

## Supporting Information

“Diazene (HN=NH) Is a Substrate for Nitrogenase: Insights into the Pathway of N<sub>2</sub> Reduction” By Brett M. Barney, Jammi McClead, Dmitriy Lukoyanov, Mikhail Laryukhin, T. C. Yang, Brian M. Hoffman, Dennis R. Dean, and Lance C. Seefeldt

### Figure Legends

**Figure S1. Power dependence of 2K Q-band EPR spectra of hydrazine- and diazene-dependent intermediates in the  $\alpha$ -70<sup>Ala</sup>/ $\alpha$ -195<sup>Gln</sup> MoFe protein variant.**

**Figure S2. pH dependence of the diazene and hydrazine EPR signals.** The EPR signal intensity (measured as peak height of the  $g = 2.07$  and  $g = 2.09$  signals) for the  $\alpha$ -70<sup>Ala</sup> /  $\alpha$ -195<sup>Gln</sup> MoFe protein trapped during turnover with azodiformate ( $\diamond$ ) or hydrazine ( $\blacktriangle$ ) are shown as a function of the pH of the turnover solution. Conditions are as described in the **Materials and Methods** section.

**Figure S3. Microwave power dependence of the diazene and hydrazine EPR signals.** The microwave power dependence for the resting state ( $\blacklozenge$ ) EPR inflection at  $g = 4.43$  or the diazene turnover ( $\triangle$ ) EPR inflection at  $g = 2.07$  or the hydrazine turnover ( $\circ$ ) EPR inflection at  $g = 2.09$  for the  $\alpha$ -70<sup>Ala</sup>/ $\alpha$ -195<sup>His</sup> modified MoFe protein are shown against the square root of the microwave power (in  $\mu$ W). Linear fits were forced to zero and included only the lower values for the turnover species.

Figure S1

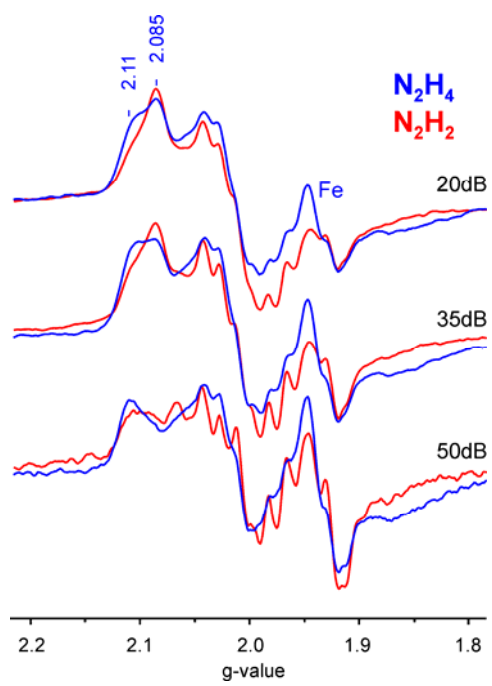


Figure S2

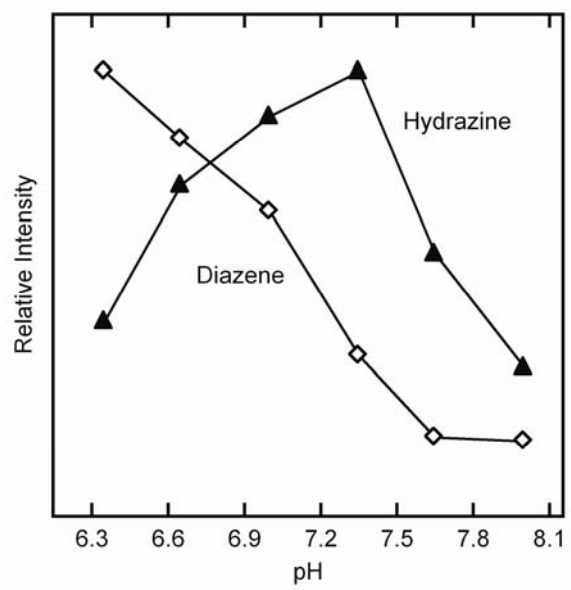


Figure S3

