

Supplementary Data — X-Ray Crystallography

Manuscript: Synthesis of Iron(II), Manganese(II) and Cobalt(II) Complexes
Containing Tetradentate Nitrogen Ligands and their Application in the
Catalytic Oxidation of Alkanes

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Fig. S1 The molecular structure of the C_2 symmetric complex Fe(**1**)OTf₂ (30% probability ellipsoids).

Fig. S2 The molecular structure of Fe(**1**)OTf₂ showing the *ca.* 90:10 disorder in the OTf₂ ligands (the dashed bonds indicate the minor occupancy 10% orientation).

Fig. S3 The molecular structure of Fe(**9**)OTf₂ (30% probability ellipsoids).

Fig. S4 The molecular structure of Fe(**9**)OTf₂ showing the *ca.* 80:20 and 90:10 disorder in the upper and lower OTf₂ ligands respectively (the dashed bonds indicate the minor occupancy orientations).

Fig. S5 The ¹H-NMR spectrum and corresponding peak assignment for [Fe(**1**)(OTf)₂], recorded in CD₂Cl₂ solution at 298 K.

Fig. S6 The COSY ¹H-NMR spectrum of [Fe(**1**)(OTf)₂] in CD₂Cl₂.

Fig. S7 The ¹H-NMR spectrum and corresponding peak assignment for [Fe(**7**)(OTf)₂] recorded in CDCl₃ solution at 298 K.

Fig. S8 The ¹H-NMR COSY spectrum and corresponding peak assignment for [Fe(**8**)(OTf)₂] recorded in CD₃CN solution at 298 K.

Fig. S9 The ¹H-NMR spectrum and corresponding peak assignment for [Fe(**12**)(OTf)₂], recorded in CDCl₃ solution at 298 K.

Fig. S10 UV-VIS spectra of biphenyl-bridged bis(pyridylmethyl) diamine iron(II) complexes. (Solvent: acetonitrile, c = 0.5 mM).

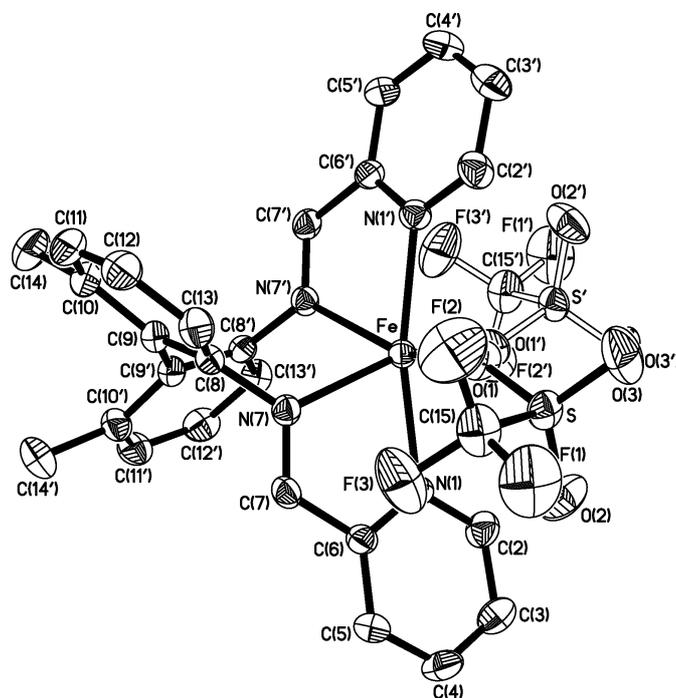


Fig. S1

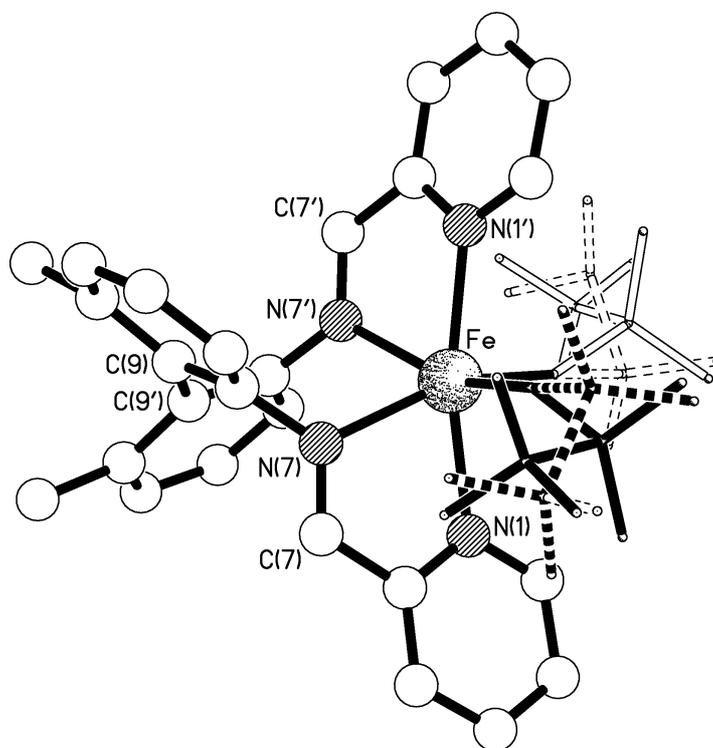


Fig. S2

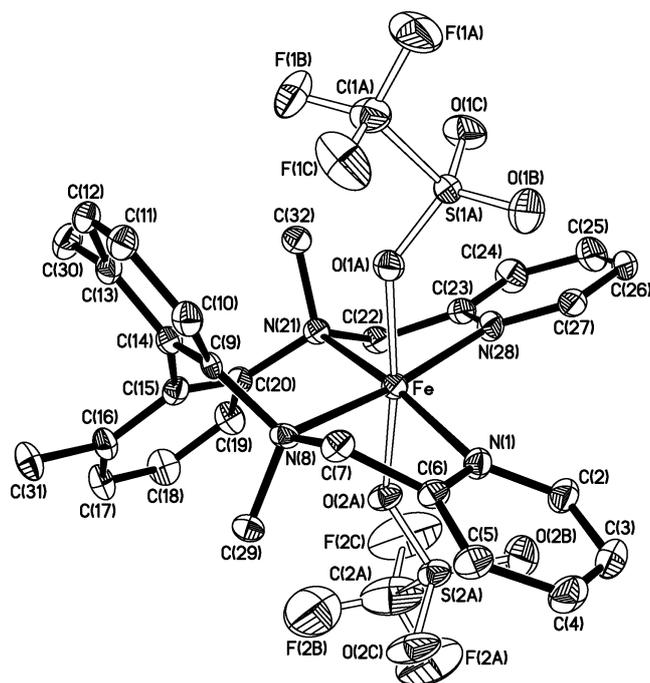


Fig. S3

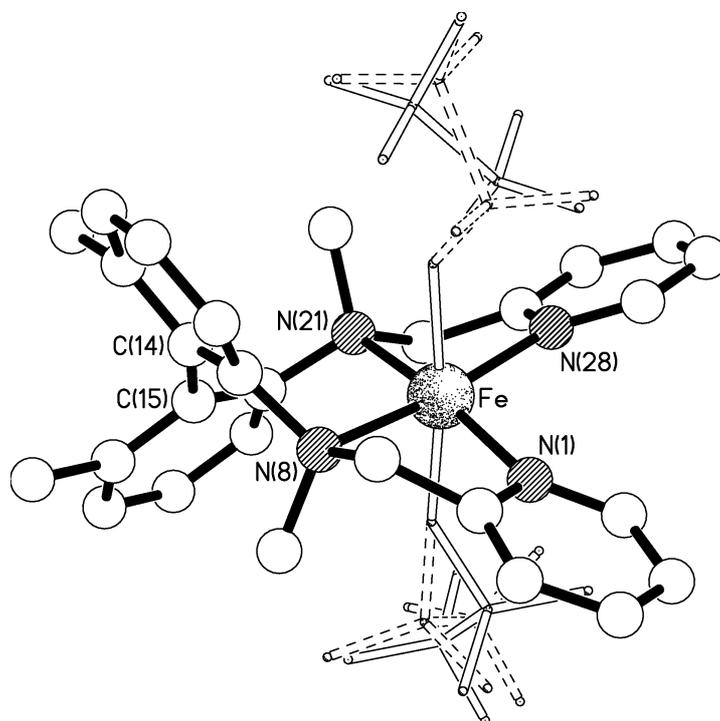


Fig. S4

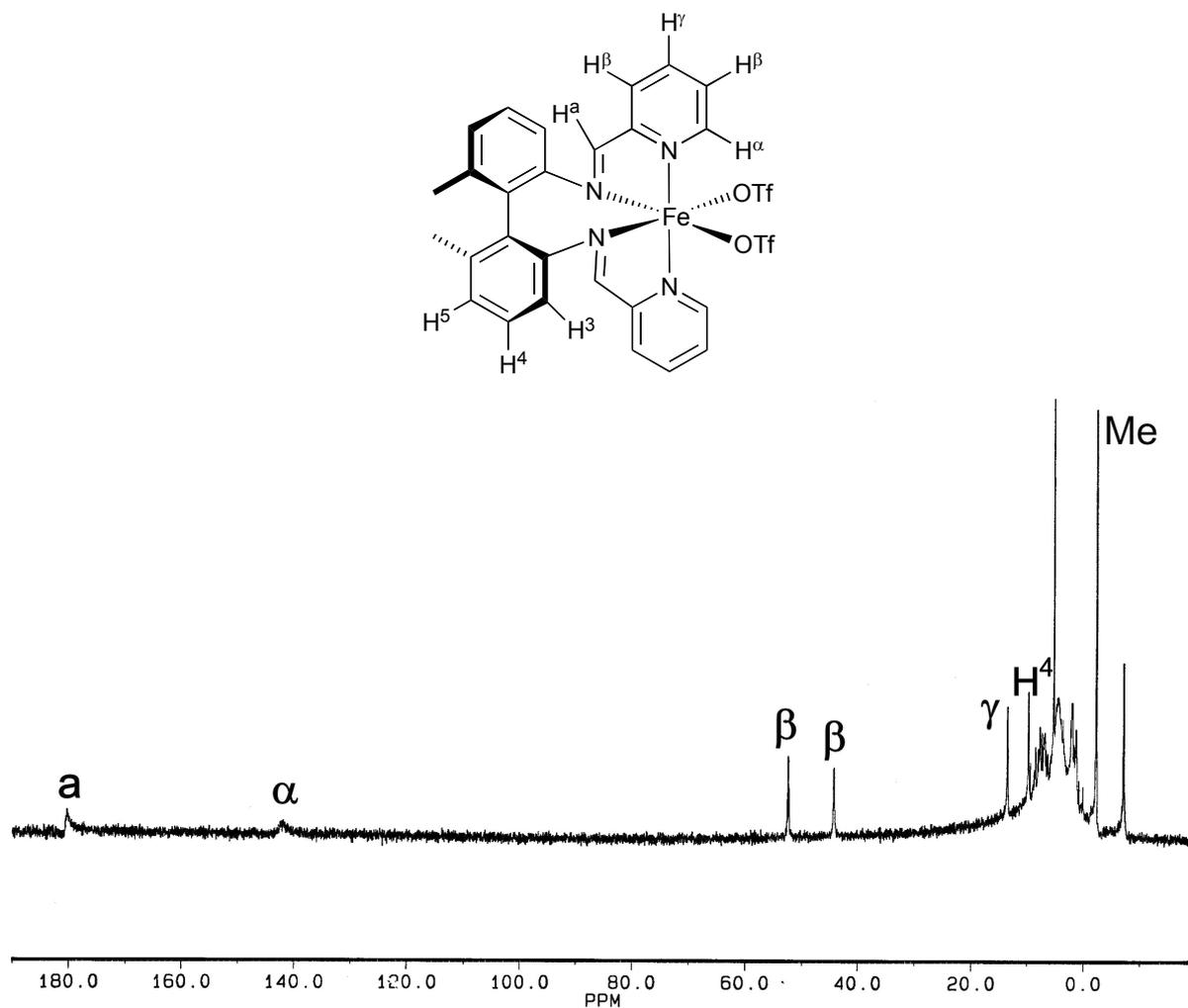


Fig. S5. The $^1\text{H-NMR}$ spectrum and corresponding peak assignment for $[\text{Fe}(\mathbf{1})(\text{OTf})_2]$, recorded in CD_2Cl_2 solution at 298 K.

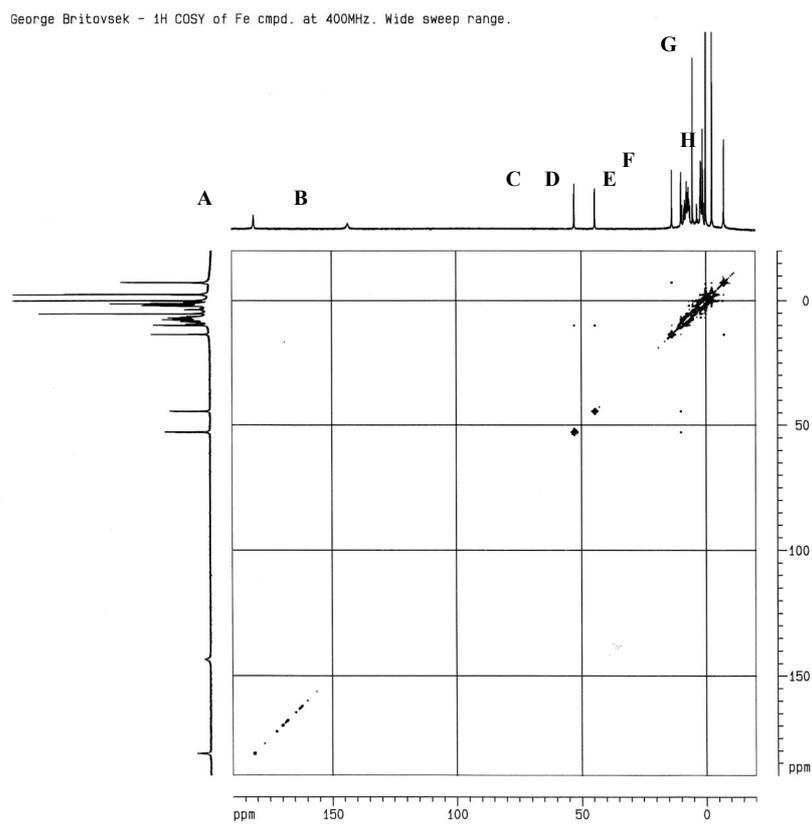


Fig. S6. The COSY ¹H-NMR spectrum of [Fe(**1**)(OTf)₂] in CD₂Cl₂.

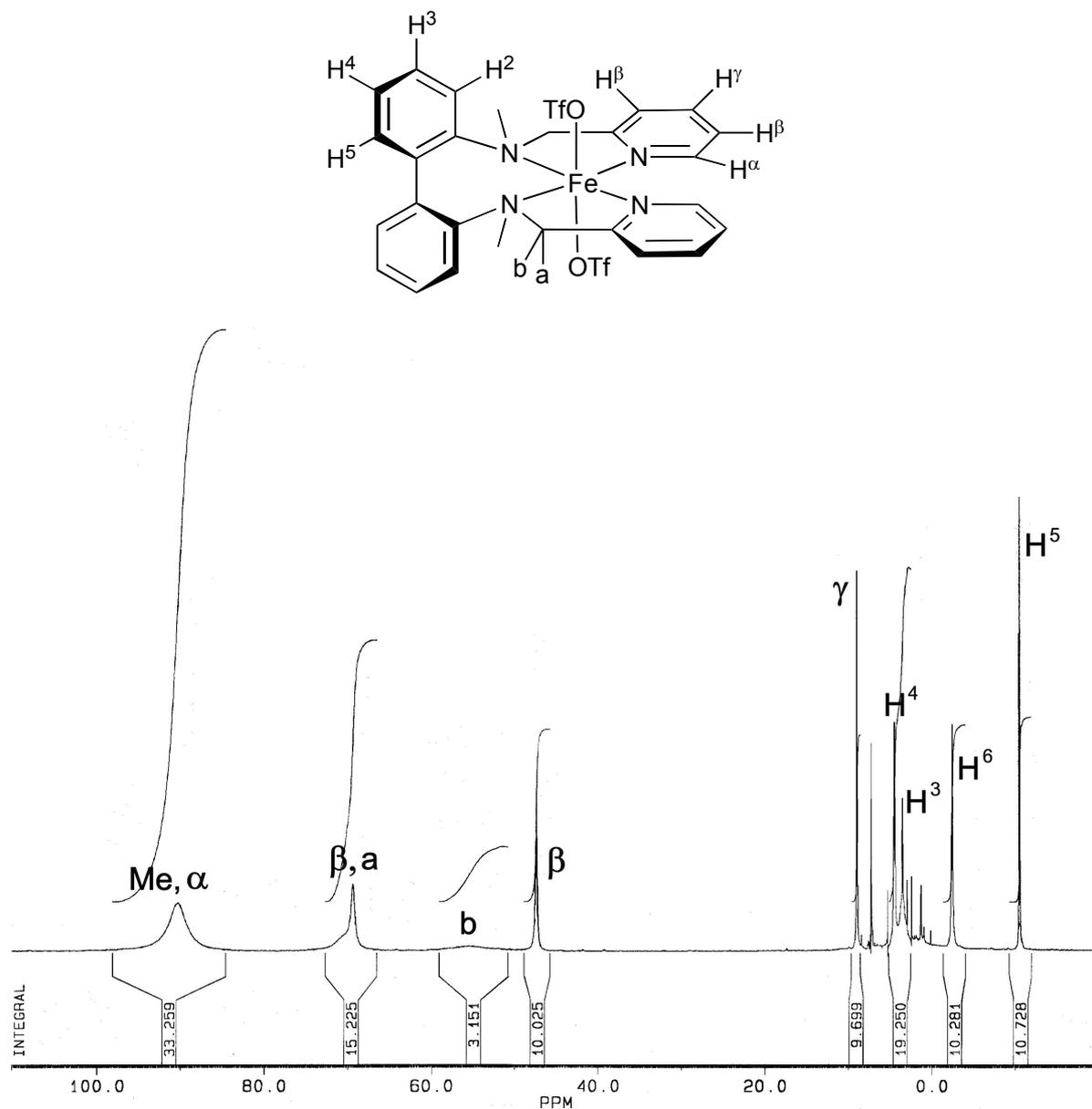


Fig. S7. The ¹H-NMR spectrum and corresponding peak assignment for [Fe(7)(OTf)₂] recorded in CDCl₃ solution at 298 K.

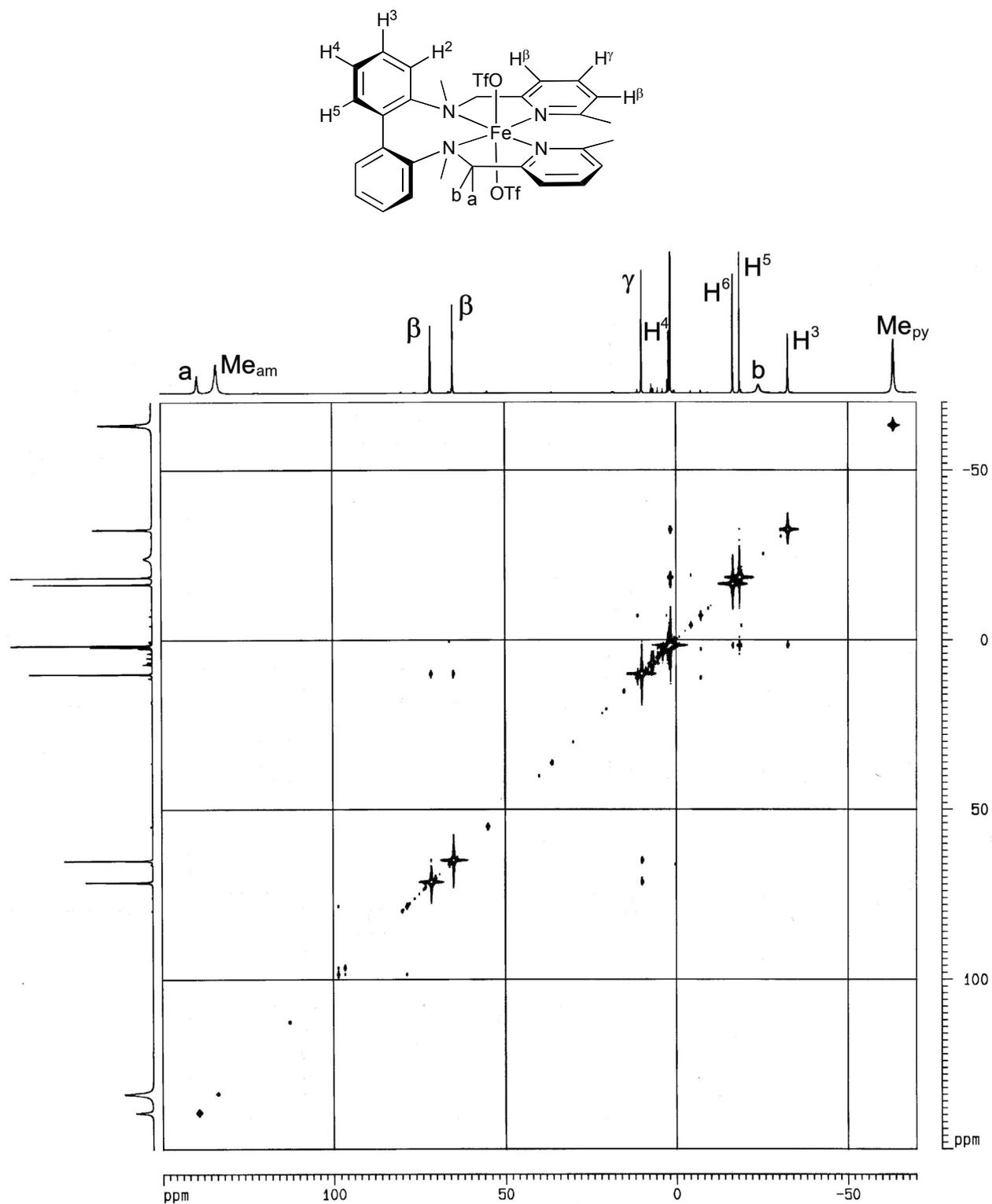


Fig. S8. The ¹H-NMR COSY spectrum and corresponding peak assignment for [Fe(8)(OTf)₂] recorded in CD₃CN solution at 298 K.

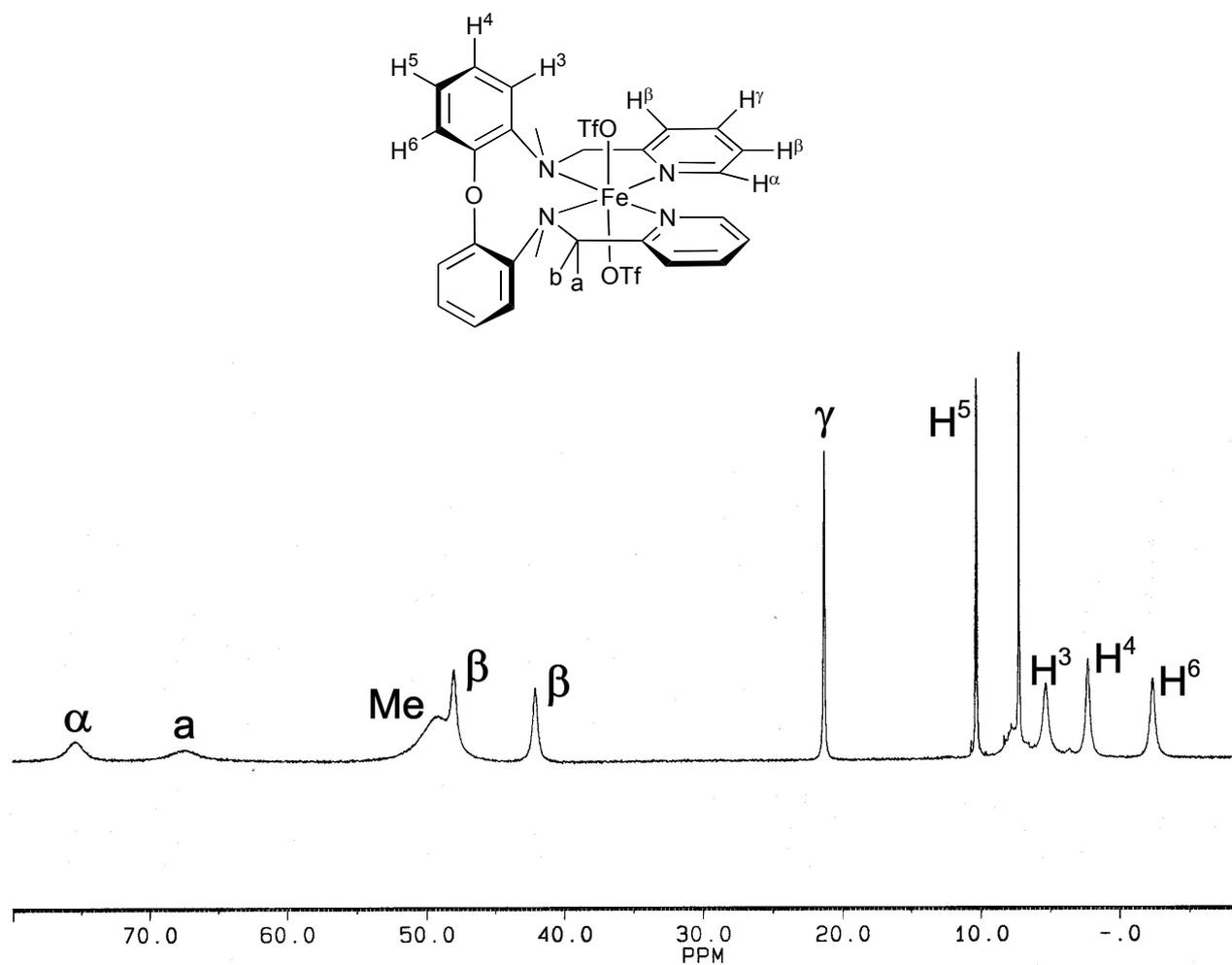


Fig. S9. The ¹H-NMR spectrum and corresponding peak assignment for [Fe(12)(OTf)₂], recorded in CDCl₃ solution at 298 K.

Biphenyl-derived series

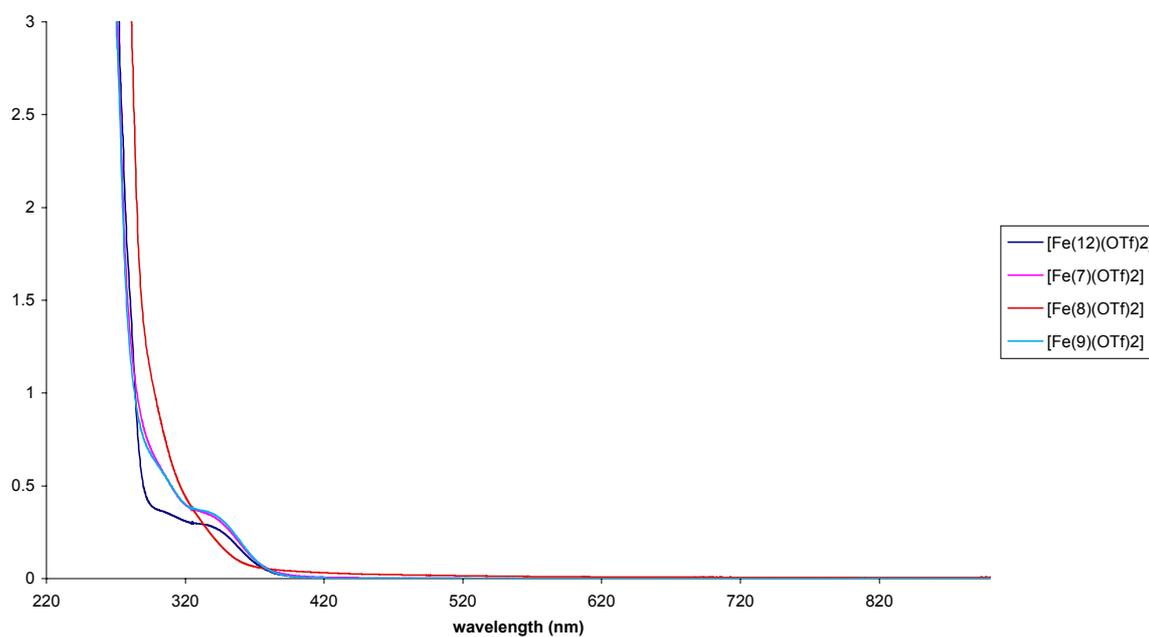


Fig. S10. UV-VIS spectra of biphenyl-bridged bis(pyridylmethyl) diamine iron(II) complexes. (Solvent: acetonitrile, $c = 0.5$ mM).