

Theoretical study of the protonation of $[Pt_3(L)_3(L^+)_3]$ ($L = CO, SO_2, CNH; L^+ = PH_3, CNH$)

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Ab initio calculations suggest that a series of clusters of the $[Pt_3(L)_3(L^+)_3(H)]^+$ type ($L = CO, SO_2, CNH; L^+ = PH_3, CNH$) are stable. We have studied these clusters at the HF, MP2, B3LYP, PBE and TPSS theory levels. The magnitude of the interaction energies and distances indicates a substantial covalent character of the Pt-H bond, confirmed by orbital diagrams. In addition, the Fukui index of electrophilic attack and electrophilicity index on the unprotonated clusters were used to explore possible sites where chemical reactivity may play a role. © 2011 Elsevier B.V. All rights reserved.