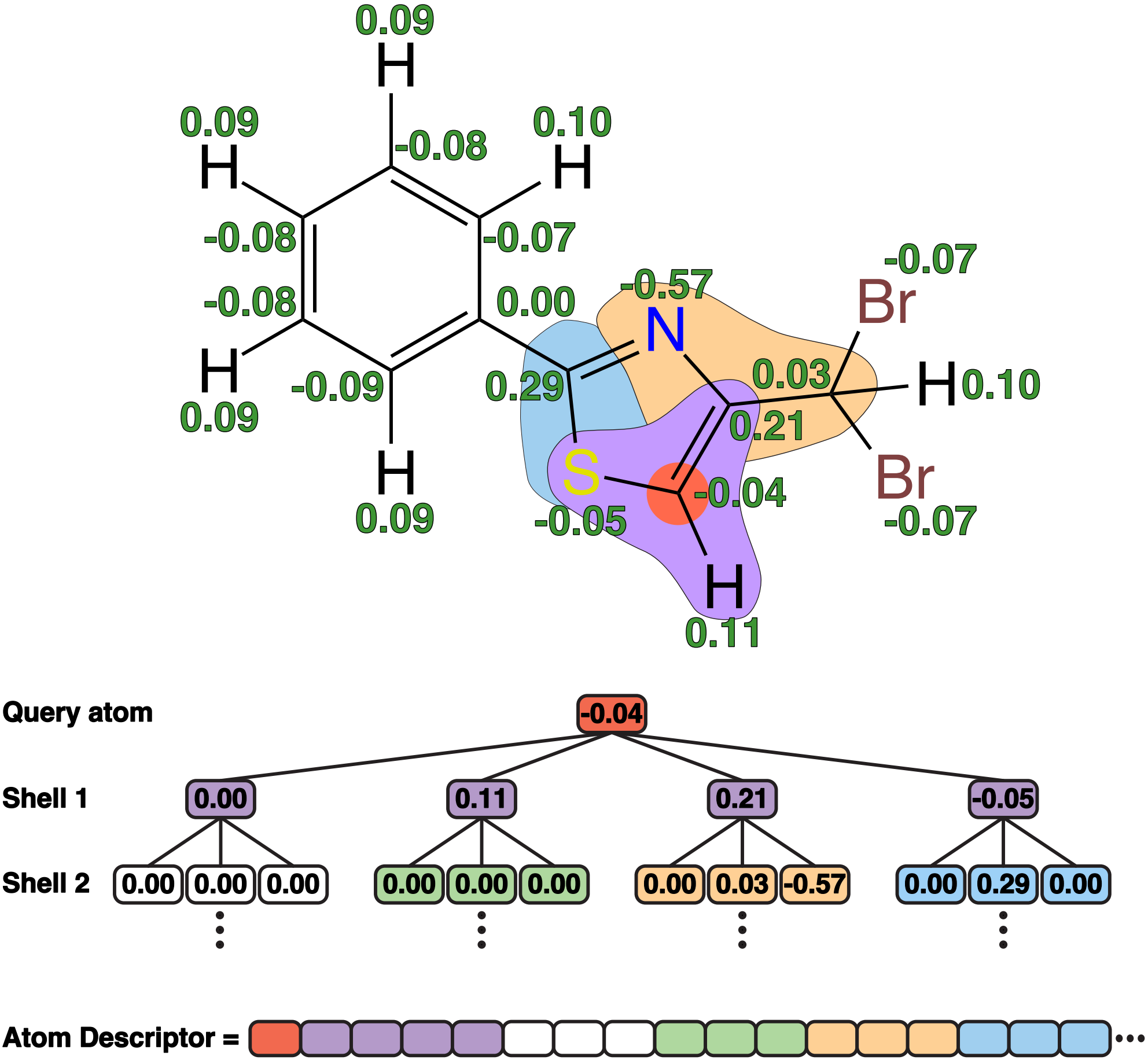
0.09
H
0.09
H
0.09
-0.08
0.10
H
-0.08
-0.07
-0.08
0.00
H
0.09
-0.09
0.29
-0.57
N
-0.07
Br
0.03
H
0.10
0.21
S
-0.04
Br
-0.07
-0.05
H
0.11
Query atom
-0.04
Shell 1
0.00
0.11
0.21
-0.05
Shell 2
0.00 0.00 0.00
0.00 0.00 0.00
0.00 0.03 -0.57
0.00 0.29 0.00
Atom Descriptor =