BeH₂ energy calculation with 2 e⁻ ccECP, single-det/2s-2p multi-det, no Tmoves -2.25-2.50Euergy -2.75 -3.00-3.252e⁻ ccECP T-moves -- 2e⁻ ccECP no T-moves -3.50200 400 600

Step numbers (proportional to walltime)