Combined computational, multiple-NMR and IR study of new phenylplatinum complexes containing monodentate silsesquioxane

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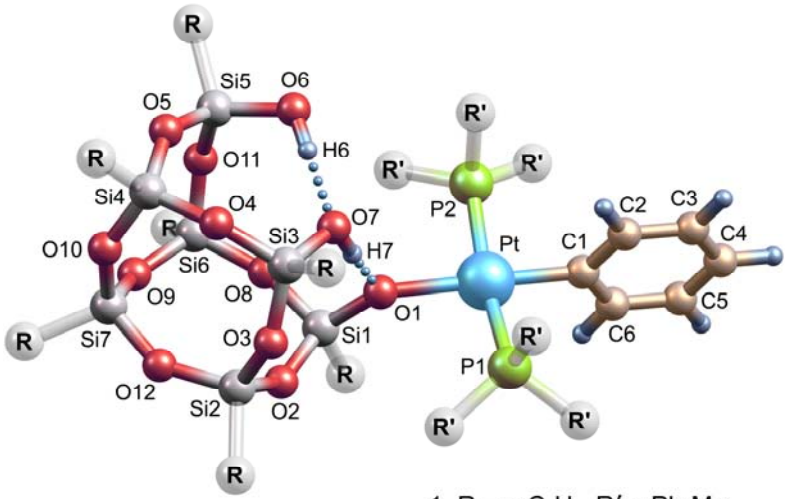
Silsesquioxanes are organosilanol compounds possessing –O–Si–O– bonds network and organic group attached to each Si atom. Incompletely condensed silsesquioxanes containing from one to four free silanol groups, Si–OH and their metal complexes are regarded as a molecular models of silica and metal silica supported catalysts.

The structure and spectroscopic properties of new synthesized platinum-silsesquioxane complex, *trans*-[Pt{$O_{10}Si_7$(*cyclo*-C_5H_9)$_7$$(OH)_2$}(Ph)$(PPh_2Me)_2$], 1 are characterized on the basis of computational, and multinuclear NMR (^{1}H, ^{13}C, ^{29}Si, ^{31}P) and IR data. Methodological DFT studies for reliable prediction of geometrical parameters, NMR chemical shifts and IR spectrum were performed for the complex *trans*-[Pt{$O_{10}Si_7$*(cyclo*-C_5H_9)$_7$$(OH)_2$}(Ph)$(PEt_3)_2$], reported in [1]. Density Functional Theory method at OPW91/6-31G(d) (6-31G(d,p)) level and small effective core potential (SDD) for Pt atom was found to be sufficient for obtaining accurate structural data, NMR and IR spectra in relatively reasonable CPU time. The theoretical approach could be further applied for better understanding of the structure and the properties of new platinum complexes of silsesquioxane.



1, R = *c*-C_5H_9, R′ = Ph_2Me
2, R = *c*-C_5H_9, R′ = Et_3

1. N. Mintcheva, M. Tanabe, K. Osakada, *Organometallics* 25 (2006) 3776.