

R(Bohr)	Theta(deg)	Energy(wavenumber)
12.00	0	-35.57406629
12.00	20	-30.50028712
12.00	40	-19.29731742
12.00	60	-7.34350182
12.00	80	0.44325170
12.00	100	16.17600984
12.00	120	21.52988298
12.00	140	4.73578765
12.00	160	-18.01843659
12.00	180	-29.23929349
11.50	0	-44.52785615
11.50	20	-37.59001000
11.50	40	-18.22548931
11.50	60	4.54791705
11.50	80	15.97742883
11.50	100	39.07776516
11.50	120	42.22347840
11.50	140	9.23535436
11.50	160	-23.92705478
11.50	180	-36.76410362
11.00	0	-56.21020313
11.00	20	-45.78162906
11.00	40	-14.28501320
11.00	60	26.97538692
11.00	80	50.39069185
11.00	100	86.72106895
11.00	120	78.14727810
11.00	140	22.25759623
11.00	160	-27.38314954
11.00	180	-46.26346446
10.50	0	-71.33652989
10.50	20	-56.92994946
10.50	40	-11.32491003
10.50	60	54.93064196
10.50	80	97.83828978
10.50	100	157.71613962
10.50	120	122.80954072
10.50	140	36.85116935
10.50	160	-32.45291231
10.50	180	-58.47173936
10.00	0	-90.86085030
10.00	20	-72.21039155
10.00	40	-10.90599806
10.00	60	87.62429636
10.00	80	180.67307099
10.00	100	278.32763826
10.00	120	176.13193574
10.00	140	51.40264716
10.00	160	-40.32170559
10.00	180	-74.11547843
9.50	0	-116.14305343
9.50	20	-93.17765033
9.50	40	-15.60309228

9.50	60	118.82857151
9.50	80	307.78884293
9.50	100	438.24241259
9.50	120	229.71315757
9.50	140	62.93074709
9.50	160	-52.19874882
9.50	180	-94.36092785
9.00	0	-148.32028323
9.00	20	-121.60964898
9.00	40	-28.28089009
9.00	60	142.01307651
9.00	80	427.77312591
9.00	100	541.08866097
9.00	120	271.09828539
9.00	140	68.55626446
9.00	160	-69.90959121
9.00	180	-120.85801294
8.50	0	-187.49850209
8.50	20	-158.46345203
8.50	40	-51.80700791
8.50	60	150.46369801
8.50	80	474.44066576
8.50	100	562.04156612
8.50	120	294.43273569
8.50	140	64.19582297
8.50	160	-95.44713160
8.50	180	-154.60073590
8.00	0	-228.03790494
8.00	20	-200.68892764
8.00	40	-87.81846590
8.00	60	139.16437878
8.00	80	468.03972128
8.00	100	539.60108136
8.00	120	292.24424072
8.00	140	46.62458866
8.00	160	-129.22404878
8.00	180	-194.90148163
7.50	0	-246.07139752
7.50	20	-231.91181425
7.50	40	-132.45803484
7.50	60	106.11664533
7.50	80	428.88178191
7.50	100	492.07221185
7.50	120	267.73535773
7.50	140	16.27297387
7.50	160	-164.80127549
7.50	180	-231.72842093
7.00	0	-166.74455101
7.00	20	-196.17454635
7.00	40	-163.27623150
7.00	60	56.25251792
7.00	80	367.29635069
7.00	100	426.30301649
7.00	120	222.76429380

7.00	140	-13.26500317
7.00	160	-172.34665043
7.00	180	-225.22019707
6.50	0	224.88578301
6.50	20	67.49876807
6.50	40	-106.28649705
6.50	60	17.42166214
6.50	80	302.34746511
6.50	100	361.44106492
6.50	120	188.71167210
6.50	140	13.46062120
6.50	160	-52.15704859
6.50	180	-53.27505422
6.00	0	1479.10909657
6.00	20	983.80842941
6.00	40	247.92104499
6.00	60	83.14204623
6.00	80	299.90951484
6.00	100	366.95640585
6.00	120	263.03389599
6.00	140	268.09751345
6.00	160	485.40021573
6.00	180	640.32590633
5.50	0	4966.48757217
5.50	20	3588.64338468
5.50	40	1428.60776736
5.50	60	519.29349854
5.50	80	560.31383695
5.50	100	655.66345581
5.50	120	733.20757271
5.50	140	1228.99661563
5.50	160	2220.51445555
5.50	180	2806.72706679
5.00	0	13851.01762670
5.00	20	10203.92047763
5.00	40	6098.70602813
5.00	60	2000.55777378
5.00	80	1627.39195926
5.00	100	1810.28473461
5.00	120	2367.28070214
5.00	140	4123.34457693
5.00	160	7126.04697263
5.00	180	8874.17039555