

Using ewald, boxsize = 83.66 x 83.66 x 41.83 A, (X x Y x Z)
 Here is what I use :

```
pair_style lj/cut/coul/long 3.3 40.0
dielectric 78.0
#pair_coeff type1 type2 epsilon sigma rcut
pair_coeff * * 1 3 3.3
kpace_style ewald 1.0e-4
kpace_modify slab 3.0
```

Correct value of Madelung constant : -1.957

| | | New version (27 Jan 2013) | | Old version (5 th September 2010) | |
|---------|----------|---------------------------|-------------------|--|-------------------|
| Rcutoff | Accuracy | E_total (kcal/mol) | Madelung Constant | E_total (kcal/mol) | Madelung Constant |
| 10 | 1e-4 | 1161.7421 | -6.63425 | 1400.0914 | -1.95000 |
| | 1e-6 | 1359.2137 | -2.75336 | 1400.0957 | -1.94490 |
| | 1e-8 | 1399.9864 | -1.95205 | 1400.0957 | -1.94490 |
| | 1e-12 | 1400.0958 | -1.94995 | 1400.0957 | -1.94490 |
| 40 | 1e-4 | 1340.1663 | -3.12770 | 1400.0894 | -1.95003 |
| | 1e-6 | 1423.4048 | -1.49181 | 1400.0957 | -1.94490 |
| | 1e-8 | 1399.9750 | -1.95228 | 1400.0958 | -1.94491 |
| | 1e-12 | 1400.0958 | -1.94995 | 1400.0958 | -1.94991 |
| 80 | 1e-4 | 1400.2481 | -1.94691 | 1400.1059 | -1.94854 |
| | 1e-6 | 1383.9974 | -2.26628 | 1400.0959 | -1.94990 |
| | 1e-8 | 1400.5308 | -1.94135 | 1400.0958 | -1.94990 |
| | 1e-12 | 1400.0958 | -1.94995 | 1400.0957 | -1.94990 |