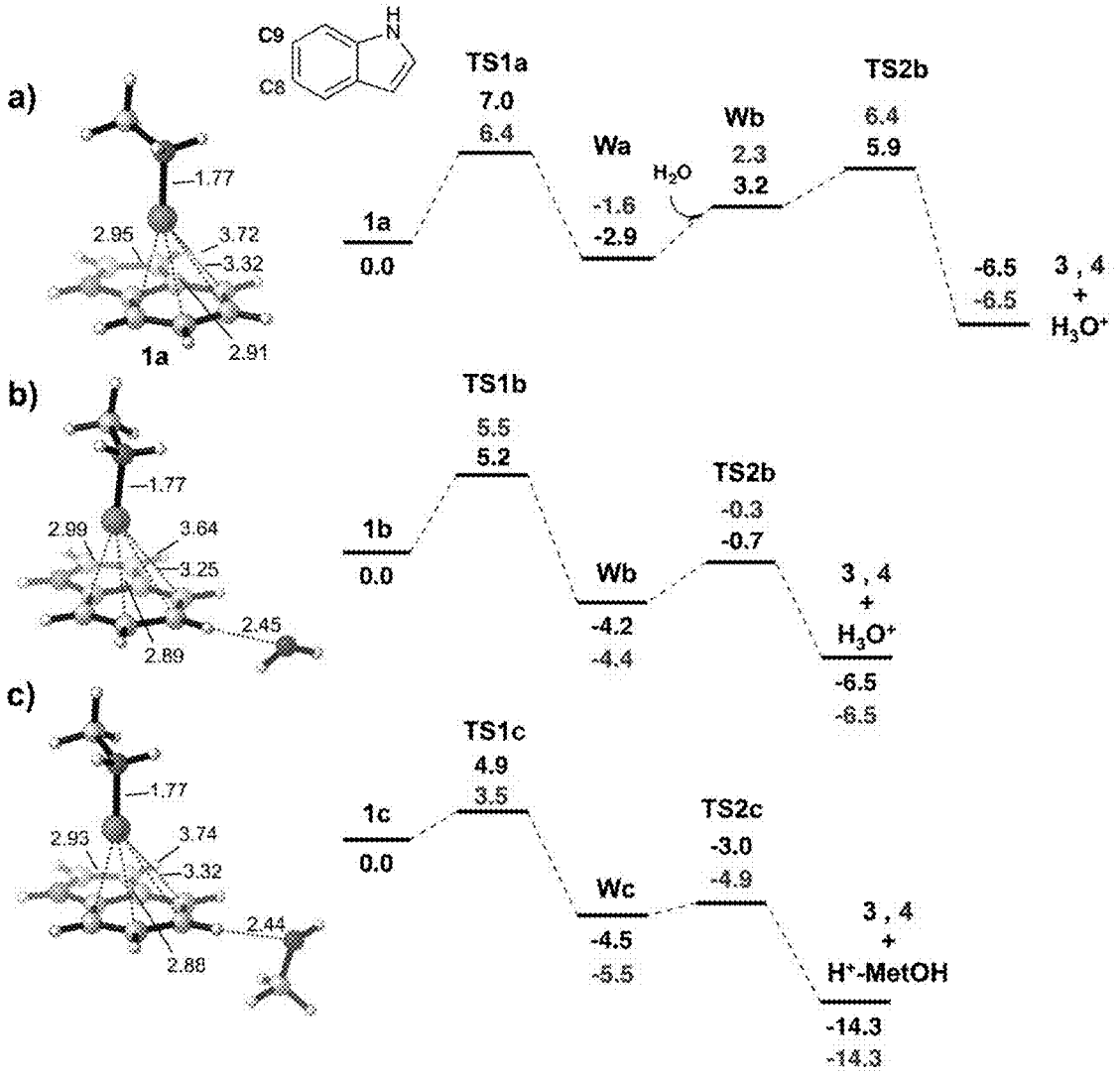
a)
C9
C8
H
N
1.77
2.95
3.72
3.32
2.91
1a
TS1a
7.0
6.4
1a
0.0
Wa
-1.6
-2.9
H2O
Wb
2.3
3.2
TS2b
6.4
5.9
-6.5
-6.5
3 , 4
+
H3O+
b)
1.77
2.99
3.64
3.25
2.45
2.89
TS1b
5.5
5.2
1b
0.0
Wb
-4.2
-4.4
TS2b
-0.3
-0.7
3 , 4
+
H3O+
-6.5
-6.5
c)
1.77
2.93
3.74
3.32
2.44
2.88
TS1c
4.9
3.5
1c
0.0
Wc
-4.5
-5.5
TS2c
-3.0
-4.9
3 , 4
+
H+-MetOH
-14.3
-14.3

Figure 21