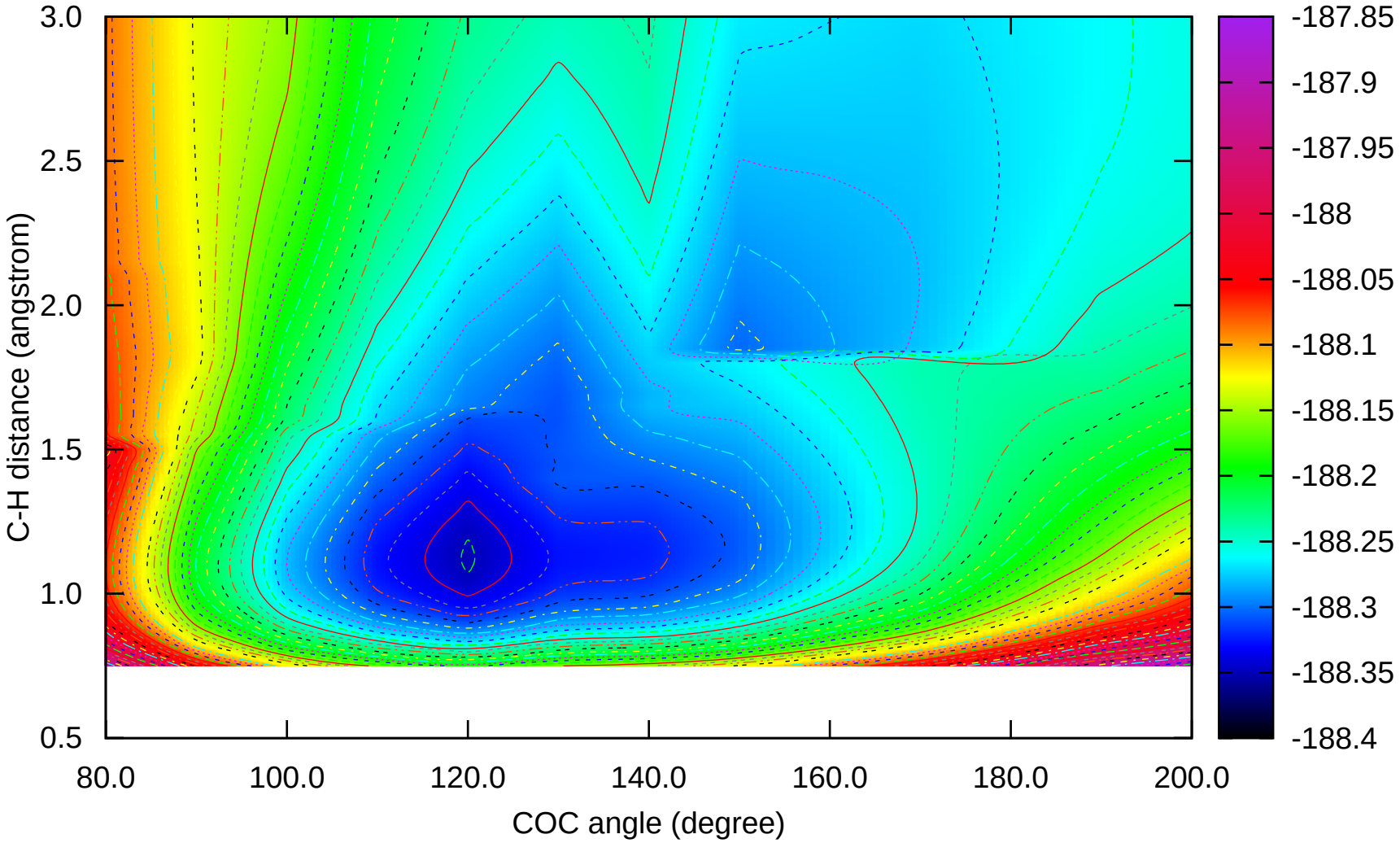
3.0
2.5
2.0
1.5
1.0
0.5
C-H distance (angstrom)
80.0
100.0
120.0
140.0
160.0
180.0
200.0
COC angle (degree)
-187.85
-187.9
-187.95
-188
-188.05
-188.1
-188.15
-188.2
-188.25
-188.3
-188.35
-188.4