

Si···H interligand interactions in cobalt(V) and iridium(V) bis(silyl)bis(hydride) complexes

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A series of bis(silyl)bis(hydride) cobalt complexes $\text{Cp}^*\text{Co}(\text{H})_2(\text{SiR}_3)_2$, ($\text{SiR}_3 = \text{SiPh}_2\text{H}$, SiMe_3 , SiH_3 , SiF_3 , SiCl_3 , SiBr_3 , $\text{Si}(\text{CF}_3)_3$; **Co1–Co7**) as well as the analogous iridium complexes $\text{Cp}^*\text{Ir}(\text{H})_2(\text{SiR}_3)_2$ ($\text{SiR}_3 = \text{SiEt}_3$, SiMe_3 , SiH_3 , SiF_3 , SiCl_3 , SiBr_3 , $\text{Si}(\text{CF}_3)_3$; **Ir1–Ir7**) were studied to detect possible residual Si···H interactions.

Tests of several density functionals by comparison with coupled-clusters results indicate that the TPSSH functional perform better than B3LYP, BP86, M06, M06L, and PBEPBE.

Based on molecular structures, as well as Wiberg bond indices and $J(\text{Si–H})$ spin-spin coupling constants as indicators of a possible Si···H interaction, at least two residual Si···H interaction in **Co2**, **Co5**, and all four possible Si···H interactions in **Co3**, **Co4** have been detected. **Co6** and **Co7** exhibit stronger Si···H bonding than the other complexes studied.

On the contrary, the iridium complexes **Ir1–Ir3**, **Ir5–Ir7** are classical iridium(V) bis(silyl) bis(hydride) complexes with only rudimentary Si···H interactions, if any.

