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Structures and spin states of small Rhodium clusters OLGA RUIZ, TUNNA BARUAH, University of Texas at El Paso — We use density functional theory to investigate the geometrical structures and spin ordering in small clusters of Rh in the size range 7-10. The calculations are performed at the all-electron level using a linear combination of atomic orbital approach. The exchange-correlation effects are treated using the generalized gradient approximation. The Gaussian basis set contains 56 basis functions per atom. For each cluster size, several isomers were studied and for each isomer all the possible ferromagnetic and anti-ferromagnetic spin orderings were studied. We find that in several isomers, the anti-ferromagnetic spin orders are competitive in energy to the ferromagnetic one.The structures, binding energies, spin magnetic moments and spin orderings of the ground and low-lying states will be presented.

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