

The Influence of Electron Delocalization upon the Stability and Structure of Potential *N*-Heterocyclic Carbene Precursors with 1,3-Diaryl-imidazolidine-4,5-dione Skeletons

Matthew G. Hobbs,^a Taryn D. Forster,^a Javier Borau-Garcia,^a Chrissy J. Knapp,^a Heiki M. Tuononen^b and Roland Roesler^{a}*

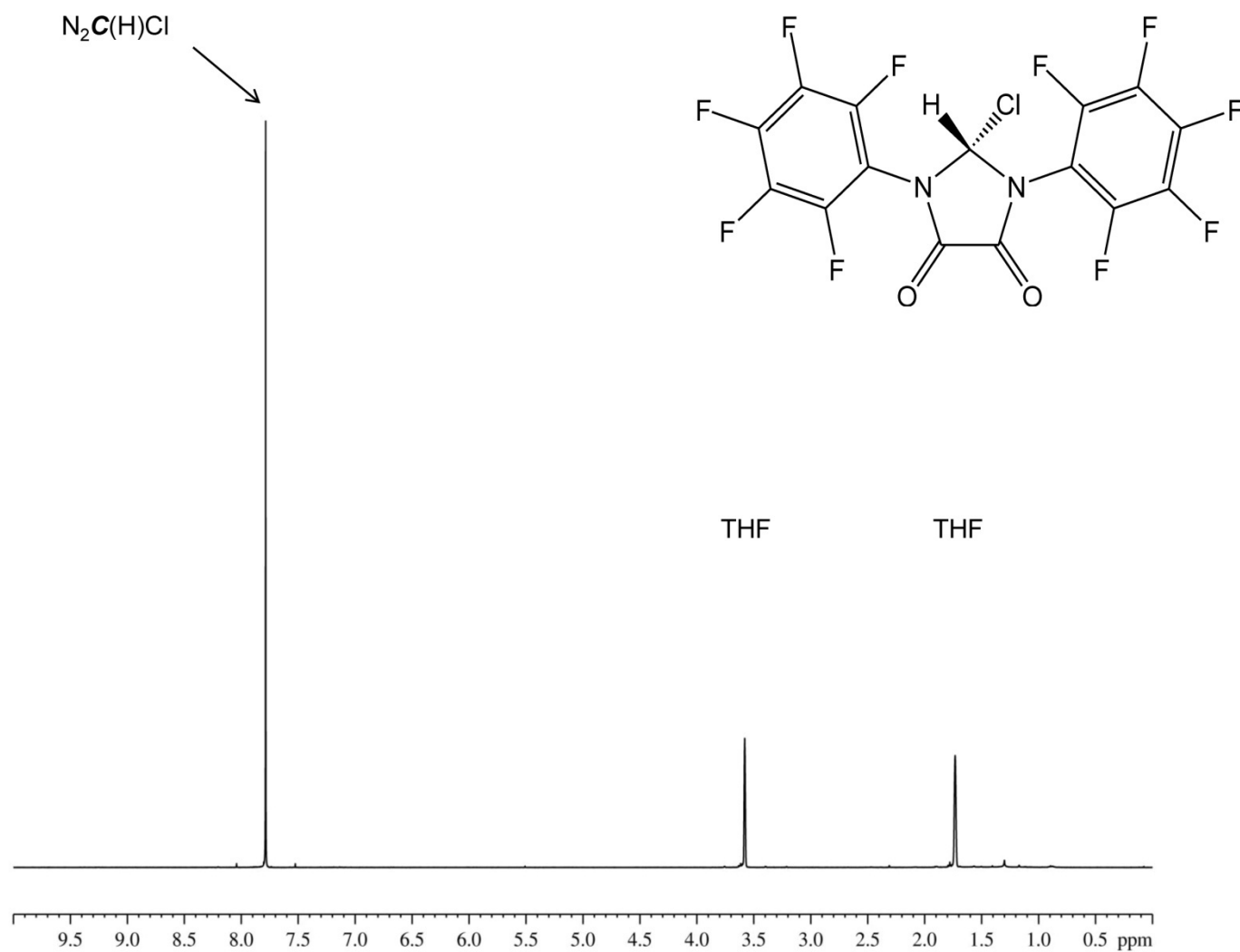
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^b Department of Chemistry, University of Jyväskylä, P.O. Box 35, F1-40014 Jyväskylä, Finland.

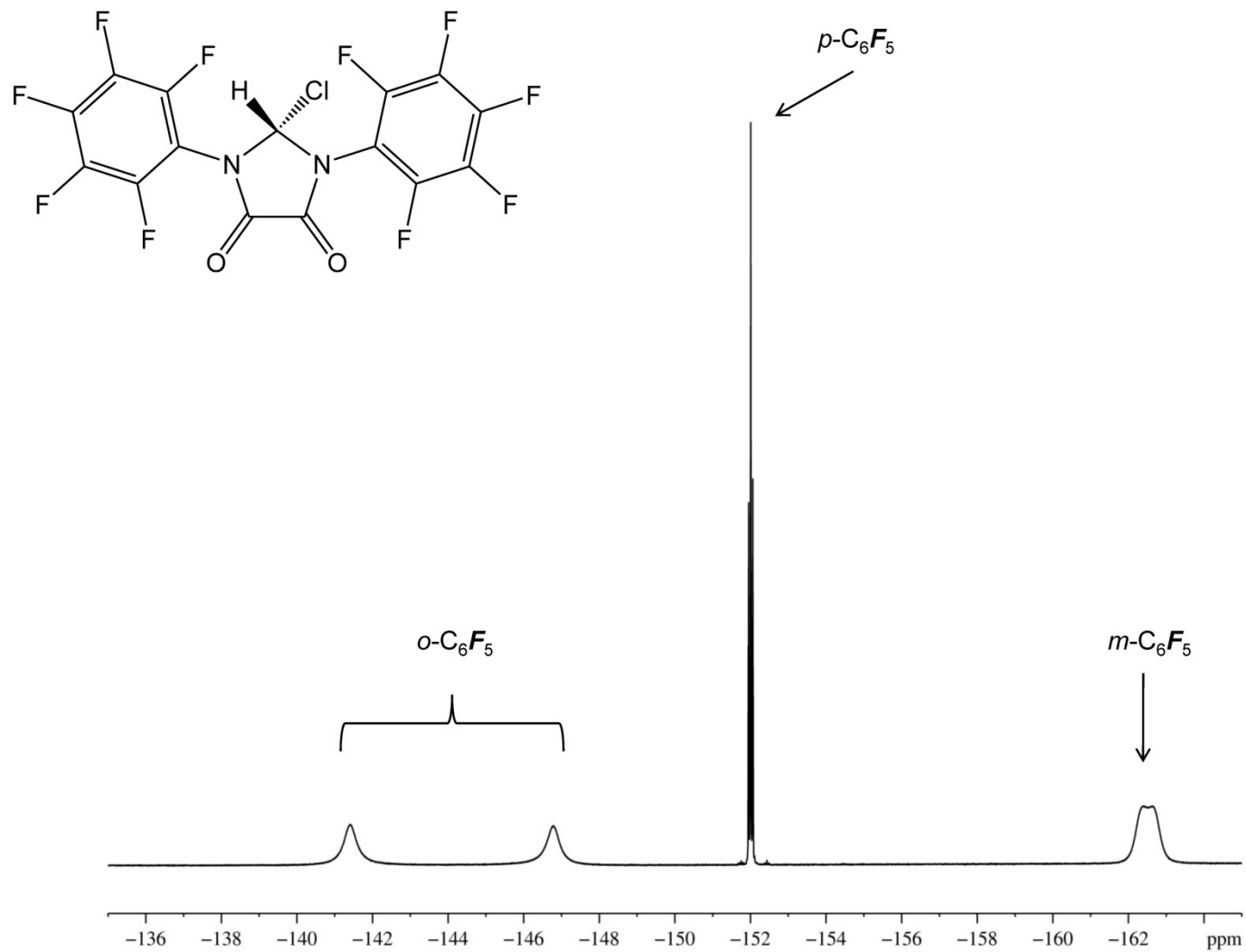
- Supporting Information –

¹H, ¹⁹F, and ¹³C NMR spectra of compounds **1a,b,c**, **3c**, **4c**, **5a,b,c**, **6a,b,c** and **7c**.

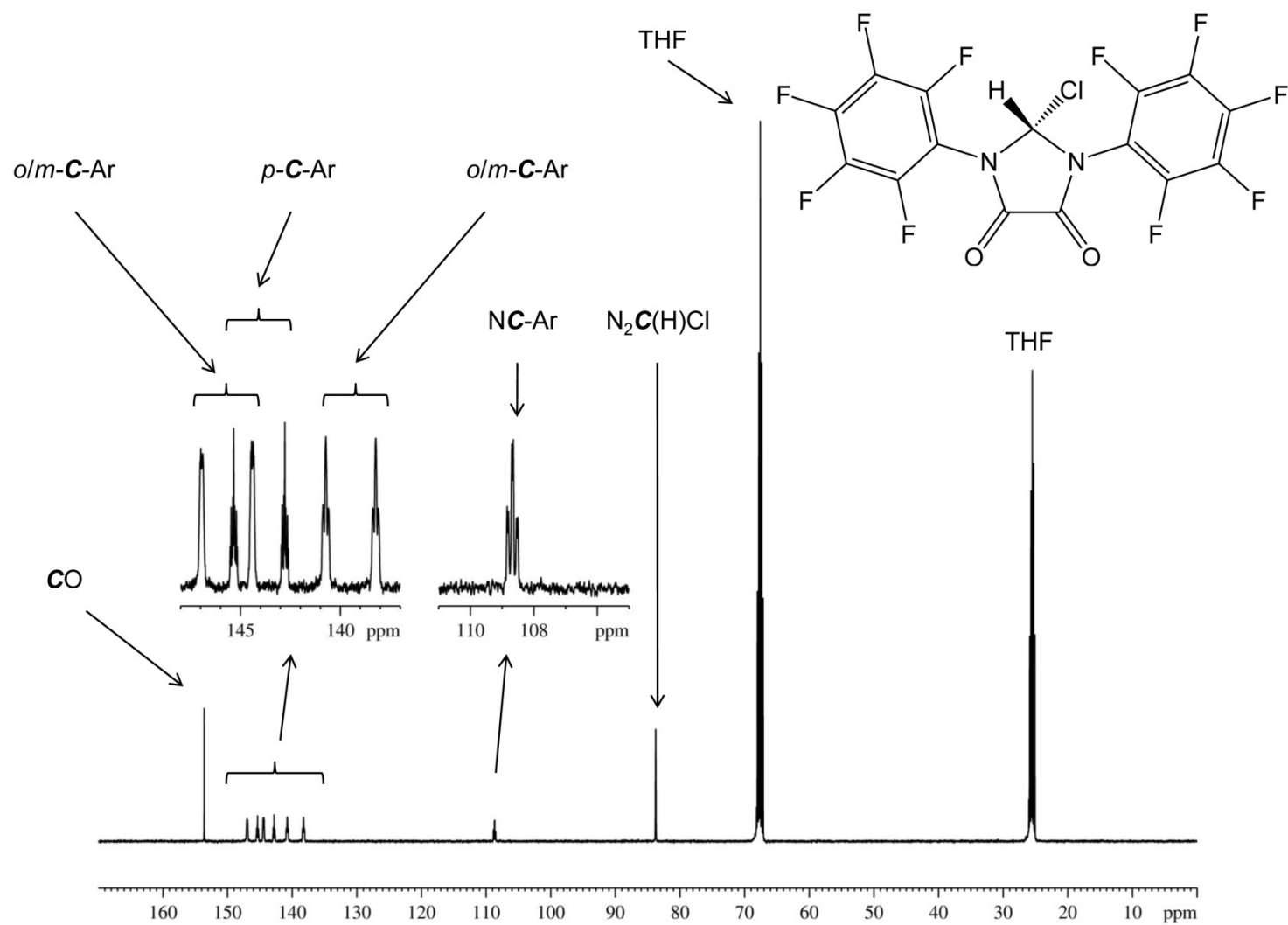
¹H NMR Spectrum of 2-chloro-1,3-bis(pentafluorophenyl)imidazolidine-4,5-dione (**1a**)



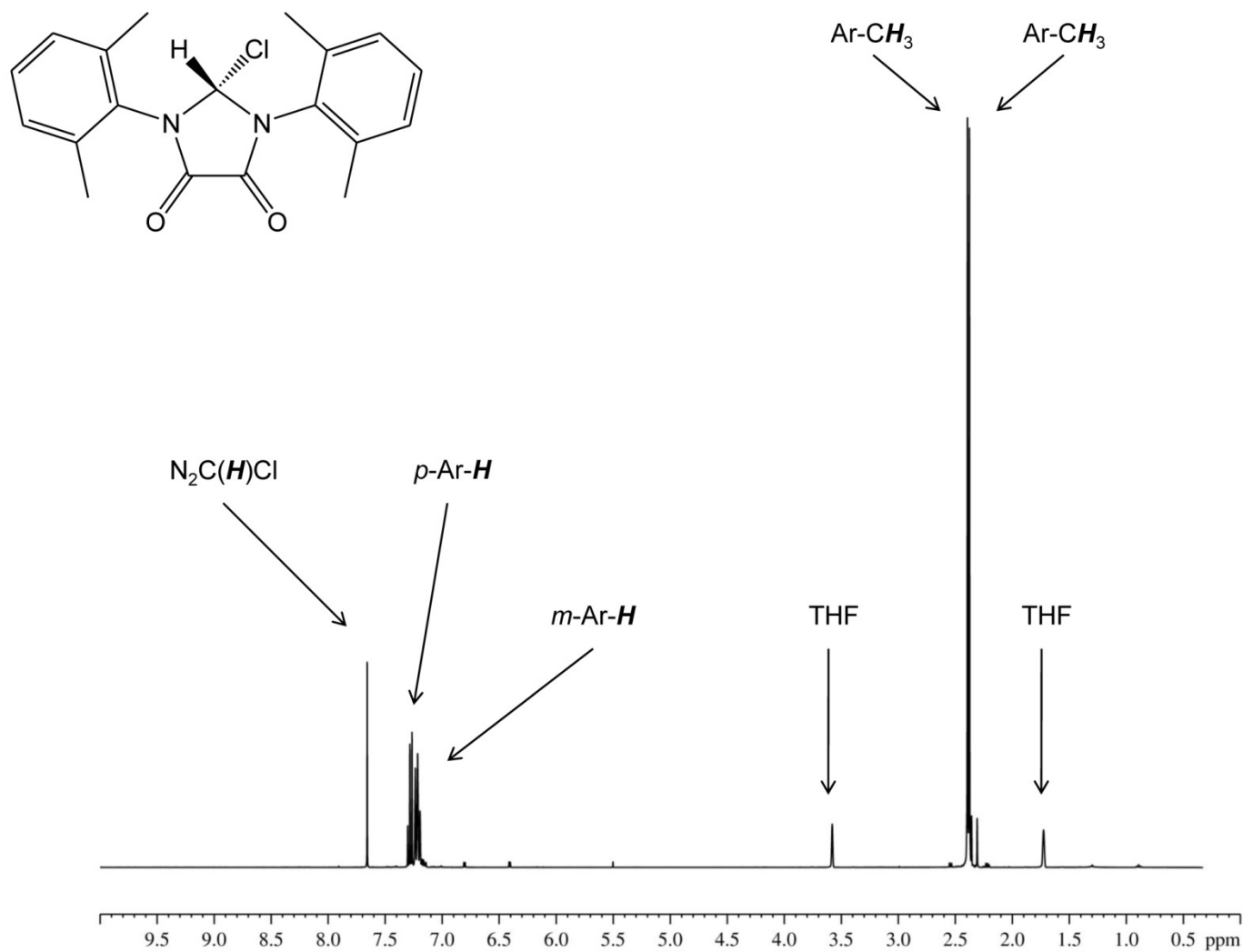
^{19}F NMR Spectrum of 2-chloro-1,3-bis(pentafluorophenyl)imidazolidine-4,5-dione (**1a**)



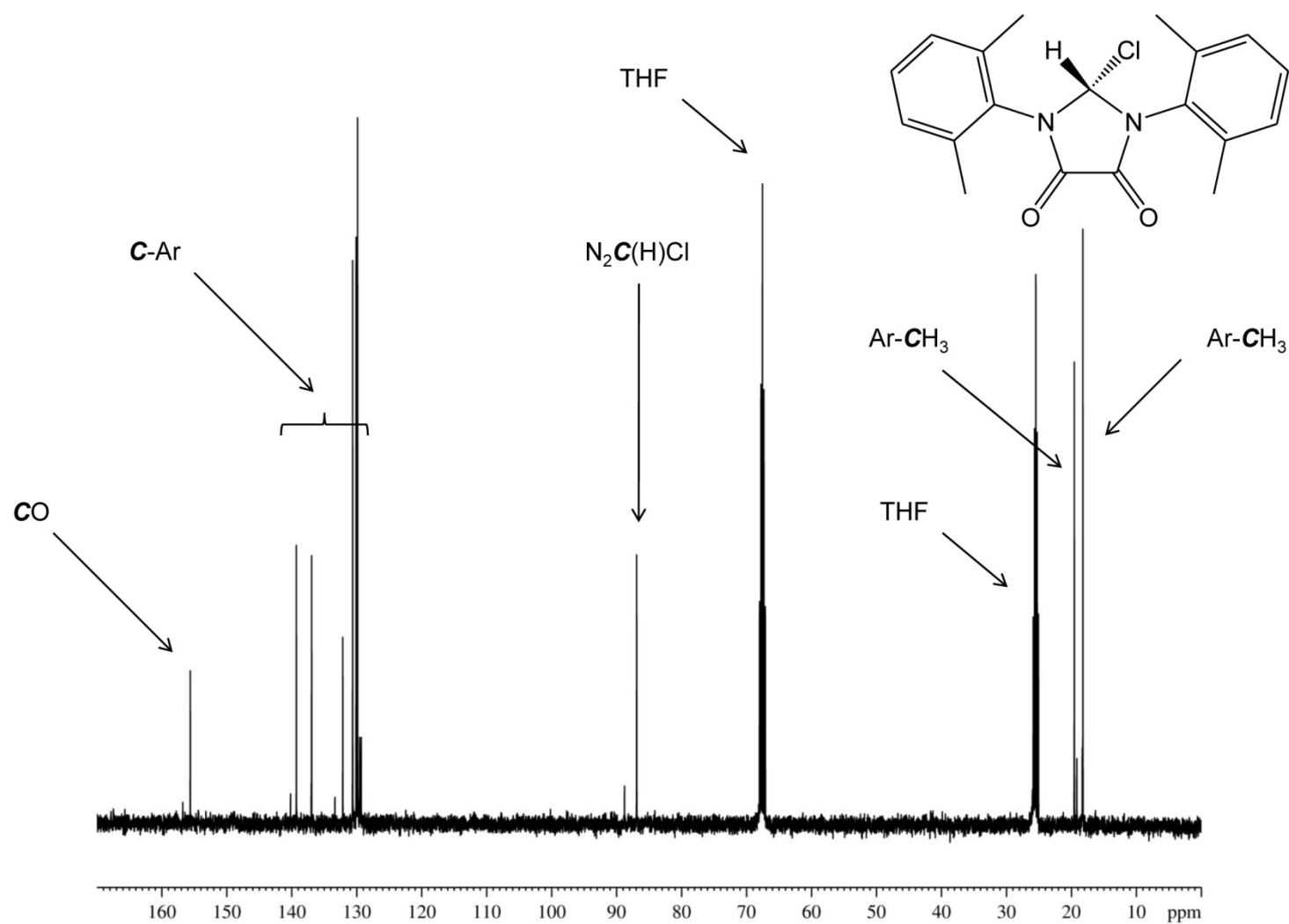
^{13}C NMR Spectrum of 2-chloro-1,3-bis(pentafluorophenyl)imidazolidine-4,5-dione (**1a**)



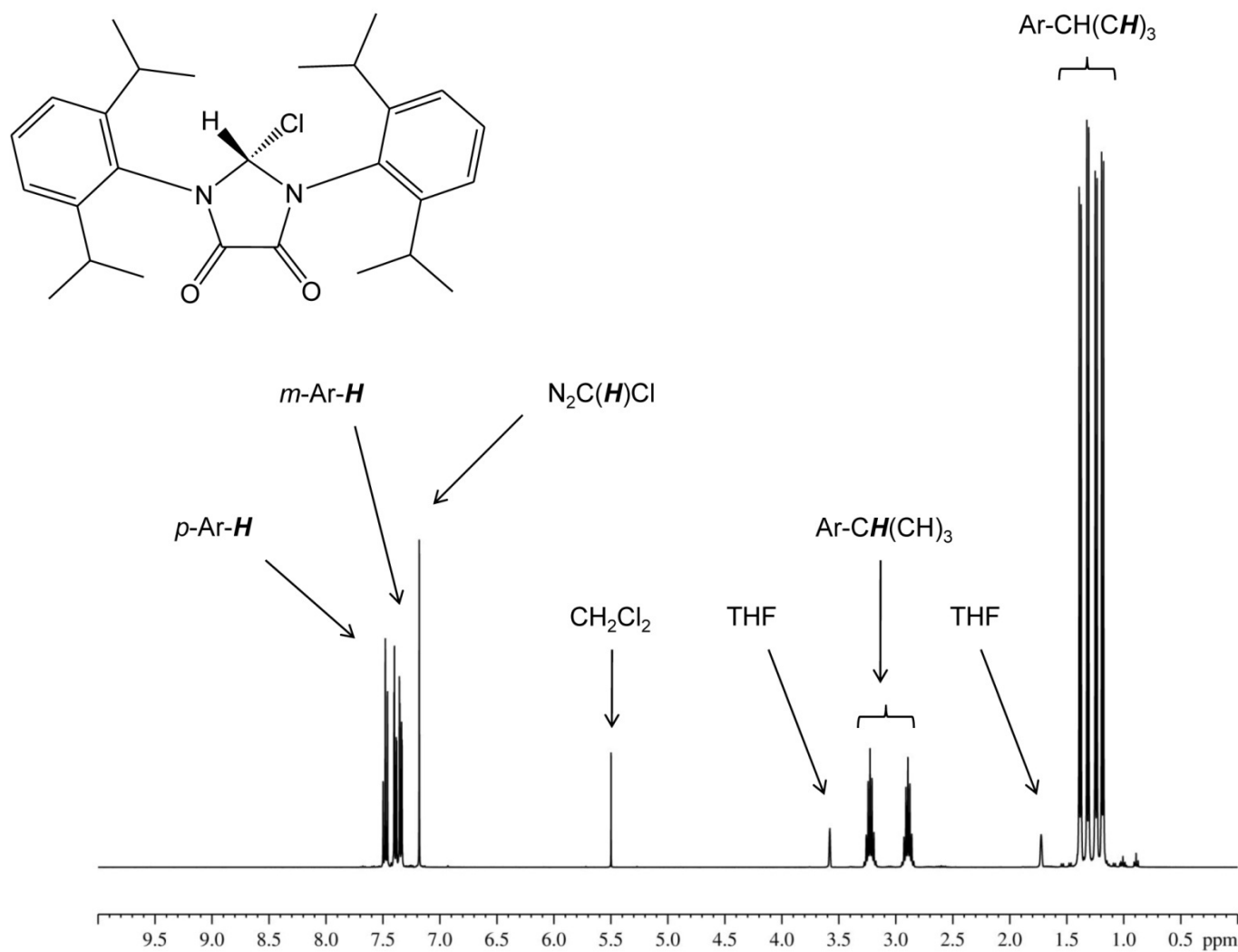
^1H NMR Spectrum of 2-chloro-1,3-bis(2,6-dimethylphenyl)imidazolidine-4,5-dione (**1b**)



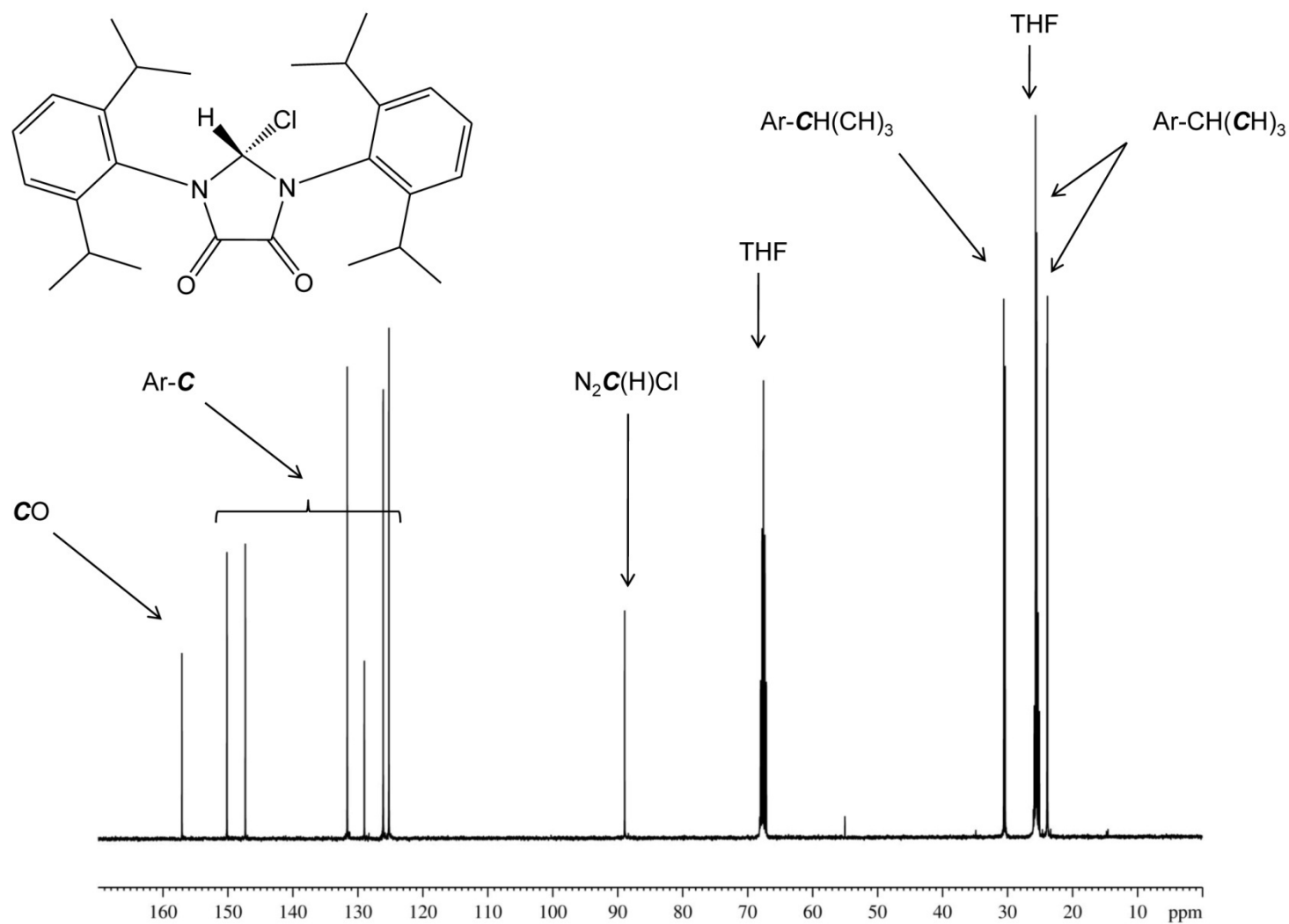
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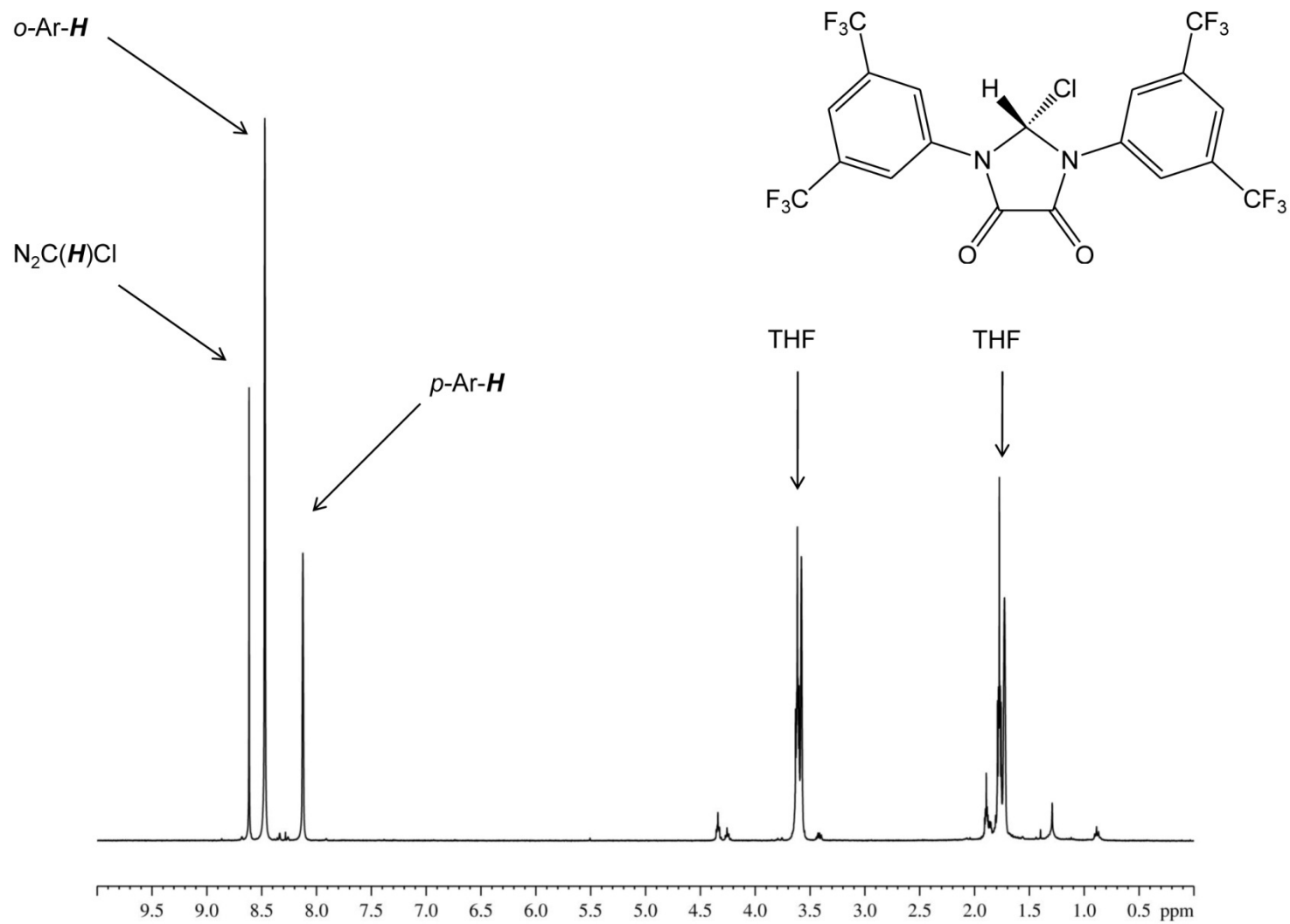
¹H NMR Spectrum of 2-chloro-1,3-bis(2,6-diisopropylphenyl)imidazolidine-4,5-dione (**1c**)



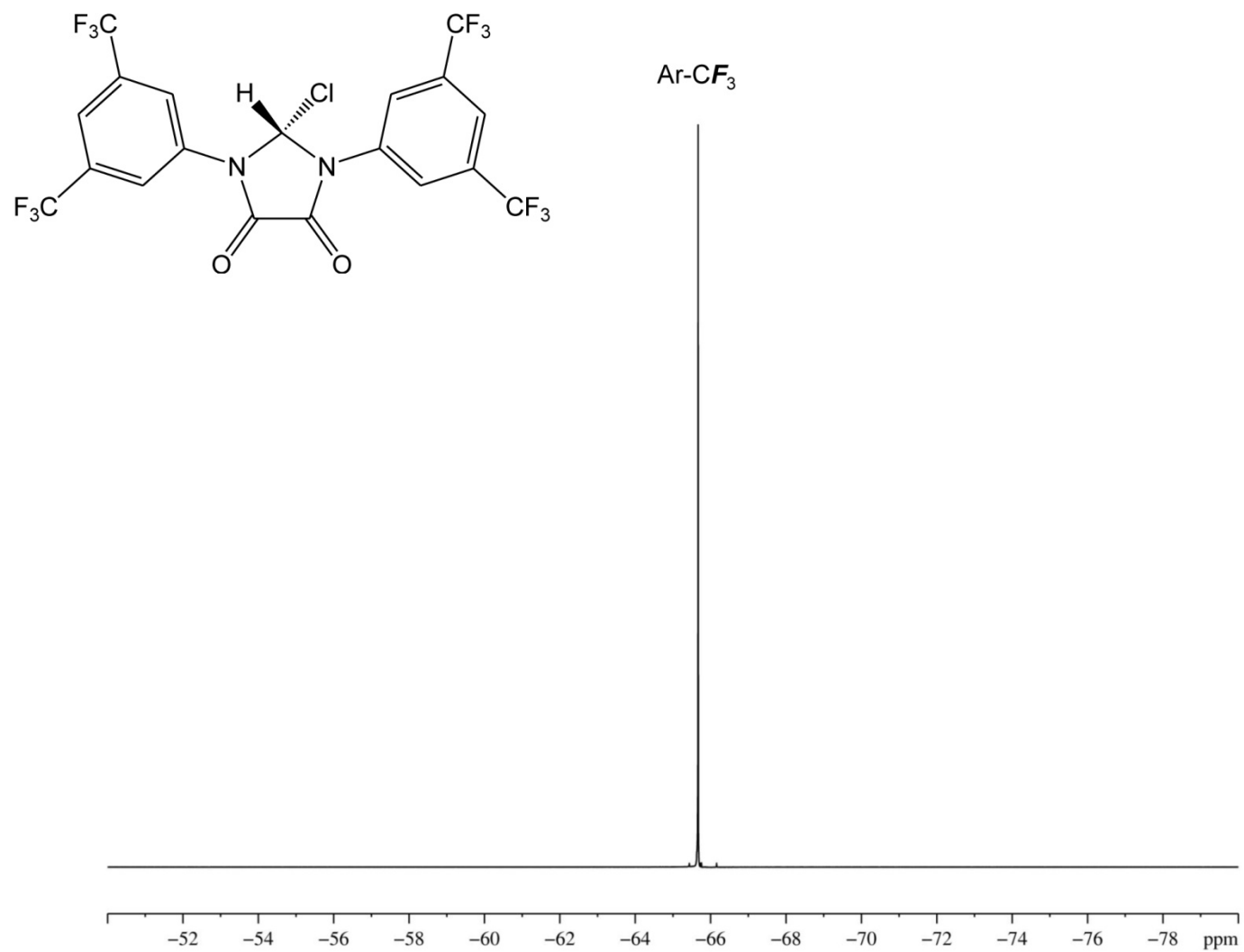
^{13}C NMR Spectrum of 2-chloro-1,3-bis(2,6-diisopropylphenyl)imidazolidine-4,5-dione (**1c**)



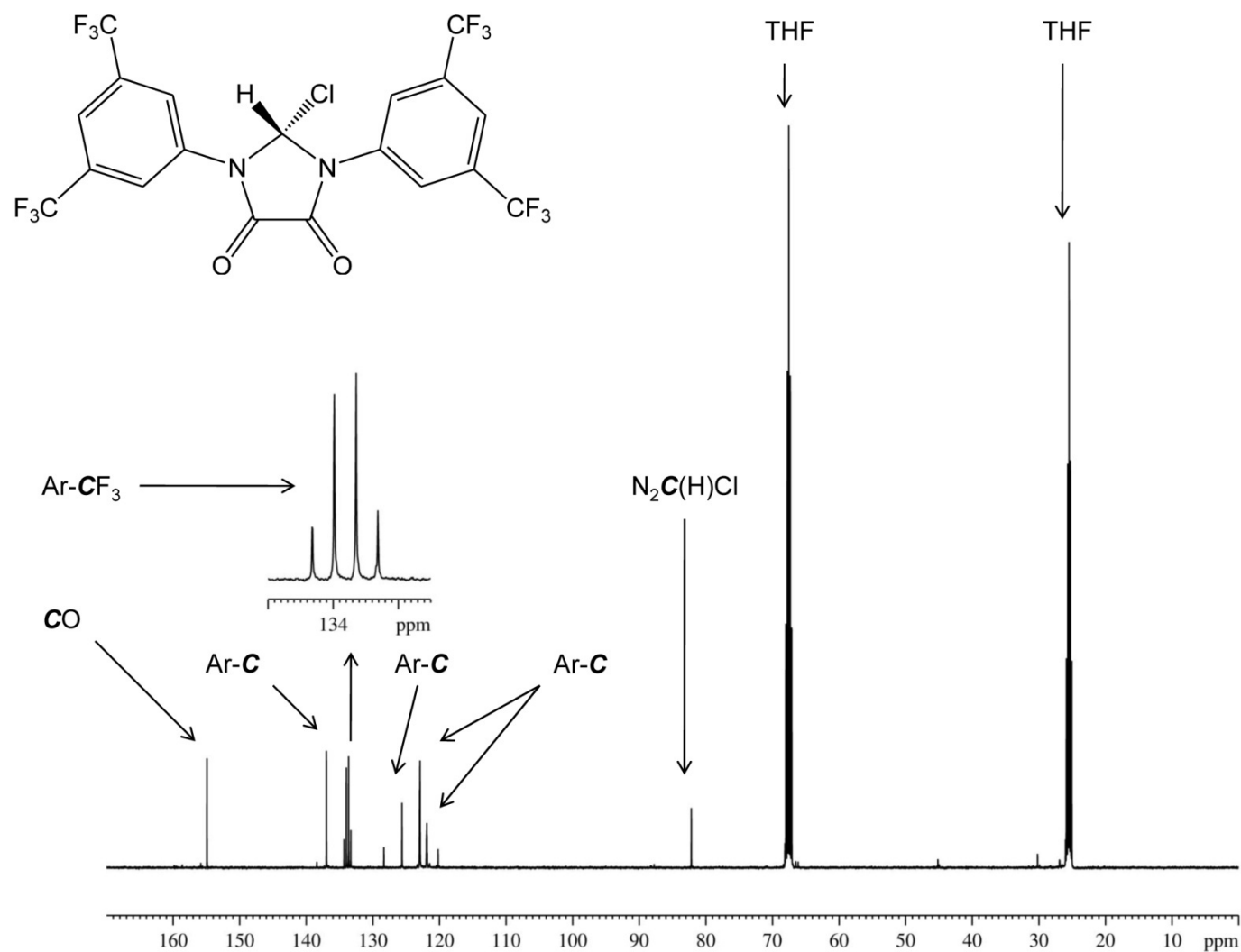
^1H NMR Spectrum of 2-chloro-1,3-bis(3,5-trifluoromethylphenyl)imidazolidine-4,5-dione



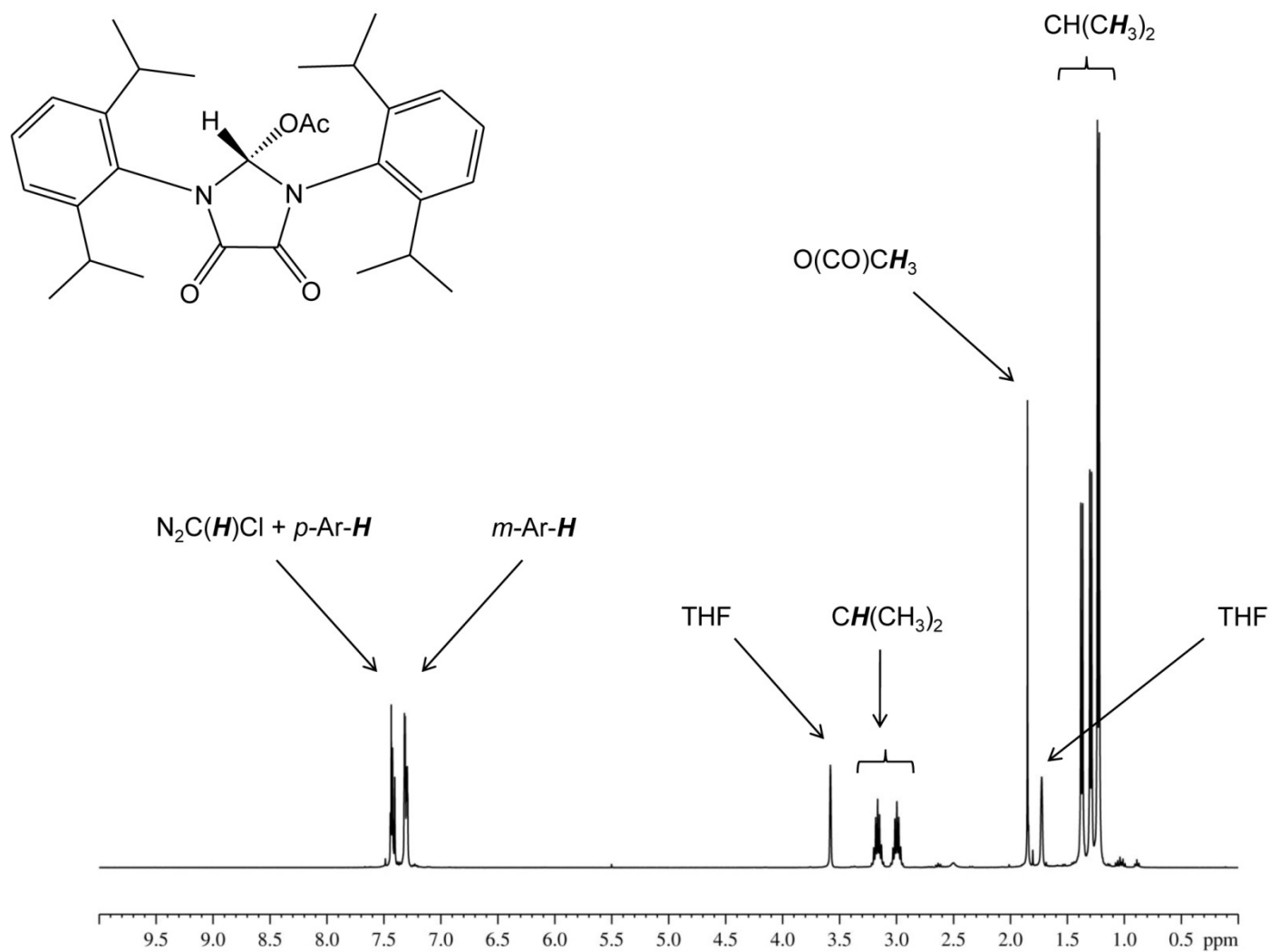
^{19}F NMR Spectrum of 2-chloro-1,3-bis(3,5-trifluoromethylphenyl)imidazolidine-4,5-dione



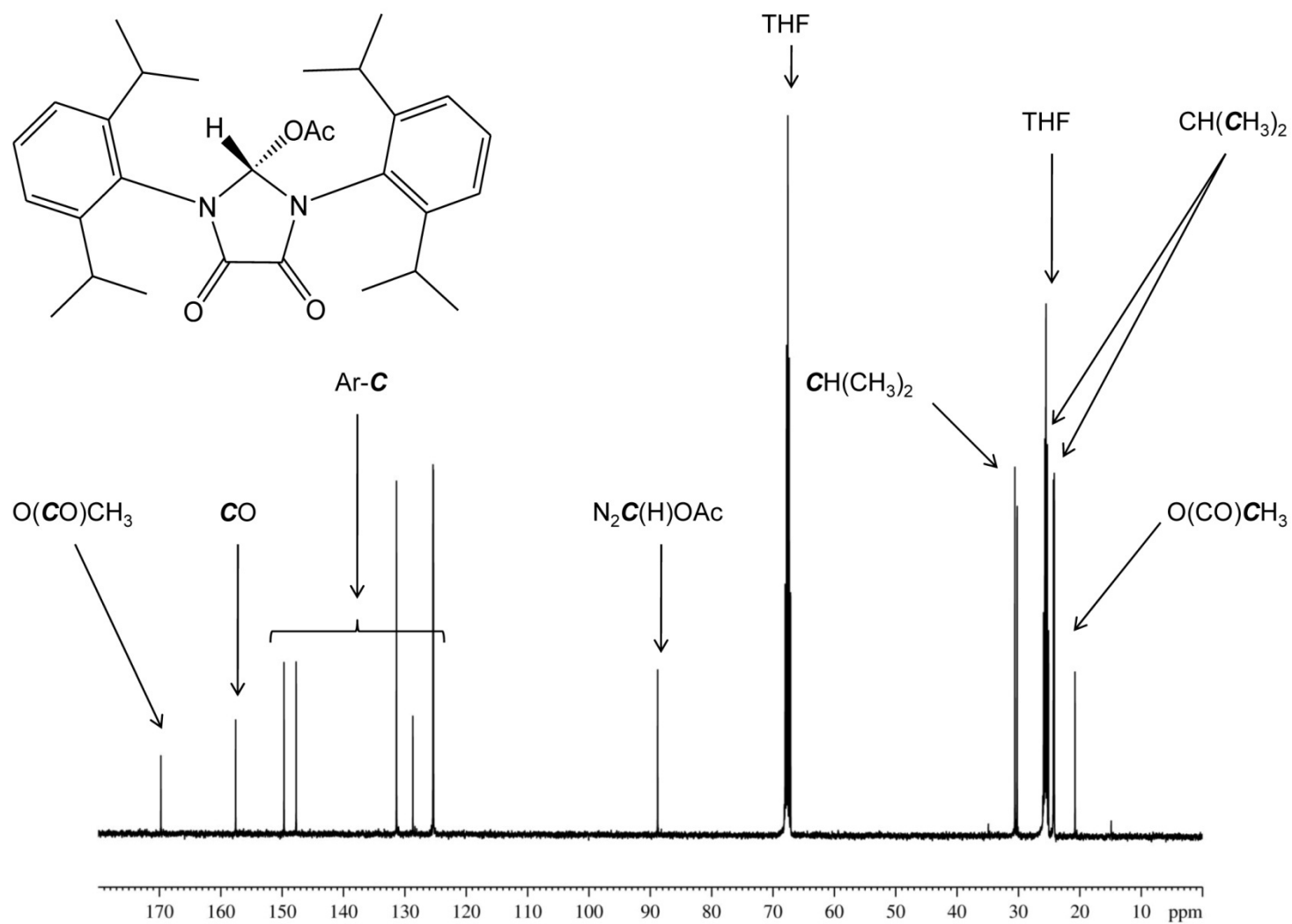
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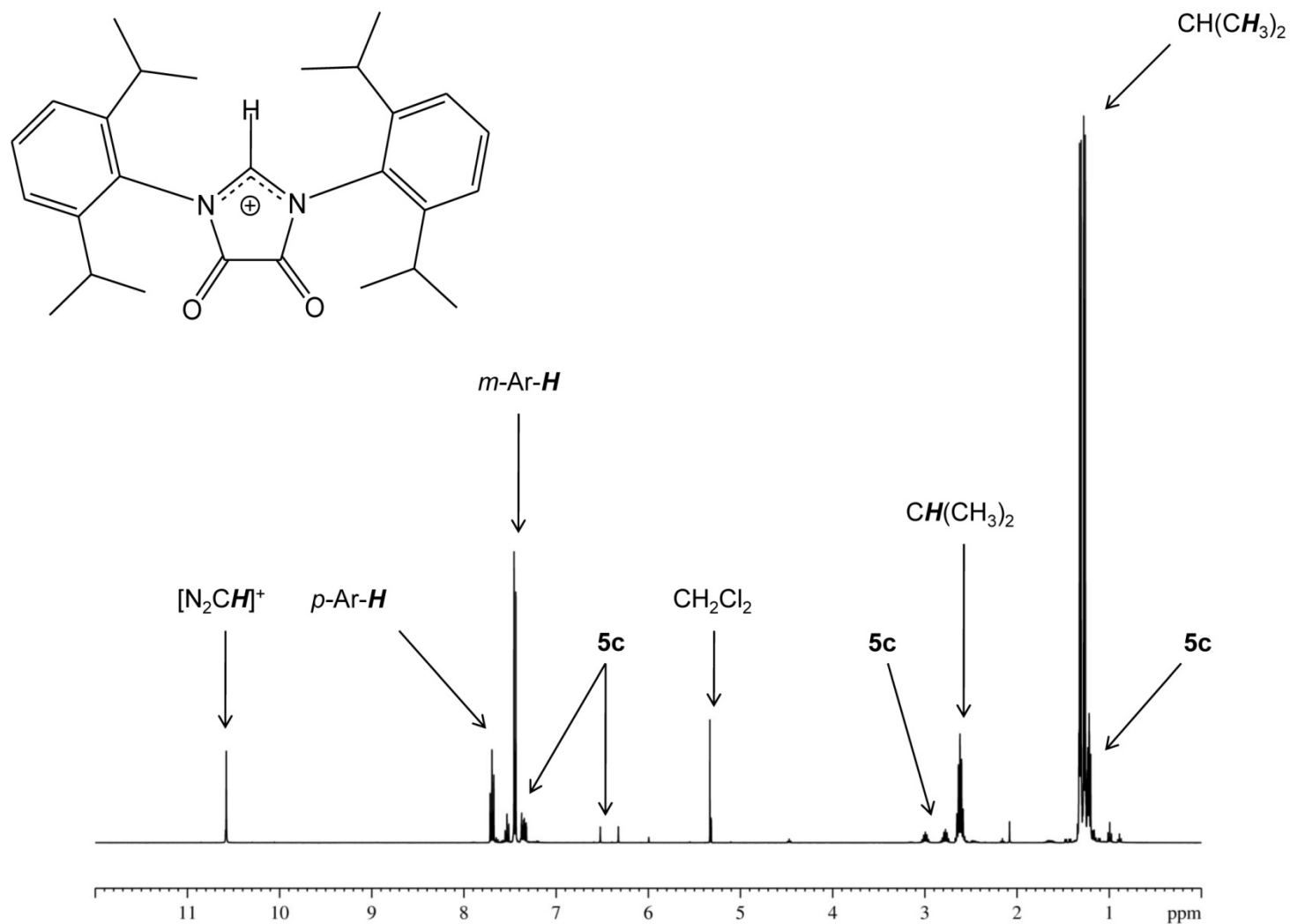
^1H NMR Spectrum of acetic acid-1,3-bis(2,6-dimethylphenyl)-4,5-dioxoimidazolidin-2-yl ester (**3c**)



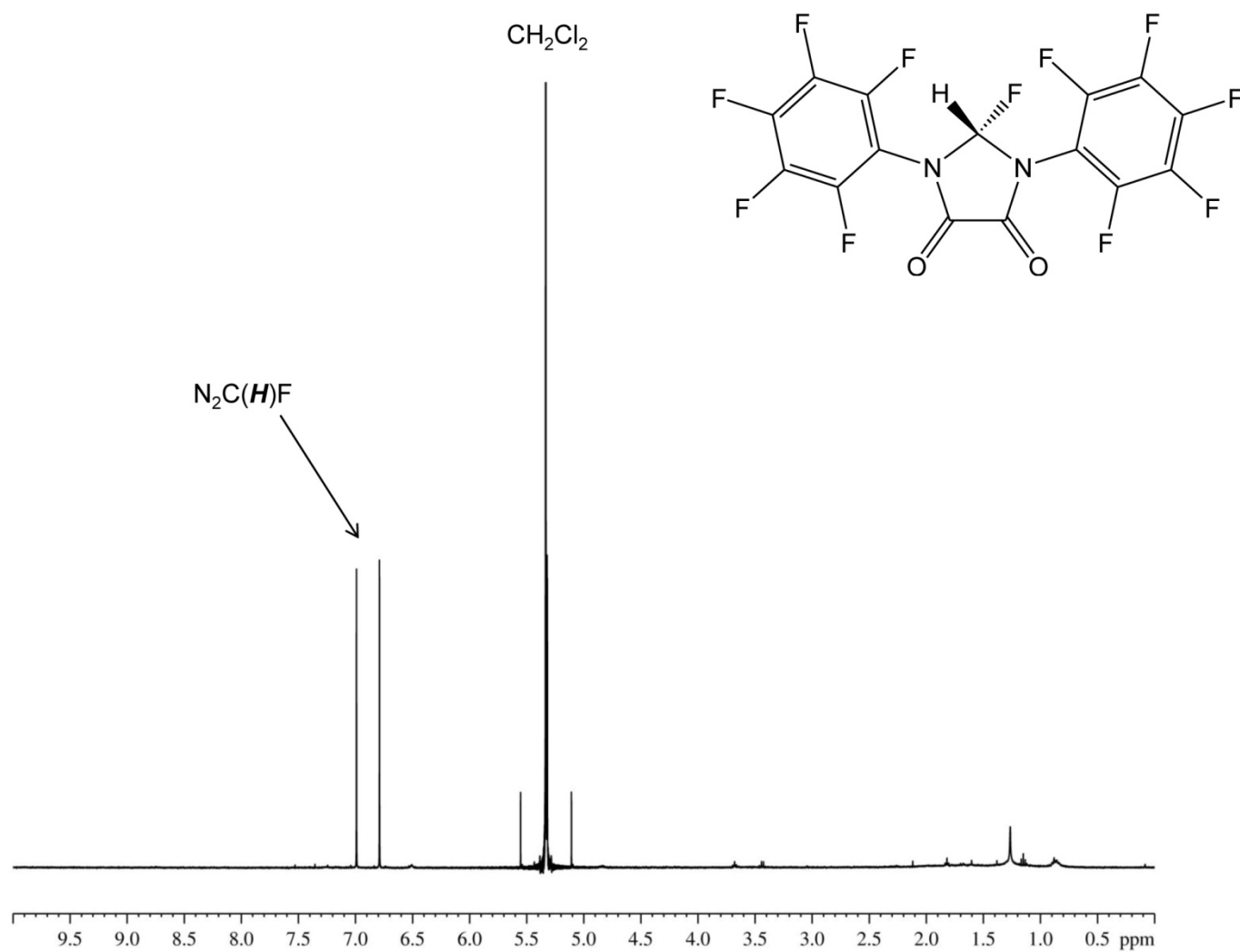
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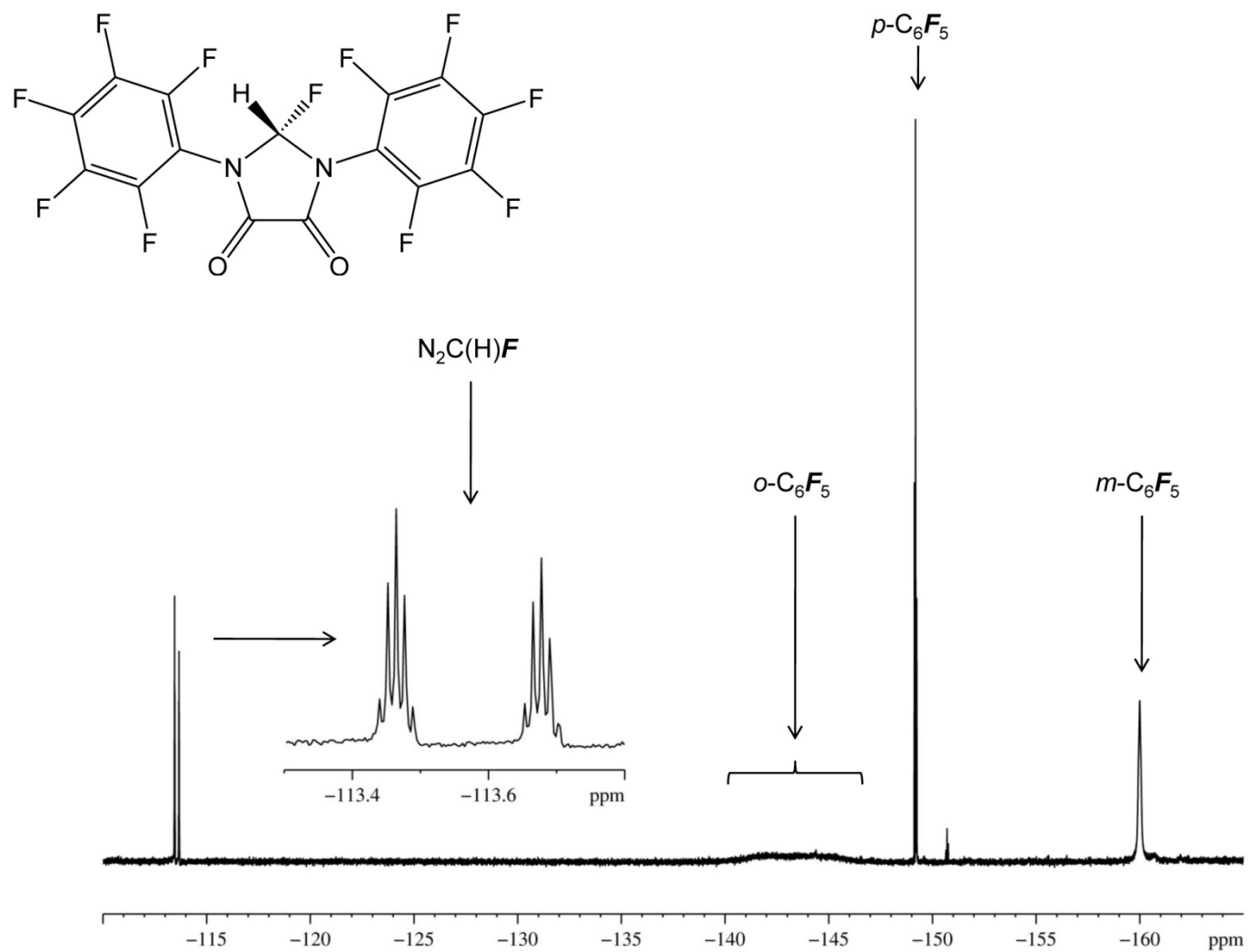
¹H NMR Spectrum of 1,3-bis(2,6diisopropylphenyl)imidazolidium-4,5-dione hexafluorophosphate
(4c)



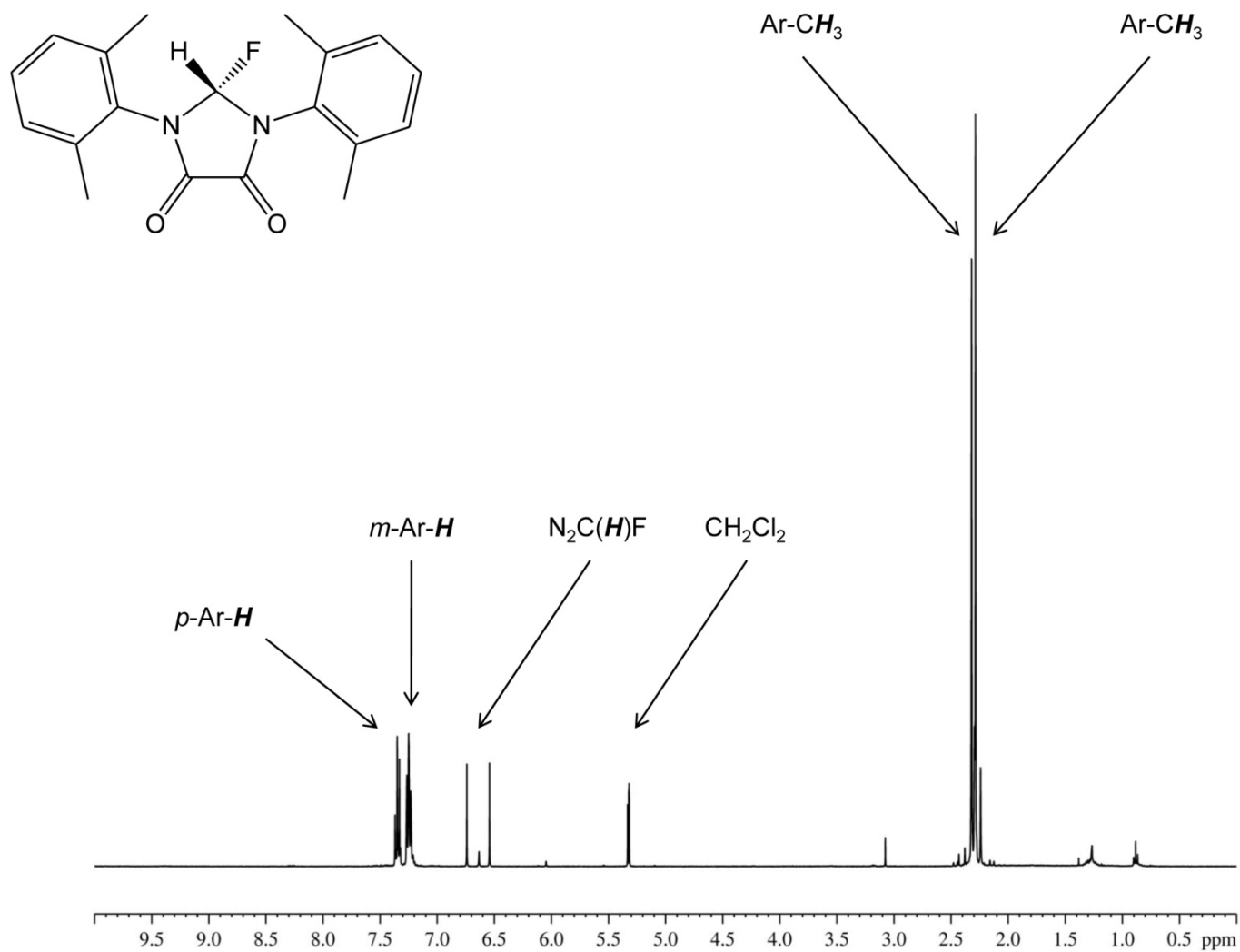
^1H NMR Spectrum of 2-fluoro-1,3-bis(pentafluorophenyl)imidazolidine-4,5-dione (**5a**)



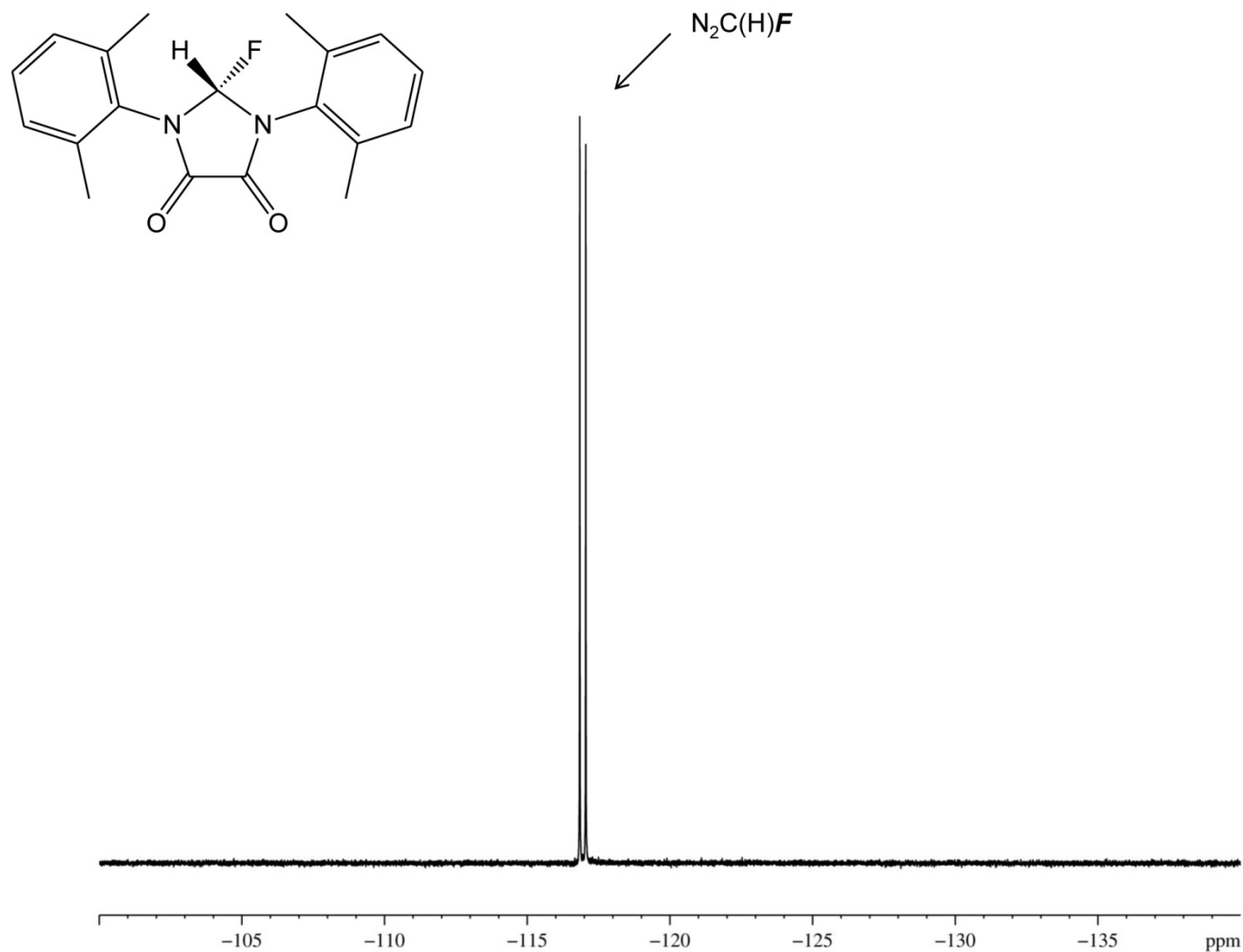
^{19}F NMR Spectrum of 2-fluoro-1,3-bis(pentafluorophenyl)imidazolidine-4,5-dione (**5a**)



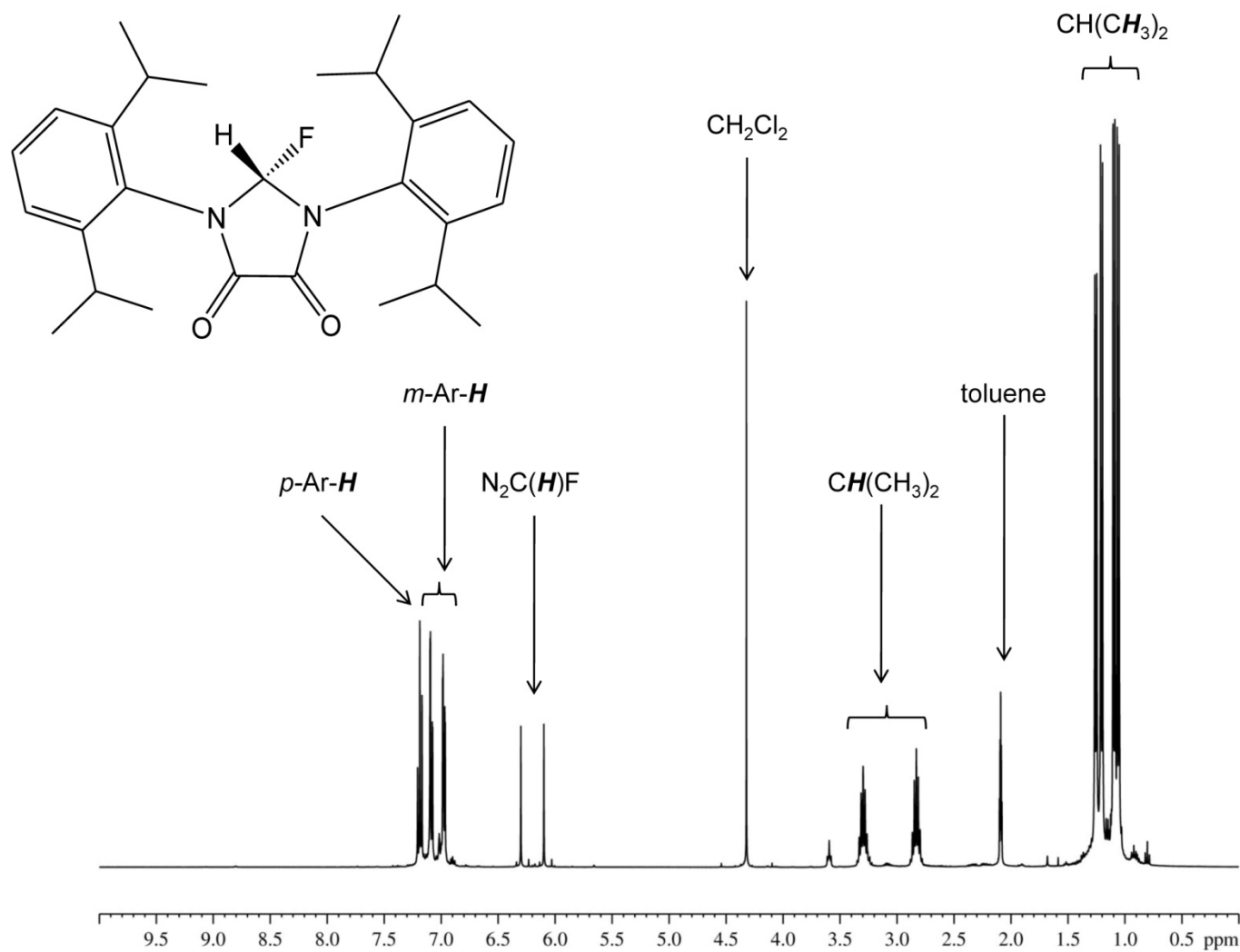
^1H NMR Spectrum of 2-fluoro-1,3-bis(2,6-dimethylphenyl)imidazolidine-4,5-dione (**5b**)



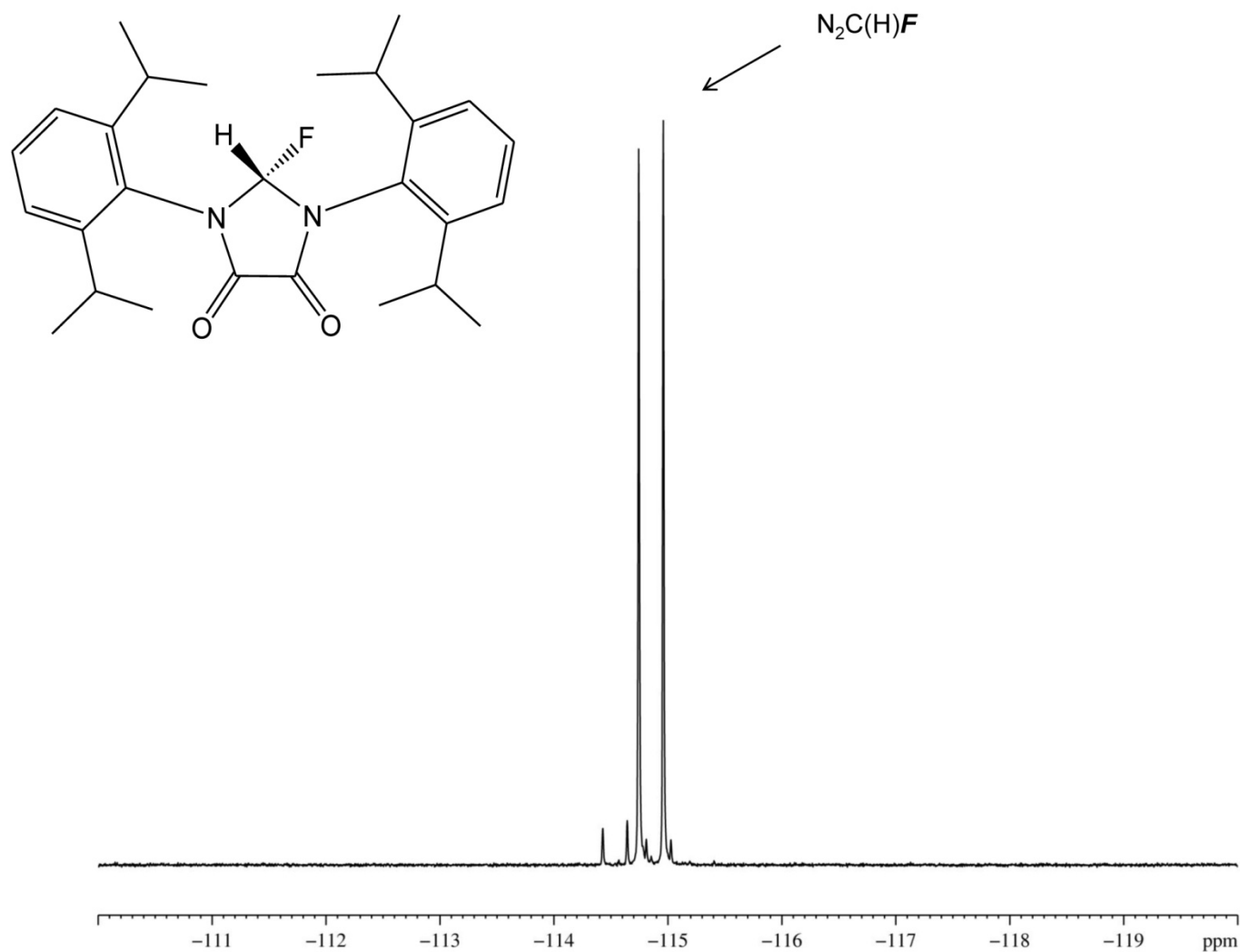
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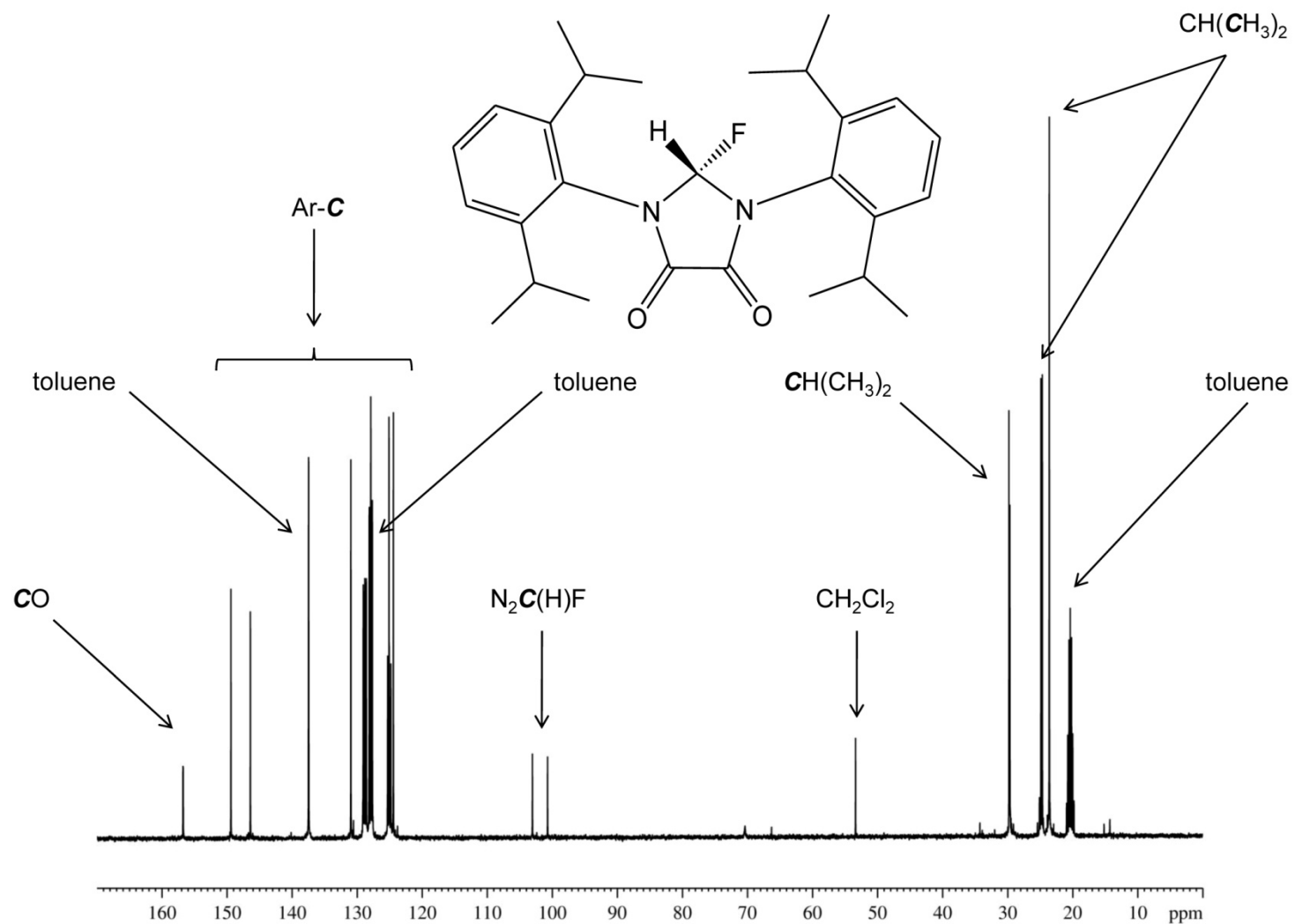
¹H NMR Spectrum of 2-fluoro-1,3-bis(2,6-diisopropylphenyl)imidazolidine-4,5-dione (**5c**)



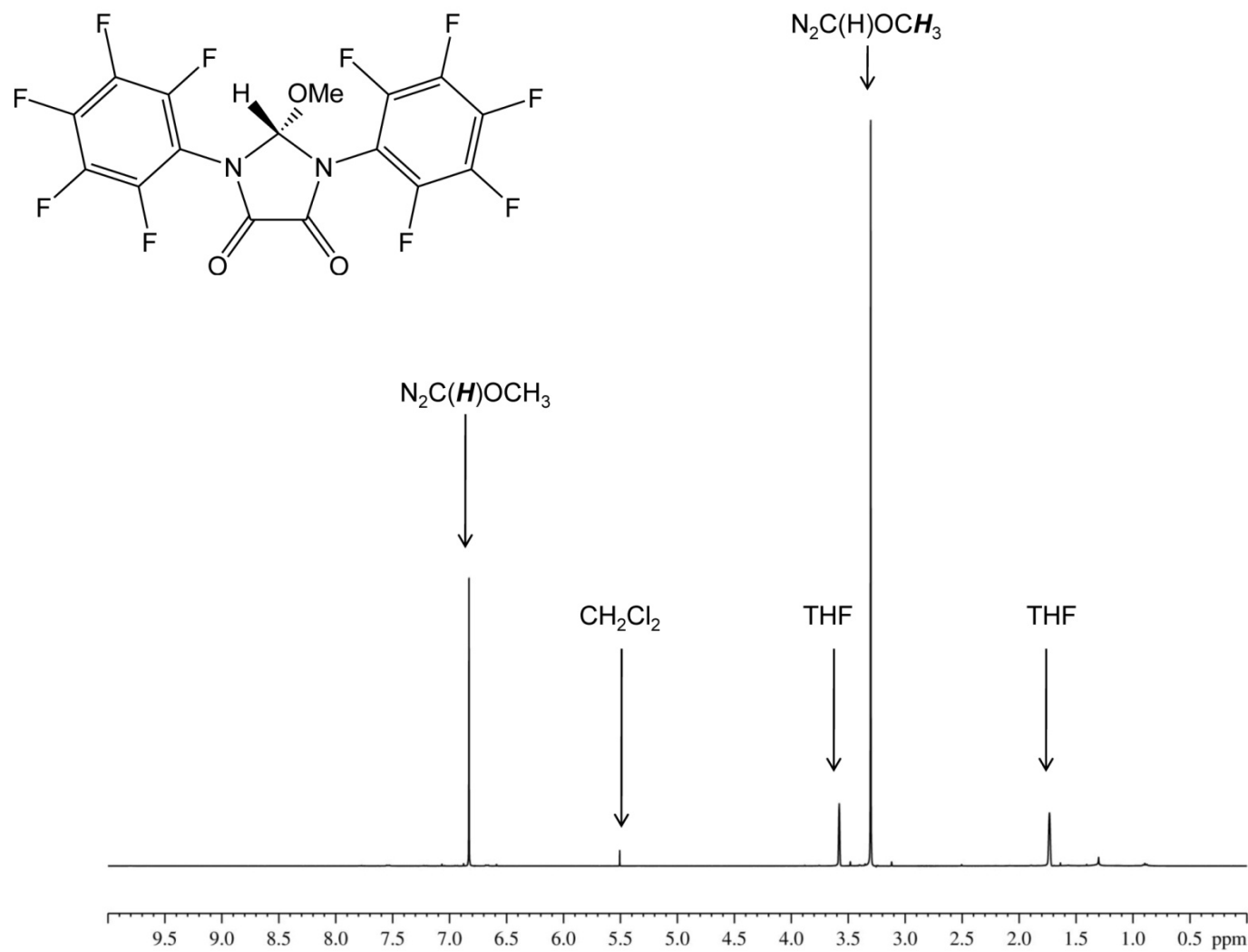
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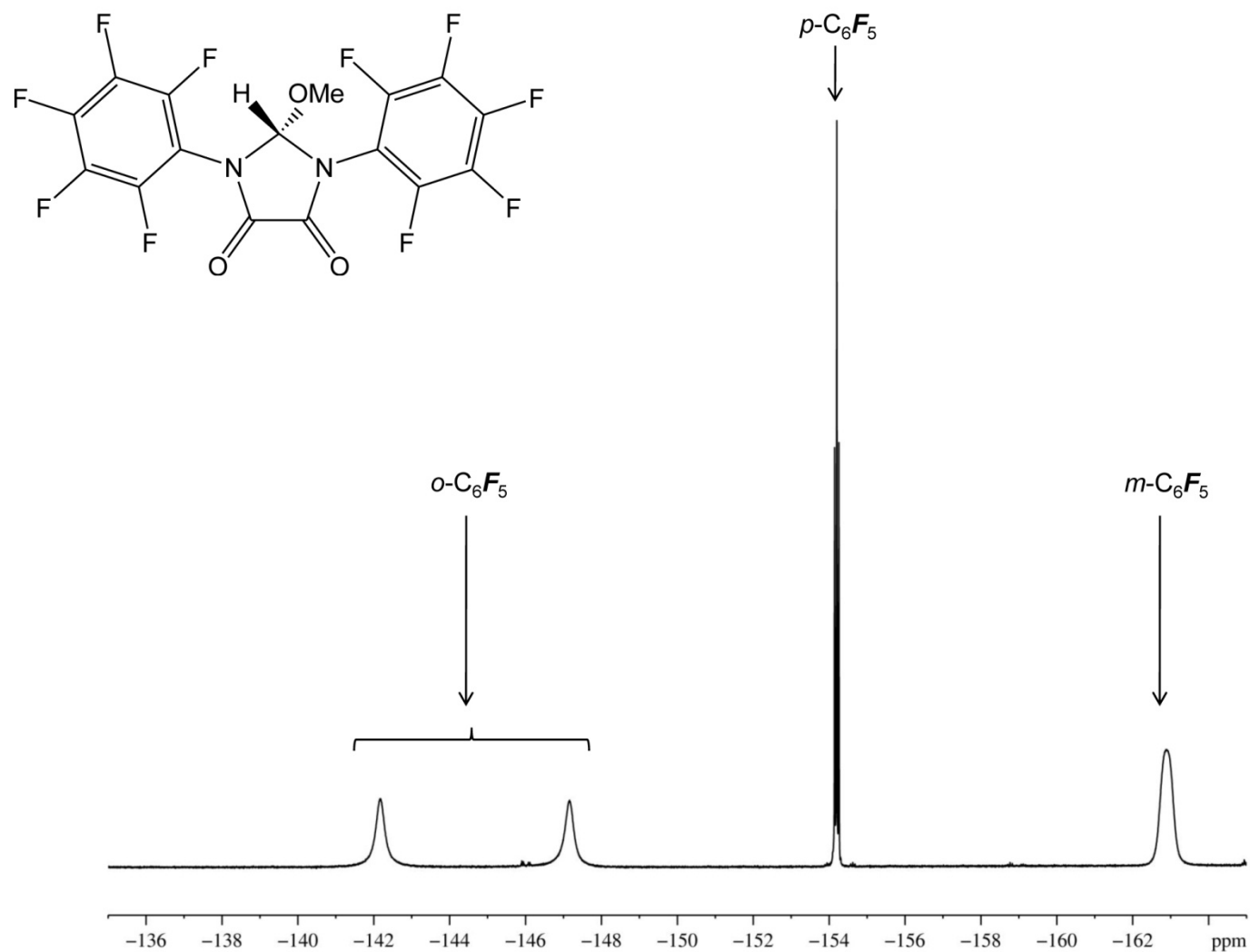
^{13}C NMR Spectrum of 2-fluoro-1,3-bis(2,6-diisopropylphenyl)imidazolidine-4,5-dione (**5c**)



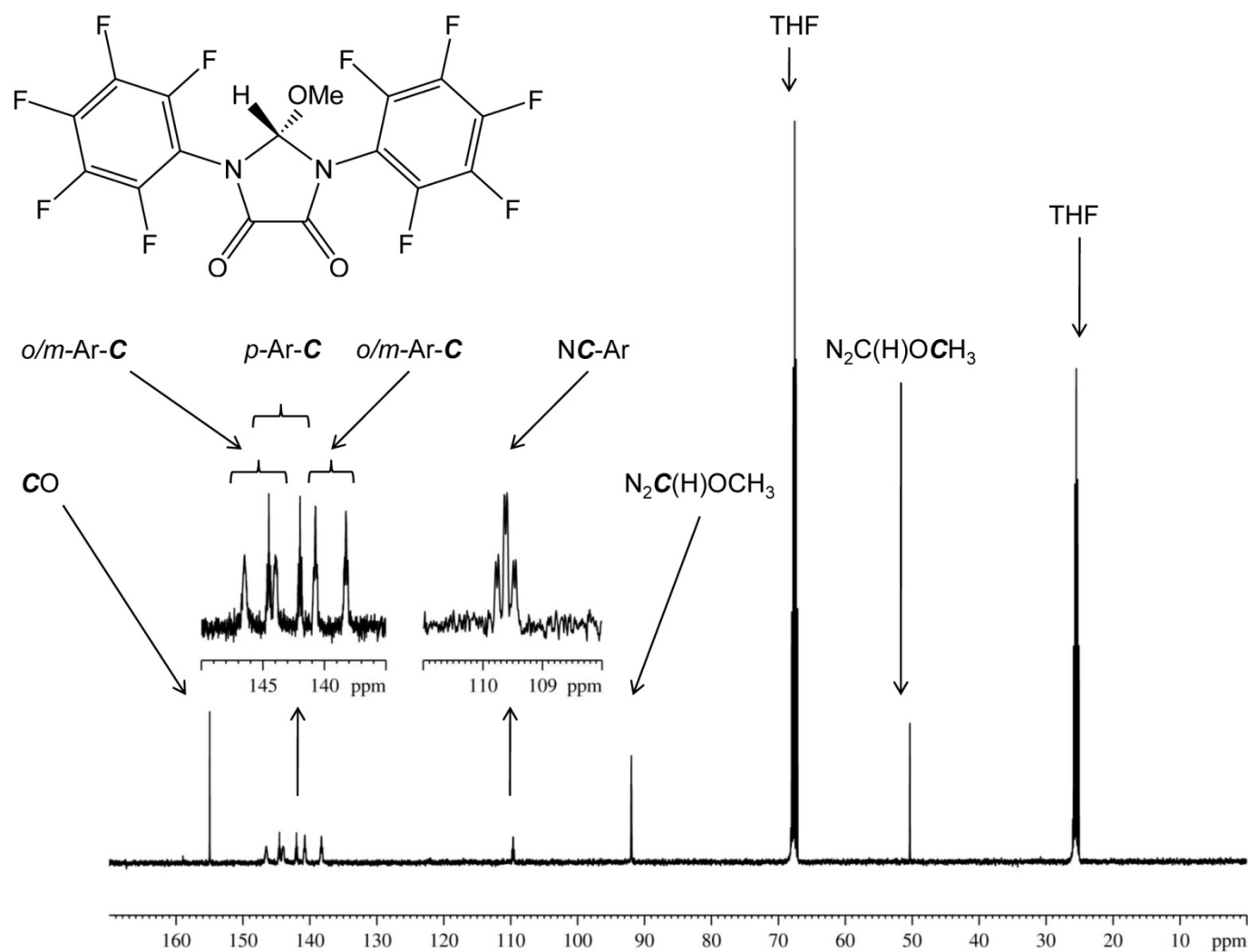
^1H NMR Spectrum of 2-methoxy-1,3-bis(pentafluorophenyl)imidazolidine-4,5-dione (**6a**)



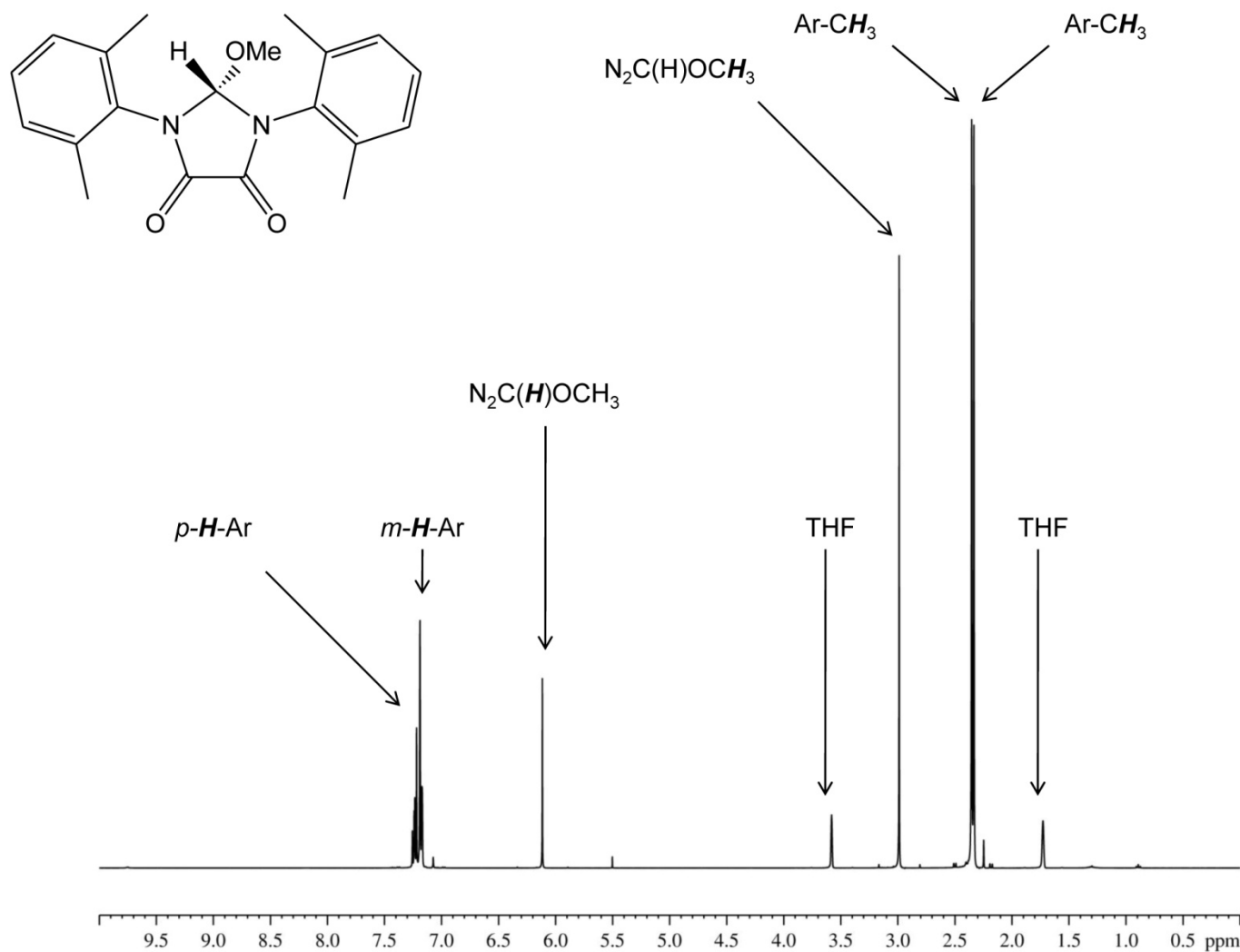
^{19}F NMR Spectrum of 2-methoxy-1,3-bis(pentafluorophenyl)imidazolidine-4,5-dione (**6a**)



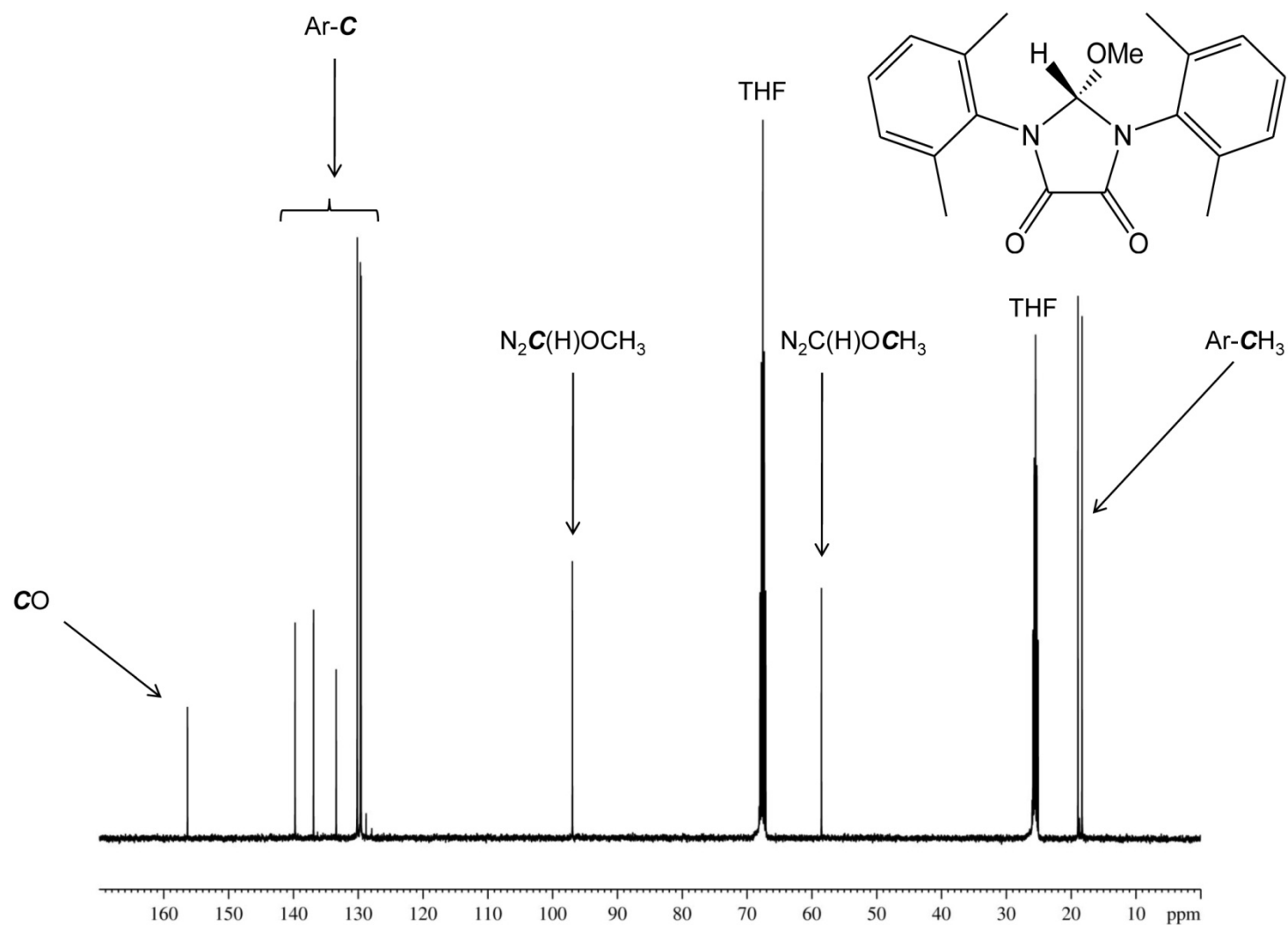
¹³C NMR Spectrum of 2-methoxy-1,3-bis(pentafluorophenyl)imidazolidine-4,5-dione (**6a**)



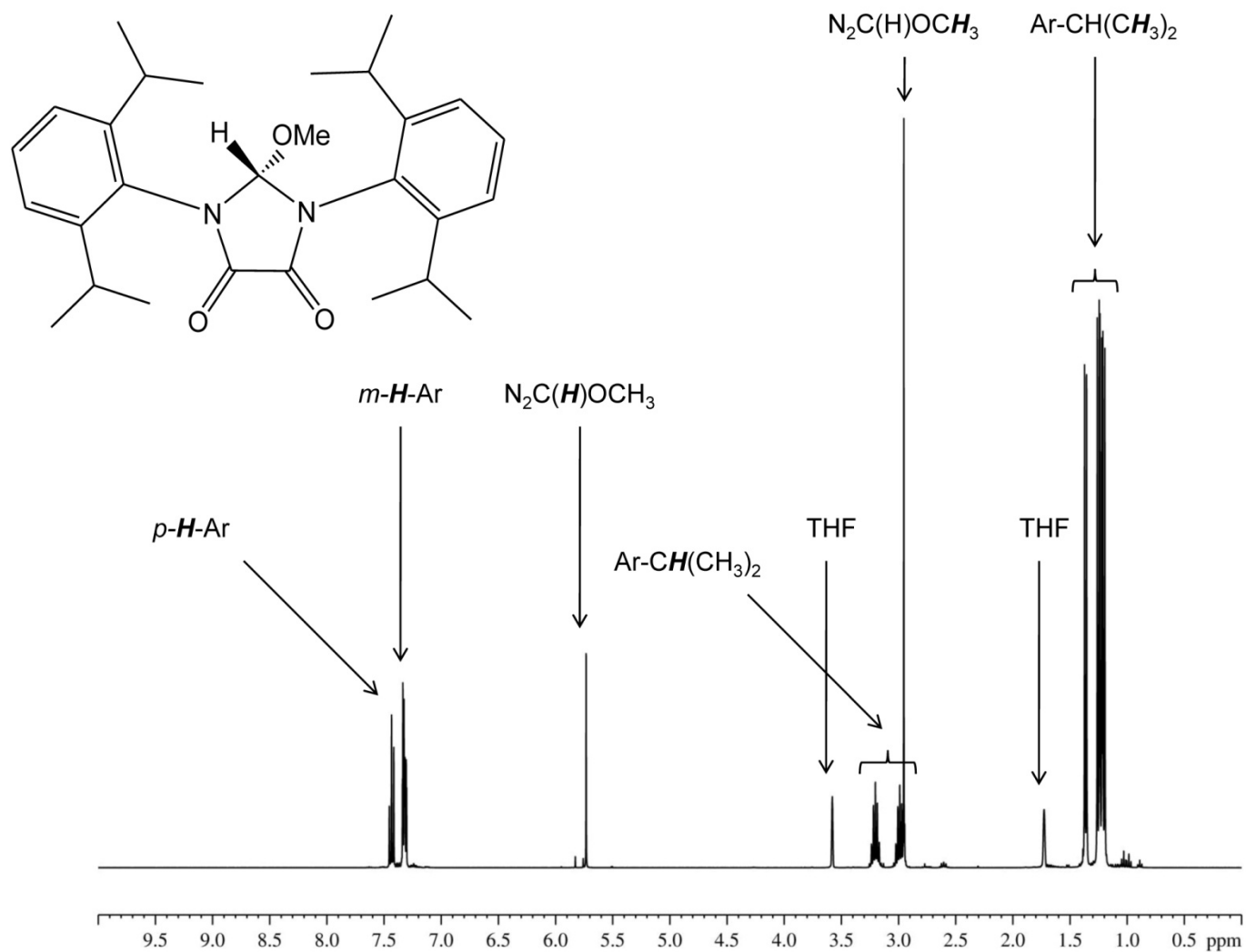
¹H NMR Spectrum of 2-methoxy-1,3-bis(2,6-dimethylphenyl)imidazolidine-4,5-dione (**6b**)



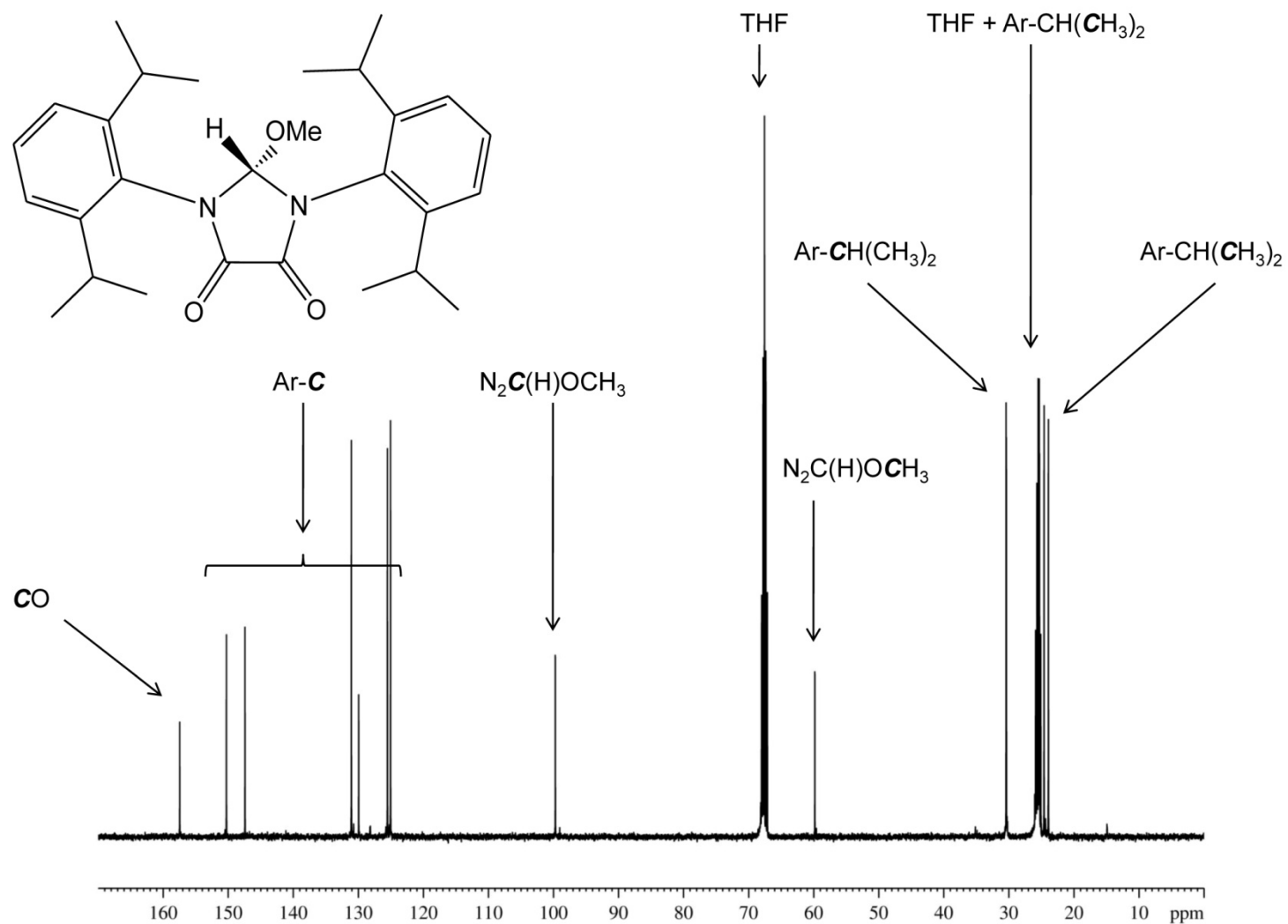
^{13}C NMR Spectrum of 2-methoxy-1,3-bis(2,6-dimethylphenyl)imidazolidine-4,5-dione (**6b**)



^1H NMR Spectrum of 2-methoxy-1,3-bis(2,6-diisopropylphenyl)imidazolidine-4,5-dione (**6c**)



^{13}C NMR Spectrum of 2-methoxy-1,3-bis(2,6-diisopropylphenyl)imidazolidine-4,5-dione (**6c**)



^1H NMR Spectrum of 1,3-bis(2,6-diisopropylphenyl)imidazolidine-4,5-dione (**7c**)

