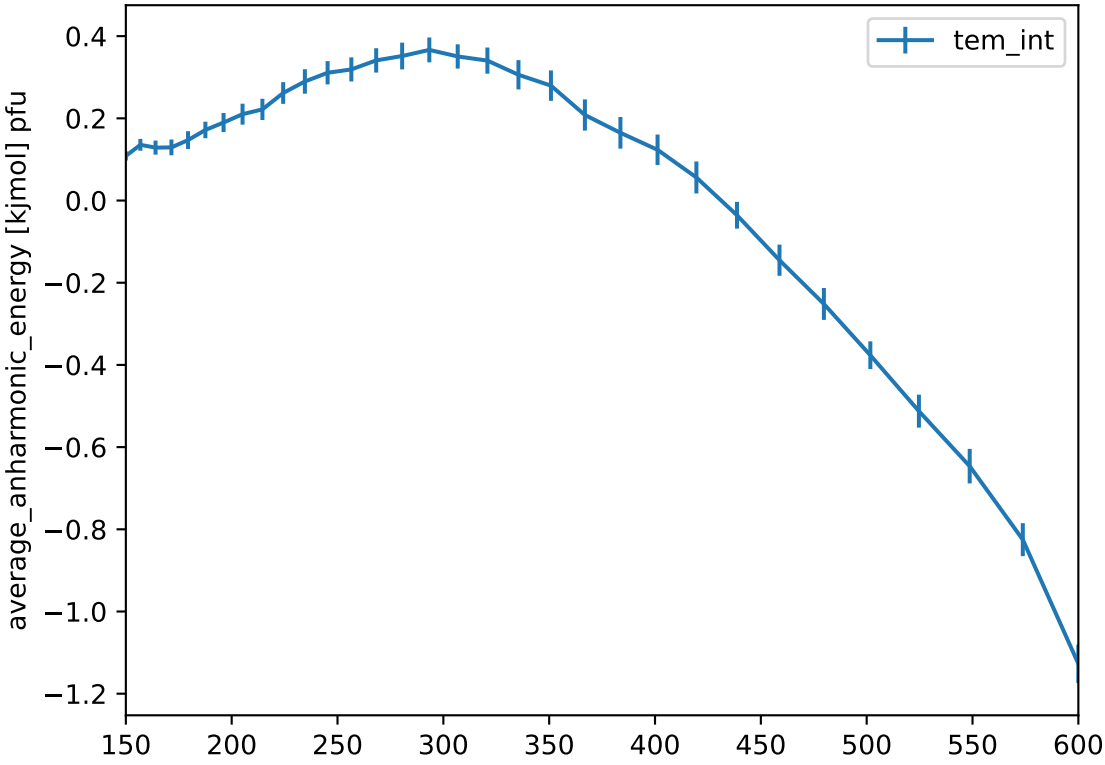
tem_int
average_anharmonic_energy [kjmol] pfu
0.4
0.2
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
−1.2
150
200
250
300
350
400
450
500
550
600