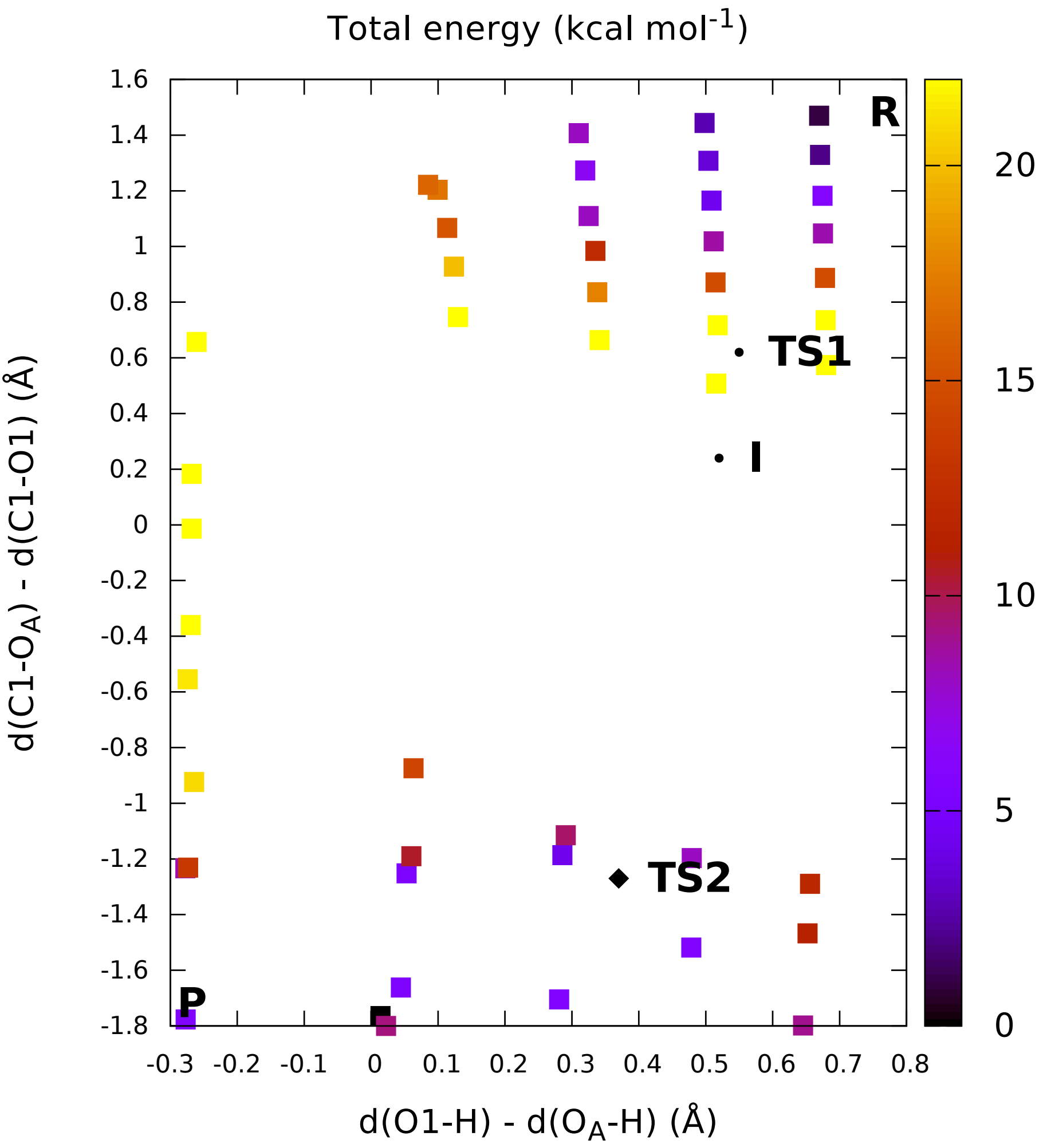
Total energy (kcal mol-1)
d(C1-OA) - d(C1-O1) (Å)
d(O1-H) - d(OA-H) (Å)
R
TS1
I
TS2
P
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-1.2
-1.4
-1.6
-1.8
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
20
15
10
5
0