Trinuclear Alkyl Hydrido Rare-Earth Complexes Supported by Amidopyridinato Ligands: Synthesis, Structures, C-Si Bond Activation and Catalytic Activity in Ethylene Polymerization

Dmitry M. Lyubov, Anton V. Cherkasov, Georgy K. Fukin, Sergey Yu. Ketkov, Andrey S. Shavyrin, Alexander A. Trifonov*

Electron Supporting Information

Fig. SI1. ^{1}H NMR spectrum of **1Lu** (400 MHz, C_6D_6, 293 K).

Fig. SI2. ^{13}C{^{1}H} NMR spectrum of **1Lu** (400 MHz, C_6D_6, 293 K).

Fig. SI3. ^{1}H NMR spectrum of **2Lu** (400 MHz, C_6D_6, 293 K).

Fig. SI4. ^{13}C{^{1}H} NMR spectrum of **2Lu** (400 MHz, C_6D_6, 293 K).

Fig. SI5. 2D NOESY spectrum of **2Lu** (400 MHz, C_7D_8, 293 K).

Fig. SI6. Variable-temperature ^{1}H NMR spectra of **2Lu** (400 MHz, C_7D_8).

Fig. SI7. 2D ^{89}Y-^{1}H HMQC NMR spectrum of **3Y** showing ^{89}Y-^{1}H spin-spin interactions (400 MHz, C_6D_6, 293 K).

Fig. SI8. Fragment of 2D ^{89}Y-^{1}H (GE) HMQC long range interactions spectrum of **3Y** (400 MHz, C_6D_6, 293 K).

Fig. SI9. Contour map of the **3Y** HOMO-4 orbital (0.002-0.01 a.u., step 0.002 a.u.) in the H(2)H(4)H(5) plane. The red and green lines correspond to the positive and negative values of the wavefunction, respectively.
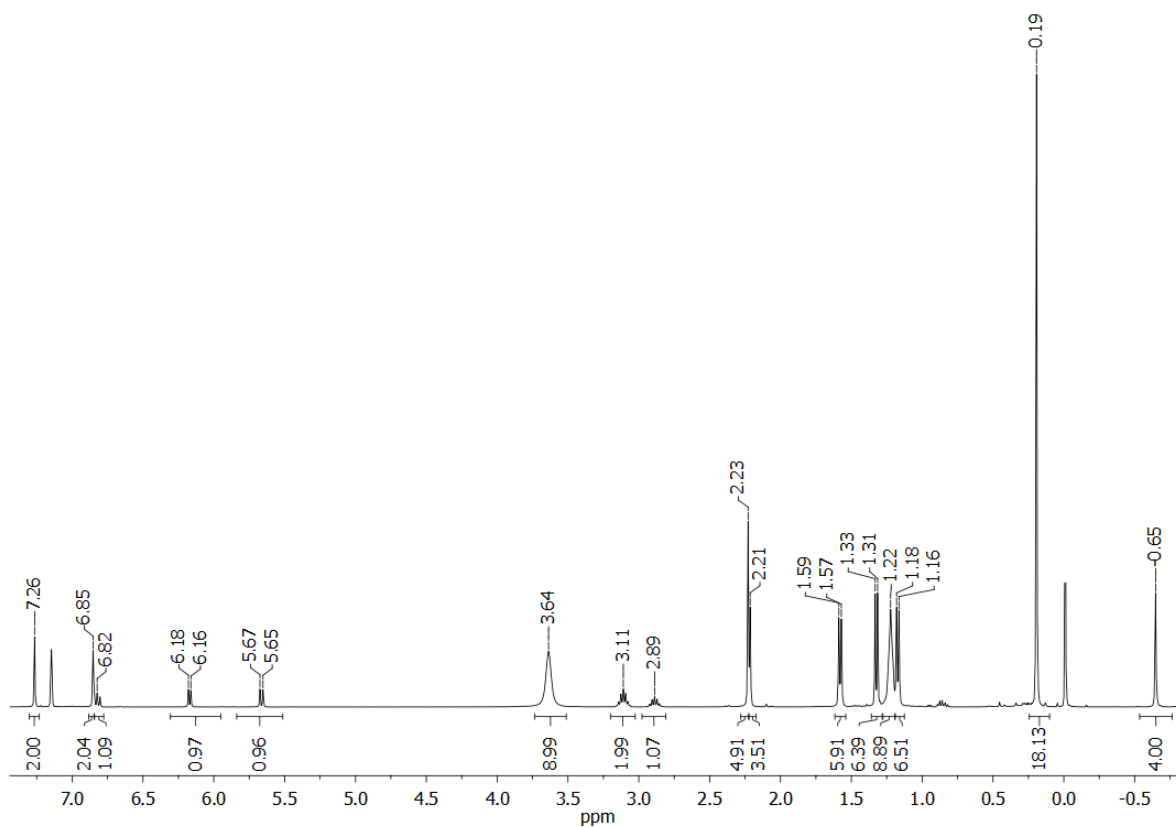
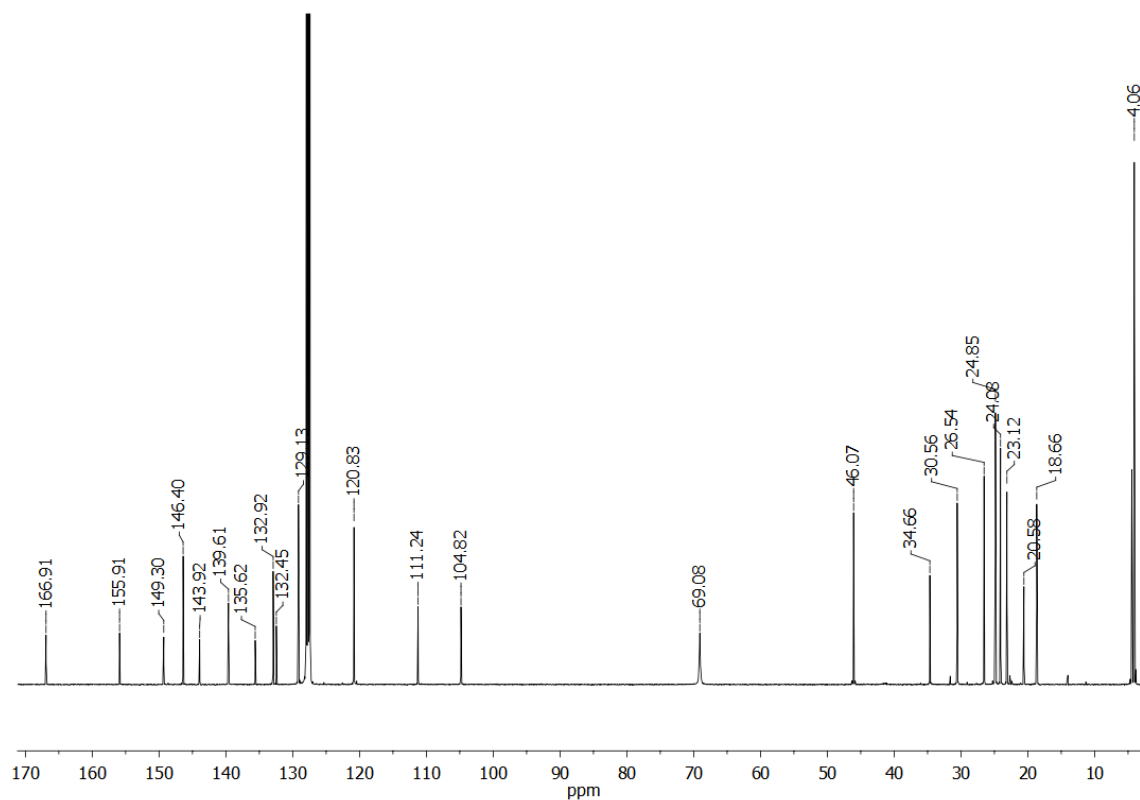**Fig. SI1.** ^{1}H NMR spectrum of **1Lu** (400 MHz, C$_6$D$_6$, 293 K).

Fig. SI2. ^{13}C{^{1}H} NMR spectrum of **1Lu** (400 MHz, C$_6$D$_6$, 293 K).
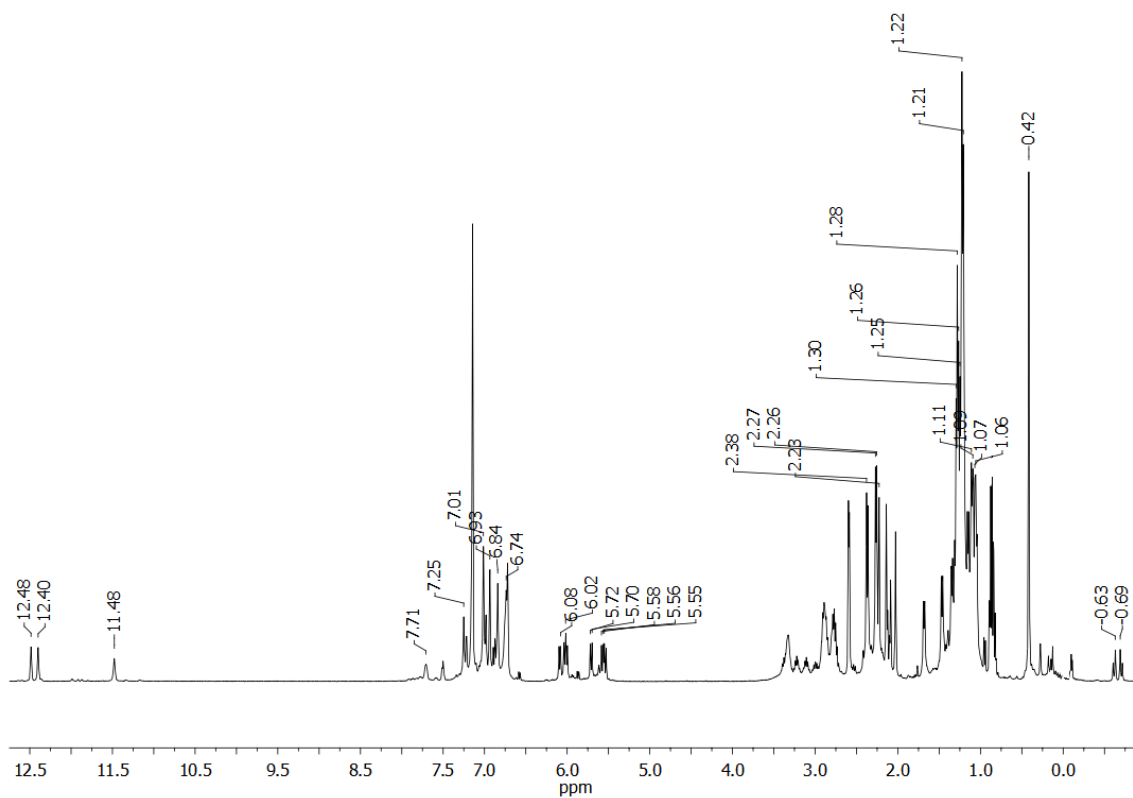
Fig. SI3. ¹H NMR spectrum of **2Lu** (400 MHz, C$_6$D$_6$, 293 K).

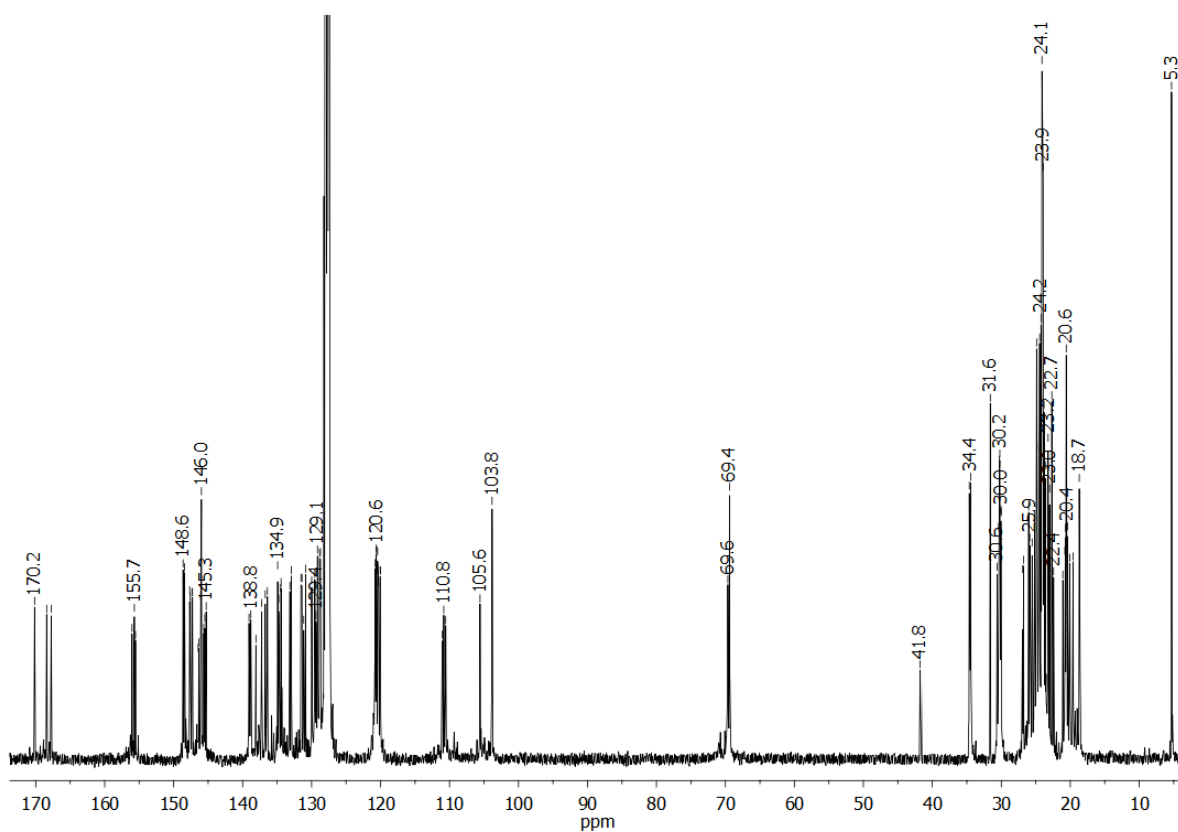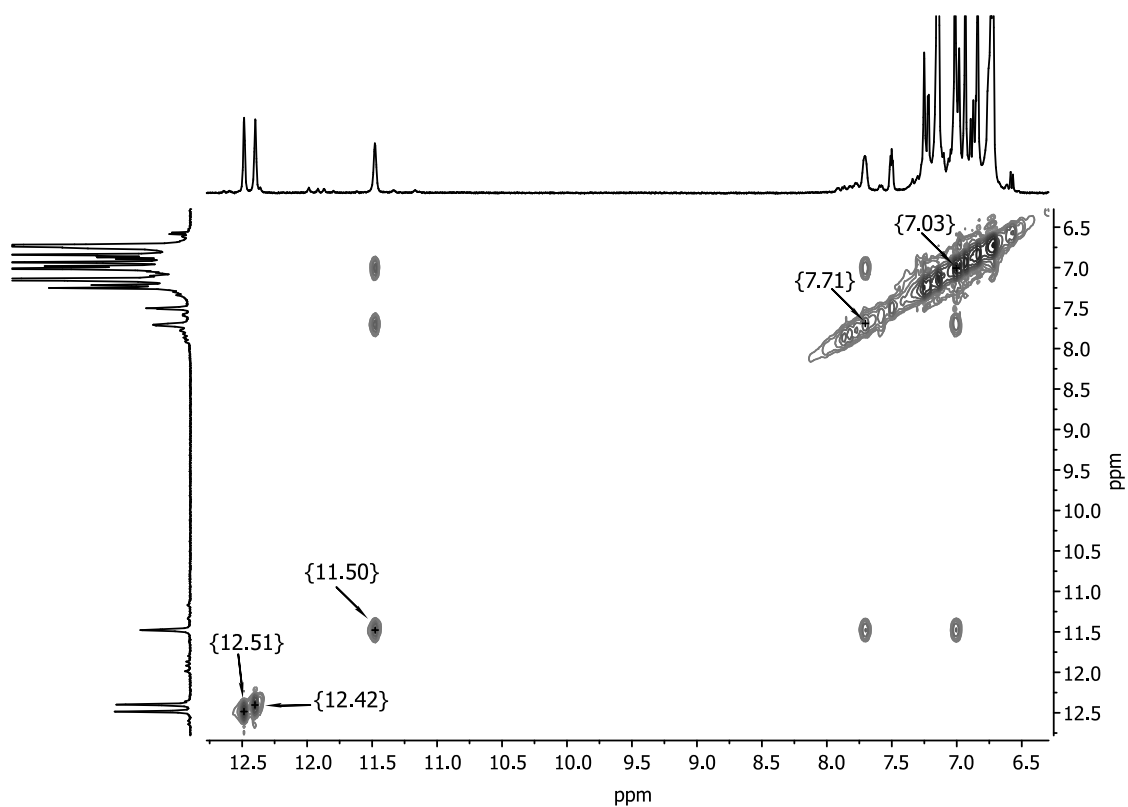**Fig. SI4.** ¹³C{¹H} NMR spectrum of **2Lu** (400 MHz, C$_6$D$_6$, 293 K).

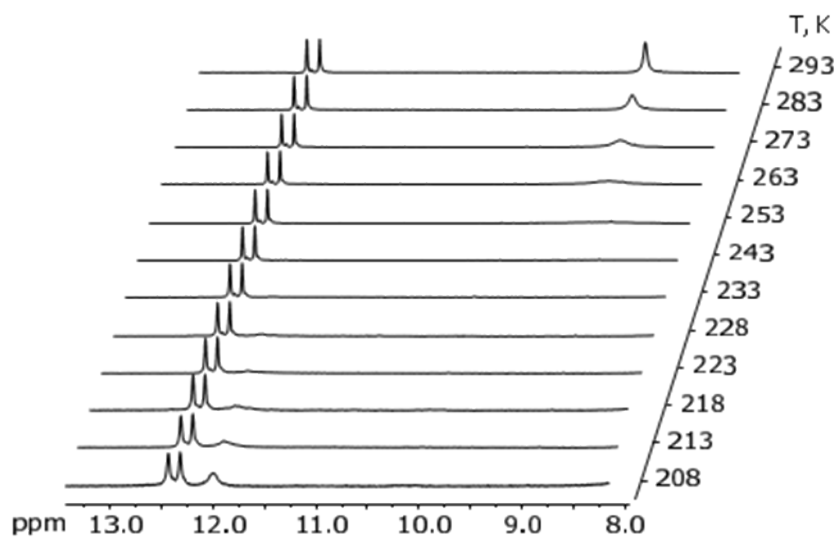**Fig. SI5.** 2D NOESY spectrum of **2Lu** (400 MHz, C₇D₈, 293 K).

Fig. SI6. Variable-temperature ¹H NMR spectra of **2Lu** (400 MHz, C₇D₈).
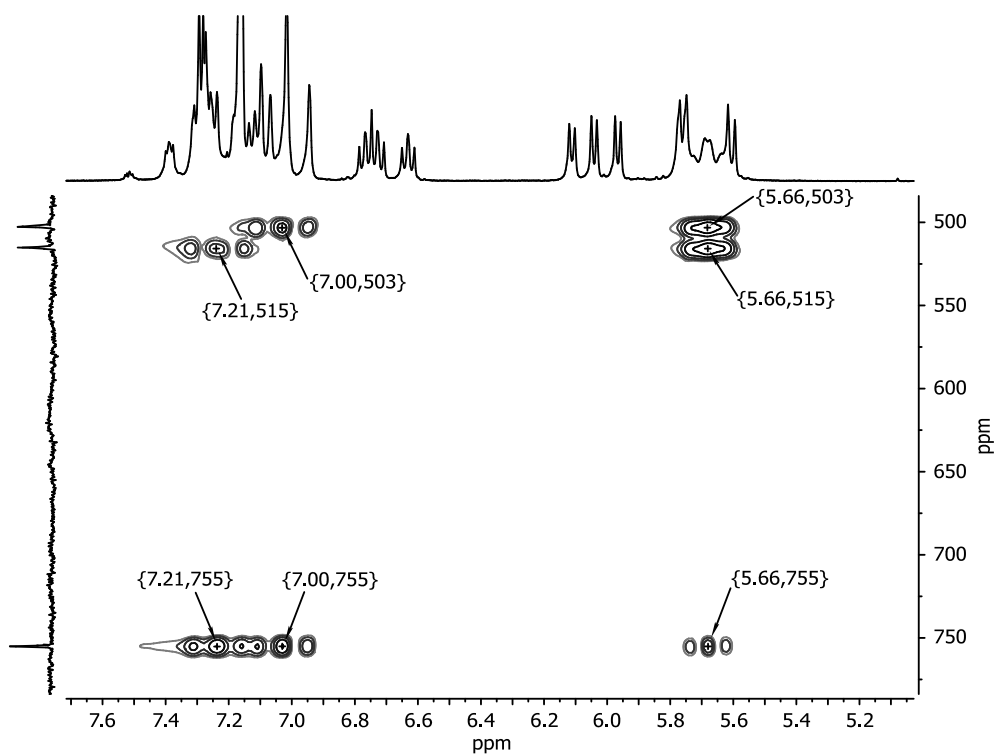
Fig. SI7. 2D ^{89}Y-^{1}H HMQC NMR spectrum of **3Y** showing ^{89}Y-^{1}H spin-spin interactions (optimized for $^{1}J_{YH} = 20Hz$, no ^{89}Y decoupling during acquisition) (400 MHz, C_6D_6, 293 K).
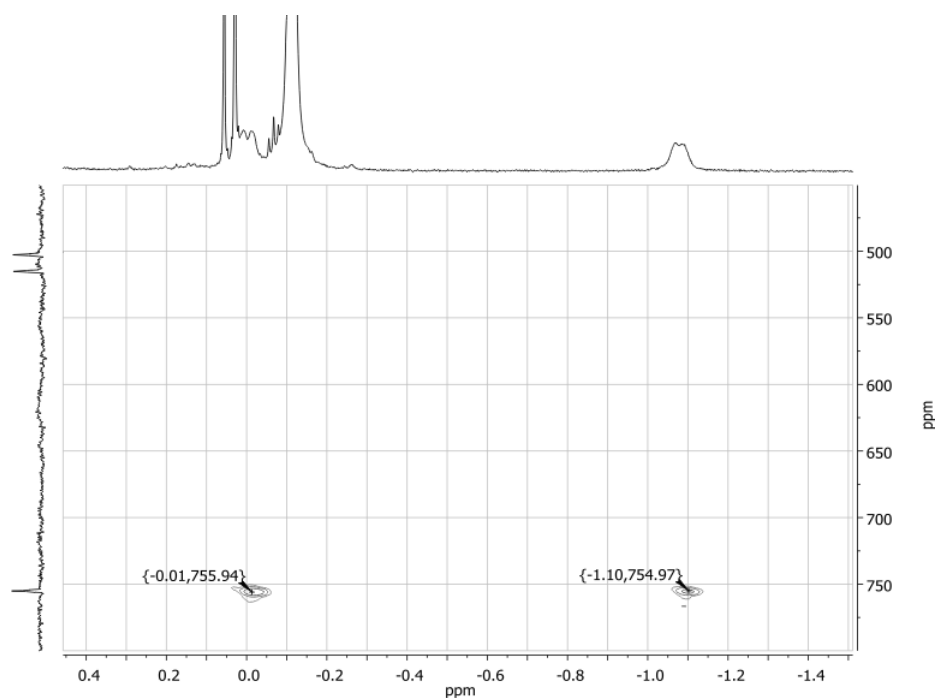

Fig. SI8. Fragment of 2D ^{89}Y-^{1}H (GE) HMQC long range interactions spectrum of **3Y** (400 MHz, C_6D_6, 293 K).
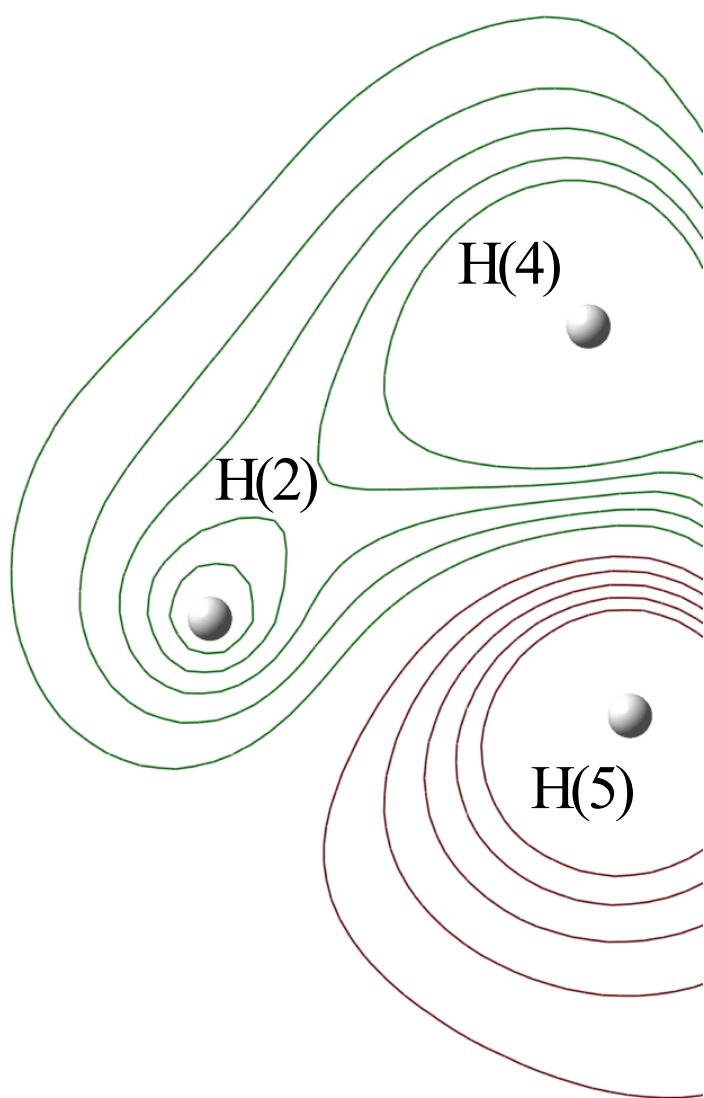
Fig. SI9. Contour map of the **3Y** HOMO-4 orbital (0.002-0.01 a.u., step 0.002 a.u.) in the H(2)H(4)H(5) plane. The red and green lines correspond to the positive and negative values of the wavefunction, respectively.