**Theoretical studies of mixed-valence organometallic species for potential utilization as quantum cellular automata**

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**Supplementary Information**



**Figure S1.** Spin orbital diagram of **16-H+**. The Fe(1)/left carbon chain/Fe(2)/right carbon chain/Cp\* and dppe percentage contributions are given in brackets. Contour values are ±0.04 (e bohr-3)1/2.

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**Figure S2.** Spin orbital diagram of **17-H+**. The Fe(1)/left carbon chain/Fe(2)/right carbon chain/Cp\* and dppe percentage contributions are given in brackets. Contour values are ±0.04 (e bohr-3)1/2.