Water Studies Lab

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In[ ]:=
```
energyscan1 =
  Import["C:\\Users\\abhardwaj24\\OneDrive - Charlotte Country Day School\\NCSSM\\Comp
    Sci\\Week 8\\energyscan1.csv"];
```

In[ ]:=
```
energyscan1 // TableForm;
Grid[energyscan1, Frame → All]
```

Out[ ]=

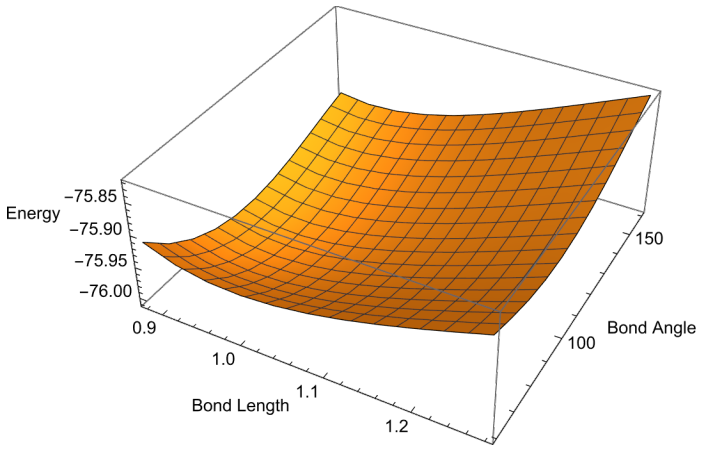
Coordinate1	Coordinate2	Energy
0.88	60.	−75.9131
0.88	70.	−75.9484
0.88	80.	−75.9732
0.88	90.	−75.9892
0.88	100.	−75.9976
0.88	110.	−75.9993
0.88	120.	−75.9954
0.88	130.	−75.9874
0.88	140.	−75.9768
0.88	150.	−75.9654
0.88	160.	−75.9552
0.92	60.	−75.9306
0.92	70.	−75.963
0.92	80.	−75.9858
0.92	90.	−76.0005
0.92	100.	−76.0078
0.92	110.	−76.0087
0.92	120.	−76.0041
0.92	130.	−75.9954
0.92	140.	−75.9841
0.92	150.	−75.9721
0.92	160.	−75.9613
0.96	60.	−75.9391
0.96	70.	−75.9688
0.96	80.	−75.9899
0.96	90.	−76.0033
0.96	100.	−76.0096
0.96	110.	−76.0097
0.96	120.	−76.0045
0.96	130.	−75.9952
0.96	140.	−75.9832
0.96	150.	−75.9705

0.96	160.	−75.9591
1.	60.	−75.9408
1.	70.	−75.9679
1.	80.	−75.9874
1.	90.	−75.9996
1.	100.	−76.0051
1.	110.	−76.0044
1.	120.	−75.9986
1.	130.	−75.9887
1.	140.	−75.9762
1.	150.	−75.9628
1.	160.	−75.9508
1.04	60.	−75.9372
1.04	70.	−75.962
1.04	80.	−75.9799
1.04	90.	−75.991
1.04	100.	−75.9956
1.04	110.	−75.9943
1.04	120.	−75.988
1.04	130.	−75.9776
1.04	140.	−75.9646
1.04	150.	−75.9506
1.04	160.	−75.938
1.08	60.	−75.9297
1.08	70.	−75.9522
1.08	80.	−75.9686
1.08	90.	−75.9787
1.08	100.	−75.9826
1.08	110.	−75.9807
1.08	120.	−75.9739
1.08	130.	−75.9631
1.08	140.	−75.9496
1.08	150.	−75.9351
1.08	160.	−75.9219
1.12	60.	−75.9191
1.12	70.	−75.9395
1.12	80.	−75.9545
1.12	90.	−75.9636
1.12	100.	−75.9668
1.12	110.	−75.9644
1.12	120.	−75.9572
1.12	130.	−75.9461
1.12	140.	−75.9322
1.12	150.	−75.9173
1.12	160.	−75.9035
1.16	60.	−75.9064
1.16	70.	−75.9247
1.16	80.	−75.9384

1.16	90.	−75.9466
1.16	100.	−75.9491
1.16	110.	−75.9463
1.16	120.	−75.9388
1.16	130.	−75.9274
1.16	140.	−75.9133
1.16	150.	−75.8979
1.16	160.	−75.8836
1.2	60.	−75.8921
1.2	70.	−75.9083
1.2	80.	−75.9208
1.2	90.	−75.9281
1.2	100.	−75.93
1.2	110.	−75.9269
1.2	120.	−75.9191
1.2	130.	−75.9076
1.2	140.	−75.8932
1.2	150.	−75.8776
1.2	160.	−75.8628
1.24	60.	−75.8766
1.24	70.	−75.8909
1.24	80.	−75.9021
1.24	90.	−75.9086
1.24	100.	−75.9101
1.24	110.	−75.9066
1.24	120.	−75.8987
1.24	130.	−75.8871
1.24	140.	−75.8726
1.24	150.	−75.8567
1.24	160.	−75.8415
1.28	60.	−75.8605
1.28	70.	−75.8728
1.28	80.	−75.8828
1.28	90.	−75.8886
1.28	100.	−75.8895
1.28	110.	−75.8858
1.28	120.	−75.8779
1.28	130.	−75.8662
1.28	140.	−75.8517
1.28	150.	−75.8357
1.28	160.	−75.8201

In[ ]:= **ListPlot3D[energyscan1, AxesLabel → {"Bond Length", "Bond Angle", "Energy"}]**

Out[ ]=



In[ ]:=
```
energyscan1 = Delete[energyscan1, 1];
{bondLength, bondAngle, energy} = Transpose[energyscan1];
results = {{"Bond Length", "Bond Angle", "Energy"}};
Do[
  If[
   Min[energy] == energy[[row]],
   results = Append[results, {bondLength[[row]], bondAngle[[row]], energy[[row]]}]
  ],
  {row, 1, Length[energyscan1]}
 ];
```

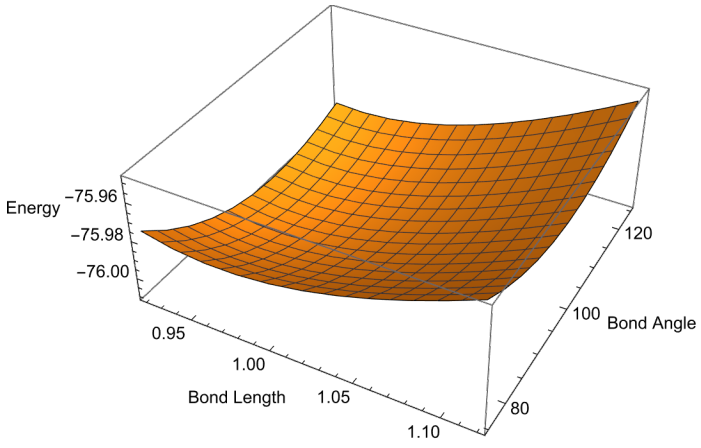
In[ ]:=
```
Grid[results, Frame → All]
```

Out[ ]=

Bond Length	Bond Angle	Energy
0.96	110.	−76.0097

In[ ]:=
```
energyscan2 =
  Import["C:\\Users\\abhardwaj24\\OneDrive - Charlotte Country Day School\\NCSSM\\Comp
     Sci\\Week 8\\energyscan2.csv"];
ListPlot3D[energyscan2, AxesLabel → {"Bond Length", "Bond Angle", "Energy"}]
```

Out[ ]=



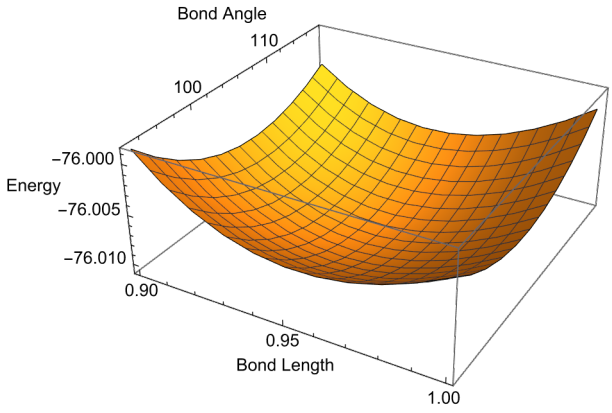
In[ ]:=
```
energyscan2 = Delete[energyscan2, 1];
{bondLength, bondAngle, energy} = Transpose[energyscan2];
results2 = {{"Bond Length", "Bond Angle", "Energy"}};
Do[
  If[
   Min[energy] == energy[[row]],
   results2 = Append[results2, {bondLength[[row]], bondAngle[[row]], energy[[row]]}]
  ],
  {row, 1, Length[energyscan2]}
 ];
Grid[results2, Frame → All]
```

Out[ ]=

Bond Length	Bond Angle	Energy
0.94	105.	−76.0106

In[ ]:=
```
energyscan3 =
  Import["C:\\Users\\abhardwaj24\\OneDrive - Charlotte Country Day School\\NCSSM\\Comp
     Sci\\Week 8\\energyscan3.csv"];
ListPlot3D[energyscan3, AxesLabel → {"Bond Length", "Bond Angle", "Energy"}]
```

Out[ ]=



In[ ]:=
```
energyscan3 = Delete[energyscan3, 1];
{bondLength, bondAngle, energy} = Transpose[energyscan3];
results3 = {{"Bond Length", "Bond Angle", "Energy"}};
Do[
  If[
   Min[energy] == energy[[row]],
   results3 = Append[results3, {bondLength[[row]], bondAngle[[row]], energy[[row]]}]
  ],
  {row, 1, Length[energyscan3]}
 ];
Grid[results3, Frame → All]
```

Out[ ]=

Bond Length	Bond Angle	Energy
0.95	105.	−76.0107