Bimetallic Lanthanide and Actinide Metallocene Hydrides

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Structure	HOMO-LUMO Gap (eV)
Anion	+0.74691
Neutral Singlet	+4.29684
Neutral Triplet	-2.38537
Neutral Closed	+4.29805
Structure	Y-Y Distance (pm)
Neutral	354.55
Neutral Exp	352
Anion	347.19
Anion Exp	346



84a α (-0.555 eV)



83a α (-1.302 eV)