The structure of small platinum clusters

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Using molecular dynamics and thermal quenching simulation techniques, we have studied the global minima and energetics of free Pt clusters in the size range of N=22−56. The Voter and Chen version of an embedded−atom model, derived by fitting to experimental data of both the diatomic molecule and bulk platinum simultaneously, has been employed in the study. The results show that the predicted global minima are based on octahedral, decahedral and icosahedral structures. Some of the icosahedral global minima do not have a central atom. The 54 atom icosahedron without a central atom is found to be more stable than the 55−atom complete icosahedron.

References

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