

## **Misconception of reductive elimination of H<sub>2</sub>, in the context of the mechanism of nitrogenase**

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### **Electronic supplementary information**

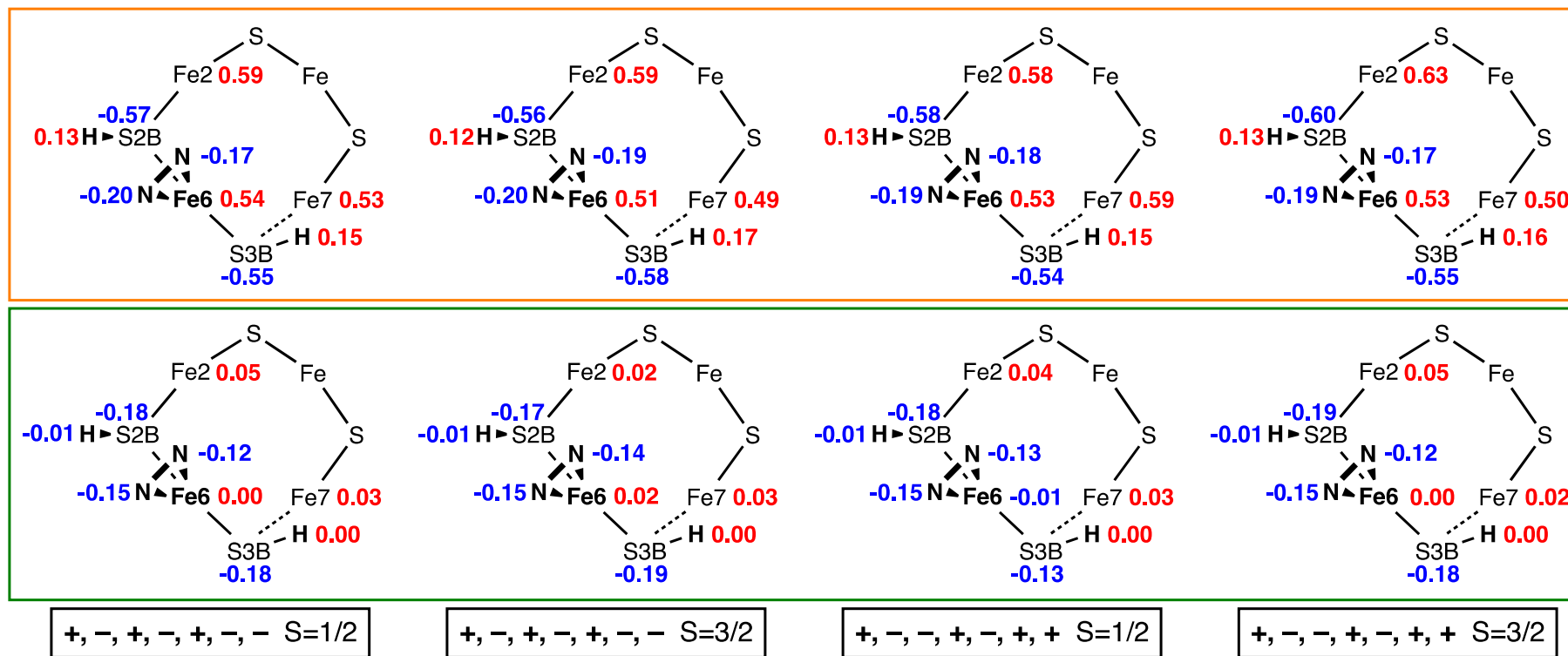


Fig S1. Calculated charges (Mulliken, orange box; Hirshfeld green box; red positive; blue negative) for the same structure in two electronic states and two net spin  $S$  states. The boxed labels list the signs of the spin densities on Fe atoms Fe1 - Fe7.

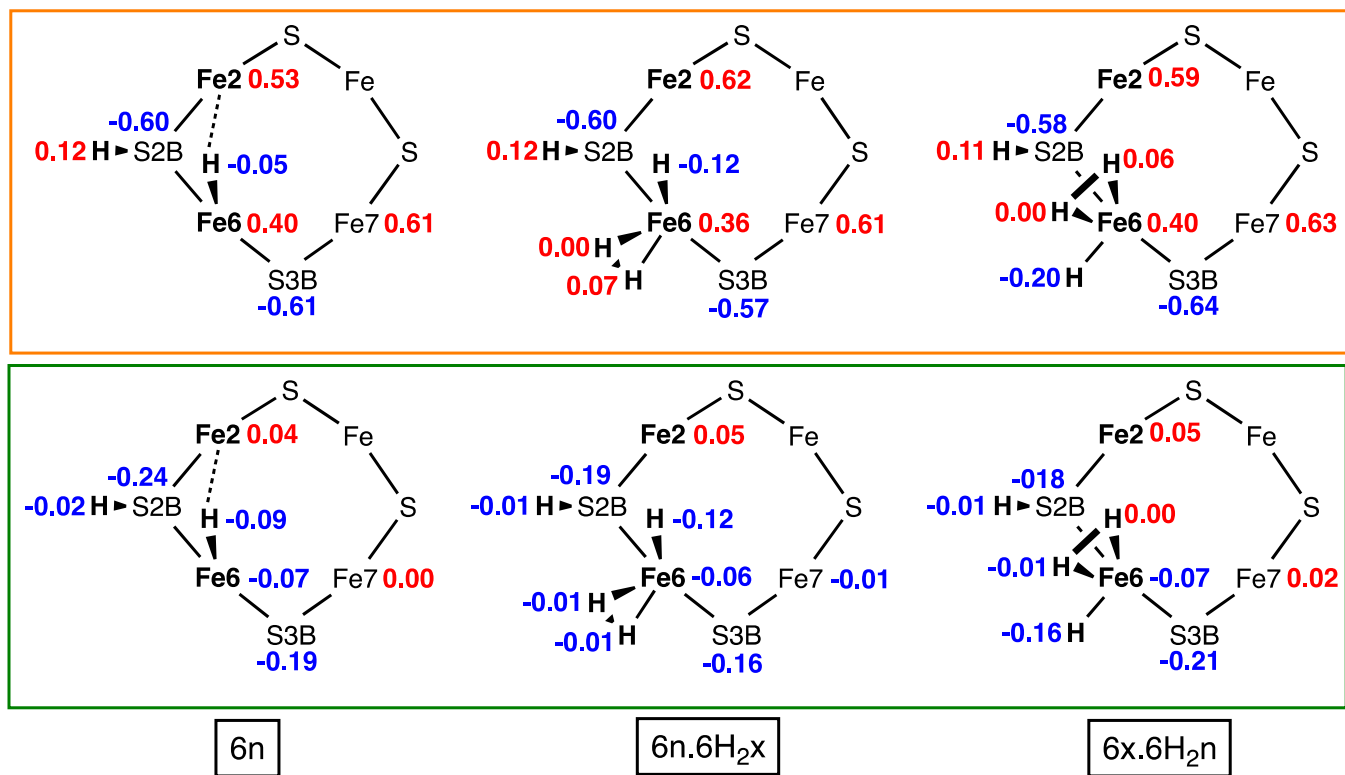


Fig. S2. Calculated charges (Mulliken, orange box; Hirshfeld green box; red positive; blue negative) for models without H on S<sub>3</sub>B.

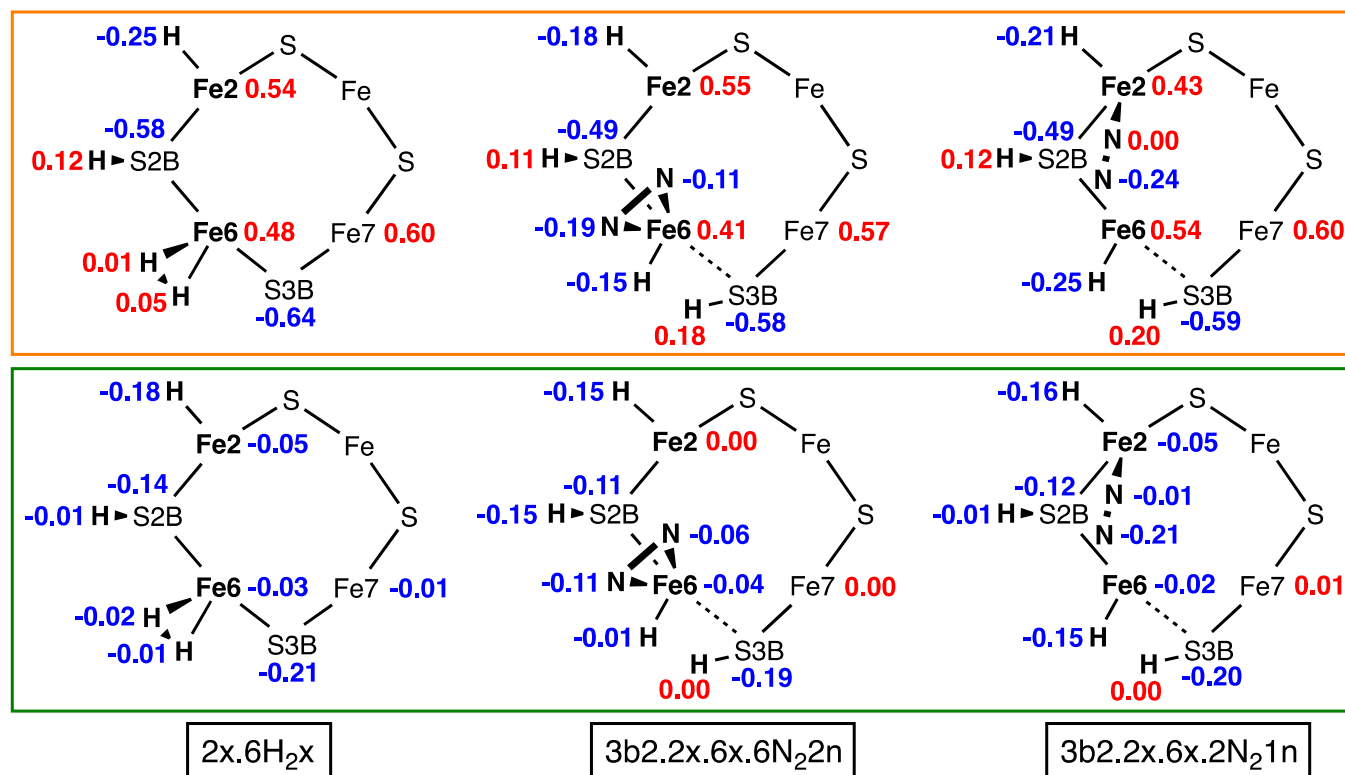


Fig. S3. Calculated charges (Mulliken, orange box; Hirshfeld green box; red positive; blue negative) for models with *exo* H on Fe2.