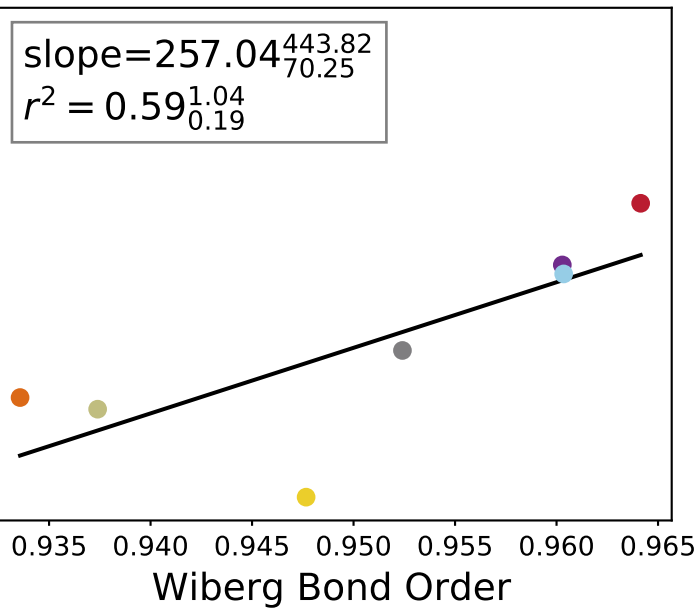


TIG2

Energy Barrier height (kJ/mol)

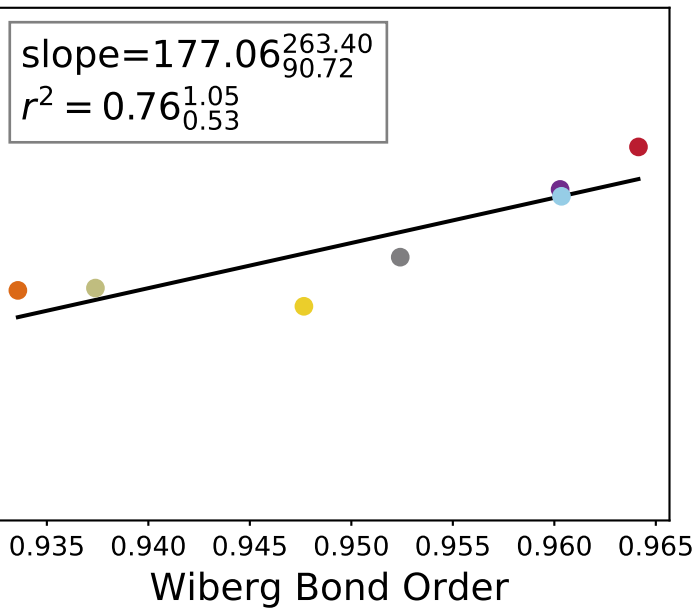
QM

slope=257.04^{443.82}_{70.25}
 $r^2 = 0.59$ ^{1.04}_{0.19}



Interpolated Fit

slope=177.06^{263.40}_{90.72}
 $r^2 = 0.76$ ^{1.05}_{0.53}



OpenFF v1.3.0

slope=-109.39^{-30.94}_{-187.83}
 $r^2 = 0.60$ ^{0.98}_{0.23}

