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Ni_4 clusters. Spectra in solid xenon and quantum-chemical calculations

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Abstract

The matrix spectra of system Ni_n have been studied and structures of Ni_4 clusters have been computed by quantum-chemical methods. It was showed that Ni_4 is a structurally flexible system regarding shifting of the fourth Ni atom into the area of Ni_3 rigid triangle. Electron transitions of two Ni_4 main isomers have been calculated and it was showed that the transition observed in the IR-spectrum is in agreement with the calculations.