621/E2

Computer simulation study of structure and stability of CO_2-N_2 dimers

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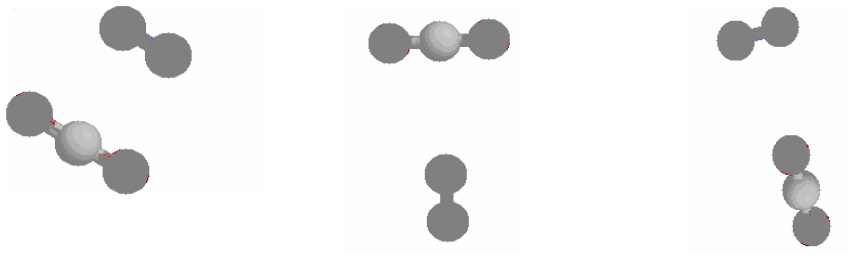
CO_2-N_2 dimers have been investigated using the realistic pair potential. Lennard-Jones potential was used to represent the attractive forces and repulsive forces while electrostatic interaction was taken into account through quadrupole - quardupole interactions. We first confirmed our simulation method by modeling the N_2-N_2 and CO_2-CO_2 neat dimers with comparison of the results with literature. Potential parameters for CO_2-N_2 dimer was generated by using the Lorentz-Berthelot (LB) mixing rules.
Three stable dimer structures have been obtained for the nitrogen-carbon dioxide dimer in excellent agreement with the dimer configurations obtained in the experimental Infrared spectroscopy. Two T-shaped structures and canted parallel structures are the observed configurations as given in the following Figure. The energies and equilibrium bond distances of these three configurations are reported. Since in our study, we used the realistic potential rather a non-realistic potential and the three structures obtained are similar to the experimentally observed structures, we report that the realistic pair potential we used in this calculation is more suitable to model the N_2-CO_2 system for further simulation studies.



a) b) c)

Figure. Three lowest energy structures of CO_2-N_2 dimers. **(a)** canted-parallel structure, **(b)** T-shaped 1 structure (N pointing to C in CO_2 molecule), **(c)** T-shape 2 structure (O pointing to the center of N_2 molecule)

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