■ Concepts and Methods of 2D Infrared Spectroscopy

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This progam was used to produce Fig. 10.10.

Set working directory (you will have to change it)

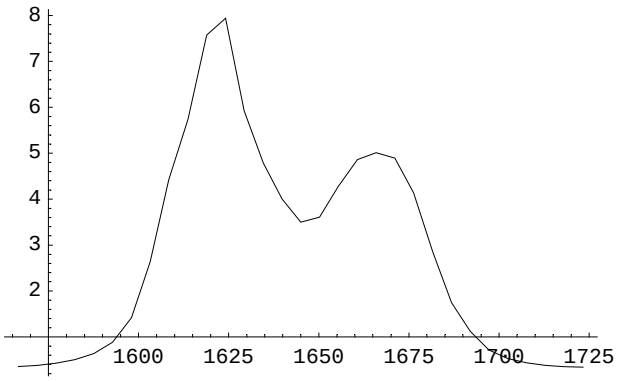
```
In[1]:= SetDirectory["C:\Dokumente und Einstellungen\p.hamm\Eigene
            Dateien/PCI/projekte/2010/2D-IR Book/SecSimul/SimulPeptide"];
```

Read data from 1LE1_lin.dat and 1LE1_2D.dat

```
In[2]:= spek1D = Import["1LE1_lin.dat"];
        spek2D = Import["1LE1_2D.dat"];
        n = Sqrt[Length[spek2D]];
        spek2D = Table[spek2D[[i + (j - 1) * n, 3]], {j, 1, n}, {i, 1, n}];
```

Plot linear absorption spectrum

```
In[6]:= ListPlot[spek1D, PlotJoined → True, PlotRange → All]
```




```
Out[6]= - Graphics -
```

Plot purely absorptive spectrm

```
In[7]:= wmin = spek1D[[1, 1]];
        wmax = spek1D[[n, 1]];
        ticks = Table[{(w - wmin) / (wmax - wmin) * (n - 1) + 1, w}, {w, 1600, 1700, 50}];
        max = Max[{Max[Re[spek2D]], -Min[Re[spek2D]]}] / 2;
        p1 = ListContourPlot[Re[spek2D], PlotRange → {0, max},
           ContourShading → False, Contours → 20, Ticks → None,
           ContourStyle → {RGBColor[1, 0, 0]}, DisplayFunction -> Identity];
        p2 = ListContourPlot[Re[spek2D], PlotRange → {-max, 0},
           ContourShading → False, Contours → 20, Ticks → None,
           ContourStyle → {RGBColor[0, 0, 1]}, DisplayFunction -> Identity];
        Show[{p1, p2}, FrameTicks → {ticks, ticks, None, None},
          PlotRange → {{1, n}, {1, n}}, DisplayFunction → $DisplayFunction];
```