Supporting information

Attempted Isolation and Characterization of Diazirinone (N_2CO)

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General Information.

Acetonitrile was distilled from CaH_2 and $CDCl_3$ from $CaCl_2$ shortly before use. 3-Chloro-3-(*p*-nitrophenoxy)diazirine (**5**) was prepared according to Moss et al. (*J. Am. Chem. Soc.* **2005**, 127, 2408-2409). Of note is the sensitivity of diazirine **5** to acid. When stored at −25 °C in the presence of a small amount of chloroform, decomposition was observed within one month. These problems were minimized by not reusing whatever material had been dedicated to spectroscopy.

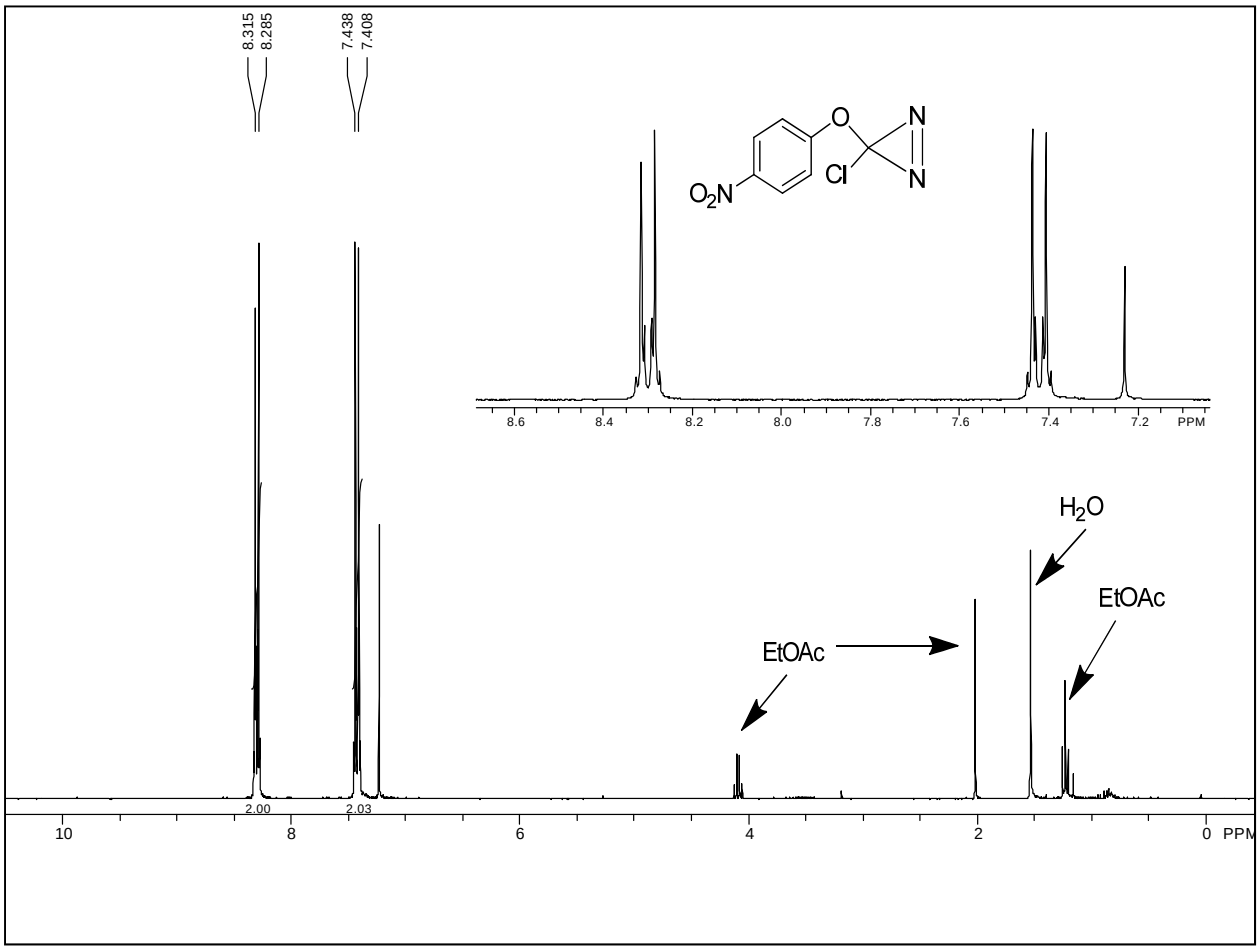
NMR spectra (^1H, 500 MHz or 300 MHz; ^{19}F, 282 MHz) were obtained in $CDCl_3$ or CD_2Cl_2 and referenced to residual solvent (NSF CHE-8813550, CHE-9208463, CHE-9629688; NIH 1 S10 RR04981-10, 1 S10 RR08389-01). Mass spectra were obtained using either electrospray ionization with time-of-flight analyzer (NSF CHE-9974739) or electron impact ionization (NSF CHE-9304546).

Cartesian Coordinates.

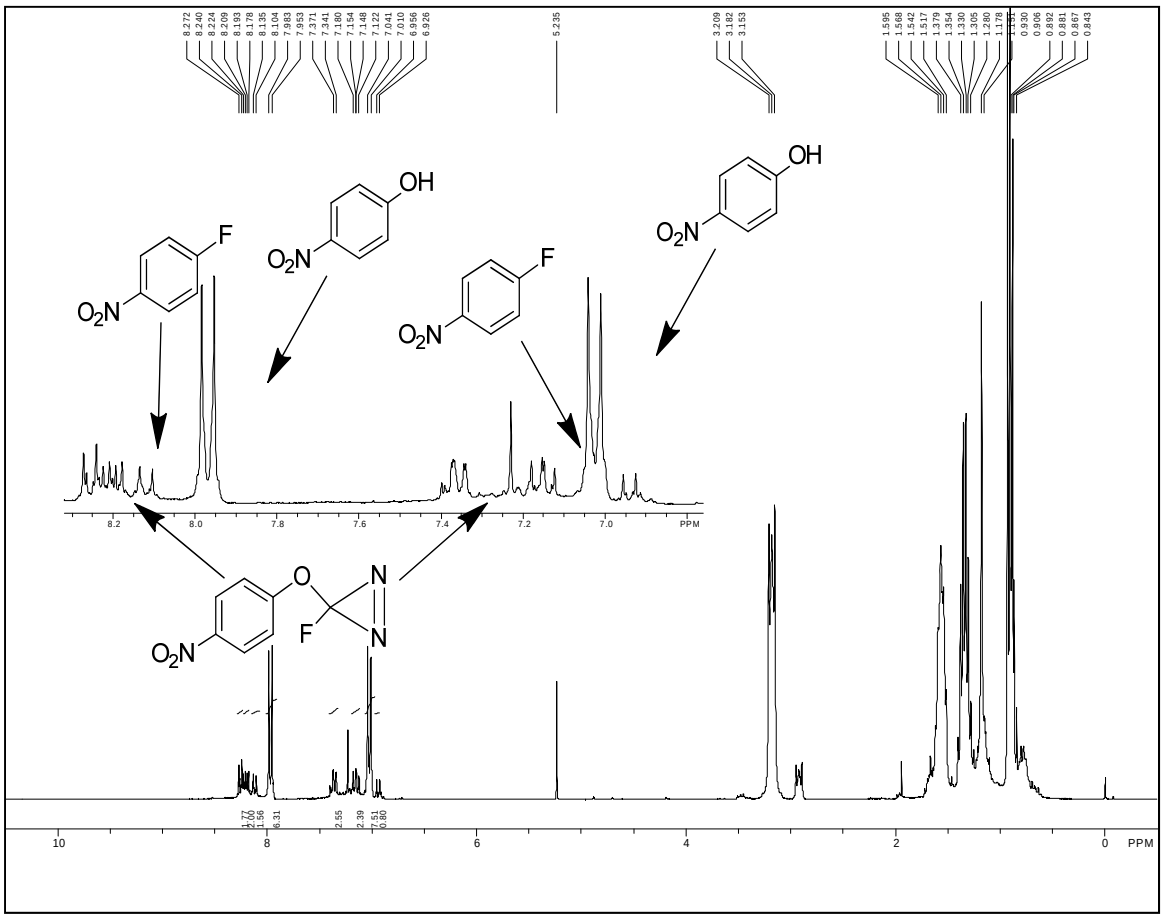
Diazirinone (**1**); CCSD(T)/ANO2

Z-matrix Symbol	Atomic Number	Coordinates (in bohr) X	Y	Z
O	8	0.00000000	0.00000000	-2.75110880
C	6	0.00000000	0.00000000	-0.50938536
N	7	0.00000000	1.24562519	1.78947761
N	7	0.00000000	-1.24562519	1.78947761

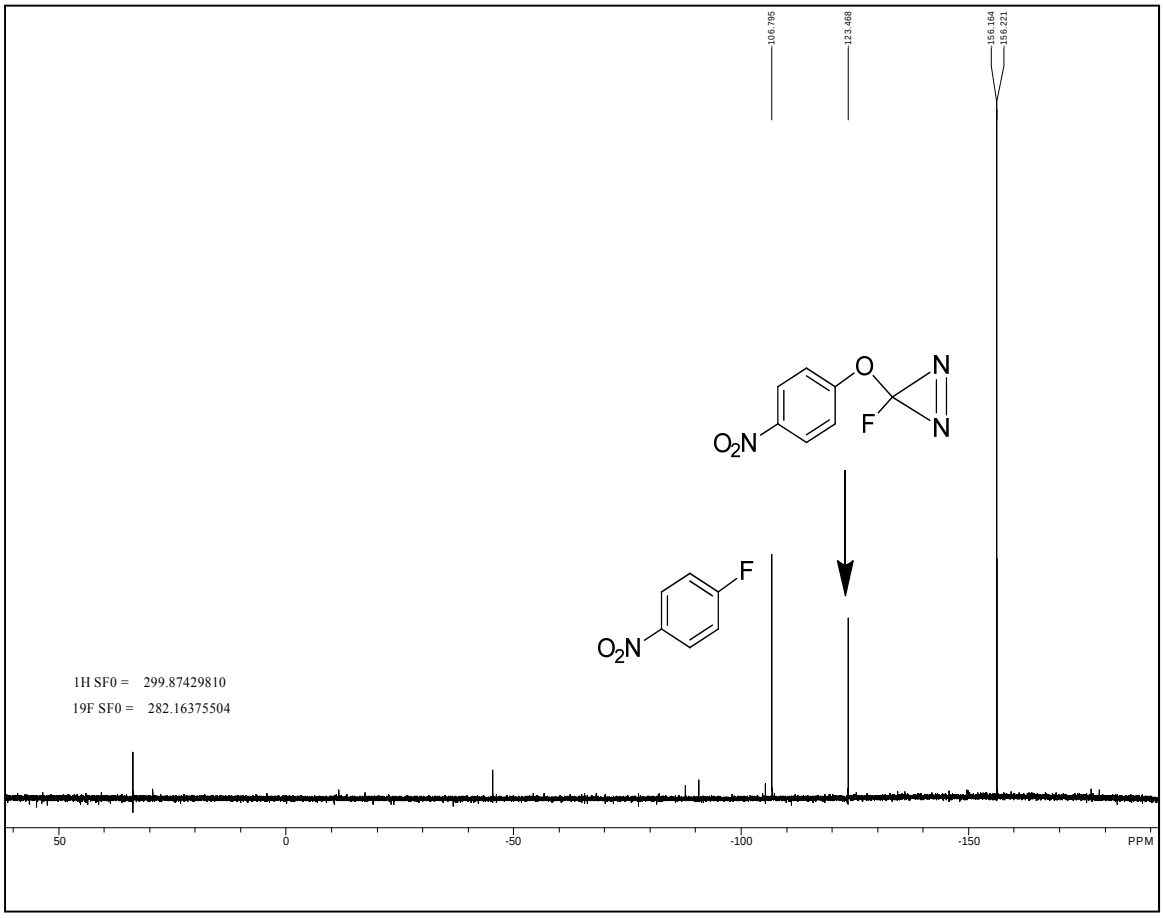
3-Chloro-3-(*p*-nitrophenoxy)diazirine (**5**)
(^{1}H NMR, 300 MHz)



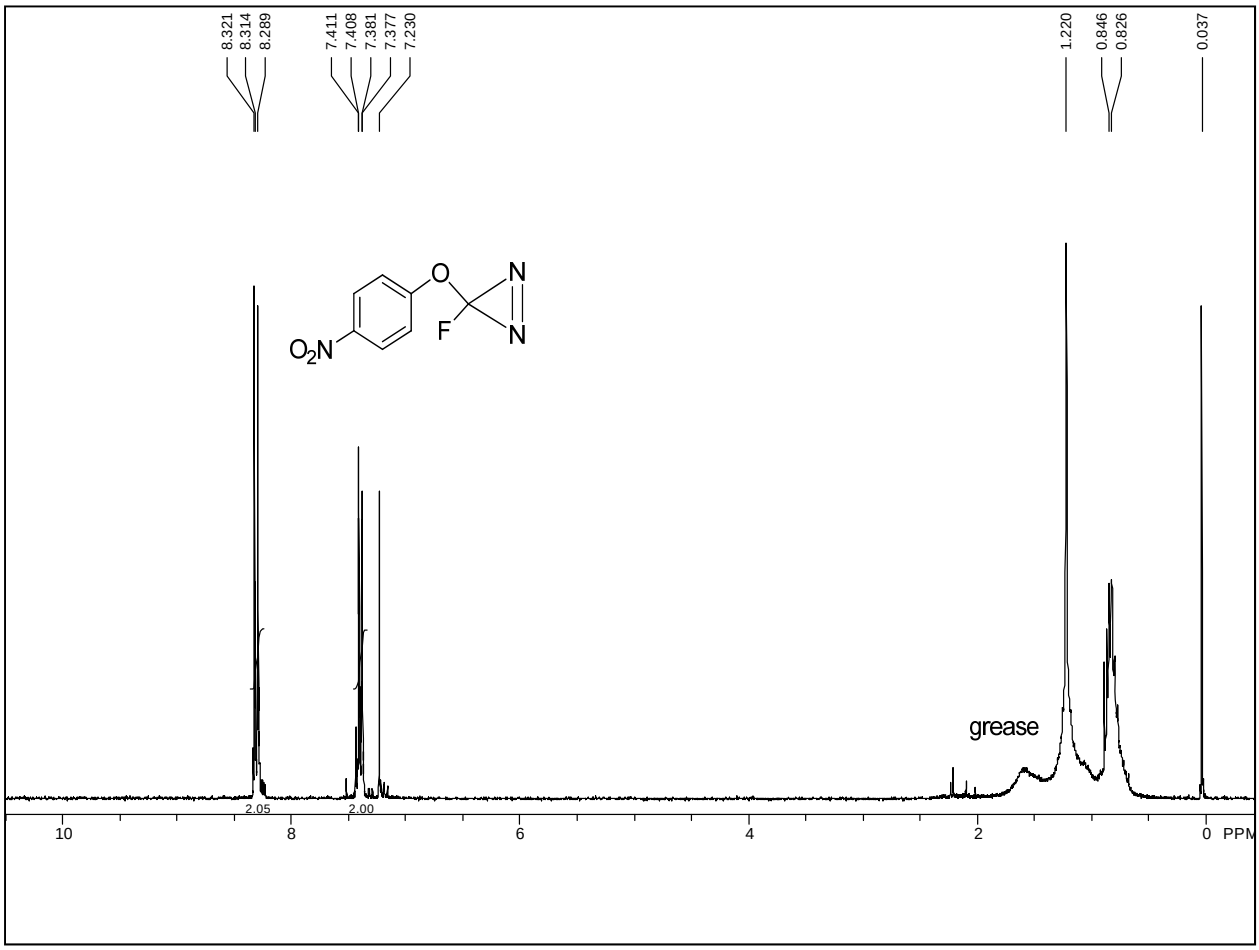
^{1}H NMR (300 MHz) spectrum of the residual reaction mixture from an attempted matrix isolation experiment using 3-chloro-3-(*p*-nitrophenoxy)diazirine (**5**) and TBAF followed by solvation in CH_2Cl_2 and two aqueous washes as described in the main paper. In this crude mixture can be identified 3-fluoro-3-(*p*-nitrophenoxy)diazirine (**9**), *p*-fluoronitrobenzene (**7**), and *p*-nitrophenol.



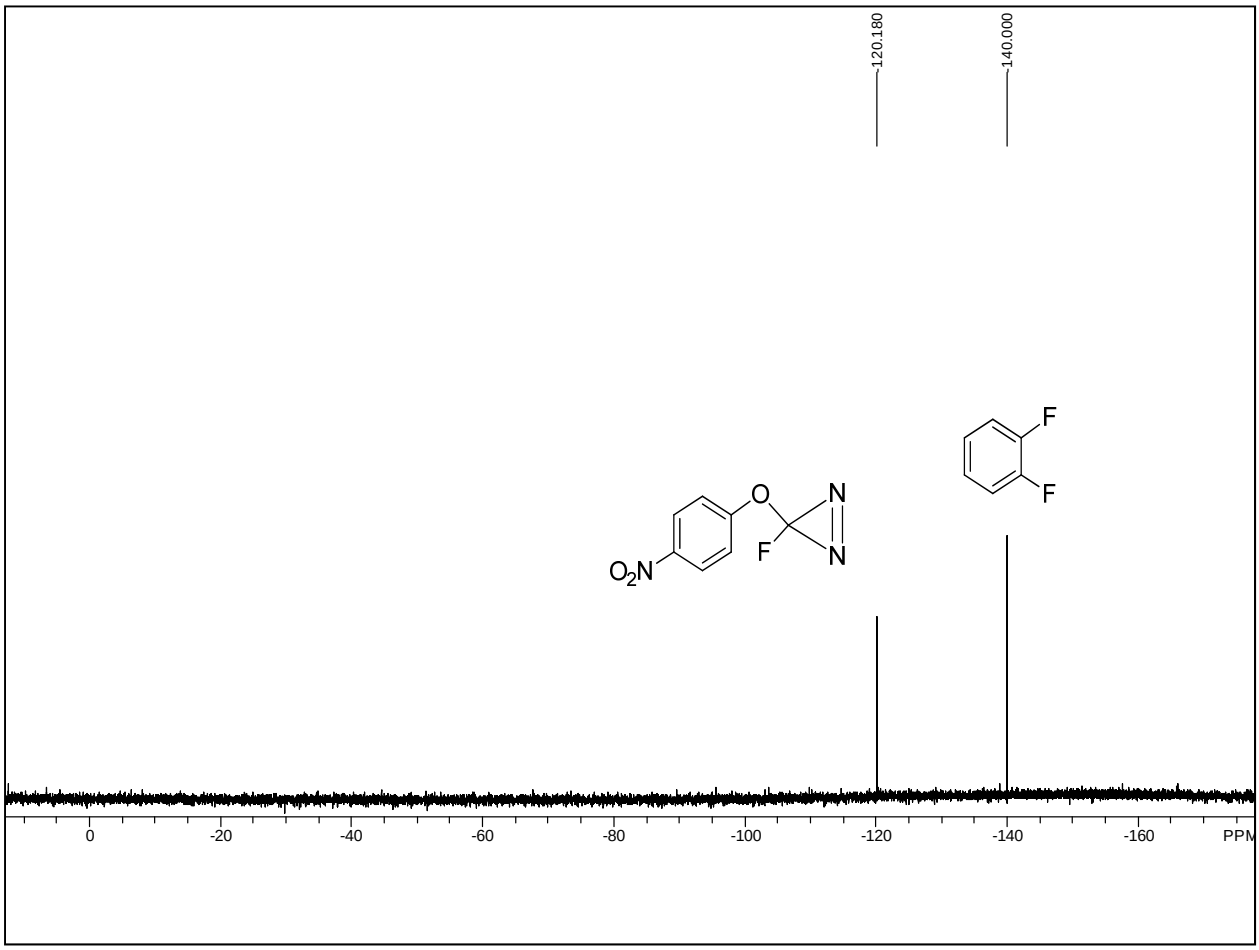
^{19}F NMR (282 MHz) spectrum of the above reaction mixture.



3-Fluoro-3-(*p*-nitrophenoxy)diazirine (**9**)
(^{1}H NMR, 300 MHz)



3-Fluoro-3-(*p*-nitrophenoxy)diazirine (**9**)
(^{19}F NMR, 282 MHz)



p-Nitrophenol
(^{1}H NMR, 300 MHz)