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LAMMPS data file. CGCMM style. atom_style charge generated by VMD/TopoTools v1.5 on
Thu Oct 15 16:26:32 +0800 2015
 76 atoms
 0 bonds
 0 angles
 0 dihedrals
 0 impropers
 3 atom types
 0 bond types
 0 angle types
 0 dihedral types
 0 improper types
 -1.409680 14.028220  xlo xhi
 0.195764 15.633664  ylo yhi
 0.018574 15.456474  zlo zhi

# Pair Coeffs
#
# 1  C
# 2  H
# 3  O

 Masses

 1 12.011000 # C
 2 1.008000 # H
 3 15.999000 # O

 Atoms

1 1 0.000000 8.816114 6.592156 5.036654 # C
2 1 0.000000 7.548607 6.979781 5.526767 # C
3 1 0.000000 7.131384 8.322307 5.411195 # C
4 1 0.000000 7.975259 9.278990 4.805583 # C
5 1 -0.127000 9.223746 8.858491 4.302831 # C
6 1 -0.127000 9.631163 7.559935 4.418040 # C
7 1 -0.127000 7.578664 10.626180 4.780387 # C
8 1 -0.127000 6.393869 11.022928 5.339705 # C
9 1 0.000000 5.484379 10.076526 5.875604 # C
10 1 0.000000 5.880890 8.723223 5.931580 # C
11 1 -0.127000 9.221865 5.253270 5.187848 # C
12 1 -0.127000 8.425649 4.341981 5.823139 # C
13 1 0.000000 7.166091 4.707626 6.335305 # C
14 1 0.000000 6.712070 6.032385 6.159105 # C
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15 1 0.000000 5.031409 7.770081 6.536748 # C
16 1 0.000000 5.449476 6.426739 6.654092 # C
17 1 0.000000 4.621198 5.483862 7.300367 # C
18 1 -0.127000 5.096775 4.176940 7.494007 # C
19 1 -0.127000 6.345479 3.822850 7.068540 # C
20 1 0.000000 3.781863 8.165652 7.063081 # C
21 1 -0.127000 3.401107 9.515493 6.962528 # C
22 1 -0.127000 4.228094 10.442021 6.392255 # C
23 1 -0.127000 2.968752 7.201967 7.693543 # C
24 1 -0.127000 3.376124 5.905121 7.811264 # C
25 2 0.127000 9.870119 9.602119 3.827235 # H
26 2 0.127000 10.605690 7.248969 4.029348 # H
27 2 0.127000 8.247416 11.388974 4.372128 # H
28 3 0.127000 6.118980 12.346618 5.388833 # O
29 2 0.127000 10.192131 4.951503 4.782595 # H
30 2 0.127000 8.791372 3.309713 5.900224 # H
31 2 0.127000 4.506446 3.458197 8.069557 # H
32 3 0.127000 6.826916 2.603186 7.461350 # O
33 2 0.127000 2.440674 9.821197 7.386900 # H
34 2 0.127000 3.897490 11.485461 6.343766 # H
35 2 0.127000 2.018219 7.525242 8.127917 # H
36 2 0.127000 2.755759 5.174070 8.338054 # H
37 2 0.000000 7.719883 2.492691 7.079508 # H
38 2 0.000000 5.500148 12.511350 6.135300 # H
39 1 0.000000 8.834976 7.332720 8.440724 # C
40 1 0.000000 7.590015 7.763093 8.950150 # C
41 1 0.000000 7.202785 9.114731 8.815551 # C
42 1 0.000000 8.058242 10.031225 8.168689 # C
43 1 -0.127000 9.289097 9.572646 7.656411 # C
44 1 -0.127000 9.666351 8.268007 7.791873 # C
45 1 -0.127000 7.623318 11.356324 7.992661 # C
46 1 -0.127000 6.391566 11.756481 8.430341 # C
47 1 0.000000 5.529222 10.882076 9.124656 # C
48 1 0.000000 5.946685 9.545847 9.298230 # C
49 1 -0.127000 9.195882 5.980633 8.586492 # C
50 1 -0.127000 8.349195 5.082072 9.174430 # C
51 1 0.000000 7.088026 5.478569 9.655912 # C
52 1 0.000000 6.717595 6.838212 9.566588 # C
53 1 0.000000 5.083176 8.623839 9.930537 # C
54 1 0.000000 5.472241 7.274641 10.070292 # C
55 1 0.000000 4.607718 6.347547 10.691835 # C
56 1 -0.127000 4.978962 4.993517 10.746477 # C
57 1 -0.127000 6.157326 4.556283 10.201104 # C
58 1 0.000000 3.819866 9.048127 10.400847 # C

59 1 -0.127000 3.444711 10.394698 10.227070 # C
60 1 -0.127000 4.269968 11.288432 9.604073 # C
61 1 -0.127000 2.979531 8.105202 11.024818 # C
62 1 -0.127000 3.362257 6.801872 11.172217 # C
63 2 0.127000 9.928199 10.281145 7.120571 # H
64 2 0.127000 10.611592 7.918743 7.365519 # H
65 2 0.127000 8.252210 12.048687 7.419717 # H
66 3 0.127000 5.894666 13.001162 8.150336 # O
67 2 0.127000 10.163731 5.654319 8.194722 # H
68 2 0.127000 8.651869 4.035794 9.285340 # H
69 2 0.127000 4.294720 4.251363 11.167252 # H
70 3 0.127000 6.406776 3.226411 10.191367 # O
71 2 0.127000 2.468952 10.715658 10.604493 # H
72 2 0.127000 3.970367 12.329521 9.462948 # H
73 2 0.127000 2.006947 8.441650 11.397038 # H
74 2 0.127000 2.697562 6.080338 11.657249 # H
75 2 0.000000 6.800632 2.965292 9.322617 # H
76 2 0.000000 6.614929 13.526241 7.750869 # H