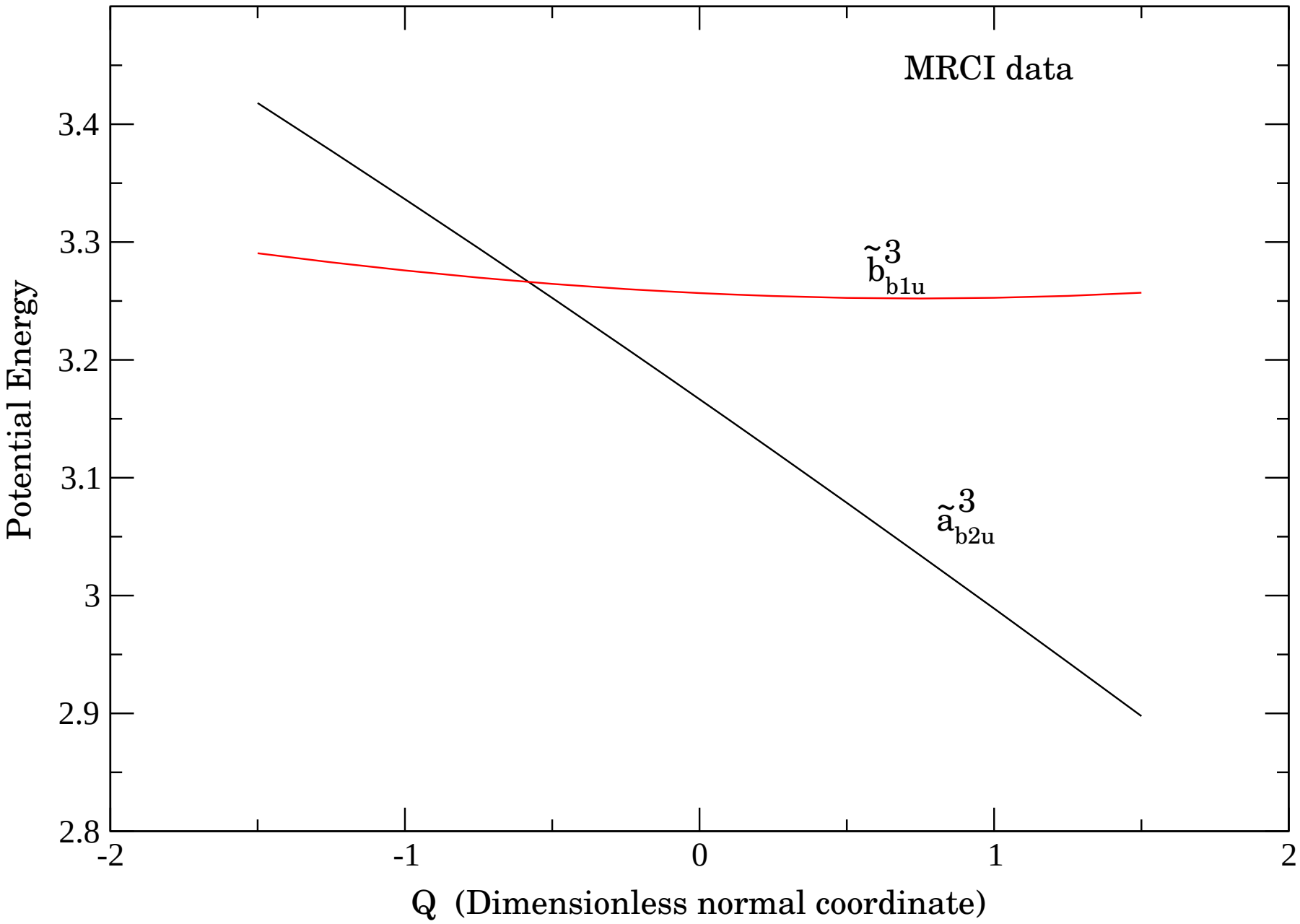

MRCI data
$\tilde{b}^3_{b1u}$
$\tilde{a}^3_{b2u}$
Potential Energy
3.4
3.3
3.2
3.1
3
2.9
2.8
-2
-1
0
1
2
Q (Dimensionless normal coordinate)