Simulação do CO_2 - Topologia

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LAMMPS Description

         3 atoms
         2 bonds
         1 angles

           2 atom types
           1 bond types
           1 angle types

           0.0   4.900  xlo xhi
           0.0   4.900  ylo yhi
           0.0   4.900  zlo zhi

 Masses

           1   12.01100
           2   15.99900

 Pair Coeffs

           1  5.589912416020577E-002   2.75699996948242        10.00000
           2  0.159986883525221        3.03299999237061        10.00000

 Bond Coeffs

           1        1284.6   1.149000

 Angle Coeffs

           1   147.8400       180.0000

 Atoms

    1    1    1   0.65120   1.14900   0.00000   0.00000
    2    2    2   -0.3256   2.29800   0.00000   0.00000
    3    3    2   -0.3256   0.00000   0.00000   0.00000

 Bonds

    1    1    1  2
    2    1    1  3

 Angles

    1    1   3  1  2
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