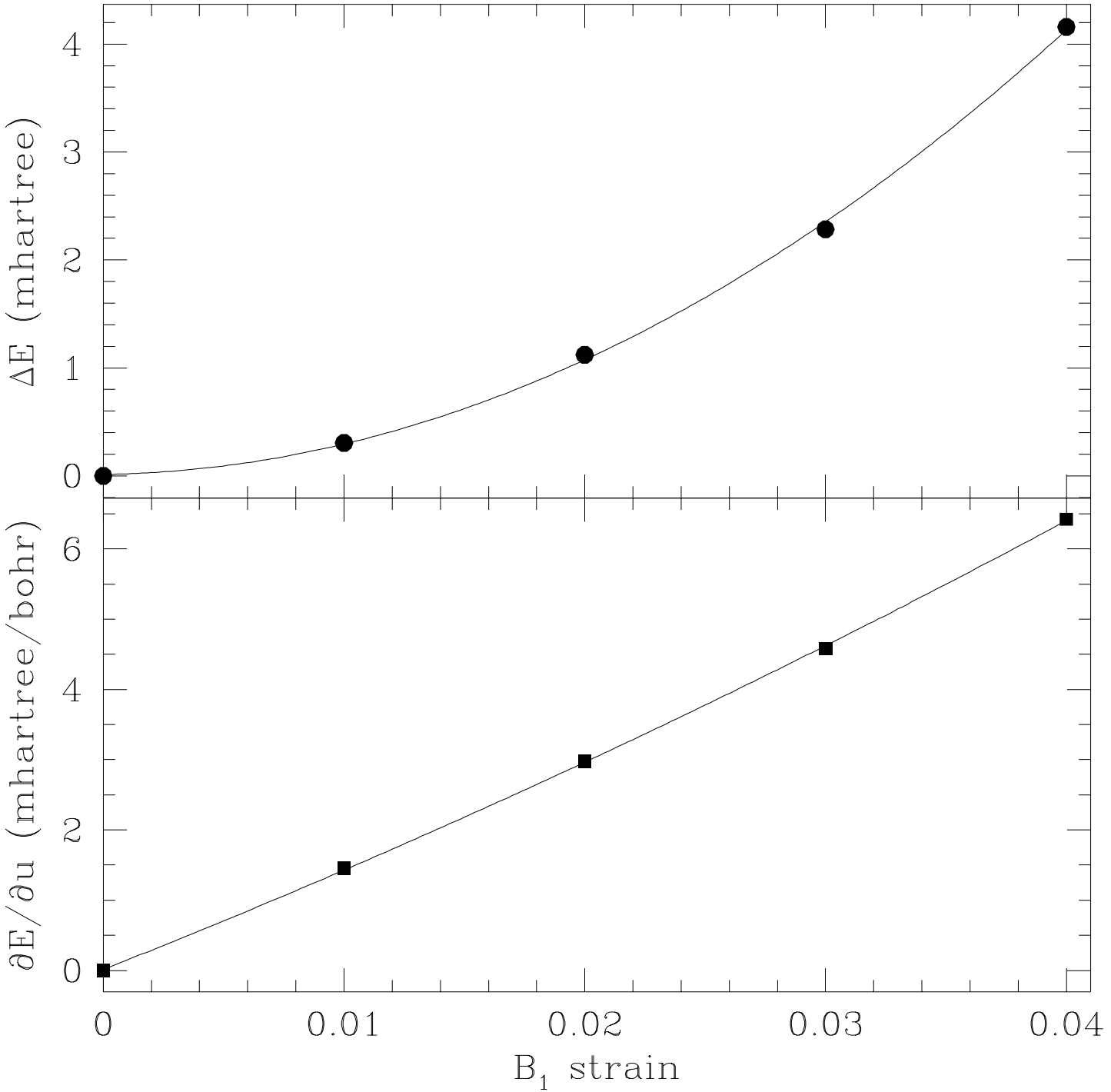
ΔE (mhartree)
0
1
2
3
4
∂E/∂u (mhartree/bohr)
0
2
4
6
0
0.01
0.02
0.03
0.04
B1 strain