The Effects of Atomic Data Choices on Calibration Uncertainty

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What we are and aren't talking about

- **Not discussing (but probably should!)**

  Calibration sources

  Absorption of materials

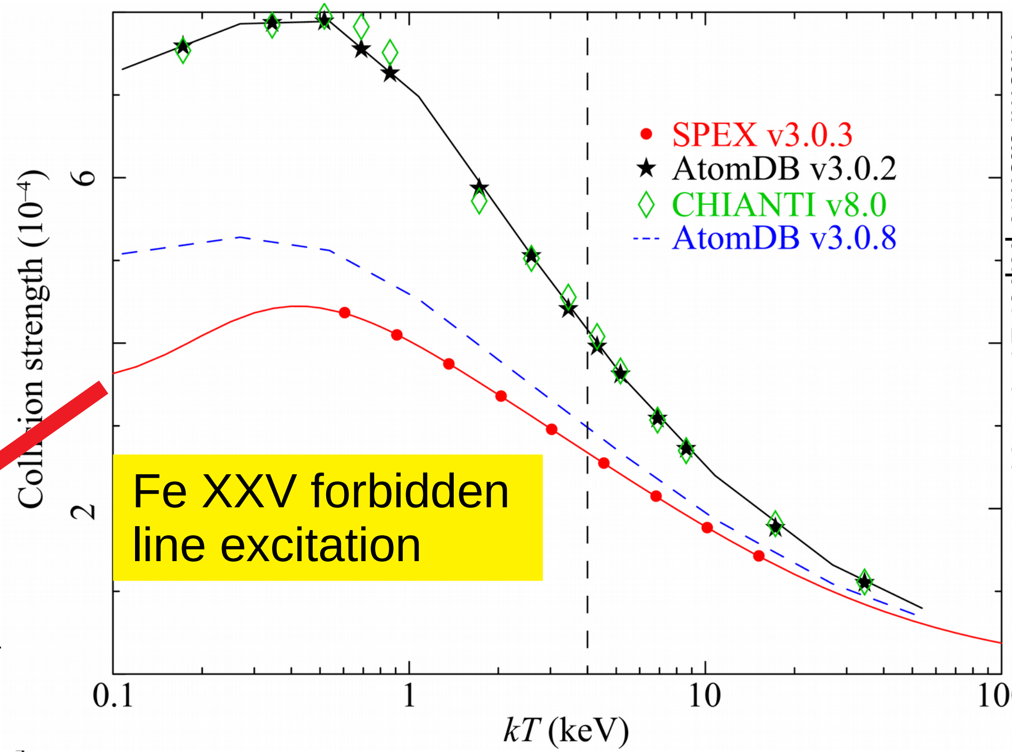
- **Are discussing (but possibly shouldn't?)**

  Estimates of atomic data uncertainty

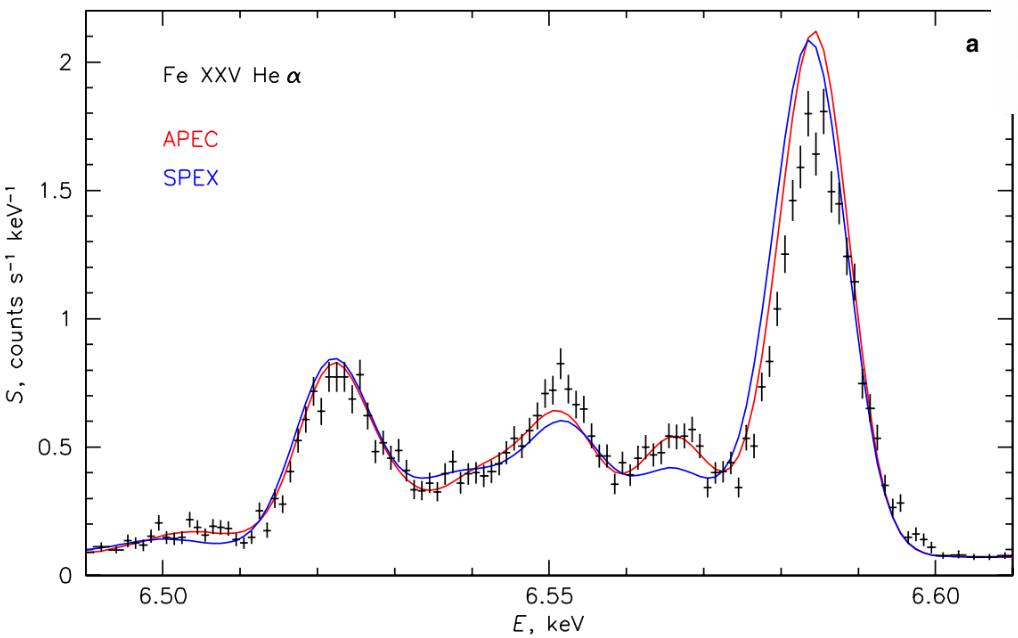
  Using uncertainties in modeling

Variation in atomic data

- Which is correct?
- How do we know?
- Do we need to care?



Hitomi atomic paper 2018PASJ...70...12H



“We obtain consistent best-fit parameters, with both APEC and SPEX predicting a temperature of 4.1 ± 0.1 keV.”

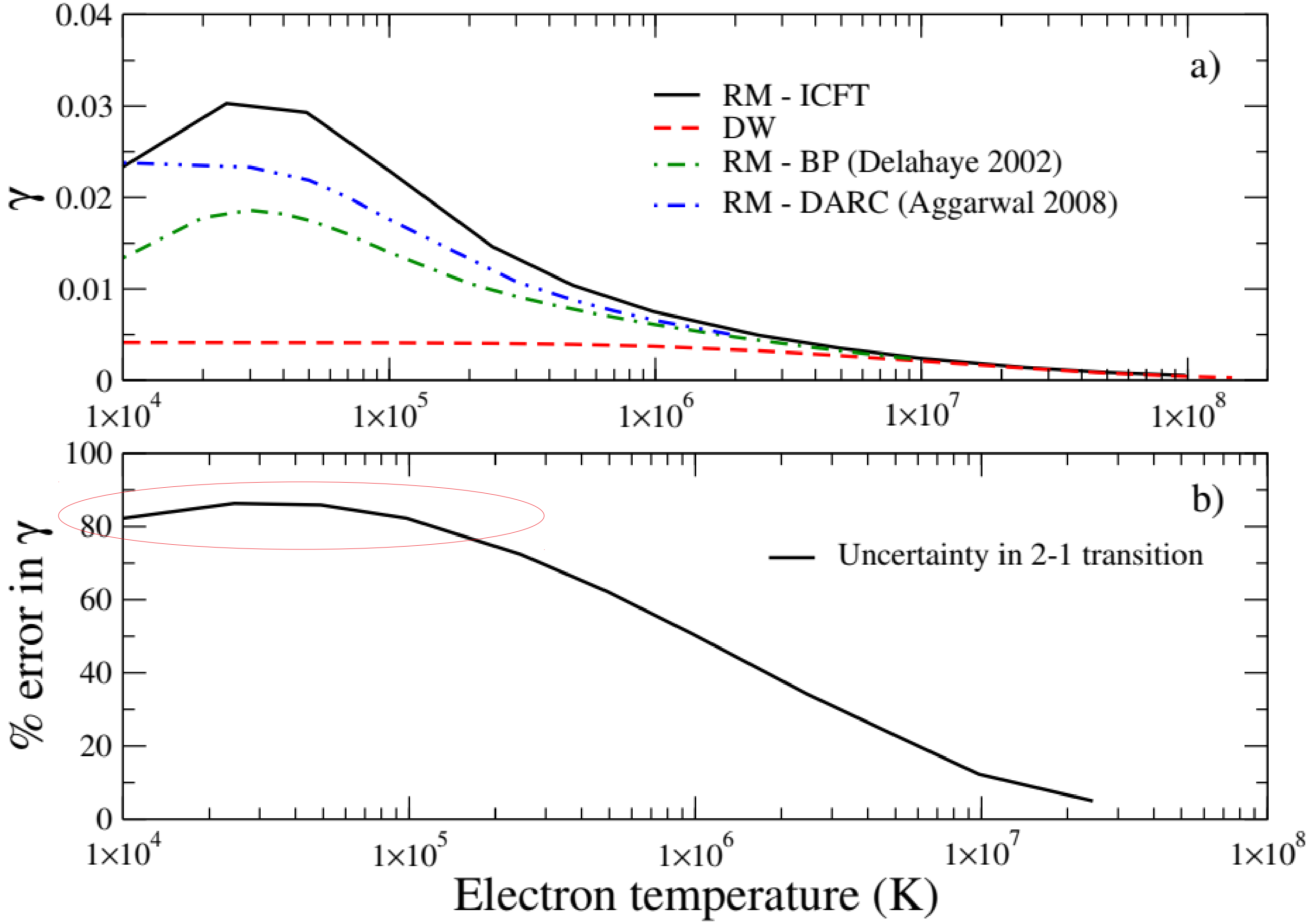
What *are* the Uncertainties?

Approach	Pros	Cons
Experimental Measurement	“Real” uncertainty Get real underlying data too	Difficult Limited data Expensive
Delta of Literature Values	Reasonable estimate Fast (if literature exists)	Comparing apples and oranges Not always multiple calculations available
Comparison with Observations	Excellent data, unavailable in lab	Hard to extract fundamental uncertainties Limited datasets
1st Principle Calculations	“Real” uncertainty Correlation effects	Difficult Few results (so far!)

Add Uncertainties to AtomDB Machinery

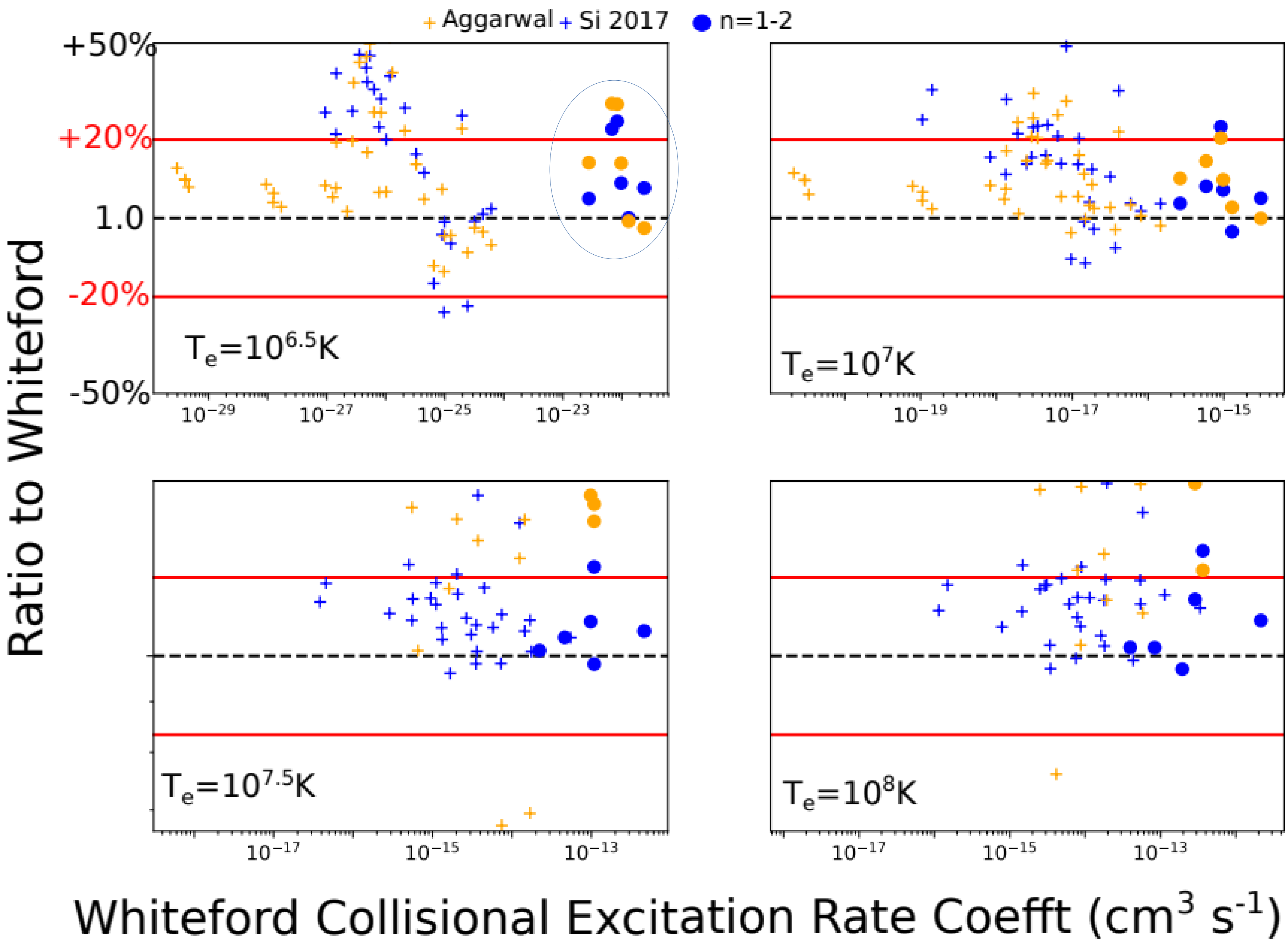
- Supply input limits for uncertainties
- $C_{var} = C_{orig} * A$, where A is generated from a truncated Gaussian between $1-2\sigma < A < 1+2\sigma$.
- Tie together values from same term transitions (doublets affected similarly)
- Reduce collisional uncertainties at high T

He-like O

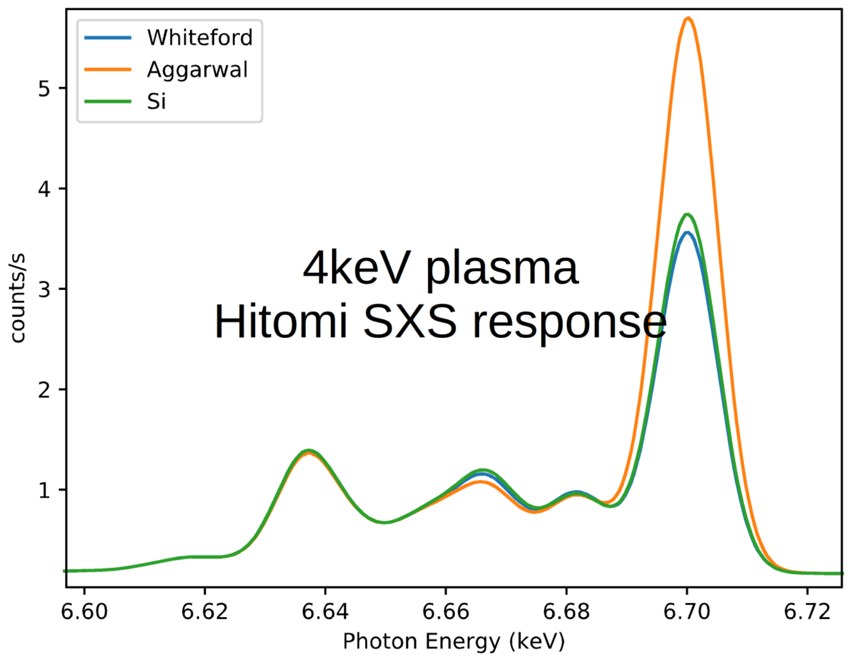


Fe XXV

Uncertainties of order 10 % for strong transitions, higher for weaker



Significant Spectral Change



Fit to 6.4-8keV range of Hitomi Perseus spectrum

Model: bapec + gauss
(-ve, to model scattering)

	CSTAT	Te (keV)	Abund
ATOMDB	3402.02	3.93 (-0.07,+0.04)	0.324 (-.009,+.006)
Aggarwal	3832.24	3.74 (-0.01,+0.02)	0.295 (-.006,+.008)
Si	3415.49	3.92 (-0.04,+0.06)	0.318 (-.008,+.008)

Production runs!

Parameter	sigma
Eff. Colln Str (dipole)	10%
Eff. Colln Str (other)	40%
Einstein A (dipole)	5%
Einstein A (others)	10%
CI Rates	10%
RR Rates	5%
DR Rates	30%
Satellite line intensity	20%
Autoionization	20%

There is an infinite parameter space to explore. I have started with these values, but they are **not** definitive in any way shape or form

Use non-equilibrium formats to separate out the ionization balance from the rest of the data.

Also performed one set with only the uncertainties on the collision strengths.

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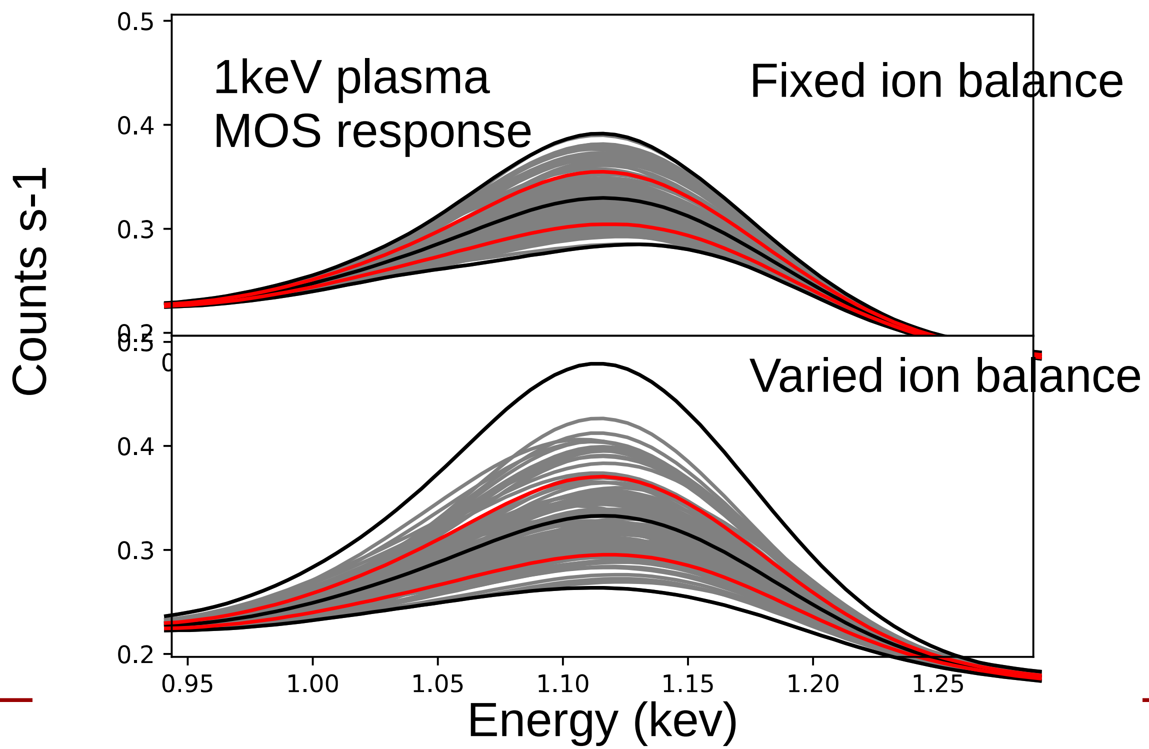
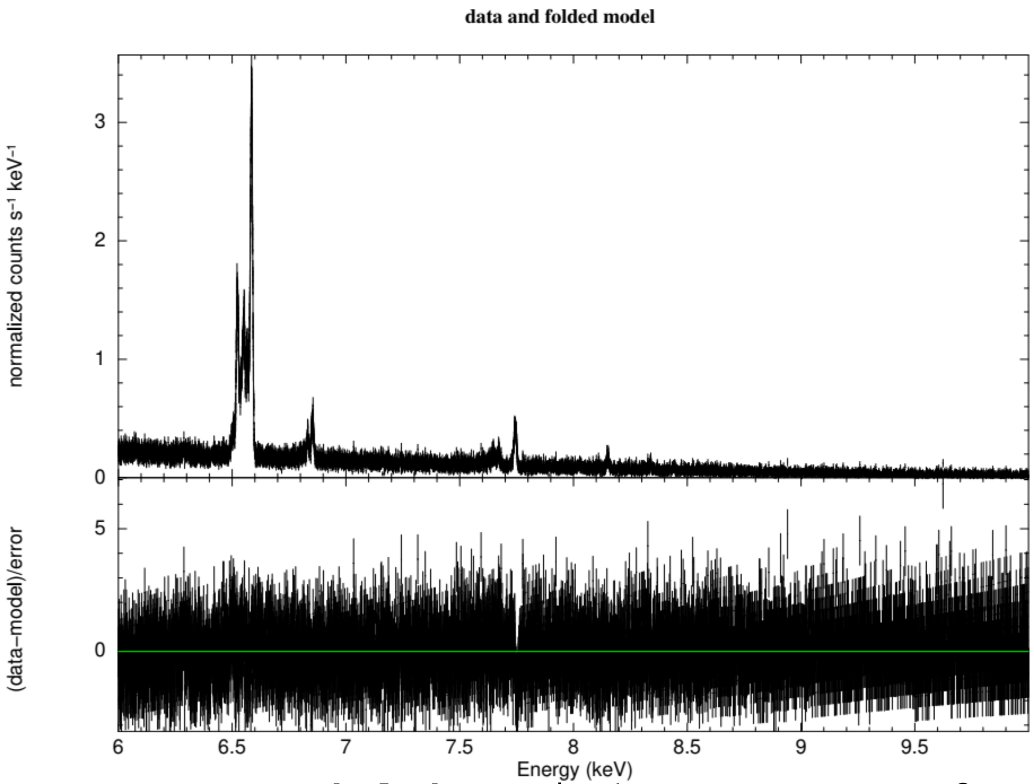
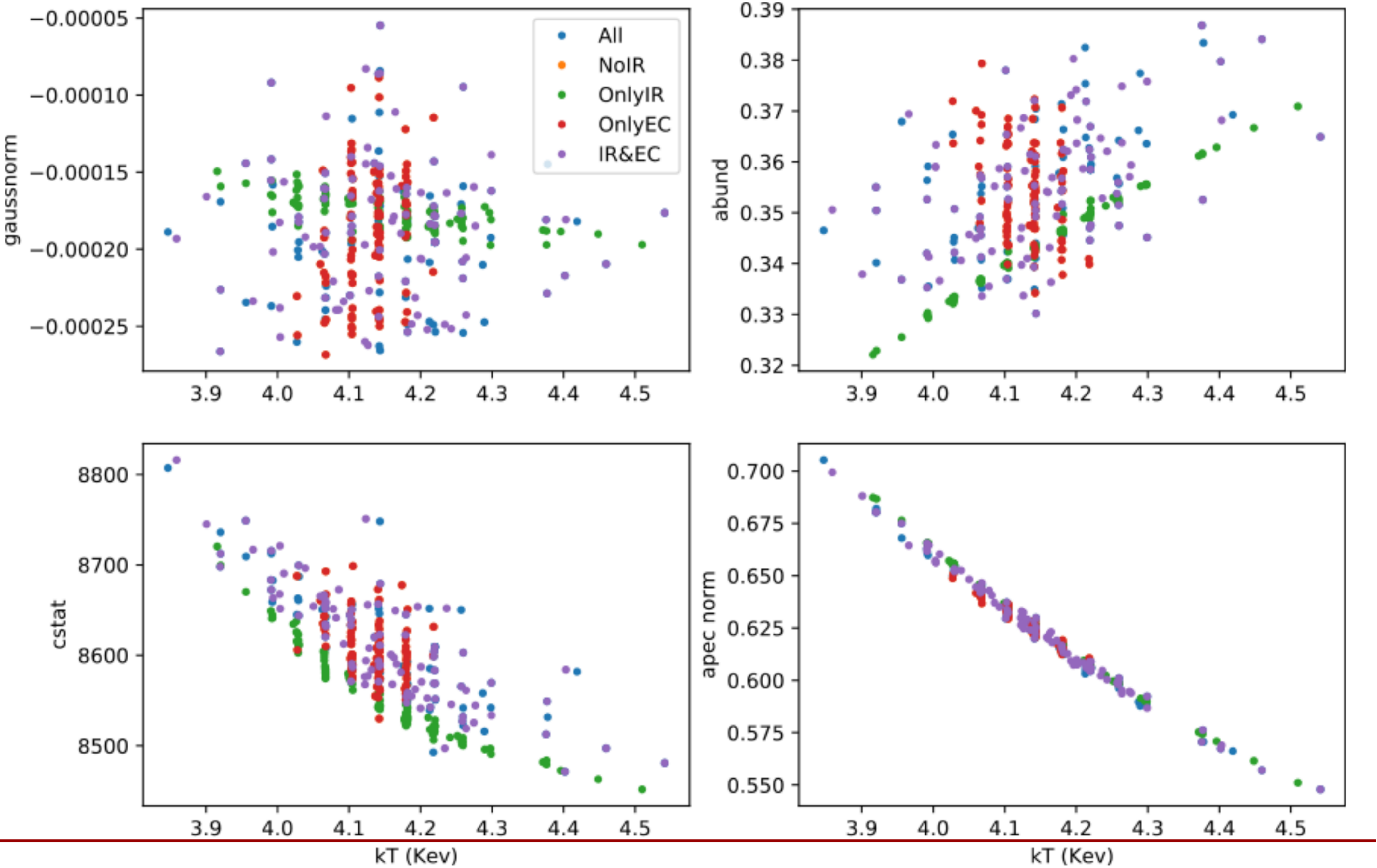


Fitting Perseus Data



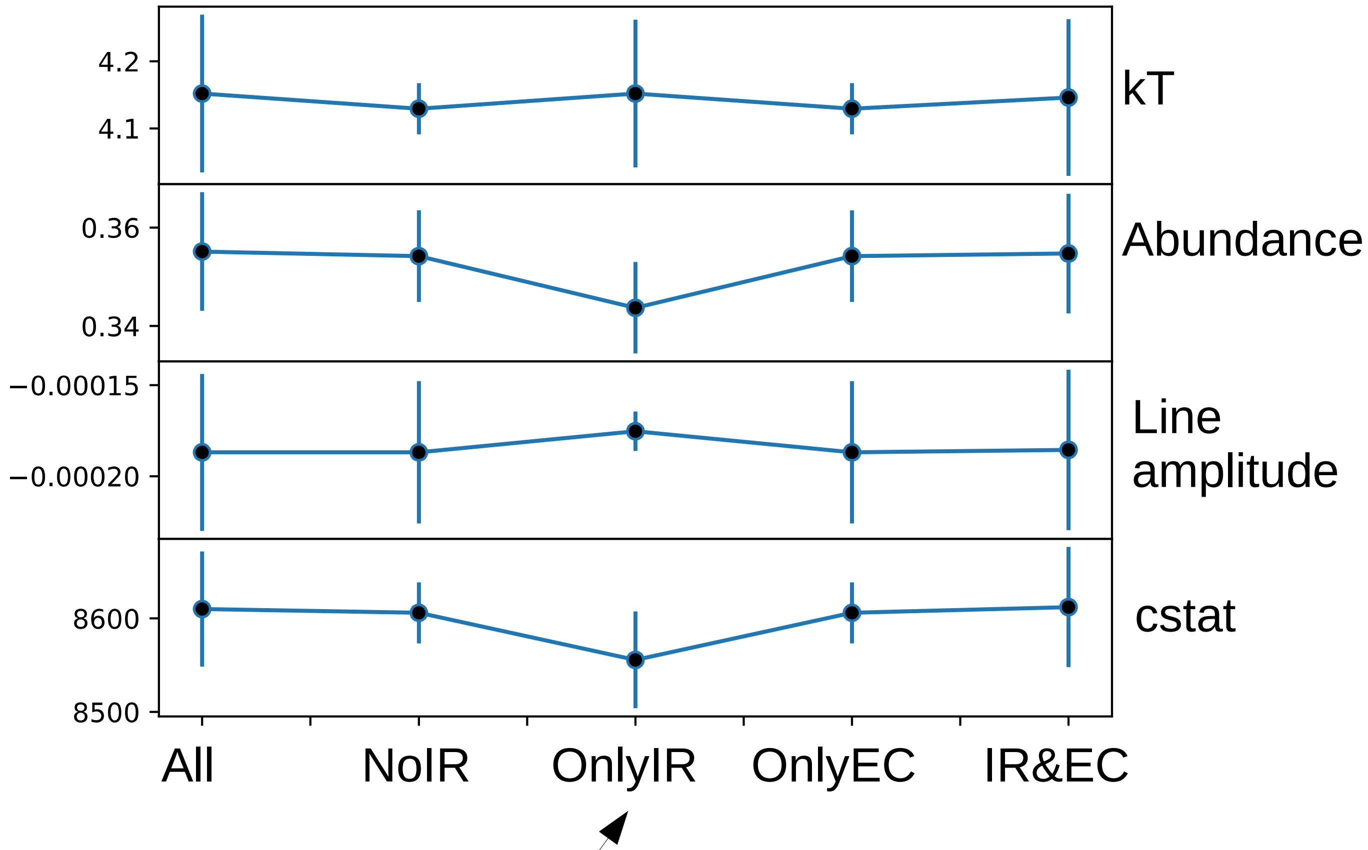

```
Model brnei<1> + zgauss<2> Source No.: 1   Active/On
Model Model Component  Parameter  Unit     Value
 par  comp
   1    1   brnei      kT         keV      4.13638
   3    1   brnei      Abundanc            0.342672
   6    1   brnei      Velocity   km/s     175.047
   7    1   brnei      norm                0.627371
  11    2   zgauss     norm                -1.73634E-04
CSTAT 8555 for 7992 dof
```

Results!



gaussnorm
−0.00005
−0.00010
−0.00015
−0.00020
−0.00025
All
NoIR
OnlyIR
OnlyEC
IR&EC
abund
0.39
0.38
0.37
0.36
0.35
0.34
0.33
0.32
cstat
8800
8700
8600
8500
apec norm
0.700
0.675
0.650
0.625
0.600
0.575
0.550
3.9
4.0
4.1
4.2
4.3
4.4
4.5
kT (Kev)
kT (Kev)

Results 2



Random ionization and recombination rates → improved fit?

ACIS example

Simple 1keV plasma,

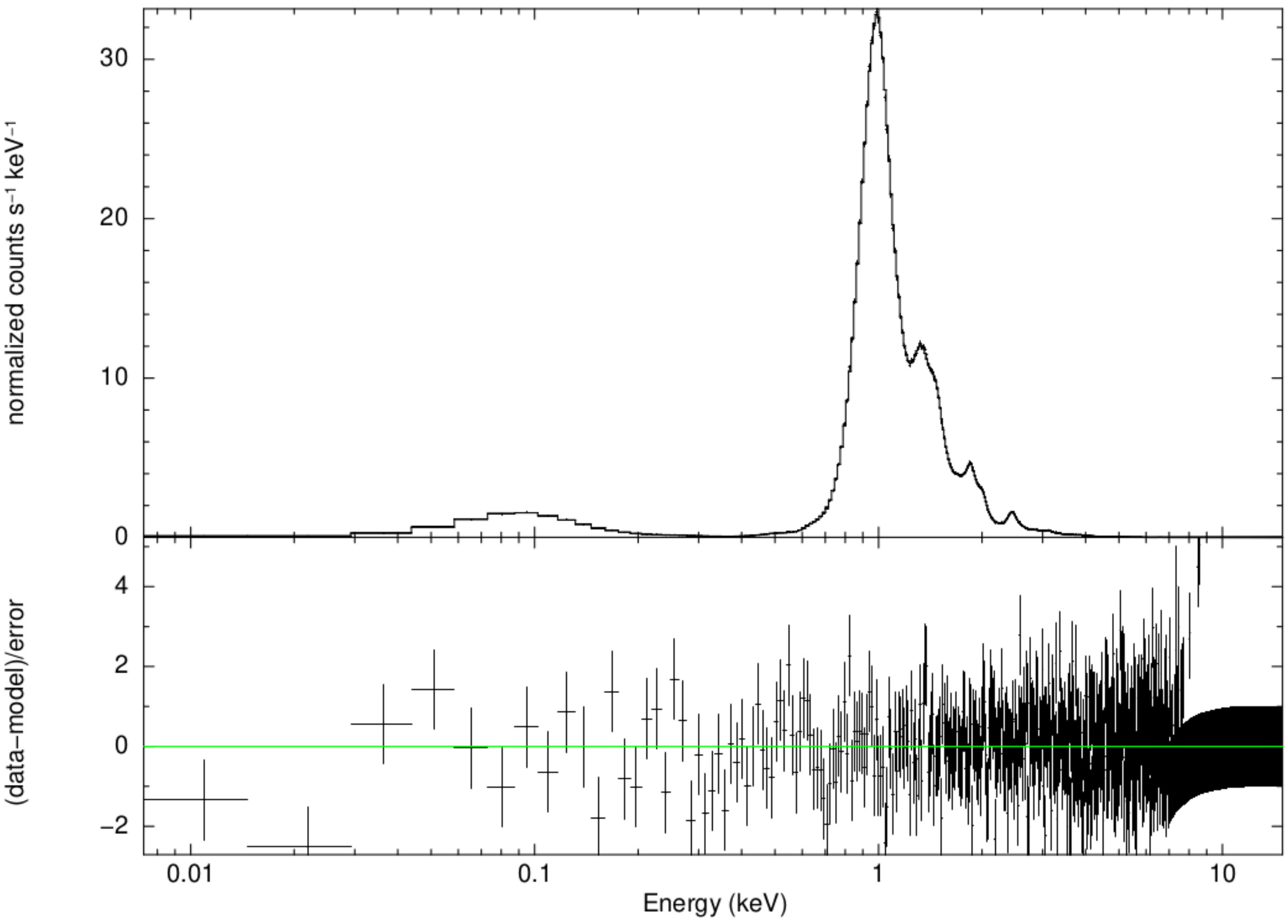
phabs*vnei

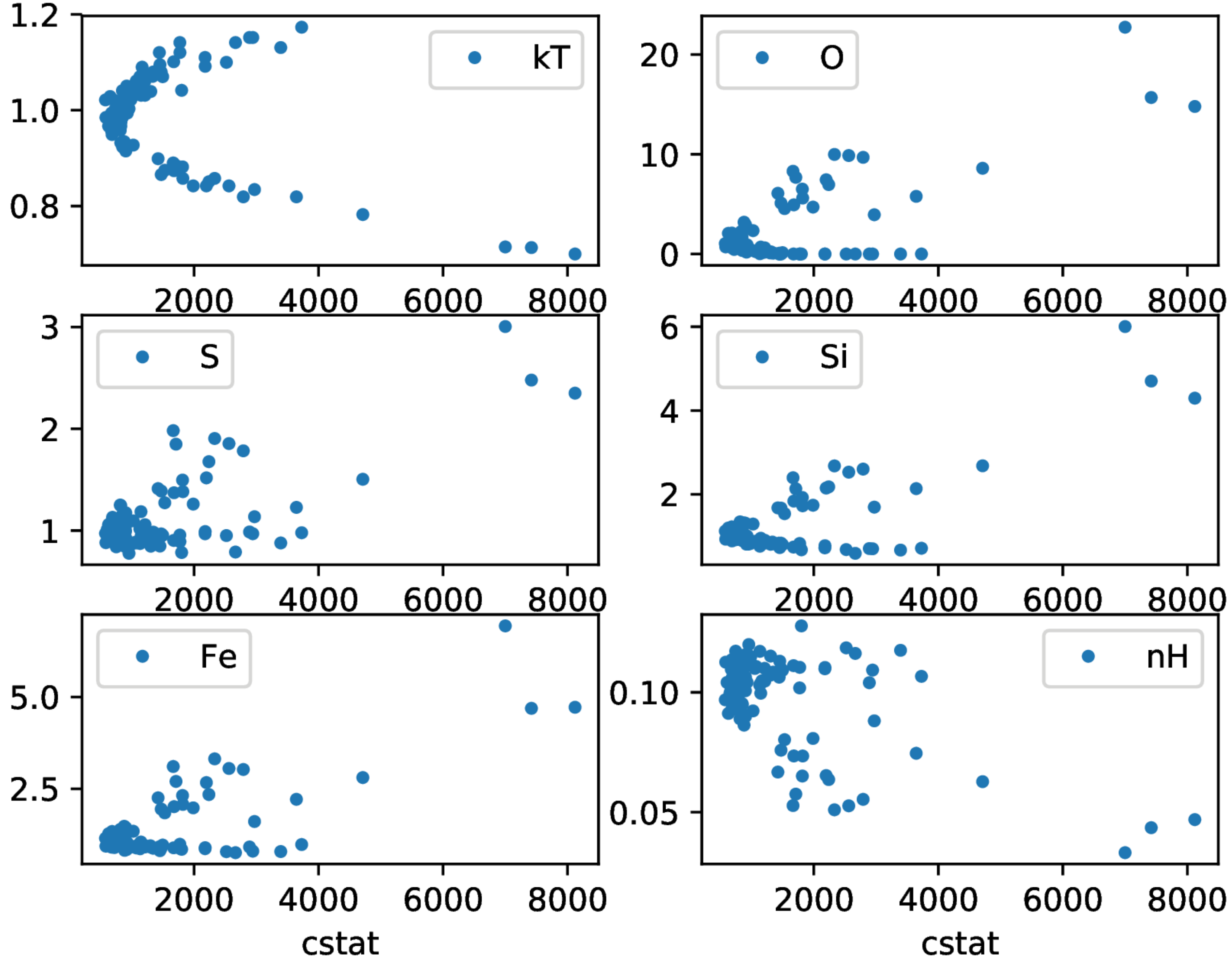
Abundance =1 for all elements

Tau = 1e13
(so actually equilibrium)

ACIS-I aimpoint response

Free O, Si, S, Fe, norm, nH





kT
O
S
Si
Fe
nH
1.2
1.0
0.8
20
10
0
3
2
1
6
4
2
5.0
2.5
0.10
0.05
2000
4000
6000
8000
cstat
cstat

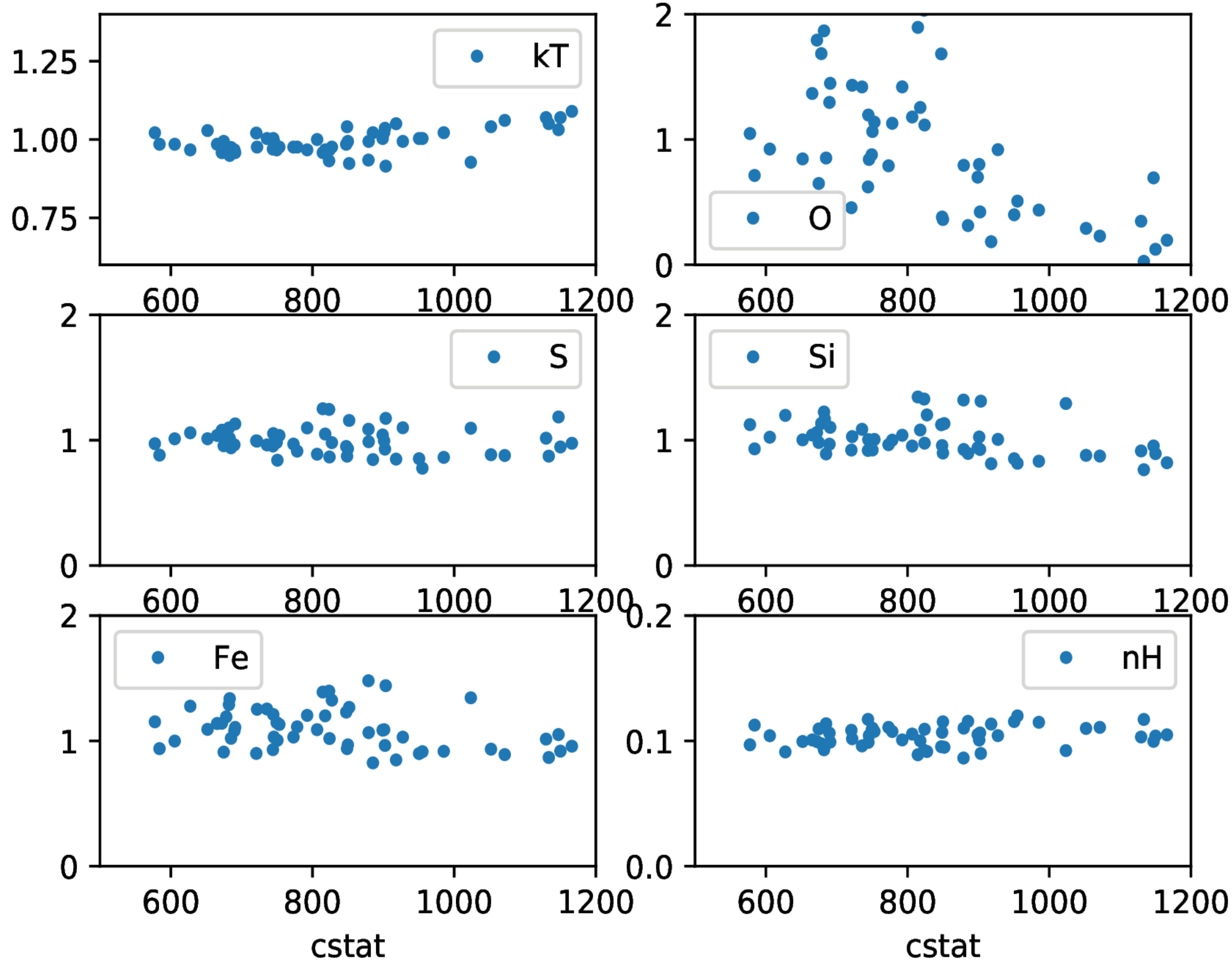
43 of 100 runs produce cstat > 1200

Data can wander off to garbage quickly.

This is **2-hours-ago** preliminary, not a result

BUT

Indicative of future issues to address?



Summary

- Atomic data errors are coming (eventually)
- This is an initial framework anticipating their arrival
- Suggestive of expected issues with using atomic data uncertainties

- Lots of work still to do!