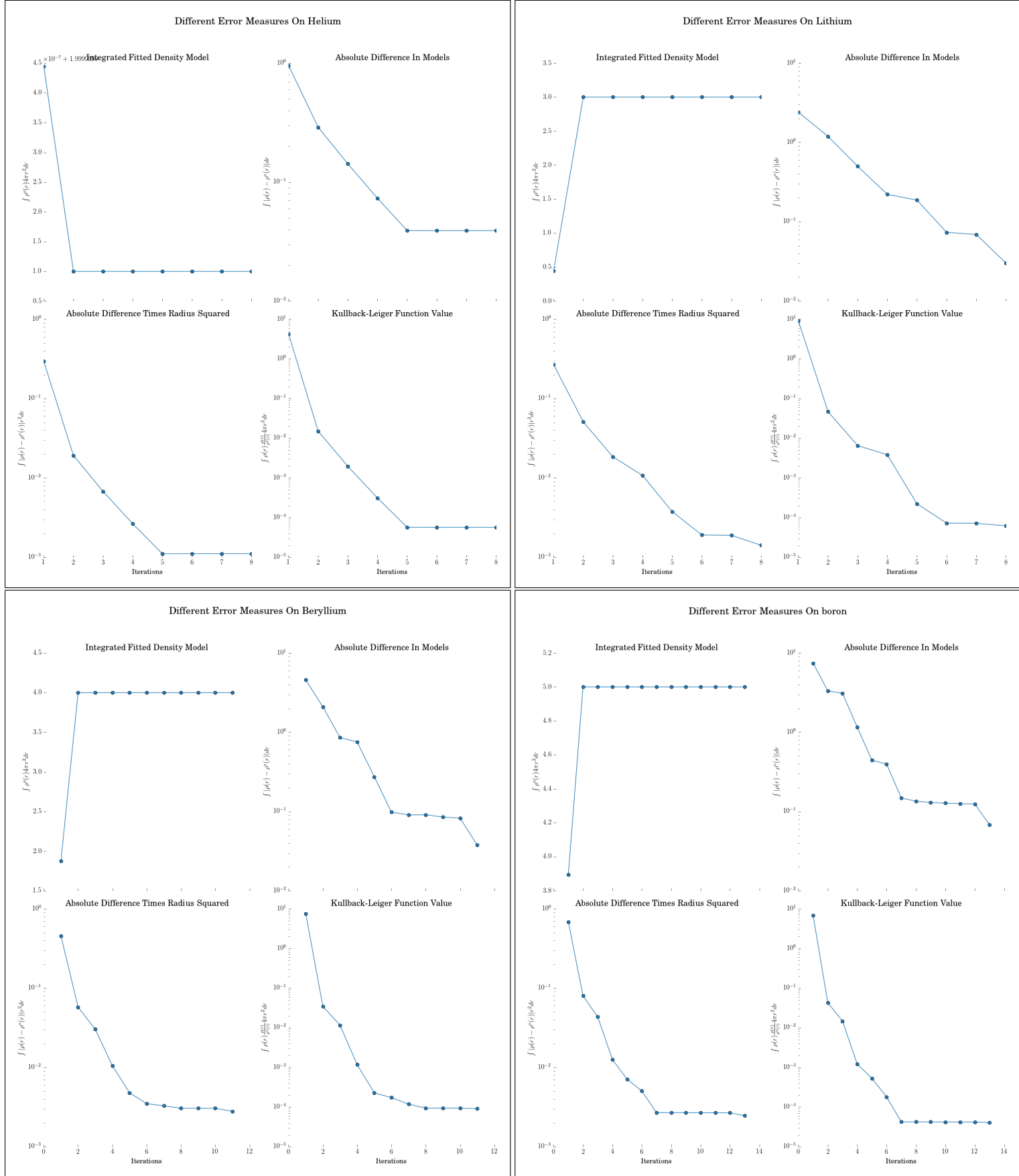


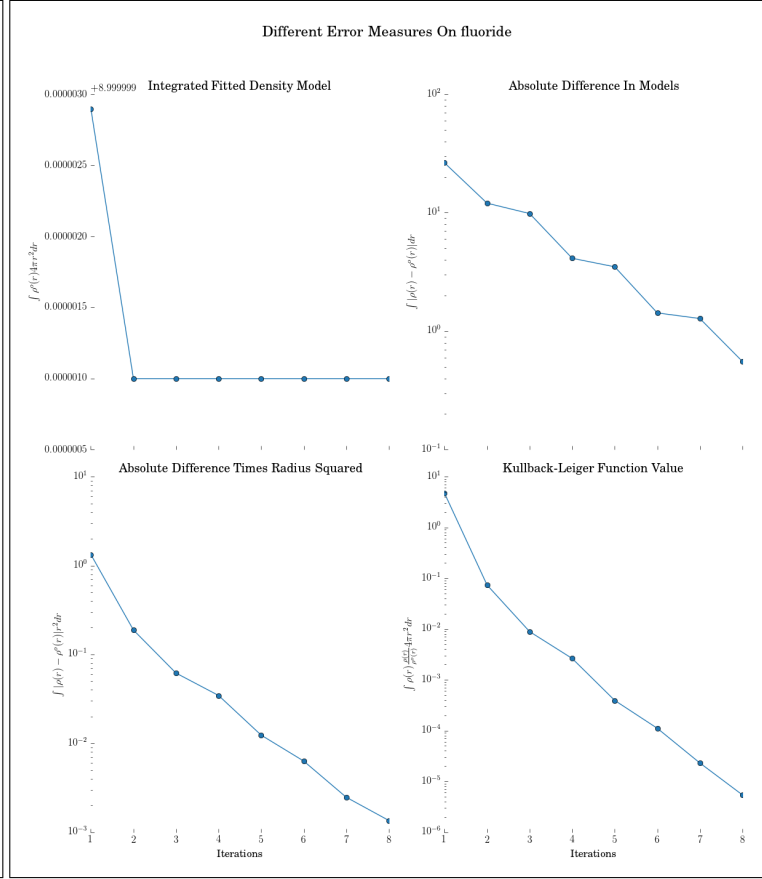
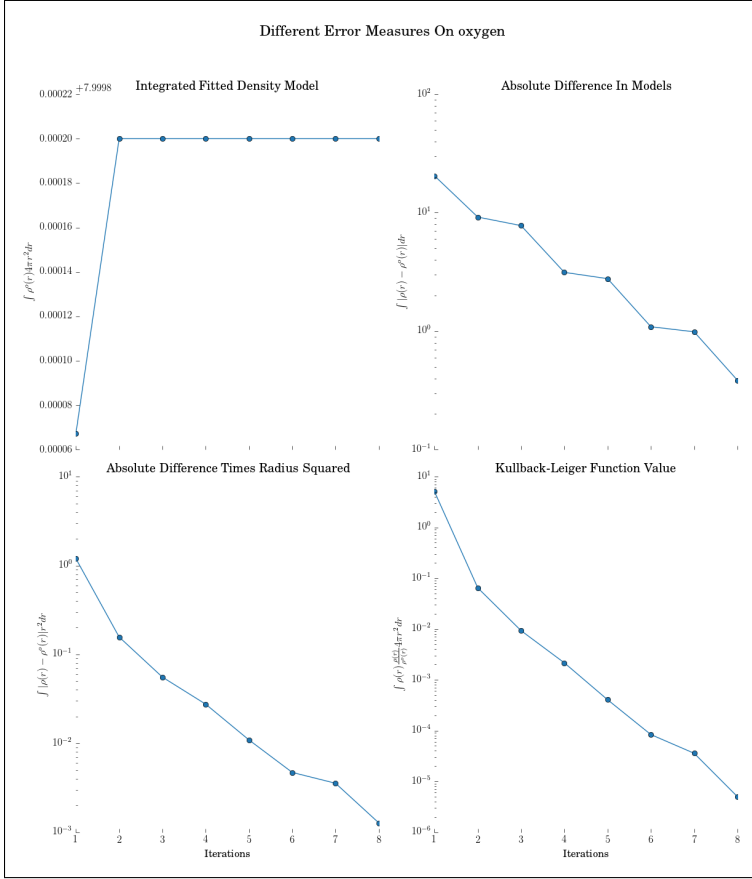
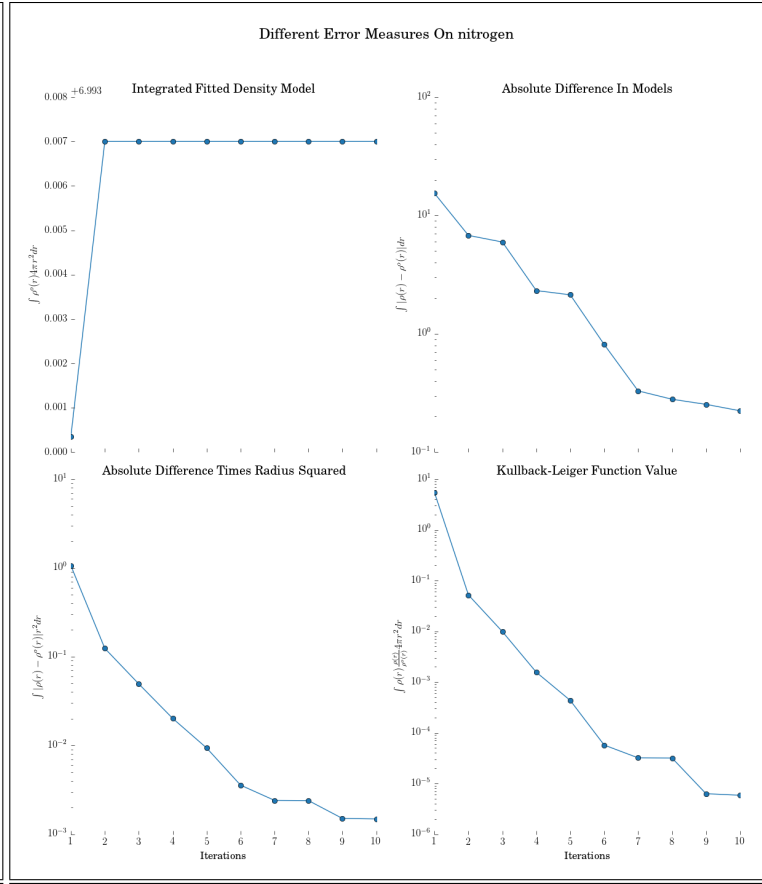
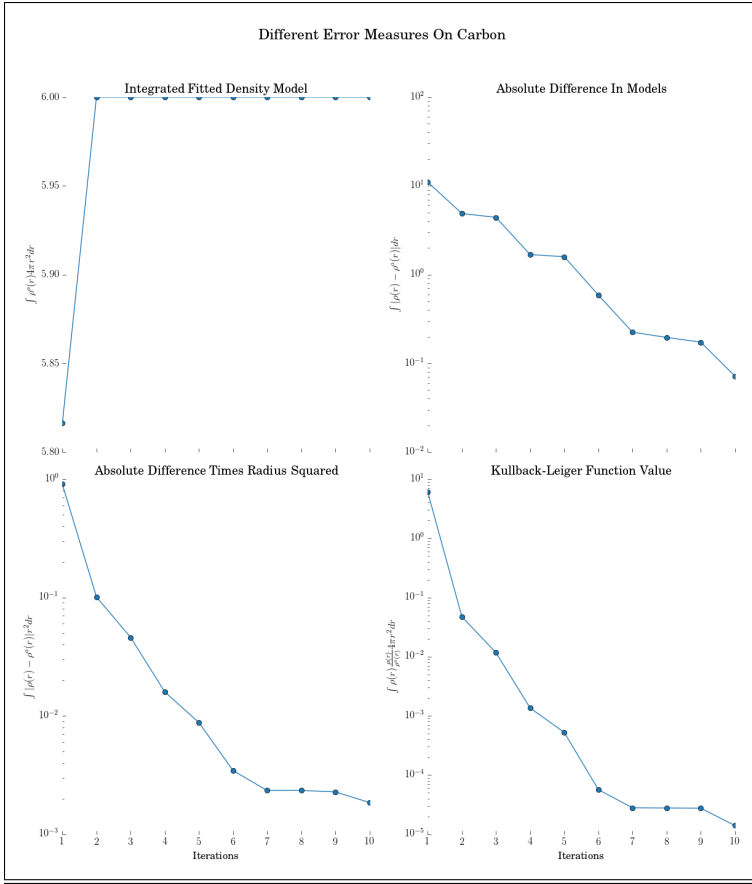




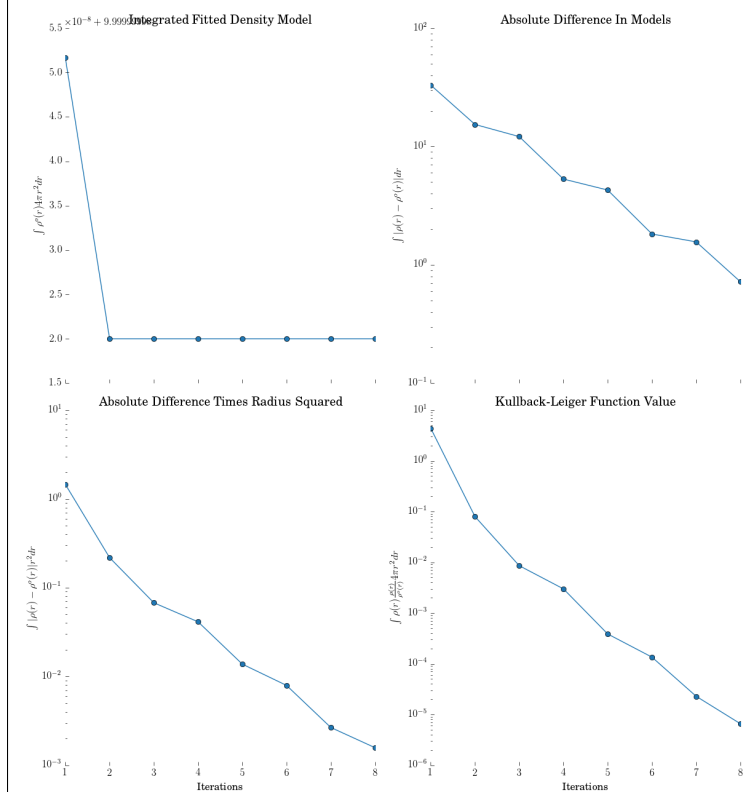
# 5 Plotting Grouped By Method

## 5.1 Results Plots

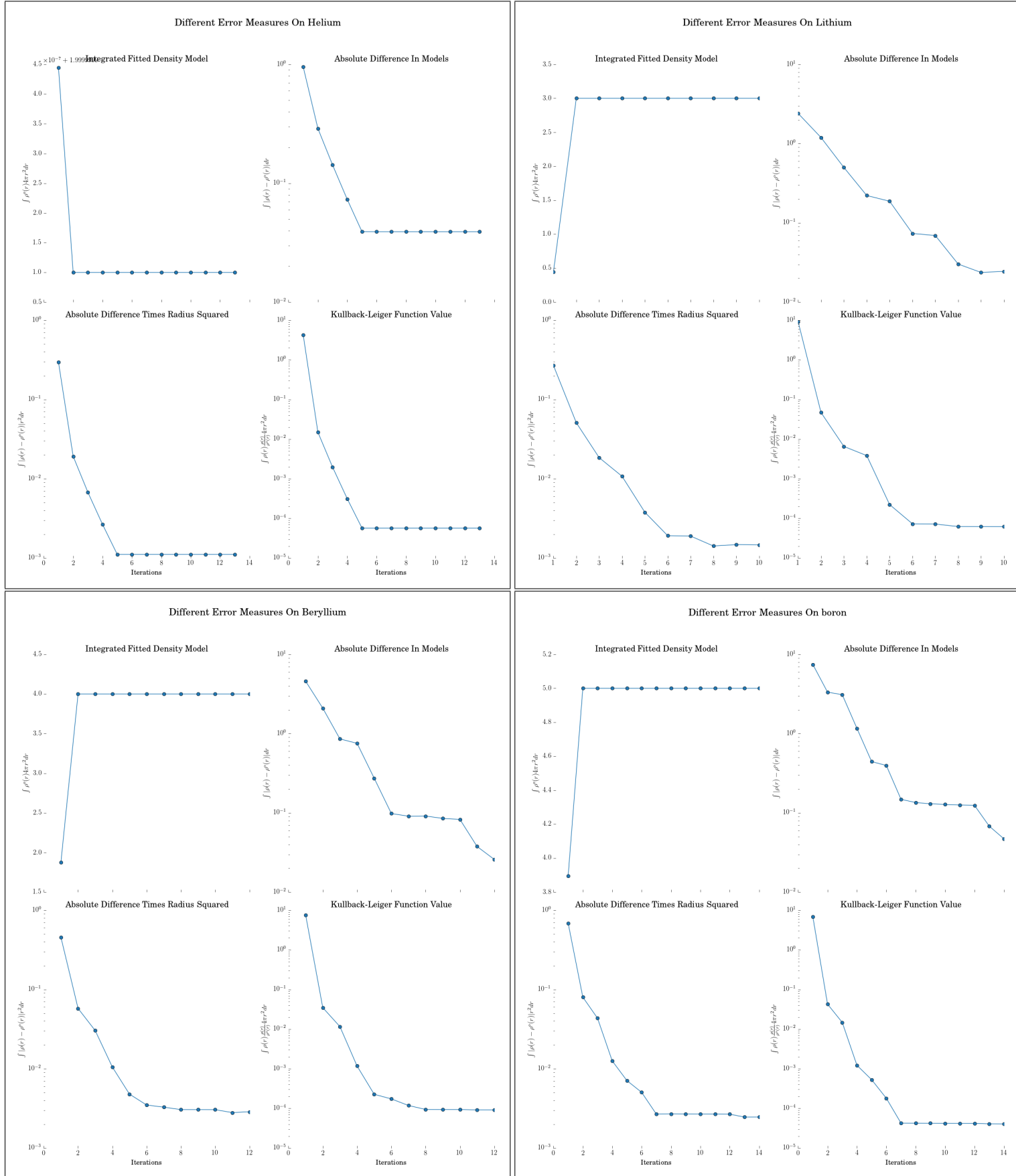


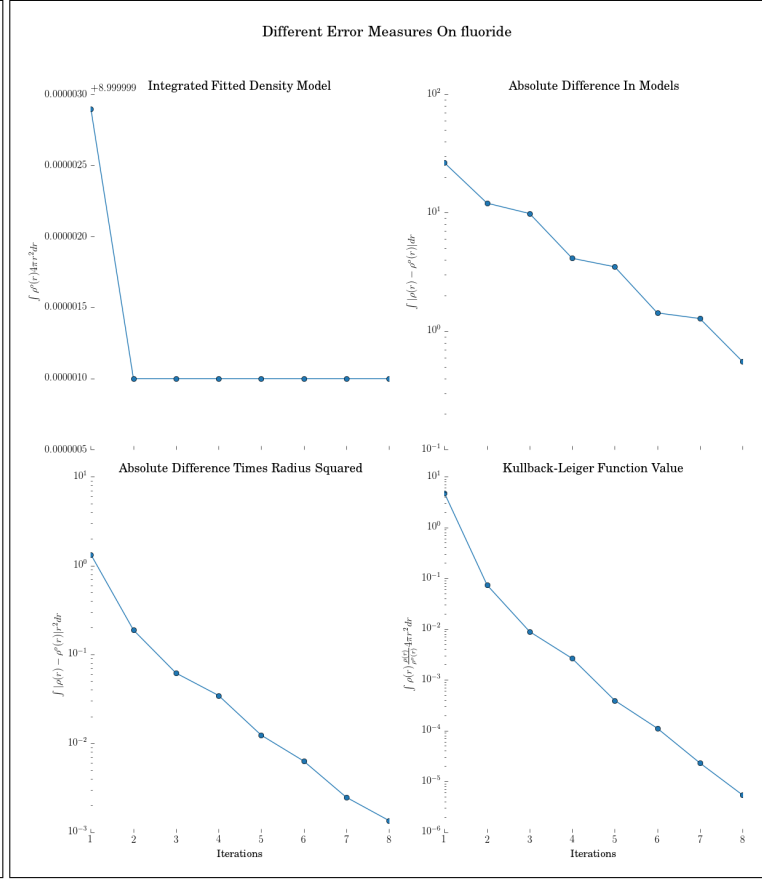
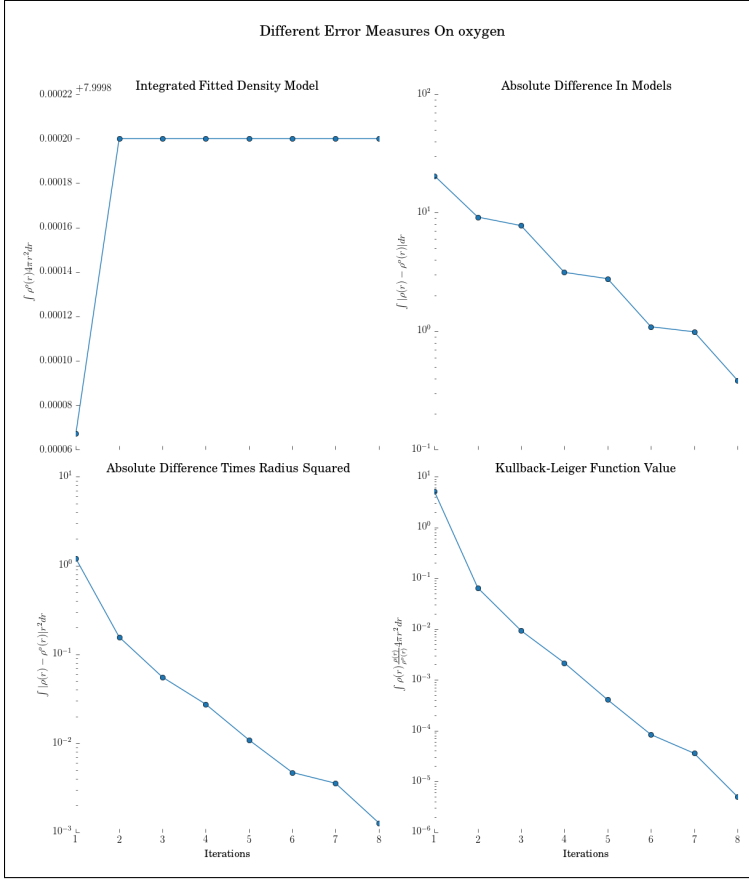
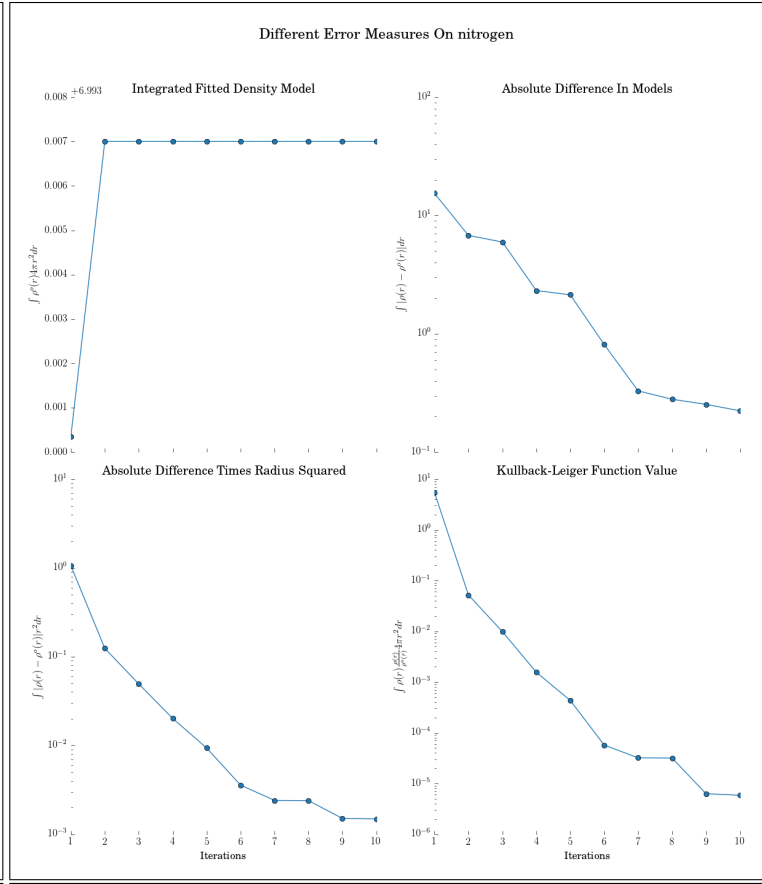
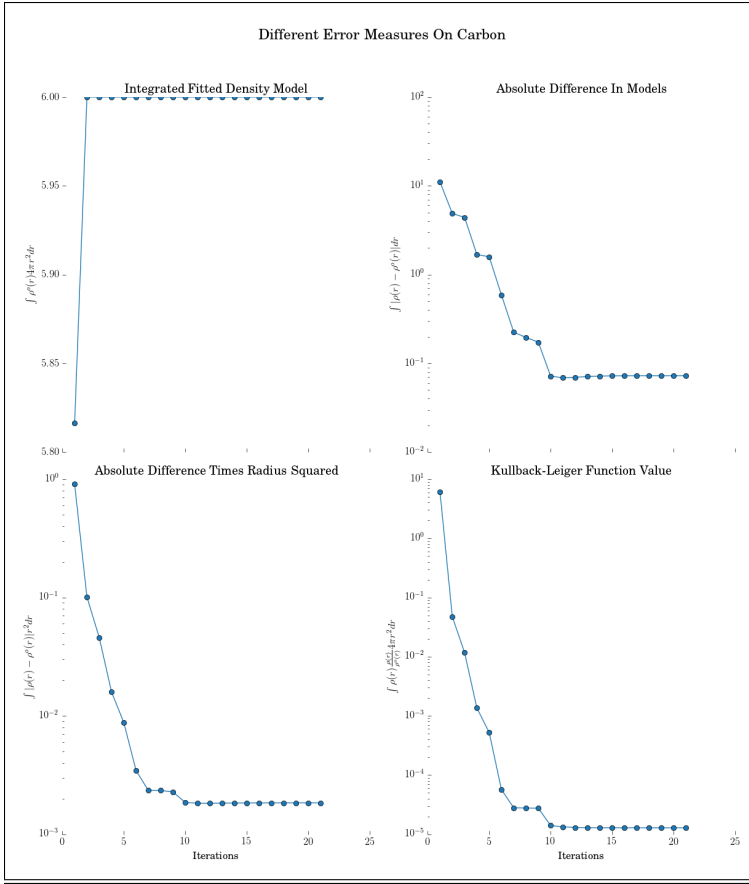


Different Error Measures On neon

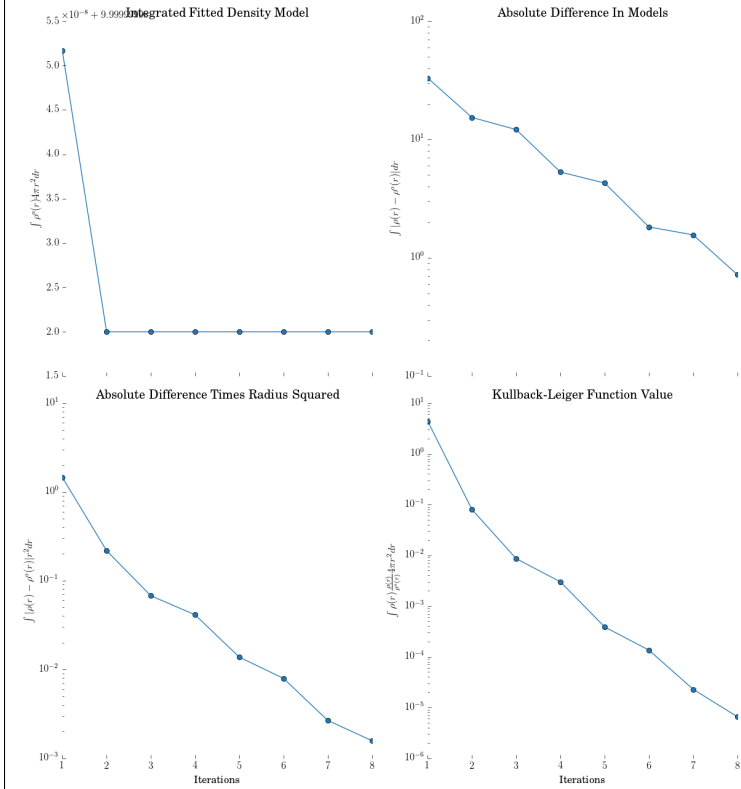


## 5.2 Results\_Original Plots (X-Axis is Number of Basis Functions)



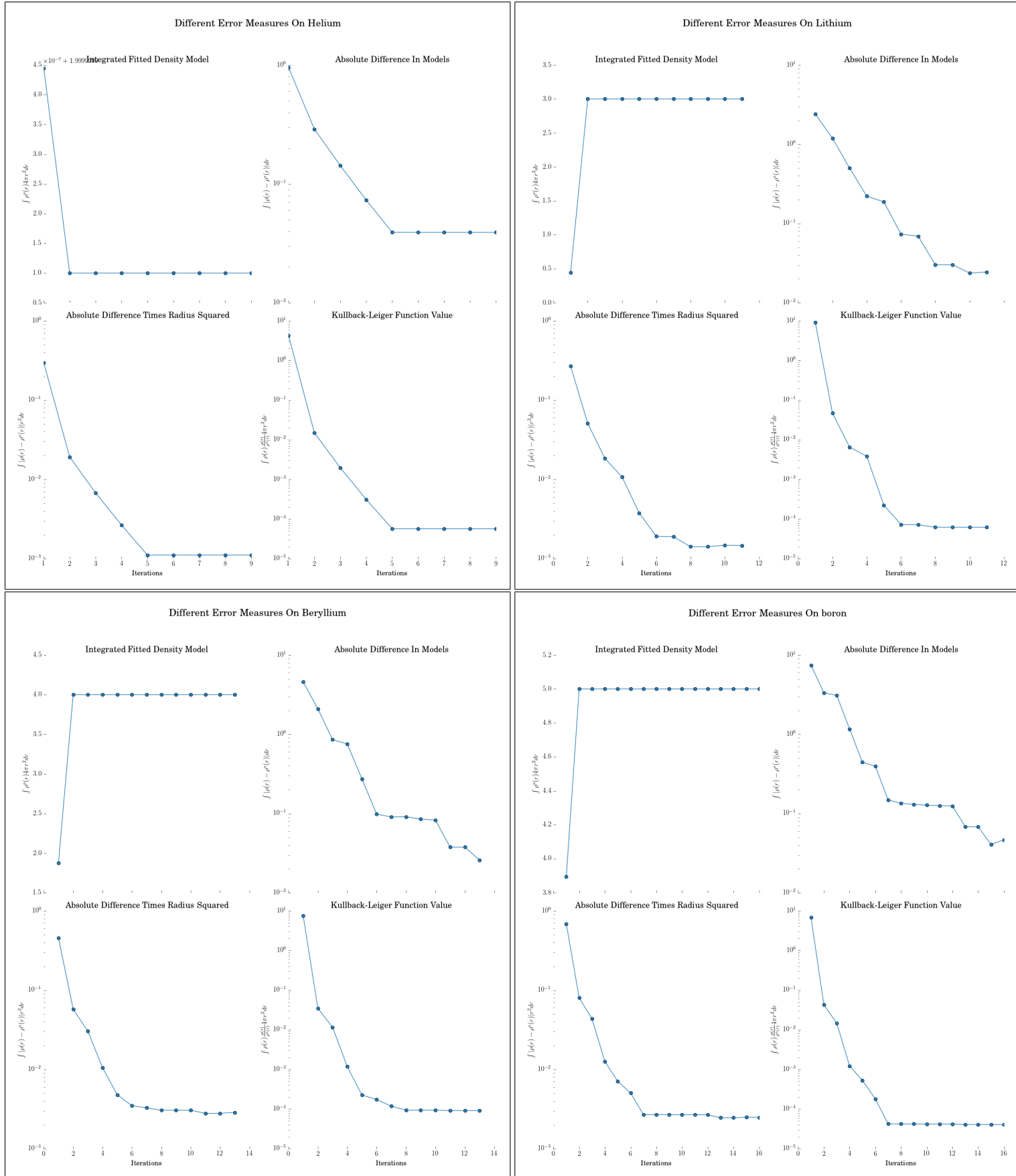


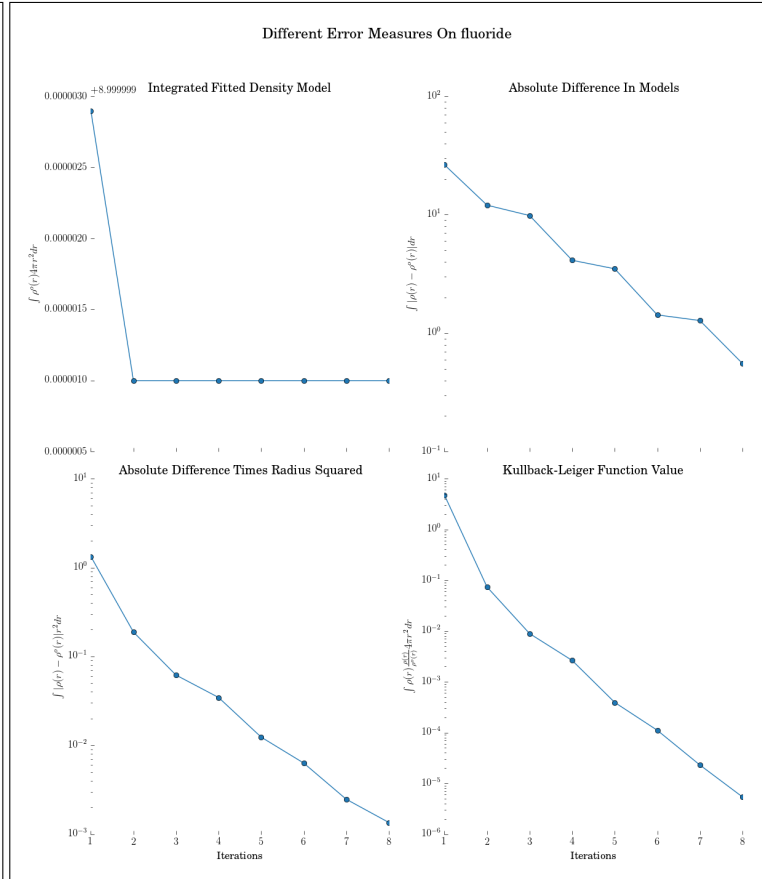
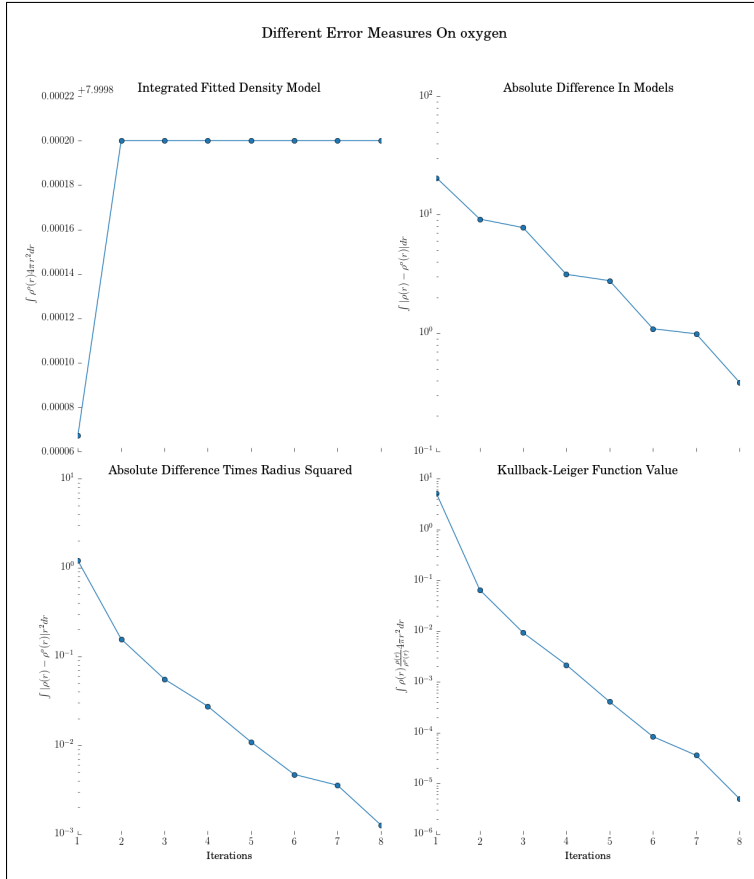
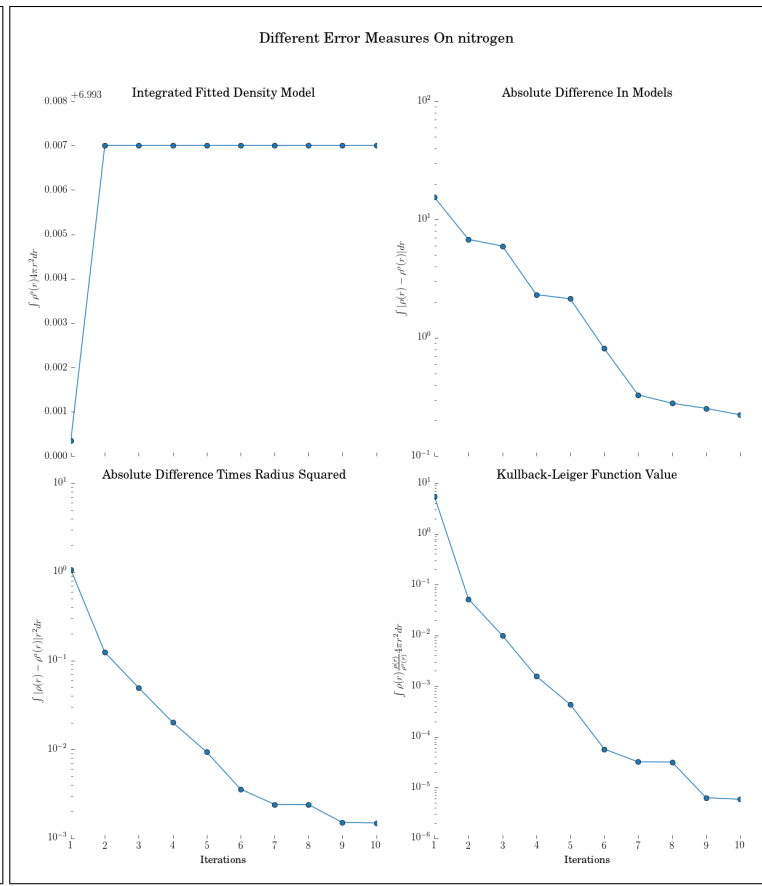
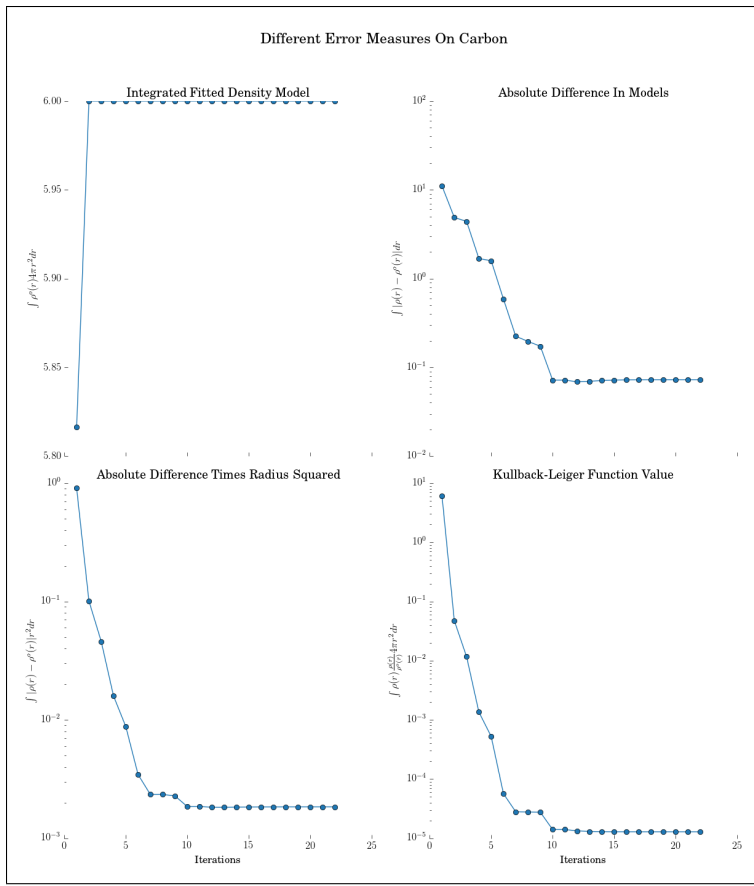
Different Error Measures On neon





### 5.3 Results\_Redundancies Plots





Different Error Measures On neon

