PyNeb_manual_6

October 15, 2017

0.1 The EmissionLine class

This is the class characterizing emission lines. An emission line is identified by an element and a spectrum (which identify the emitting ion), a wavelength in Angstrom, a blend flag, a label in the standard PyNeb format, an observed intensity, a reddening-corrected intensity, an expression describing how the intensity depends on the included wavelengths, an observational error and an error on the corrected intensity. Other programs determine one or more of these values.

To instantiate an Emission Line object, use the following:

obsIntens is a value, a list or a numpy array of values corresponding to the observed intensity of the given emission line.

```
In [3]: print(line)
Line 03 03_5007A
```

To know how the label of a given line is exactly spelled, you can print the dictionary pn.LINE_LABEL_LIST

```
In [4]: print(pn.LINE_LABEL_LIST['03'])
['4931A', '4959A', '5007A', '2315A', '2321A', '2331A', '4363A', '1658A', '1661A', '
```

It is possible to instantiate a line not contained in the pn.LINE_LABEL_LIST. In this case a warning is issued, but the code doesn't stop.

The observed intensity is stored in **line.obsIntens** and the extinction-corrected intensity is stored in **line.corrIntens**. **line.corrIntens** is set to 0.0 when the line is instantiated, unless the parameter corrected is set to **True**, in which case the observed value **obsIntens** is copied to the **corrIntens** slot (the same applies for **corrError**, which is set to **obsError**).

The **corrIntens** value can also be computed using an instantiation of the **pn.RedCorr** class:

```
In [5]: redcorr = pn.RedCorr(E_BV = 0.87, law = 'F99')
In [6]: line.correctIntens(redcorr) #redcorr is used to compute line.corrIntens
```

The line information is printed using:

```
In [7]: line.printLine()
Line O3 O3_5007A evaluated as L(5007)
Observed intensity: [ 1.4  1.3]
Observed error: [ 0.  0.]
Corrected intensity: [ 22.58352855  20.97041937]
Corrected error: [ 0.  0.]
```

Most of the times, users will not need to define or manipulate EmissionLine objects, since most of the work on the EmissionLine objects will be performed from the Observation class (read data, extinction correction); see next section.

WARNING: Note that the wavelengths assigned to EmissionLine objects are simply the numerical part of the label:

whereas pn. Atom computes them as the difference from energy levels:

This can cause small errors when both methods are used simultaneously. For instance, the extinction correction at Hb1 is slightly different from the expected value of 1:

This happens because the ExtCorr uses the precise $H\beta$ value computed from energy levels. If this roundoff error exceeds your tolerance, a possible workaround is forcing the emission line to have exactly the wavelength computed from the energy levels:

0.2 The Observation class: reading and dealing with observations

0.2.1 Reading observation from a file

pn.Observation is the class characterizing observation records. An observation record is composed of an object identifier, the observed intensity of one or more emission lines, and, optionally, the dereddened line intensities and the identifier of the extinction law used, and the value of c(Hbeta).

Observations can be initialized by reading data files, which can be organized with different emission lines either in rows or columns (usually, in a survey of many objects with few emission lines emission lines change across columns; and in a high-resolution observation of a small sample of objects lines change across rows).

The following is an example of how to define an observation:

```
In [13]: obs = pn.Observation()
In [14]: %%writefile observations1.dat
        LINE SMC 24
        S4_10.5m 7.00000
        Ne2 12.8m 8.3000
        Ne3 15.6m 34.10
        S3_18.7m 10.
        02_3726A 39.700
        02_3729A 18.600
        Ne3_3869A 18.90
        Ne3_3968A 6.4
        S2_4069A
                   0.85
        S2_4076A
                  0.450
        O3_4363A
                  4.36
        H1r_4861A 100.00
        O3_5007A 435.09
        N2_5755A 0.510000
                  0.76
        S3 6312A
        O1_6300A 1.69
        O1_6364A 0.54
        N2 6548A 6.840000
        H1r_6563A 345.00
```

```
N2_6584A 19.00

S2_6716A 1.220000

S2_6731A 2.180000

Ar3_7136A 4.91

O2_7319A+ 6.540000

O2_7330A+ 5.17
```

Overwriting observations1.dat

obs.correctData()

```
In [15]: obs.readData('observations1.dat', fileFormat='lines_in_rows', err_default=
In [16]: obs.printIntens(returnObs=True)
S4_10.5m
              7.000
Ne2 12.8m
             8.300
Ne3_15.6m
             34.100
S3_18.7m
            10.000
02_3726A
             39.700
02_3729A
            18.600
Ne3_3869A
            18.900
Ne3_3968A
             6.400
S2_4069A
              0.850
S2_4076A
             0.450
03_4363A
             4.360
H1r_4861A 100.000
03_5007A
            435.090
N2_5755A
              0.510
              0.760
S3_6312A
01_6300A
              1.690
O1 6364A
              0.540
N2_6548A
              6.840
H1r_6563A 345.000
N2_6584A
            19.000
S2_6716A
             1.220
              2.180
S2_6731A
Ar3_7136A
              4.910
02_7319A+
              6.540
02_7330A+
              5.170
In [17]: obs.extinction.law = 'CCM89' # define the extinction law from Cardelli ex
```

The data can be read by the readData method as above or directly while instantiating the object:

```
In [18]: obs = pn.Observation('observations1.dat', fileFormat='lines_in_rows', corn
```

the dereddened data are computed

The format of the data file from which the emission line intensities are read can be one of three kinds: "lines_in_rows" as above, or "lines_in_cols" like this one:

Overwriting observations2.dat

```
In [20]: obs2 = pn.Observation('observations2.dat', fileFormat='lines_in_cols', con
```

or fileFormat='lines_in_rows_err_cols' (errors labeled "err". Don't name an observation "err"!) like this one:

```
In [21]: %%writefile observations3.dat
    LINE     TT     err     TT2     err     TT3     err
    cHbeta     1.2     0.0     1.5     0.2     1.1     0.2
          03_5007A     1.5     0.15     1.3     .2     1.1     0.1
          H1_6563A     2.89     0.05     1.6     0.3     1.3     0.1
          N2_6584A     1.     0.20     0.3     0.5     1.5     0.1
```

Overwriting observations3.dat

```
In [22]: #obs3 = pn.Observation('observations3.dat', fileFormat='lines_in_rows_err_
```

The delimiter between the columns is any sequence of spaces or TAB, but it can be changed using the delimiter parameter. The line names are defined by a label starting with the name of the atom ('O2'), followed by an underscore, followed by a wavelength and ending with a unit ('A' or 'm'). The list of all the lines managed by PyNeb, ordered by atoms, is obtained by entering:

Br3 ['6646A', '6133A', '3714A', '8420A', '9419A', '3498A', '7385A', '8142A', '7.94r

```
C1 ['9808A', '9824A', '9850A', '4618A', '4621A', '4627A', '8728A', '2963A', '2965A'
C2 ['2325A', '2328A', '2323A', '2327A', '2322A', '2325A', '1335A', '1336A', '3131A'
C3 ['1910A', '1909A', '1907A', '977A', '2000A', '2001A', '2003A', '422.0m', '124.9r
C4 ['1551A', '1548A', '92.8m']
Ca2 ['7292A', '7324A']
Ca5 ['5309A', '6087A', '6428A', '2280A', '2413A', '2464A', '3998A', '4.16m', '3.05r
C12 ['8579A', '9124A', '9381A', '3586A', '3678A', '3719A', '6162A', '14.4m', '10.0r
Cl3 ['5538A', '5518A', '3353A', '8500A', '8548A', '3343A', '8434A', '8481A', '151.5
C14 ['7261A', '7531A', '8046A', '3071A', '3119A', '3204A', '5323A', '1463A', '1474A
Fe3 ['4009A', '4659A', '4668A', '4701A', '4734A', '4755A', '5011A', '5085A', '5270A
Fe4 ['4491A', '5685A', '5735A', '6740A']
Fe5 ['3783A', '3795A', '3822A', '3891A', '3895A', '3911A', '4071A', '4181A', '4227A
Fe6 ['3556A', '3929A', '5146A', '5176A', '5278A', '5335A', '5370A', '5424A', '5427A
Fe7 ['5159A', '5276A', '5721A', '6087A']
K4 ['6102A', '6796A', '7109A', '2594A', '2711A', '2760A', '4511A', '6.0m', '4.3m',
K5 ['4163A', '4123A', '2514A', '6349A', '6446A', '2495A', '6222A', '6316A', '42.2m
K6 ['5602A', '6229A']
Kr3 ['6827A', '9902A', '3022A', '3504A', '3600A', '5423A', '2.2m', '1.88m', '13.1m
Kr4 ['5868A', '5346A', '3219A', '7131A', '8091A', '2993A', '6108A', '6798A', '6.0m
Kr5 ['5069A', '6256A', '8243A', '2550A', '2819A', '3163A', '5132A', '2.67m', '1.32r
Mg5 ['2783A', '2929A', '2992A', '1294A', '1325A', '1338A', '2418A', '5.6m', '3.96m'
Mg7 ['2441A', '2509A', '2629A', '1174A', '1190A', '1216A', '2261A', '943A', '953A',
N1 ['5200A', '5198A', '3467A', '3466A']
N2 ['6527A', '6548A', '6584A', '3058A', '3063A', '3071A', '5755A', '2137A', '2139A'
N3 ['1749A', '1754A', '1747A', '1752A', '1744A', '1750A', '990A', '992A', '2280A',
N4 ['1488A', '1487A', '1483A', '765A', '1575A', '1576A', '1580A', '158.4m', '48.3m
Na4 ['3242A', '3362A', '3416A', '1504A', '1529A', '1540A', '2804A', '9.0m', '6.34m
Na6 ['2816A', '2872A', '2972A', '1343A', '1356A', '1378A', '2569A', '14.39m', '5.4r
Ne2 ['12.8m']
Ne3 ['3869A', '3968A', '4012A', '1794A', '1815A', '1824A', '3343A', '15.6m', '10.9r
Ne4 ['2425A', '2422A', '1602A', '4716A', '4726A', '1601A', '4714A', '4724A', '224.9
Ne5 ['3300A', '3346A', '3426A', '1565A', '1575A', '1592A', '2973A', '1132A', '1137A'
Ne6 ['997A', '1010A', '993A', '1006A', '986A', '999A', '559A', '563A', '1271A', '12
Ni3 ['7890A', '8500A', '6000A', '6401A', '6534A', '6682A', '6797A', '7125A', '6946A
O1 ['6300A', '6364A', '6392A', '2959A', '2973A', '2979A', '5577A', '63.2m', '44.1m
02 ['3729A', '3726A', '2470A', '7319A', '7320A', '7330A', '7331A', '2470A', '834A',
o2r ['4638.86A', '4641.81A', '4649.13A', '4650.84A', '4661.63A', '4673.73A', '4676
03 ['4931A', '4959A', '5007A', '2315A', '2321A', '2331A', '4363A', '1658A', '1661A
04 ['1400A', '1407A', '1397A', '1405A', '1394A', '1401A', '788A', '1801A', '1806A',
O5 ['1220A', '1218A', '1214A', '630A', '1301A', '1303A', '1309A', '73.5m', '22.6m',
Rb4 ['5760A', '9009A', '9604A', '2603A', '3110A', '3178A', '4750A', '1.6m', '1.44m
Rb5 ['5364A', '4742A', '2873A', '6188A', '7290A', '2609A', '5080A', '5800A', '4.1m
Rb6 ['4210A', '5373A', '7220A', '2212A', '2495A', '2832A', '4660A', '1.95m', '1.01r
S2 ['6731A', '6716A', '4076A', '4069A', '1260A', '1549A', '1550A', '1823A', '1824A'
S3 ['8829A', '9069A', '9531A', '3681A', '3722A', '3798A', '6312A', '33.5m', '12.0m'
S4 ['1405A', '1424A', '1398A', '1417A', '1387A', '1406A', '10.5m', '29.0m', '11.2m
```

```
Se3 ['7671A', '8854A', '3516A', '3746A', '4082A', '6493A', '5.74m', '2.54m', '4.55r Se4 ['2.28m']
Si2 ['2335A', '2351A', '2329A', '2345A', '2320A', '1808A', '1817A', '8007A', '8077A', Si3 ['1897A', '1892A', '1883A', '1206A', '3315A', '3329A', '3359A', '77.7m', '25.7r Xe3 ['5847A', '2769A', '3574A', '3800A', '5261A', '1.23m', '1.02m', '6.0m', '1.11m Xe4 ['7535A', '5709A', '3566A', '6769A', '9498A', '2804A', '4467A', '5511A', '2.36r Xe6 ['6409A']
```

The presence of a trailing "e" at the end of the label points to the error associated to the line. The error is considered to be relative to the intensity (i.e., 0.05 means 5% of the intensity), unless the parameter errIsRelative is set to False. A common value for all the errors can be defined by the parameter **err_default** (0.10 is the default value).

0.2.2 Extinction correction in Observation class

Once the data have been read, they have to be corrected from extinction. An instantiation of **RedCorr()** is available inside the **Observation** object as **obs.extinction**.

If the data file contains **cHbeta** or **E(B-V)** alongside of line labels, the corresponding information on extinction is transmitted to the extinction correction object. Otherwise, the extinction parameters must be set manually; for example:

An extinction law has to be specified in either case:

```
In [25]: obs.extinction.law = 'F99'
  To correct all the lines at once:
In [26]: obs.correctData()
In [27]: obs.printIntens(returnObs=True)
S4_10.5m
               7.000
Ne2_{12.8m}
               8.300
Ne3_{15.6m}
              34.100
S3_18.7m
              10.000
02_3726A
              39.700
02_3729A
              18.600
Ne3_3869A
              18.900
Ne3_3968A
               6.400
S2_4069A
               0.850
S2_4076A
               0.450
O3_4363A
               4.360
H1r_4861A
             100.000
```

435.090

03_5007A

```
N2_5755A
              0.510
S3_6312A
              0.760
01_6300A
              1.690
01_6364A
              0.540
N2 6548A
               6.840
H1r_6563A
            345.000
N2 6584A
             19.000
S2_6716A
              1.220
S2_6731A
              2.180
Ar3_7136A
              4.910
02_7319A+
              6.540
02_7330A+
              5.170
In [28]: obs.printIntens()
              7.120
S4\_10.5m
Ne2_12.8m
              8.415
             34.483
Ne3_{15.6m}
S3_18.7m
             10.093
02_3726A
            171.242
02_3729A
             80.156
Ne3_3869A
             78.134
Ne3_3968A
             25.717
S2_4069A
              3.320
S2_4076A
              1.754
03_4363A
             15.704
H1r_4861A
            310.254
03_5007A
           1289.851
N2_5755A
              1.244
S3_6312A
              1.662
01_6300A
              3.704
01_6364A
              1.170
N2_6548A
             14.346
            721.747
H1r_6563A
N2_6584A
             39.607
              2.488
S2_6716A
S2_6731A
              4.435
Ar3_7136A
              9.384
02_7319A+
             12.180
02_7330A+
              9.614
```

If you want the corrected line intensities to be normalized to a given wavelength, use the following:

```
In [29]: obs.correctData(normWave=4861.)
```

The extinction correction can be determined by comparing the observed values to a theoretical ratio, as in the following:

```
In [30]: obs.printIntens()
S4_10.5m
              2.295
Ne2_12.8m
              2.712
Ne3_15.6m
             11.115
S3_18.7m
             3.253
02_3726A
             55.194
02_3729A
             25.836
Ne3_3869A
             25.184
Ne3_3968A
             8.289
S2_4069A
              1.070
S2_4076A
              0.565
O3 4363A
              5.062
H1r_4861A
            100.000
O3 5007A
            415.740
N2_5755A
              0.401
S3_6312A
              0.536
01_6300A
              1.194
01_6364A
              0.377
N2_6548A
              4.624
H1r_6563A
          232.631
N2_6584A
            12.766
S2_6716A
              0.802
S2_6731A
              1.429
Ar3_7136A
              3.025
02_7319A+
              3.926
02_7330A+
              3.099
In [31]: obs.def_EBV(label1="H1r_6563A", label2="H1r_4861A", r_theo=2.85)
         print(obs.extinction.E_BV)
         obs.correctData(normWave=4861.)
[ 0.16483175]
In [32]: obs.printIntens()
S4_10.5m
              4.076
Ne2_12.8m
             4.826
Ne3_15.6m
             19.803
S3_18.7m
             5.802
02_3726A
             46.576
O2_3729A
             21.812
Ne3_3869A
             21.722
Ne3_3968A
             7.255
S2_4069A
              0.950
S2_4076A
              0.503
O3_4363A
              4.687
```

```
H1r_4861A
            100.000
03_5007A
            425.599
N2_5755A
               0.454
S3_6312A
               0.641
O1 6300A
              1.428
O1 6364A
               0.454
N2 6548A
               5.657
H1r 6563A
            285.000
N2 6584A
             15.668
S2_6716A
               0.995
               1.777
S2_6731A
Ar3_7136A
               3.882
02_7319A+
               5.106
02_7330A+
               4.034
```

By default, this method prints out the corrected intensities. To print the observed intensities, use the **returnObs=True** parameter.

The method **getSortedLines** returns the lines sorted in alphabetical order according to either the emitting atoms (default) or the wavelength (using the **crit='wave'** parameter):

```
In [33]: for line in obs.getSortedLines():
             print(line.label, line.corrIntens[0])
Ar3_7136A 3.88214978929
H1r 4861A 100.0
H1r 6563A 285.0
N2_5755A 0.453846550278
N2_6548A 5.65746807125
N2_6584A 15.6684748528
Ne2_12.8m 4.82602971256
Ne3_15.6m 19.8027022262
Ne3_3869A 21.7218621627
Ne3_3968A 7.25498470993
O1_6300A 1.42792388246
O1_6364A 0.45369747694
O2_3726A 46.5764398853
O2_3729A 21.8120580007
02_7319A+ 5.1064244648
02 7330A+ 4.03377032255
O3 4363A 4.68705107403
O3 5007A 425.599154595
S2_4069A 0.95040451703
S2 4076A 0.502681231482
S2_6716A 0.995405412218
S2_6731A 1.77656378862
S3_18.7m 5.80184591117
S3_6312A 0.641461012117
```

```
S4_10.5m 4.07647872134
```

The following method, which gives the list of all the atoms implied in the observed emission lines, will be useful later:

```
In [34]: atomList = obs.getUniqueAtoms()
In [35]: atomList
Out[35]: array(['Ar3', 'H1r', 'N2', 'Ne2', 'Ne3', 'O1', 'O2', 'O3', 'S2', 'S3', 'S4' dtype='<U3')</pre>
```

0.2.3 Adding observations and lines

Once an **Observation** object is instantiated, you can add a new observation (corresponding, e.g., to a new object or a new fiber) by using:

```
In [36]: obs.addObs('test', np.random.rand(25))
```

where 'test' is the name of the new observation. The new observation must have the same size of **obs**, that is, it must contain **obs.n_lines** lines.

```
In [37]: obs.printIntens()
S4\_10.5m
               4.076
                         0.192
               4.826
Ne2_12.8m
                         0.023
Ne3_15.6m
              19.803
                         0.427
S3_{18.7m}
               5.802
                         0.337
02_3726A
              46.576
                         0.548
02_3729A
             21.812
                         0.576
Ne3_3869A
             21.722
                        0.975
Ne3_3968A
              7.255
                        0.532
S2_4069A
               0.950
                         0.235
S2_4076A
               0.503
                         0.971
03_4363A
               4.687
                         0.519
H1r_4861A
            100.000
                         0.709
O3 5007A
             425.599
                         0.616
N2_5755A
               0.454
                         0.884
S3_6312A
               0.641
                         0.522
01_6300A
               1.428
                         0.391
01_6364A
               0.454
                         0.297
N2_6548A
               5.657
                         0.624
H1r_6563A
            285.000
                         0.251
                         0.926
N2_6584A
             15.668
S2_6716A
               0.995
                         0.728
               1.777
S2_6731A
                         0.452
Ar3_7136A
               3.882
                         0.448
02_7319A+
               5.106
                         0.160
02_7330A+
               4.034
                         0.715
```

```
In [38]: line = pn.EmissionLine(label='C13_5518A', obsIntens=[3.5, 2.5])
         obs.addLine(line)
In [39]: obs.printIntens()
S4_{10.5m}
              4.076
                        0.192
Ne2_12.8m
              4.826
                        0.023
Ne3_{15.6m}
             19.803
                        0.427
                        0.337
S3_18.7m
              5.802
02_3726A
             46.576
                        0.548
02_3729A
             21.812
                        0.576
Ne3_3869A
             21.722
                        0.975
Ne3_3968A
              7.255
                       0.532
S2_4069A
              0.950
                        0.235
S2 4076A
              0.503
                        0.971
O3 4363A
                        0.519
              4.687
H1r 4861A
            100.000
                        0.709
03_5007A
            425.599
                        0.616
N2 5755A
              0.454
                        0.884
S3_6312A
              0.641
                        0.522
01_6300A
              1.428
                        0.391
01_6364A
              0.454
                        0.297
N2_6548A
              5.657
                        0.624
H1r_6563A
            285.000
                        0.251
N2_6584A
             15.668
                        0.926
              0.995
                        0.728
S2_6716A
S2_6731A
              1.777
                        0.452
Ar3_7136A
              3.882
                        0.448
02_7319A+
              5.106
                        0.160
02 7330A+
                        0.715
              4.034
Cl3 5518A
              5.534
                        3.953
```

0.2.4 Getting line intensities

You can extract the line intensities from an **Observation** object by, for example:

```
'N2_6584A': 15.668474852815743,
          'Ne2_12.8m': 4.8260297125551359,
          'Ne3_15.6m': 19.802702226158502,
          'Ne3_3869A': 21.721862162658756,
          'Ne3 3968A': 7.2549847099308185,
          'O1_6300A': 1.4279238824617235,
          '01_6364A': 0.45369747693998408,
          'O2_3726A': 46.576439885253663,
          '02_3729A': 21.812058000703153,
          '02_7319A+': 5.1064244648045349,
          '02_7330A+': 4.0337703225472392,
          '03_4363A': 4.6870510740329472,
          '03_5007A': 425.59915459530959,
          'S2_4069A': 0.95040451703046003,
          'S2_4076A': 0.50268123148205257,
          'S2_6716A': 0.99540541221817869,
          'S2_6731A': 1.7765637886180774,
          'S3_18.7m': 5.8018459111708029,
          'S3_6312A': 0.64146101211689832,
          'S4_10.5m': 4.0764787213393321}
In [42]: obs.getIntens()['02_7330A+']
Out[42]: array([ 4.03377032, 0.71466343])
```

0.3 Using Observation to determine ionic abundances

Once the electron temperature and density are determined, it is easy to obtain the ionic abundances from a set of emission lines included in an **Observation** object:

```
In [43]: obs = pn.Observation()
         obs.readData('observations1.dat', fileFormat='lines_in_rows', err_default=
         obs.def_EBV(label1="H1r_6563A", label2="H1r_4861A", r_theo=2.85)
         obs.correctData(normWave=4861.)
         Te = [10000.]
         Ne = [1e3]
         # Define a dictionary to hold all the Atom objects needed
         all_atoms = pn.getAtomDict(atom_list=obs.getUniqueAtoms())
         # define a dictionary to store the abundances
         ab\_dict = \{\}
         # we use the following lines to determine the ionic abundances
         ab_labels = ['N2_6584A', 'O2_3726A', 'O3_5007A', 'S2_6716A',
                      'S3_6312A', 'Ar3_7136A', 'Ne3_3869A']
         for line in obs.getSortedLines():
             if line.label in ab_labels:
                 ab = all_atoms[line.atom].getIonAbundance(line.corrIntens, Te, Ne,
                                                            to_eval=line.to_eval, Hk
                 ab_dict[line.atom] = ab
```

```
warng _ManageAtomicData: rec data not available for Ar3
warng _ManageAtomicData: atom data not available for H1
warng _ManageAtomicData: coll data not available for H1
warng _ManageAtomicData: rec data not available for Ne2
warng ManageAtomicData: rec data not available for Ne3
warng _ManageAtomicData: rec data not available for S2
warng _ManageAtomicData: rec data not available for S3
warng _ManageAtomicData: rec data not available for S4
In [44]: ab_dict
Out[44]: {'Ar3': array([ 3.21287725e-07]),
          'N2': array([ 3.22649264e-06]),
          'Ne3': array([ 2.36596811e-05]),
          '02': array([ 3.64228102e-05]),
          '03': array([ 0.00014833]),
          'S2': array([ 6.71633117e-08]),
          'S3': array([ 1.42901804e-06])}
```