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# Pair potential for the n-CG-PI modified para-hydrogen system
# First row = index for each row
# Second row = distance (Å)
# Third row = potential (kcal/mol)
# Fourth row = force (kcal/mol/Å)
1 0.050000 35.185309 24.590893
2 0.100000 33.966561 24.159044
3 0.150000 32.769405 23.727195
4 0.200000 31.593841 23.295346
5 0.250000 30.439870 22.863498
6 0.300000 29.307491 22.431649
7 0.350000 28.196705 21.999800
8 0.400000 27.107511 21.567951
9 0.450000 26.039910 21.136102
10 0.500000 24.993901 20.704253
11 0.550000 23.969485 20.272404
12 0.600000 22.966661 19.840555
13 0.650000 21.985429 19.408706
14 0.700000 21.025790 18.976857
15 0.750000 20.087744 18.545008
16 0.800000 19.171290 18.113159
17 0.850000 18.276428 17.681310
18 0.900000 17.403159 17.249461
19 0.950000 16.551482 16.817612
20 1.000000 15.721397 16.385763
21 1.050000 14.912905 15.953914
22 1.100000 14.126006 15.522065
23 1.150000 13.360699 15.090216
24 1.200000 12.616984 14.658367
25 1.250000 11.894862 14.226518
26 1.300000 11.194333 13.794669
27 1.350000 10.515395 13.362820
28 1.400000 9.858050 12.930971
29 1.450000 9.222298 12.499122
30 1.500000 8.608138 12.067273
31 1.550000 8.015571 11.635424
32 1.600000 7.444596 11.203575
33 1.650000 6.895213 10.771726
34 1.700000 6.367423 10.339877
35 1.750000 5.861226 9.908029
36 1.800000 5.376620 9.476180
37 1.850000 4.913608 9.044331
38 1.900000 4.472187 8.612482
39 1.950000 4.052359 8.180633
40 2.000000 3.654124 7.748784
41 2.050000 3.277481 7.316935
42 2.100000 2.922431 6.885086
43 2.150000 2.588972 6.453237
44 2.200000 2.277107 6.021388
45 2.250000 1.986834 5.589539
46 2.300000 1.718153 5.157690
47 2.350000 1.471065 4.725841
48 2.400000 1.245569 4.293992
49 2.450000 1.041666 3.862143
50 2.500000 0.859355 3.430294
51 2.550000 0.698636 2.998445
52 2.600000 0.559510 2.566596
53 2.650000 0.441977 2.134747
54 2.700000 0.346358 1.689985

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55 2.750000 0.268982 1.405083
56 2.800000 0.204851 1.160151
57 2.850000 0.151434 0.976509
58 2.900000 0.107225 0.791852
59 2.950000 0.071034 0.655808
60 3.000000 0.041265 0.534947
61 3.050000 0.017059 0.433281
62 3.100000 -0.002451 0.347111
63 3.150000 -0.017921 0.271704
64 3.200000 -0.029972 0.210316
65 3.250000 -0.039161 0.157249
66 3.300000 -0.046012 0.116813
67 3.350000 -0.050998 0.082602
68 3.400000 -0.054455 0.055703
69 3.450000 -0.056592 0.029777
70 3.500000 -0.057656 0.012783
71 3.550000 -0.057899 -0.003059
72 3.600000 -0.057448 -0.014990
73 3.650000 -0.056428 -0.025819
74 3.700000 -0.055018 -0.030564
75 3.750000 -0.053398 -0.034245
76 3.800000 -0.051565 -0.039082
77 3.850000 -0.049555 -0.041318
78 3.900000 -0.047432 -0.043587
79 3.950000 -0.045182 -0.046426
80 4.000000 -0.042945 -0.043066
81 4.050000 -0.040805 -0.042520
82 4.100000 -0.038655 -0.043499
83 4.150000 -0.036538 -0.041161
84 4.200000 -0.034553 -0.038254
85 4.250000 -0.032660 -0.037443
86 4.300000 -0.030829 -0.035798
87 4.350000 -0.029074 -0.034420
88 4.400000 -0.027406 -0.032303
89 4.450000 -0.025757 -0.033636
90 4.500000 -0.024185 -0.029260
91 4.550000 -0.022823 -0.025216
92 4.600000 -0.021487 -0.028241
93 4.650000 -0.020181 -0.023990
94 4.700000 -0.018945 -0.025451
95 4.750000 -0.017836 -0.018901
96 4.800000 -0.016813 -0.022006
97 4.850000 -0.015824 -0.017579
98 4.900000 -0.014936 -0.017918
99 4.950000 -0.014034 -0.018188
100 5.000000 -0.013198 -0.015227
101 5.050000 -0.012450 -0.014713
102 5.100000 -0.011633 -0.017936
103 5.150000 -0.010719 -0.018625
104 5.200000 -0.009772 -0.019282
105 5.250000 -0.009064 -0.009021
106 5.300000 -0.008607 -0.009269
107 5.350000 -0.008169 -0.008244
108 5.400000 -0.007764 -0.007972
109 5.450000 -0.007330 -0.009388
110 5.500000 -0.006809 -0.011424
111 5.550000 -0.006369 -0.006175
112 5.600000 -0.006040 -0.007012
113 5.650000 -0.005715 -0.005989

114	5.700000	-0.005432	-0.005319
115	5.750000	-0.005153	-0.005837
116	5.800000	-0.004882	-0.005025
117	5.850000	-0.004623	-0.005332
118	5.900000	-0.004351	-0.005541
119	5.950000	-0.004085	-0.005084
120	6.000000	-0.003830	-0.005106
121	6.050000	-0.003608	-0.003805
122	6.100000	-0.003442	-0.002824
123	6.150000	-0.003165	-0.008239
124	6.200000	-0.002832	-0.005100
125	6.250000	-0.002579	-0.004998
126	6.300000	-0.002356	-0.003935
127	6.350000	-0.002192	-0.002616
128	6.400000	-0.002082	-0.001782
129	6.450000	-0.001986	-0.002082
130	6.500000	-0.001862	-0.002855
131	6.550000	-0.001732	-0.002362
132	6.600000	-0.001570	-0.004117
133	6.650000	-0.001449	-0.000709
134	6.700000	-0.001342	-0.003585
135	6.750000	-0.001174	-0.003114
136	6.800000	-0.001033	-0.002535
137	6.850000	-0.000928	-0.001671
138	6.900000	-0.000837	-0.001960
139	6.950000	-0.000769	-0.000783
140	7.000000	-0.000674	-0.003016
141	7.050000	-0.000581	-0.000698
142	7.100000	-0.000503	-0.002425
143	7.150000	-0.000426	-0.000650
144	7.200000	-0.000384	-0.001013
145	7.250000	-0.000322	-0.001464
146	7.300000	-0.000261	-0.000985
147	7.350000	-0.000230	-0.000272
148	7.400000	-0.000206	-0.000680
149	7.450000	-0.000171	-0.000723
150	7.500000	-0.000167	0.000574
151	7.550000	-0.000150	-0.001263
152	7.600000	-0.000095	-0.000944
153	7.650000	-0.000041	-0.001221
154	7.700000	-0.000013	0.000125
155	7.750000	-0.000023	0.000284
156	7.800000	0.000020	-0.002016
157	7.850000	0.000069	0.000034
158	7.900000	0.000073	-0.000193
159	7.950000	0.000050	0.001141
160	8.000000	0.000000	0.000845