Forcefield = oplsaal constraint tolerance = 1.00e-04 8.7 ×10⁴ -5.12 ×10⁵ 8.65 -5.14 8.6 -5.16 Kinetic energy (kJ/mol) 8 27 27 28 29 8.5 -5.2 -5.24

-5.26

2000

4000

6000

8000

number of steps

10000

12000

16000

14000

8.35

2000

4000

6000

8000

number of steps

10000

12000

14000

16000