Unconventional Distribution of Hydrides in Hydrido Rhenium Carbonyl Clusters

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We have recently shown that coupling stereochemical considerations to potential energy (PE) calculations it is possible to retrieve hydrides locations in hydrido carbonyl clusters as large as $[H_{6-x}Os_{10}(CO)_{24}]^{x-}$ (x = 1,2). [1] However, when the ratio between the number of hydrides and that of carbonyls increases, such as in $[H_{7-x}Re_5(CO)_{15}]^{x-}$ (x = 1,2) and $[H_7Re_5(CO)_{15}]^{2-}$, the 'empty' space to be 'filled' with the hydrides becomes more evenly distributed about the cluster surface and the localisation of the hydrido ligands becomes more elusive thus requiring additional theoretical tools.

[1] Beringhelli T., Cariati E., Dragonetti C., Galli S., Lucenti E., Roberto D., Sironi A., Ugo R., *Inorg. Chim. Acta*, 2003, **354**, 79-89.

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