











Transmission & absorption spectra

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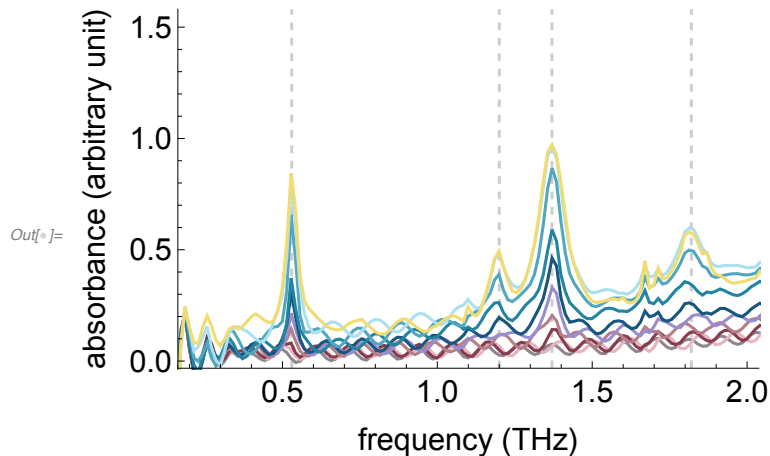
In[ ]:= dataset = "set2_N2_5"; (*choose dataset folder here*)
col = 3; (*choose column number: 2 for transmission, 3 for absorption*)
path = NotebookDirectory[] <> "../data/" <> dataset <> "/frequency_domain/";
(*path for importing files containing frequency domain data*)
colour = Reverse[{, , , , , , , , , , , }];
data0 = Import[path <> "Ref.csv"][[All, {1, col}]];
(*import transmittance/absorbance values for each sample*)
Ref = ListPlot[Table[{data0[[i]][1], data[[i]][2] - data0[[i]][2]}, {i, Length[data]}],
  Joined -> True, PlotStyle -> colour[[1]]];
data = Import[path <> "L000_1.csv"][[All, {1, col}]];
L0a = ListPlot[data, Joined -> True, PlotStyle -> colour[[2]]];
data = Import[path <> "L000_2.csv"][[All, {1, col}]];
L0b = ListPlot[data, Joined -> True, PlotStyle -> colour[[2]]];
data = Import[path <> "L001.csv"][[All, {1, col}]];
L1 = ListPlot[data, Joined -> True, PlotStyle -> colour[[3]]];
data = Import[path <> "L003.csv"][[All, {1, col}]];
L3 = ListPlot[data, Joined -> True, PlotStyle -> colour[[4]]];
data = Import[path <> "L005.csv"][[All, {1, col}]];
L5 = ListPlot[data, Joined -> True, PlotStyle -> colour[[5]]];
data = Import[path <> "L010.csv"][[All, {1, col}]];
L10 = ListPlot[data, Joined -> True, PlotStyle -> colour[[6]]];
data = Import[path <> "L015.csv"][[All, {1, col}]];
L15 = ListPlot[data, Joined -> True, PlotStyle -> colour[[7]]];
data = Import[path <> "L020.csv"][[All, {1, col}]];
L20 = ListPlot[data, Joined -> True, PlotStyle -> colour[[8]]];
data = Import[path <> "L049.csv"][[All, {1, col}]];
L49 = ListPlot[data, Joined -> True, PlotStyle -> colour[[9]]];
data = Import[path <> "L080.csv"][[All, {1, col}]];
L80 = ListPlot[data, Joined -> True, PlotStyle -> colour[[10]]];
data = Import[path <> "L100_1.csv"][[All, {1, col}]];
L100a = ListPlot[data, Joined -> True, PlotStyle -> colour[[11]]];
data = Import[path <> "L100_2.csv"][[All, {1, col}]];
L100b = ListPlot[data, Joined -> True, PlotStyle -> colour[[11]]];
data = Import[path <> "S001.csv"][[All, {1, col}]];
S1 = ListPlot[data, Joined -> True, PlotStyle -> colour[[12]]];
data = Import[path <> "S002.csv"][[All, {1, col}]];
S2 = ListPlot[data, Joined -> True, PlotStyle -> colour[[13]]];
data = Import[path <> "S003.csv"][[All, {1, col}]];
S3 = ListPlot[data, Joined -> True, PlotStyle -> colour[[14]]];

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In[ ]:= (*show selected samples on the same plot - all pure standard samples*)
Show[Ref, L0b, L1, L3, L5, L10, L15, L20, L49, L80, L100b,
  PlotRange → {{0.2, 2}, {0, 1.5}}, Frame → {{True, False}, {True, False}},
  GridLines → {{{0.53, Directive[Dashed, Thickness[0.005]]},
    {1.20, Directive[Dashed, Thickness[0.005]]},
    {1.37, Directive[Dashed, Thickness[0.005]]},
    {1.82, Directive[Dashed, Thickness[0.005]]}}, None},
  FrameLabel → {"absorbance (arbitrary unit)", None}, {"frequency (THz)", None}},
  FrameTicks → All, LabelStyle → Directive[FontSize → 16]]

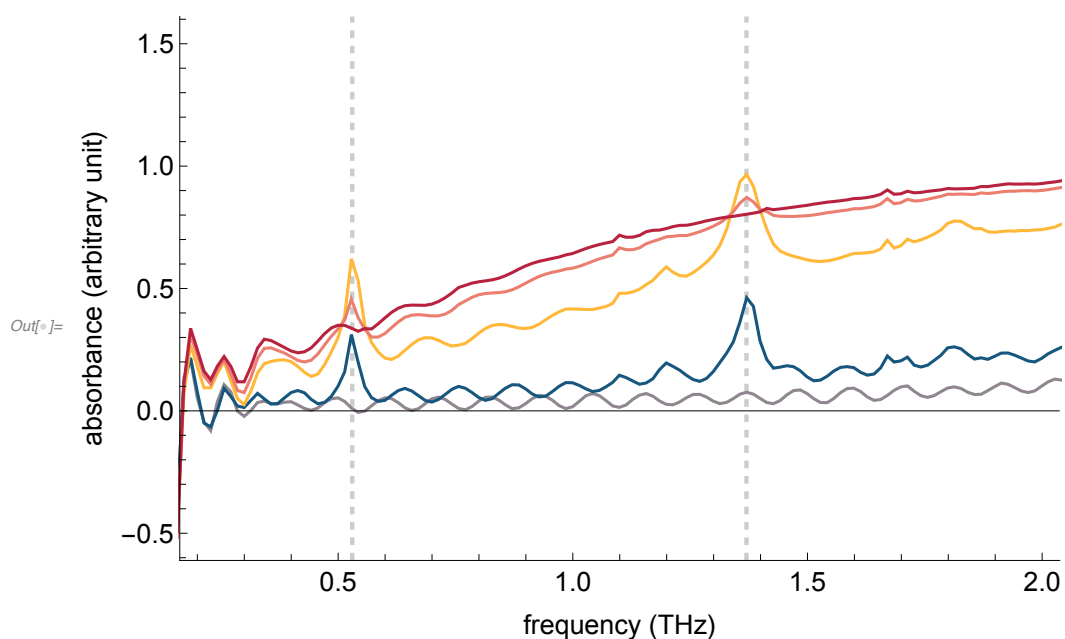
```



```

In[ ]:= (*show selected samples on the same plot -
  pure standard and all real samples*)
Show[L0b, L15, S1, S2, S3, PlotRange → {{0.2, 2}, {-0.5, 1.5}},
  Frame → {{True, False}, {True, False}},
  FrameLabel → {"absorbance (arbitrary unit)", None}, {"frequency (THz)", None}},
  FrameTicks → All, GridLines → {{{0.53, Directive[Dashed, Thickness[0.005]]},
    {1.37, Directive[Dashed, Thickness[0.005]]}}, None},
  LabelStyle → Directive[FontSize → 14]]

```



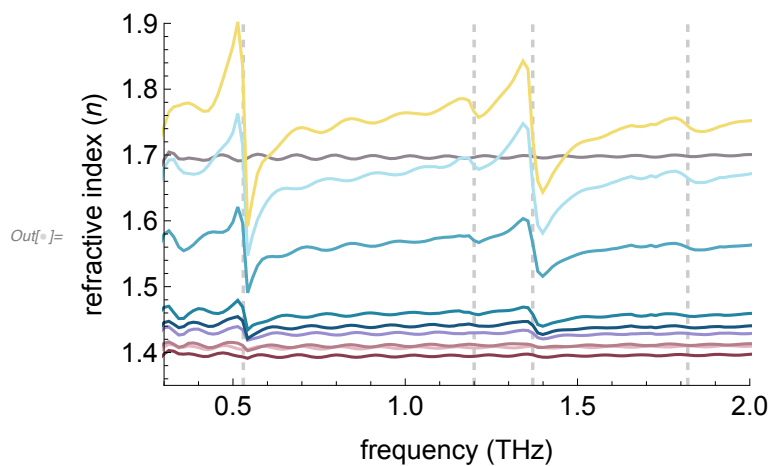
Refractive index spectra

```

path = "../data/set2_N2_5/frequency_domain/";
ri = Import[NotebookDirectory[] <> path <> "refractive-index.csv"];
Length[ri]
colour = Reverse[{{Red, Orange, Yellow, LightBlue, Blue, DarkBlue, Purple, Maroon, Pink, Grey, Black}}];
list = {3, 4, 5, 6, 7, 8, 9, 10, 11, 17};
(*choose columns of data - only pure standards are chosen here*)
ListPlot[Table[ri[[All, {1, i}]], {i, list}],
  PlotStyle -> colour[[2 ;; 11]], Joined -> True,
  PlotRange -> {{0.3, 2}, {1.35, 1.9}}, Frame -> {{True, False}, {True, False}},
  FrameLabel -> {{ "refractive index (n)", None}, {"frequency (THz)", None}},
  FrameTicks -> All, GridLines -> {{ {0.53, Directive[Dashed, Thickness[0.006]]},
    {1.20, Directive[Dashed, Thickness[0.006]]}, {1.37, Directive[Dashed,
    Thickness[0.006]]}, {1.82, Directive[Dashed, Thickness[0.006]]}},
    None}, LabelStyle -> Directive[FontSize -> 14]]

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Out[]= 702



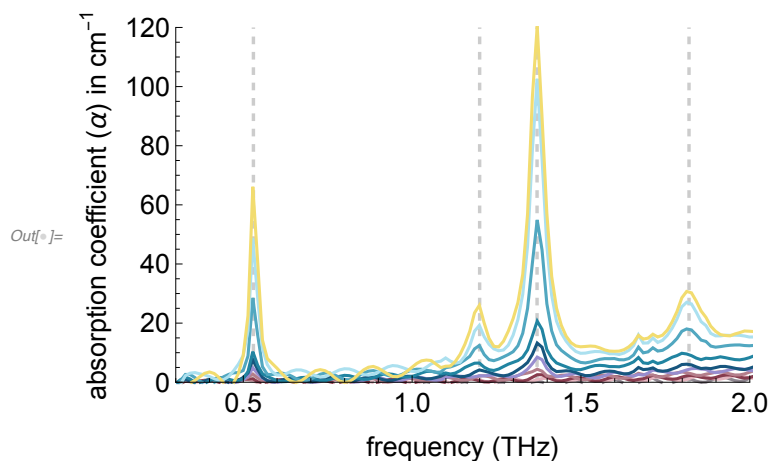
Absorption coefficient spectra

```

path = "../data/set2_N2_5/frequency_domain/";
ac = Import[NotebookDirectory[] <> path <> "absorption-coefficient.csv"];
Length[ac]
colour = Reverse[{Red, Orange, Yellow, LightBlue, Blue, DarkBlue, Purple, Maroon, Pink, Grey, Black}];
list = {3, 4, 5, 6, 7, 8, 9, 10, 11, 17};
(*choose columns of data - only pure standards are chosen here*)
ListPlot[Table[ac[[All, {1, i}]], {i, list}],
  PlotStyle -> colour[[2 ;; 11]], Joined -> True, PlotRange -> {{0.3, 2}, {0, 120}},
  Frame -> {{True, False}, {True, False}}, FrameLabel ->
    {"absorption coefficient ( $\alpha$ ) in cm-1", None}, {"frequency (THz)", None},
  FrameTicks -> All, GridLines -> {{0.53, Directive[Dashed, Thickness[0.006]]},
    {1.20, Directive[Dashed, Thickness[0.006]]}, {1.37, Directive[Dashed,
    Thickness[0.006]]}, {1.82, Directive[Dashed, Thickness[0.006]]}},
  None}, LabelStyle -> Directive[FontSize -> 14]]

```

Out[]= 702



```

list = {3, 8, 12, 15, 16}; (*choose columns of data - real samples,
0% and 15% (w/w) pure standards are chosen here*)
ListPlot[Table[ac[[All, {1, i}]], {i, list}], PlotStyle → colour[{{2, 7, 12, 13, 14}},
Joined → True, PlotRange → {{0.3, 2}, {0, 120}},
Frame → {{True, False}, {True, False}}, FrameLabel →
{{"absorption coefficient ( $\alpha$ ) in  $\text{cm}^{-1}$ ", None}, {"frequency (THz)", None}},
FrameTicks → All, GridLines → {{{0.53, Directive[Dashed, Thickness[0.006]]},
{1.20, Directive[Dashed, Thickness[0.006]]},
{1.37, Directive[Dashed, Thickness[0.006]]},
{1.82, Directive[Dashed, Thickness[0.006]]}}, None},
LabelStyle → Directive[FontSize → 14]]

```

