

Supporting Information

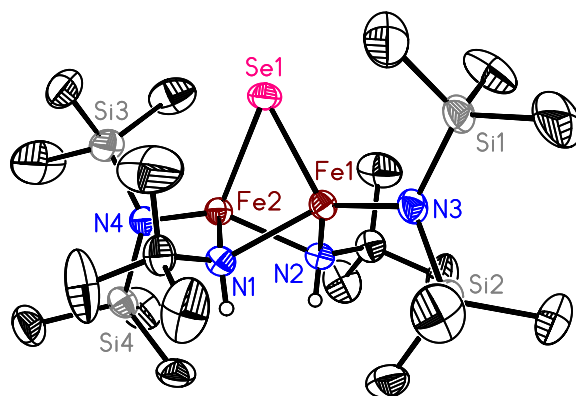
**Iron-Amide-Sulfide and Iron-Imide-Sulfide Clusters: Heteroligated
Core Environments Relevant to the Nitrogenase FeMo Cofactor**

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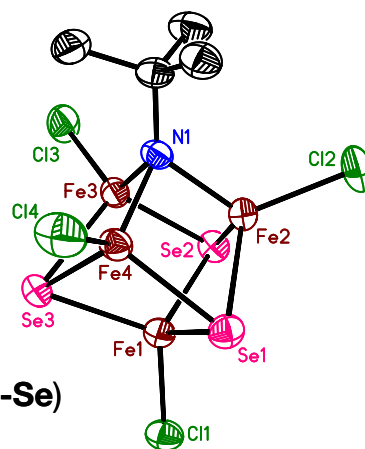
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$\text{Fe}_2(\text{NH}^t\text{Bu})_2\text{Se}[\text{N}(\text{SiMe}_3)_2]_2$ (**7-Se**)



$[\text{Fe}_4(\text{N}^t\text{Bu})\text{Se}_3\text{Cl}_4]^{2-}$ (**10-Se**)

Figure S1 Structures of selenide-substituted clusters **7-Se** and **10-Se**, showing non-hydrogen atoms (50% probability thermal ellipsoids), amide hydrogens (as small open circles), and selected atom labels.