Dihydrogen Complexes of Rhodium: $[RhH_2(H_2)_x(PR_3)_2]^+$ (R = Cy, ^iPr,; x = 1, 2)

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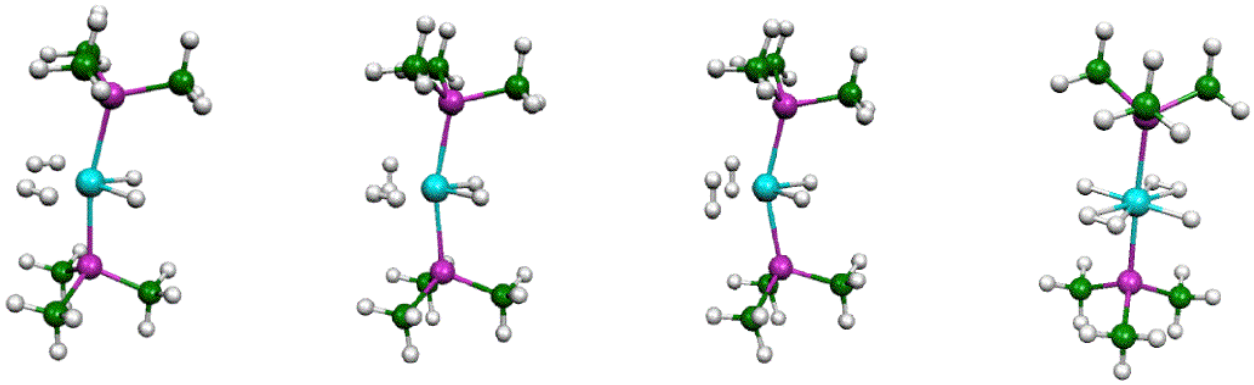
SUPPORTING INFORMATION

DFT CALCULATED STRUCTURES FOR $[RhH_6(PMe_3)_2]^+$

DFT (B3LYP/DZVP) Calculated structures for $[RhH_6(PMe_3)_2]^+$



A B C D

Relative Energies ($kcalmol^{-1}$) and selected bond distances and angles:

	A	**B**	**C**	**D**
Relative Energy ($kcal\ mol^{-1}$)	+0.3	0	+0.1	+27.2
Rh-P (Å)	2.399, 2.398	2.400, 2.400	2.403, 2.401	2.403, 2.403
Rh-H (Å)	1.557, 1.558	1.554, 1.557	155.1, 155.4	1.664, 1.657
H-H	0.771, 0.772	0.769, 0.773	0.771, 0.773	0.852, 0.852
P-Rh-P	167.3	164.9	163.7	177.7