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Abstract:	The interaction of different rare gas dimers (He2, Ne2, Ar2 and Kr2) in the confines of a carbon nanotube, along the tube axis and perpendicular to it, is examined using the density functional theoretic method, with the M05-2X functional and the 6-311++G**basis set. The equilibrium internuclear distance between the rare gas atoms is found to be reduced inside the tube, when the dimer is oriented perpendicular to the tube axis. The electron density at the bond critical point between the rare gas atoms is increased when compared to that in the isolated dimer.
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