

Info: NONZERO IMPRECISION IN COULOMB MATRIX: 1.2E-21 (7) 2.25E-21 (7)

Info: Entering startup phase 8 with 35208 kB of memory in use.

Info: Finished startup with 35208 kB of memory in use.

TCL: Minimizing for 100 steps

PRESSURE: 0 0 0 0 0 0 0 0 0 0

GPRESSURE: 0 0 0 0 0 0 0 0 0 0

ETITLE:	TS ELECT TOTAL	BOND VDW TEMP	ANGLE BOUNDARY TOTAL2	DIHED MISC TOTAL3	IMPRP KINETIC TEMPAV
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G					
ENERGY:	0	1913.4792	3008.0536	358.3486	10.7302
	-18281.1014	5217.3380	0.0000	0.0000	0.0000
	-7773.1518	0.0000	-7773.1518	-7773.1518	0.0000

0

INITIAL STEP: 1e-06

GRADIENT TOLERANCE: 15332.5

PRESSURE: 1 0 0 0 0 0 0 0 0 0

GPRESSURE: 1 0 0 0 0 0 0 0 0 0