

# Crystal Structure Investigation of a Dinuclear N-Heterocyclic Carbenes Dinitrosyl Iron Compound (iMes)Fe(NO)<sub>2</sub>(μ-BF<sub>4</sub>)(iMes)Fe(NO)<sub>2</sub> and its Reactions and Characterization with an External Ligand (L = iMe)

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By examining the single crystal structure of the complex (iMes)Fe(NO)<sub>2</sub>(μ-BF<sub>4</sub>)(iMes)Fe(NO)<sub>2</sub> (iMes = 1,3-bis(2,4,6-trimethylphenyl)imidazolium chloride), it can be observed that this crystal is an asymmetric structure bridged by BF<sub>4</sub> and connected by a dinitrosyl iron complex, exhibiting the electronically localized {Fe(NO)<sub>2</sub>}<sup>9-</sup>-{Fe(NO)<sub>2</sub>}<sup>10</sup> electronic state (Figure 1).

We investigated the reactions between (iMes)Fe(NO)<sub>2</sub>(μ-BF<sub>4</sub>)(iMes)Fe(NO)<sub>2</sub> and an external ligand iMe. (iMe = 1,3-dimethyl-2,3-dihydro-1H-imidazole). The structures of the reaction products were determined and identified through IR spectroscopy. The results indicate that iMe can undergo ligand replacement reactions with (iMes)Fe(NO)<sub>2</sub>, leading to compounds with different coordination environments.

Upon addition of the ligand iMe, the {Fe(NO)<sub>2</sub>}<sup>9-</sup>-{Fe(NO)<sub>2</sub>}<sup>10</sup> structure opens up and forms two compounds: [(iMes)iMeFe(NO)<sub>2</sub>]<sup>+</sup>BF<sub>4</sub>{Fe(NO)<sub>2</sub>}<sup>9-</sup> and [(iMes)(iMe)Fe(NO)<sub>2</sub>]{Fe(NO)<sub>2</sub>(iMe)}<sup>10</sup> (Figure 2). IR spectroscopy was used to confirm the generation of these two compounds and analyze the corresponding positions of the peaks.

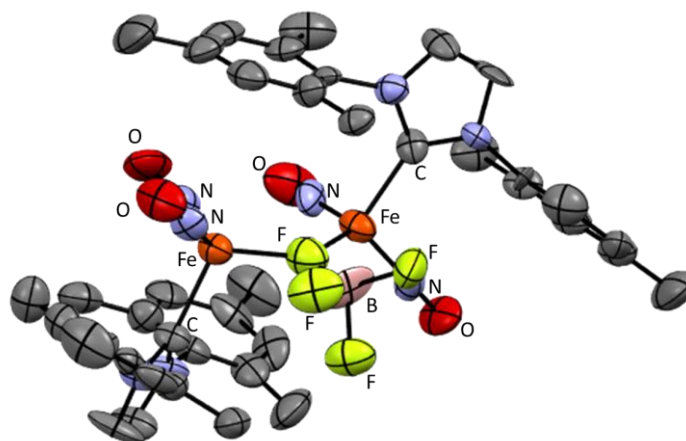


Figure 1

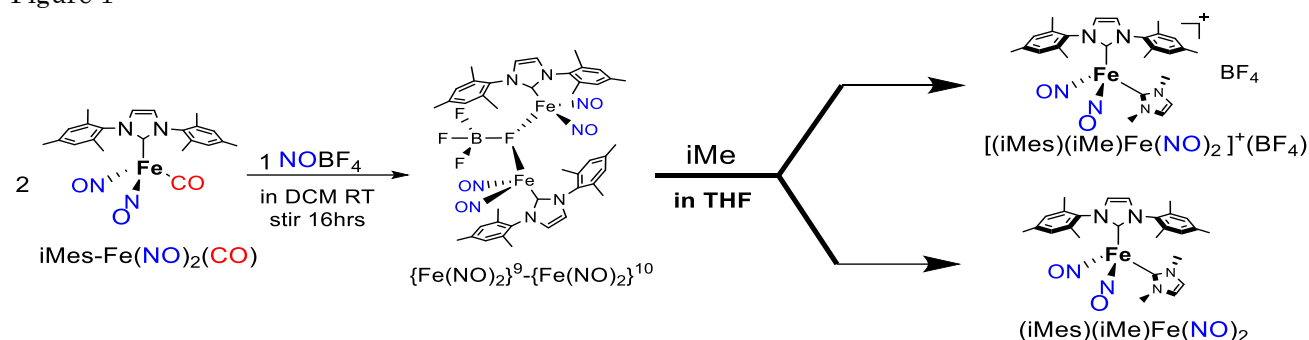


Figure 2

## References

1. A {Fe(NO)<sub>3</sub>}<sup>10</sup> Trinitosyliron Complex Stabilized by an N-Heterocyclic Carbene and the Cationic and Neutral {Fe(NO)<sub>2</sub>}<sup>9/10</sup> Products of Its NO Release  
Chung-Hung Hsieh, Marcetta Y. Darensbourg,  
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