

R(Bohr)	Theta(deg)	Energy(wavenumber)
12.00	0	-36.72145965
12.00	20	-36.28608706
12.00	40	-35.81327207
12.00	60	-33.23215829
12.00	80	-29.71057217
12.00	90	-29.36373582
12.00	100	-29.00316035
12.00	120	-25.74882892
12.00	140	-24.07489311
12.00	160	-28.93885418
12.00	180	-24.33084489
11.50	0	-45.63284694
11.50	20	-45.09214832
11.50	40	-43.99433436
11.50	60	-41.10520936
11.50	80	-37.60956520
11.50	90	-37.01634625
11.50	100	-36.51763321
11.50	120	-34.12458753
11.50	140	-33.40064923
11.50	160	-37.38221107
11.50	180	-33.78563036
11.00	0	-57.21316001
11.00	20	-56.43325559
11.00	40	-54.64815569
11.00	60	-51.17099130
11.00	80	-47.37141813
11.00	90	-46.50396517
11.00	100	-45.85952072
11.00	120	-44.01064138
11.00	140	-43.87004570
11.00	160	-47.04591480
11.00	180	-44.56762501
10.50	0	-72.13893049
10.50	20	-71.12846759
10.50	40	-68.48664701
10.50	60	-64.08577821
10.50	80	-59.61755253
10.50	90	-58.39171882
10.50	100	-57.52345376
10.50	120	-56.08685819
10.50	140	-56.49444523
10.50	160	-59.13097643
10.50	180	-57.60496675
10.00	0	-91.55873689
10.00	20	-90.21616445
10.00	40	-86.48221431
10.00	60	-80.77511810
10.00	80	-75.18096374
10.00	90	-73.47516013
10.00	100	-72.31420320
10.00	120	-71.09842147
10.00	140	-72.06198256

10.00	160	-74.57411535
10.00	180	-73.75698797
9.50	0	-116.65956592
9.50	20	-115.12633552
9.50	40	-110.14605271
9.50	60	-102.52430050
9.50	80	-95.18259835
9.50	90	-92.79150604
9.50	100	-91.23514296
9.50	120	-90.20451032
9.50	140	-91.84969493
9.50	160	-94.57489405
9.50	180	-94.36514177
9.00	0	-148.67864200
9.00	20	-147.10882509
9.00	40	-141.15141764
9.00	60	-131.13482009
9.00	80	-121.18882761
9.00	90	-117.84933988
9.00	100	-115.75104918
9.00	120	-114.98060411
9.00	140	-117.58408240
9.00	160	-120.72029236
9.00	180	-120.87862164
8.50	0	-187.75188597
8.50	20	-187.40970251
8.50	40	-181.91793320
8.50	60	-169.41145758
8.50	80	-155.59489182
8.50	90	-150.78520694
8.50	100	-147.93580690
8.50	120	-147.47008096
8.50	140	-151.19689814
8.50	160	-154.57290648
8.50	180	-154.64370913
8.00	0	-228.20808584
8.00	20	-233.03528484
8.00	40	-234.12640479
8.00	60	-220.34723754
8.00	80	-201.31544097
8.00	90	-194.44119864
8.00	100	-190.45219664
8.00	120	-190.39939095
8.00	140	-194.66324151
8.00	160	-196.23180738
8.00	180	-194.97254763
7.50	0	-246.43372875
7.50	20	-268.12040468
7.50	40	-294.28952827
7.50	60	-286.97438262
7.50	80	-261.59422775
7.50	90	-251.45151986
7.50	100	-245.67770326
7.50	120	-245.13211035

7.50	140	-246.76103185
7.50	160	-238.84105697
7.50	180	-231.84647654
7.00	0	-167.44831955
7.00	20	-237.97733510
7.00	40	-342.02918159
7.00	60	-365.98099312
7.00	80	-335.75974652
7.00	90	-320.87400828
7.00	100	-311.81511182
7.00	120	-307.10210563
7.00	140	-293.60125469
7.00	160	-252.26476252
7.00	180	-225.29459911
6.50	0	223.20715042
6.50	20	18.34448866
6.50	40	-307.03354168
6.50	60	-432.64011568
6.50	80	-408.03725352
6.50	90	-386.02957347
6.50	100	-370.36625728
6.50	120	-348.32888222
6.50	140	-279.95660366
6.50	160	-138.36404124
6.50	180	-53.45254366
6.00	0	1478.96915931
6.00	20	924.44294393
6.00	40	24.86188658
6.00	60	-395.80158812
6.00	80	-412.78897505
6.00	90	-381.04683255
6.00	100	-350.33602502
6.00	120	-271.01236094
6.00	140	-34.71008097
6.00	160	393.00846146
6.00	180	640.26677978
5.50	0	4966.48548718
5.50	20	3511.93105609
5.50	40	1166.78947759
5.50	60	11.88992642
5.50	80	-149.29376458
5.50	90	-102.75540765
5.50	100	-35.60369540
5.50	120	213.23332852
5.50	140	917.58939810
5.50	160	2117.48705253
5.50	180	2806.68993162
5.00	0	13851.47242278
5.00	20	10088.84315089
5.00	40	4324.34322770
5.00	60	1463.51041572
5.00	80	925.38396493
5.00	90	1001.96689107
5.00	100	1162.62654162

5.00	120	1874.16758620
5.00	140	3796.47793547
5.00	160	7000.49048279
5.00	180	8874.15705149