

C–H \cdots H–Fe Dihydrogen Bonding: Synthesis and Structure of *trans*-[FeH(NCS(*i*-Pr)-S)(dppe)₂]I (dppe = Ph₂PCH₂CH₂PPh₂)

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Compound *trans*-[FeH(NCS)(dppe)₂] (1) reacted with isopropyl iodide (*i*-PrI) to give an Fe(II)-organic isothiocyanide complex, *trans*-[FeH(NCS(*i*-Pr)-S)(dppe)₂]I (2). Compound 2 was structurally characterized, in which the hydride ligand appears to be involved in the “dihydrogen” bonding, M–H \cdots H–C. Crystallographic data for 2: monoclinic space group $P2_1/n$, $a = 13.490(2)$ Å, $b = 17.269(3)$ Å, $c = 21.384(3)$ Å, $\beta = 90.682(7)^\circ$, $Z = 4$, $R(wR_2) = 0.0348(0.0894)$.

