Heat Maps using Matplotlib and Seaborn

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Heat Maps using Matplotlib and Seaborn

In [1]:
```
%pylab inline
import matplotlib.pyplot as plt
import pandas as pd
import numpy as np
```

```
Populating the interactive namespace from numpy and matplotlib
```

In [2]:
```
helix = pd.read_csv('Data/helix_parameters.csv')
helix.head() # just seeing that data was imported properly by outputing first 5 cells
```

Out[2]:

	job_n	Energy	n_helices	r0_A	r0_B	r0_C	omega0	delta_omega0_A	\
0	36019	-387.167	3	6.0	6.0	6.0	0	0	
1	36022	-402.606	3	6.0	6.0	6.0	0	0	
2	36020	-395.944	3	6.0	6.0	6.0	0	0	
3	36002	-389.788	3	6.0	6.0	6.0	0	0	
4	36005	-388.016	3	6.0	6.0	6.0	0	0	

	delta_omega0_B	delta_omega0_C	...	invert_B	invert_C	z1_offset_A	\
0	120	240	...	1	0	0	
1	120	240	...	1	0	0	
2	120	240	...	1	0	0	
3	120	240	...	1	0	0	
4	120	240	...	1	0	0	

	z1_offset_B	z1_offset_C	delta_t_A	delta_t_B	delta_t_C	omega1	z1
0	0.6	-3.0	0	0	0	99.999268	1.51
1	0.6	0.6	0	0	0	99.999268	1.51
2	0.6	-1.8	0	0	0	99.999268	1.51
3	-3.0	-1.8	0	0	0	99.999268	1.51
4	-3.0	1.8	0	0	0	99.999268	1.51

[5 rows x 27 columns]

In [3]:
```
# shape of the dataframe
helix.shape
```

Out[3]:
```
(47475, 27)
```

In [4]:
```
# checking what the columns are
helix.columns
```

Out[4]:
```
Index([u'job_n', u'Energy', u'n_helices', u'r0_A', u'r0_B', u'r0_C', u'omega0',
       u'delta_omega0_A', u'delta_omega0_B', u'delta_omega0_C', u'z0_offset_A',
```

```
       u'z0_offset_B', u'z0_offset_C', u'helix1 phase', u'helix 2 phase',
       u'helix3 phase', u'invert_A', u'invert_B', u'invert_C', u'z1_offset_A',
       u'z1_offset_B', u'z1_offset_C', u'delta_t_A', u'delta_t_B',
       u'delta_t_C', u'omega1', u'z1'],
      dtype='object')
```

Selecting Columns (by different methods)

In [5]:
```
# selecting a couple columns
couple_columns = helix[['Energy','helix 2 phase', 'helix1 phase']]
couple_columns.head()
```

Out[5]:

	Energy	helix 2 phase	helix1 phase
0	-387.167	0	0
1	-402.606	0	0
2	-395.944	0	0
3	-389.788	0	0
4	-388.016	0	0

In [6]:
```
# selecting same columns a different way
helix.ix[:,['Energy','helix 2 phase', 'helix1 phase']].head()
```

Out[6]:

	Energy	helix 2 phase	helix1 phase
0	-387.167	0	0
1	-402.606	0	0
2	-395.944	0	0
3	-389.788	0	0
4	-388.016	0	0

Heat Map

In [7]:
```
# this is essentially would be taking the average of each unique combination.
# one important mention is notice how little the data varies from eachother.
phase_1_2 = couple_columns.groupby(['helix1 phase', 'helix 2 phase']).mean()
print phase_1_2.shape
phase_1_2.head(10)
```

```
(100, 1)
```

Out[7]:

		Energy
helix1 phase	helix 2 phase	
0	0	-392.419841
	20	-389.622691
	40	-390.318620
	60	-392.198537
	80	-393.661624
	100	-392.226253
	120	-390.955112
	140	-394.319969
	160	-392.594862
	180	-389.254009

In [8]:
```
phase_1_2 = phase_1_2.reset_index()
phase_1_2.head()
```

Out[8]:

	helix1 phase	helix 2 phase	Energy
0	0	0	-392.419841
1	0	20	-389.622691
2	0	40	-390.318620
3	0	60	-392.198537
4	0	80	-393.661624

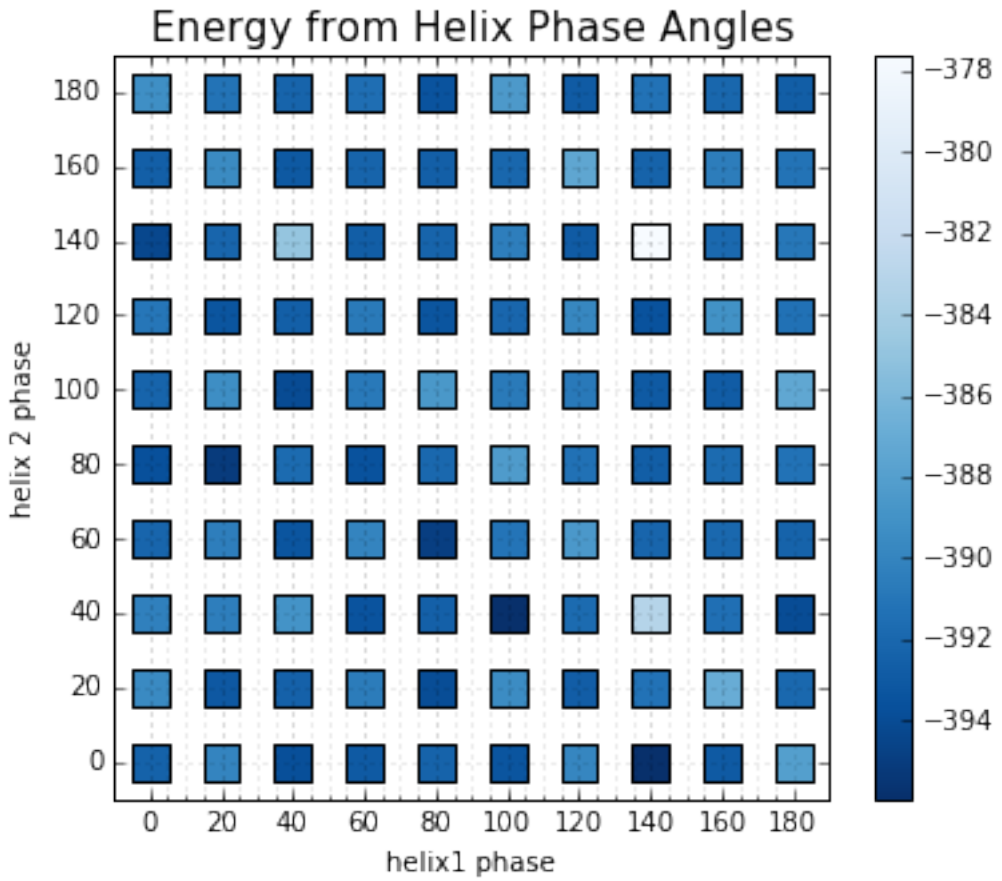
Heat Map using Matplotlib

In [9]:
```
major_ticks = np.arange(0, 200, 20)
minor_ticks = np.arange(0, 180, 5)

fig = plt.figure(figsize = (6,5))
ax = fig.add_subplot(1,1,1)
s = ax.scatter('helix1 phase', 'helix 2 phase', c = 'Energy',data = phase_1_2, cmap = 'Blues_r'
ax.axis([phase_1_2['helix1 phase'].min()-10, phase_1_2['helix1 phase'].max()+10, phase_1_2['heli
ax.set_xticks(major_ticks)
ax.set_xticks(minor_ticks, minor=True)
ax.set_yticks(major_ticks)
ax.grid(which='both', alpha = 0.3)
ax.grid(which='major', alpha=0.3)
ax.set_xlabel('helix1 phase', fontsize=10);
ax.set_ylabel('helix 2 phase', fontsize=10);
ax.set_title('Energy from Helix Phase Angles', size = 15)

# http://stackoverflow.com/questions/13943217/how-to-add-colorbars-to-scatterplots-created-like
cbar = plt.colorbar(mappable = s,ax = ax)

plt.show()
```



Heat Map using Seaborn

```
In [10]: import numpy as np;
         import seaborn as sns;

         # To translate into Excel Terms for those familiar with Excel
         # string 1 is row labels 'helix1 phase'
         # string 2 is column labels 'helix 2 phase'
         # string 3 is values 'Energy'
         # Official pivot documentation
         # http://pandas.pydata.org/pandas-docs/stable/generated/pandas.DataFrame.pivot.html

         phase_1_2.pivot('helix1 phase', 'helix 2 phase','Energy').head()
```

```
Out[10]: helix 2 phase         0           20          40          60          80   \
         helix1 phase
         0             -392.419841 -389.622691 -390.318620 -392.198537 -393.661624
         20            -390.013375 -393.121438 -390.435441 -390.489424 -395.112815
         40            -393.751152 -392.486692 -388.967952 -393.297131 -391.750444
         60            -392.960539 -390.578310 -393.441091 -390.007804 -393.577453
         80            -392.347250 -393.919370 -392.575410 -394.918433 -391.945480

         helix 2 phase         100         120         140         160         180
```

```
helix1 phase
0             -392.226253 -390.955112 -394.319969 -392.594862 -389.254009
20            -389.307695 -393.365839 -392.171938 -389.534864 -391.171958
40            -394.077600 -392.610059 -384.873483 -393.059775 -392.283178
60            -390.840711 -390.734280 -392.706732 -392.278805 -391.558888
80            -388.600299 -393.314092 -392.258363 -392.636642 -393.471684
```

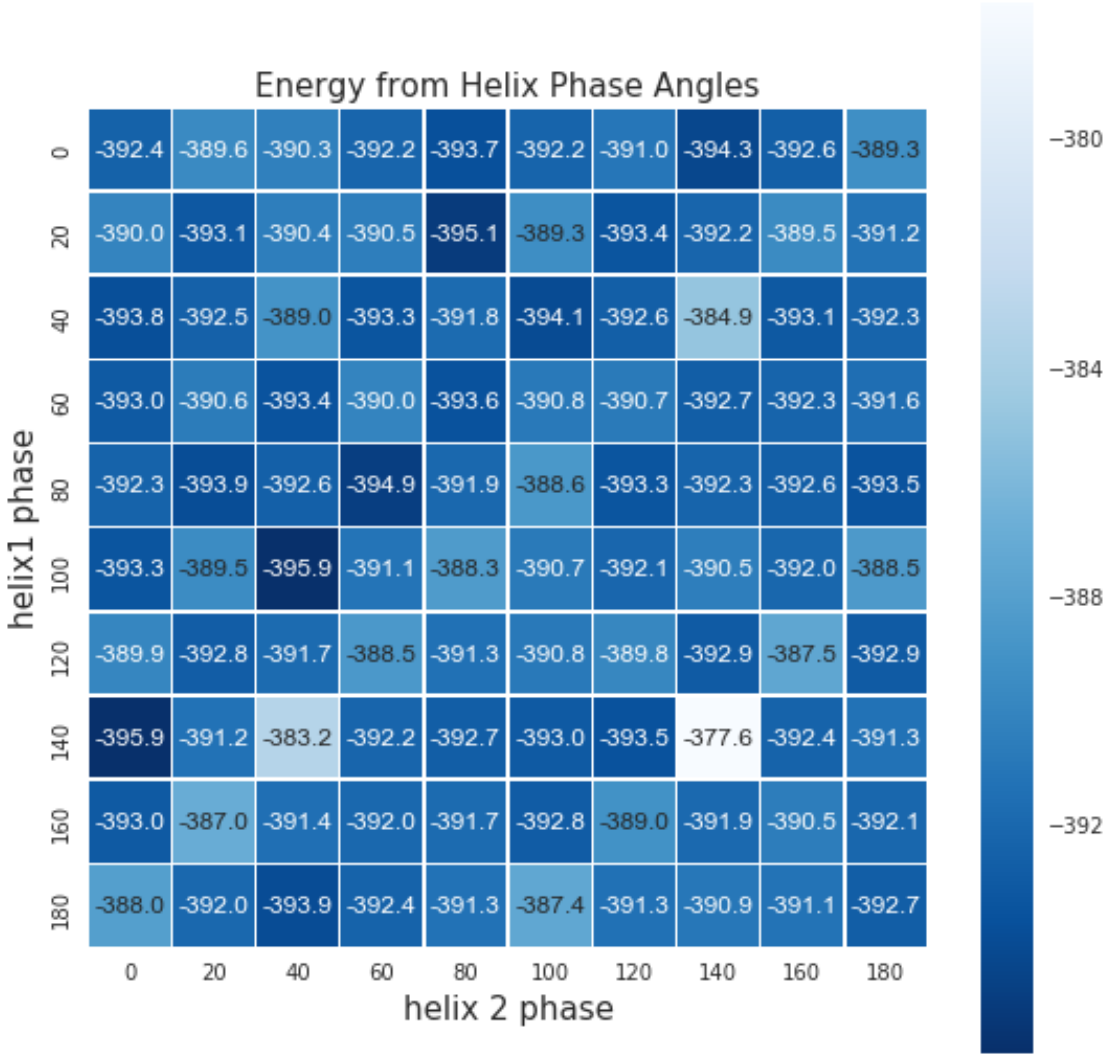
In [11]:
```
# To translate into Excel Terms for those familiar with Excel
# string 1 is row labels 'helix1 phase'
# string 2 is column labels 'helix 2 phase'
# ['Energy'] is values
phase_1_2.pivot('helix1 phase', 'helix 2 phase')['Energy'].head()
```

Out[11]:
```
helix 2 phase         0           20          40          60          80   \
helix1 phase
0             -392.419841 -389.622691 -390.318620 -392.198537 -393.661624
20            -390.013375 -393.121438 -390.435441 -390.489424 -395.112815
40            -393.751152 -392.486692 -388.967952 -393.297131 -391.750444
60            -392.960539 -390.578310 -393.441091 -390.007804 -393.577453
80            -392.347250 -393.919370 -392.575410 -394.918433 -391.945480

helix 2 phase         100         120         140         160         180
helix1 phase
0             -392.226253 -390.955112 -394.319969 -392.594862 -389.254009
20            -389.307695 -393.365839 -392.171938 -389.534864 -391.171958
40            -394.077600 -392.610059 -384.873483 -393.059775 -392.283178
60            -390.840711 -390.734280 -392.706732 -392.278805 -391.558888
80            -388.600299 -393.314092 -392.258363 -392.636642 -393.471684
```

In [12]:
```
# seaborn heatmap documentation
# https://stanford.edu/~mwaskom/software/seaborn/generated/seaborn.heatmap.html

# cmap choices: http://matplotlib.org/users/colormaps.html
plt.figure(figsize=(9,9))
pivot_table = phase_1_2.pivot('helix1 phase', 'helix 2 phase','Energy')
plt.xlabel('helix 2 phase', size = 15)
plt.ylabel('helix1 phase', size = 15)
plt.title('Energy from Helix Phase Angles', size = 15)
sns.heatmap(pivot_table, annot=True, fmt=".1f", linewidths=.5, square = True, cmap = 'Blues_r'
```


Energy from Helix Phase Angles
helix1 phase
helix 2 phase
0 20 40 60 80 100 120 140 160 180
-392.4 -389.6 -390.3 -392.2 -393.7 -392.2 -391.0 -394.3 -392.6 -389.3
-390.0 -393.1 -390.4 -390.5 -395.1 -389.3 -393.4 -392.2 -389.5 -391.2
-393.8 -392.5 -389.0 -393.3 -391.8 -394.1 -392.6 -384.9 -393.1 -392.3
-393.0 -390.6 -393.4 -390.0 -393.6 -390.8 -390.7 -392.7 -392.3 -391.6
-392.3 -393.9 -392.6 -394.9 -391.9 -388.6 -393.3 -392.3 -392.6 -393.5
-393.3 -389.5 -395.9 -391.1 -388.3 -390.7 -392.1 -390.5 -392.0 -388.5
-389.9 -392.8 -391.7 -388.5 -391.3 -390.8 -389.8 -392.9 -387.5 -392.9
-395.9 -391.2 -383.2 -392.2 -392.7 -393.0 -393.5 -377.6 -392.4 -391.3
-393.0 -387.0 -391.4 -392.0 -391.7 -392.8 -389.0 -391.9 -390.5 -392.1
-388.0 -392.0 -393.9 -392.4 -391.3 -387.4 -391.3 -390.9 -391.1 -392.7
−380
−384
−388
−392

In [ ]: