Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information for

Syntheses and structures of Li, Fe, and Mo derivatives of *N*,*N*'-bis(2,6-diisopropylphenyl)-*o*-phenylenediamine

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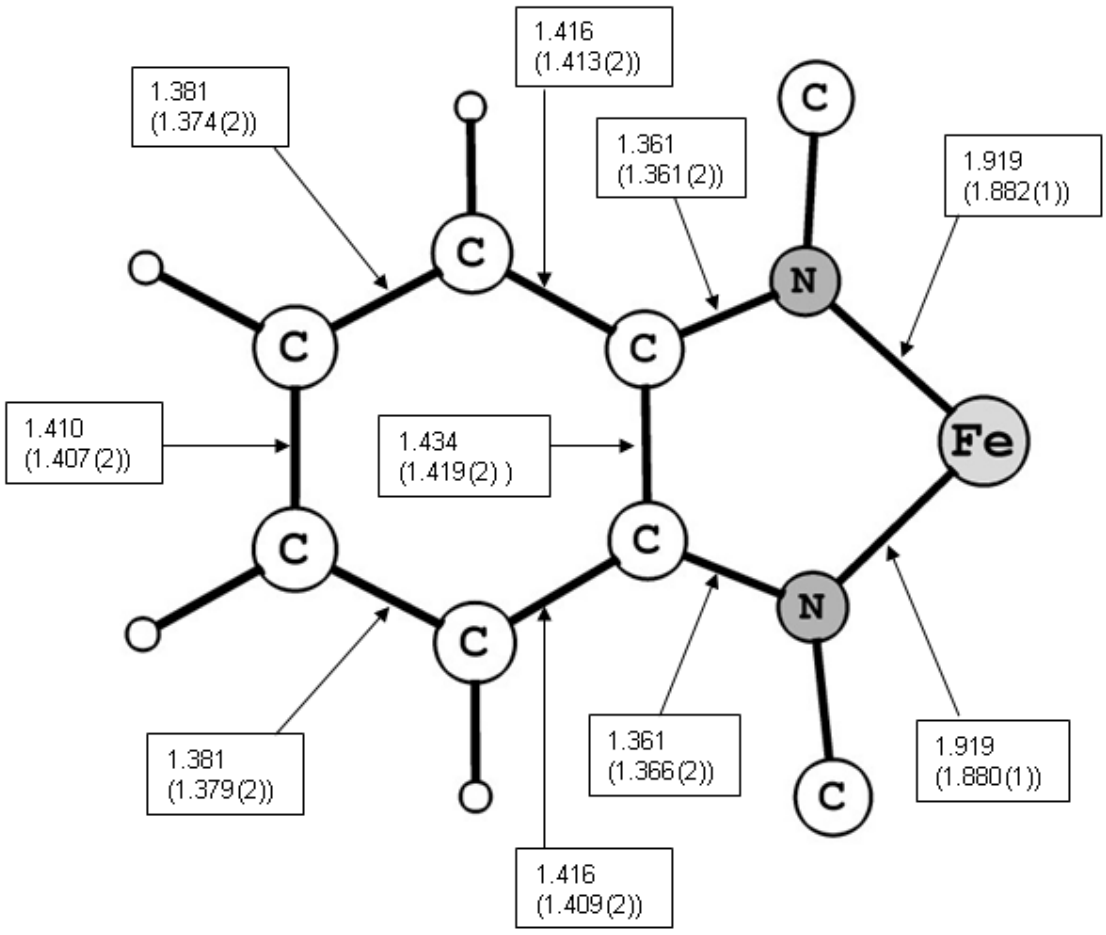
Computation Details

Gaussian 09 software package was used to define three fragments for compound **3**: N,N-chelating ligand (charge -1, multiplicity 2), Fe (charge +1, multiplicity -2), and toluene (charge 0, multiplicity 1); five fragments for compound 4: N,N-chelating ligand (charge -1, multiplicity 2), Fe (charge +1, multiplicity -2), CO (charge 0, multiplicity 1), CO (charge 0, multiplicity 1), and CO (charge 0, multiplicity 1). For further details regarding how to use Gaussian 09 to model antiferromagnetic coupling, see "Modeling Antiferromagnetic Coupling in Gaussian 09" on Gaussian website (http://gaussian.com/g_tech/afc.htm).

Optimized Geometries vs Crystal Structures

All distances are in Å. In each box, the top number is the computed distance, while the bottom number in bracket is from crystal structure.

1. Compound **3**



2. Compound **4**