

Supplementary Material

Aromatic metamorphosis of an indole into 2-quinolone, dihydrobenzazasiline, and dihydrobenzazagermine

Kazuki Nishihara, Takashi Kurogi, and Hideki Yorimitsu*

Department of Chemistry, Graduate School of Science, Kyoto University, Sakyo-ku, Kyoto, 606-8502 Japan

Email: yori@kuchem.kyoto-u.ac.jp

Table of Contents

Crystallographic Data of 5	S2
NMR Spectra	S3

Table S1. Crystallographic data of **5**

Formula	C ₂₆ H ₂₁ N ₁ Si ₁
Formula weight	375.53
Temperature / °C	−180
λ (Å)	1.54184
Crystal size / mm ³	0.20×0.05×0.02
Crystal system	<i>Monoclinic</i>
Space group	<i>C2/c</i>
<i>a</i> / Å	18.6090(4)
<i>b</i> / Å	9.38980(10)
<i>c</i> / Å	23.7552(4)
α / °	90
β / °	100.577(2)
γ / °	90
<i>V</i> / Å ³	4080.33(12)
<i>Z</i>	8
μ mm ^{−1}	1.077
D _{calcd.} / g·cm ^{−3}	1.223
F(000)	1584
Refl./restr./param.	3981/0/253
Completeness	0.980
GOF	1.073
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>))	0.0432
<i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.1109
<i>R</i> ₁ (all data)	0.0504
<i>wR</i> ₂ (all data)	0.1153
Largest diff. peak and hole / e·Å ^{−3}	0.418, −0.306
CCDC number	2261304

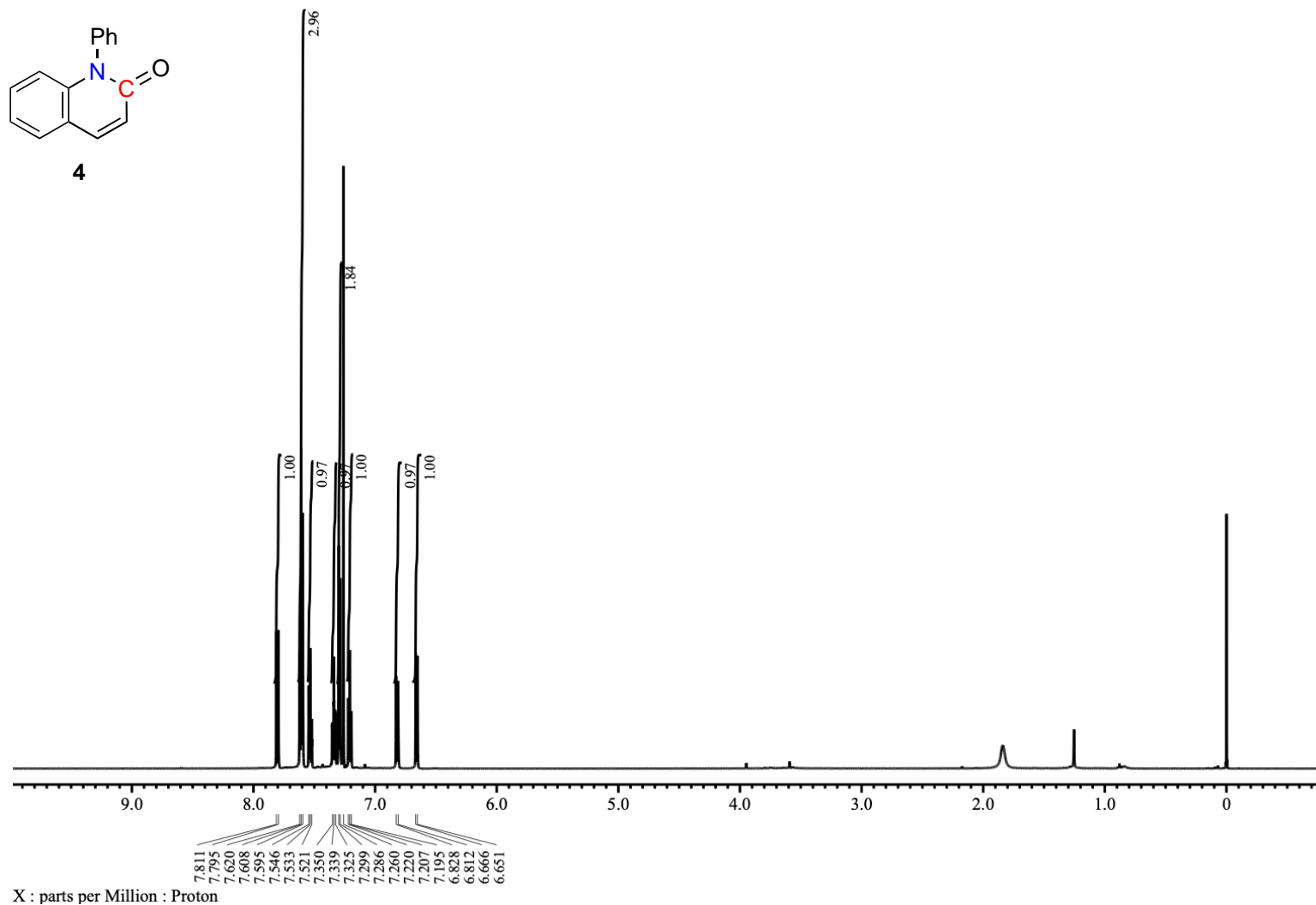


Figure S1. ^1H NMR (600 MHz, CDCl_3) spectrum of **4**.

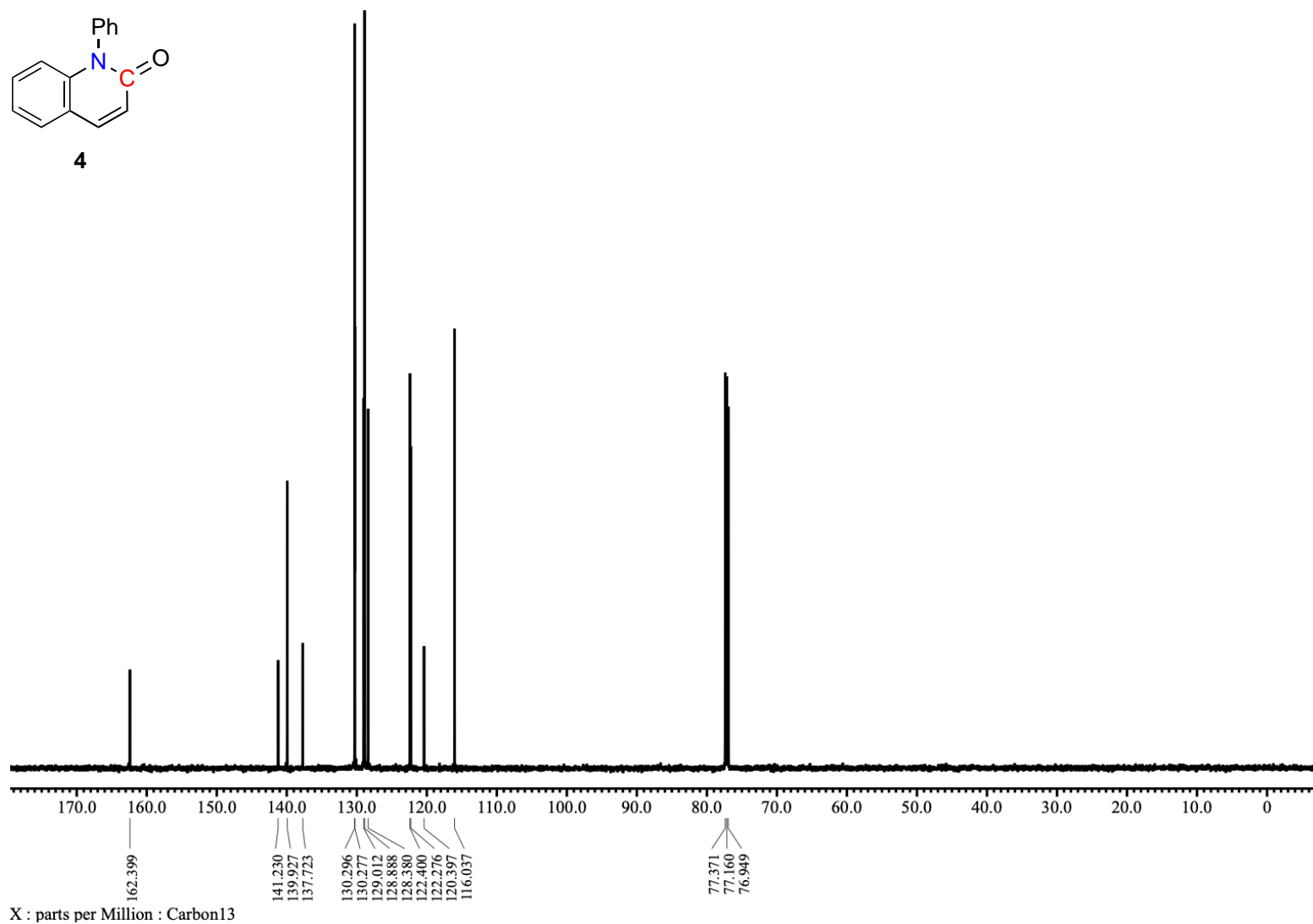
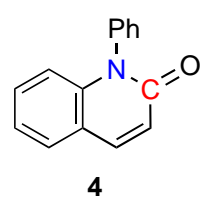


Figure S2. ^{13}C NMR (151 MHz, CDCl_3) spectrum of **4**.

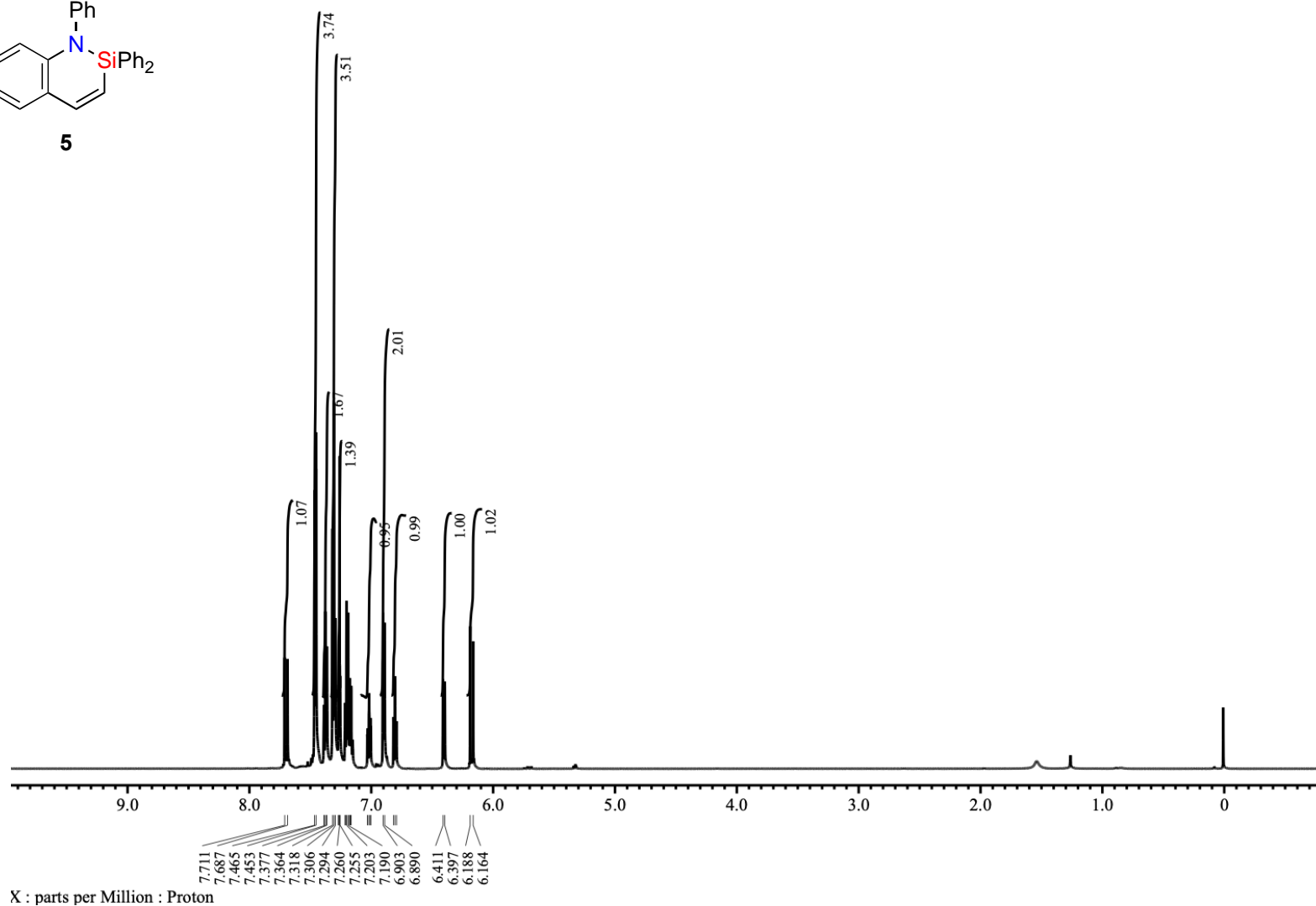
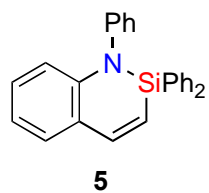


Figure S3. ^1H NMR (600 MHz, CDCl_3) spectrum of **5**.

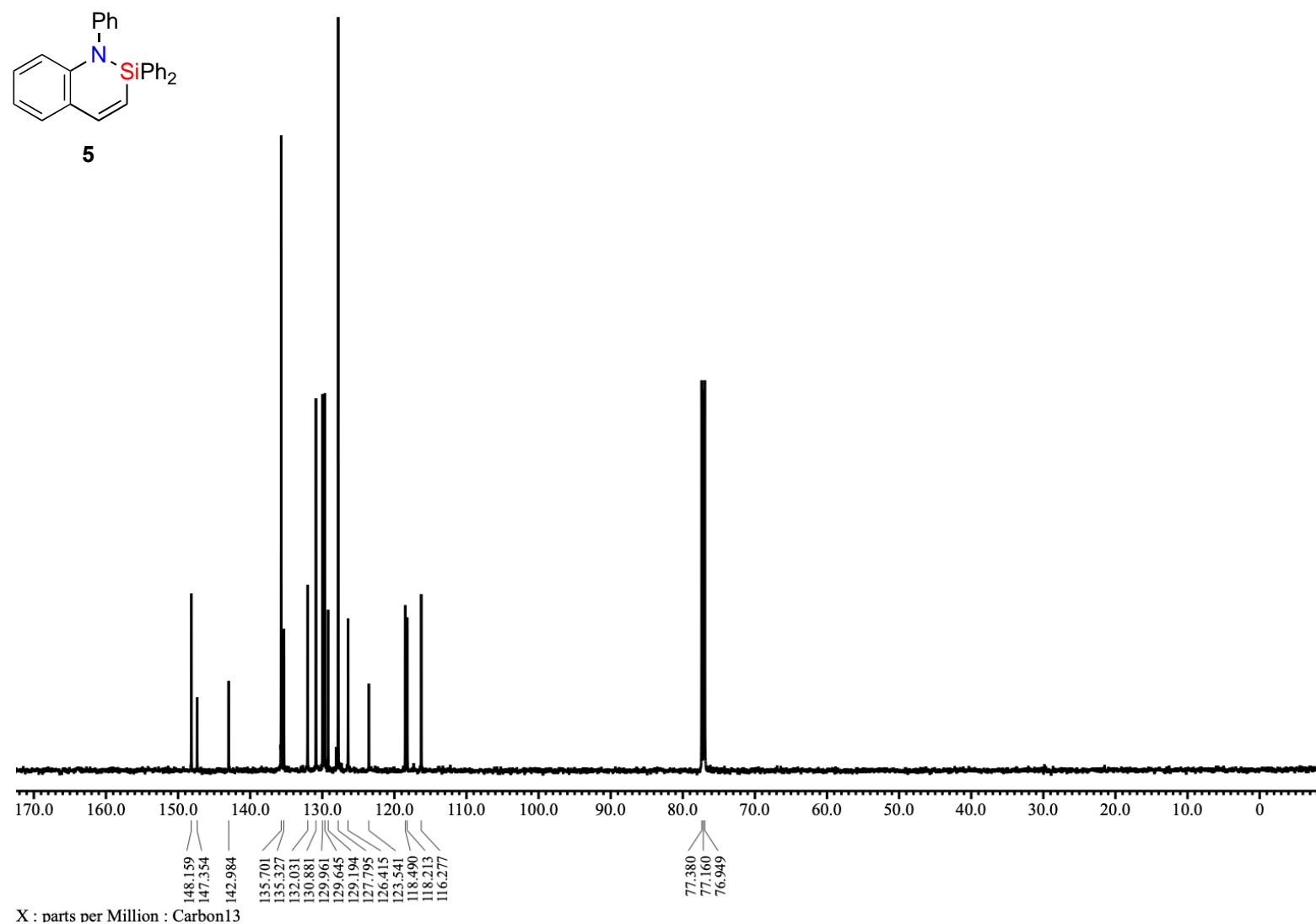


Figure S4. ^{13}C NMR (151 MHz, CDCl_3) spectrum of **5**.

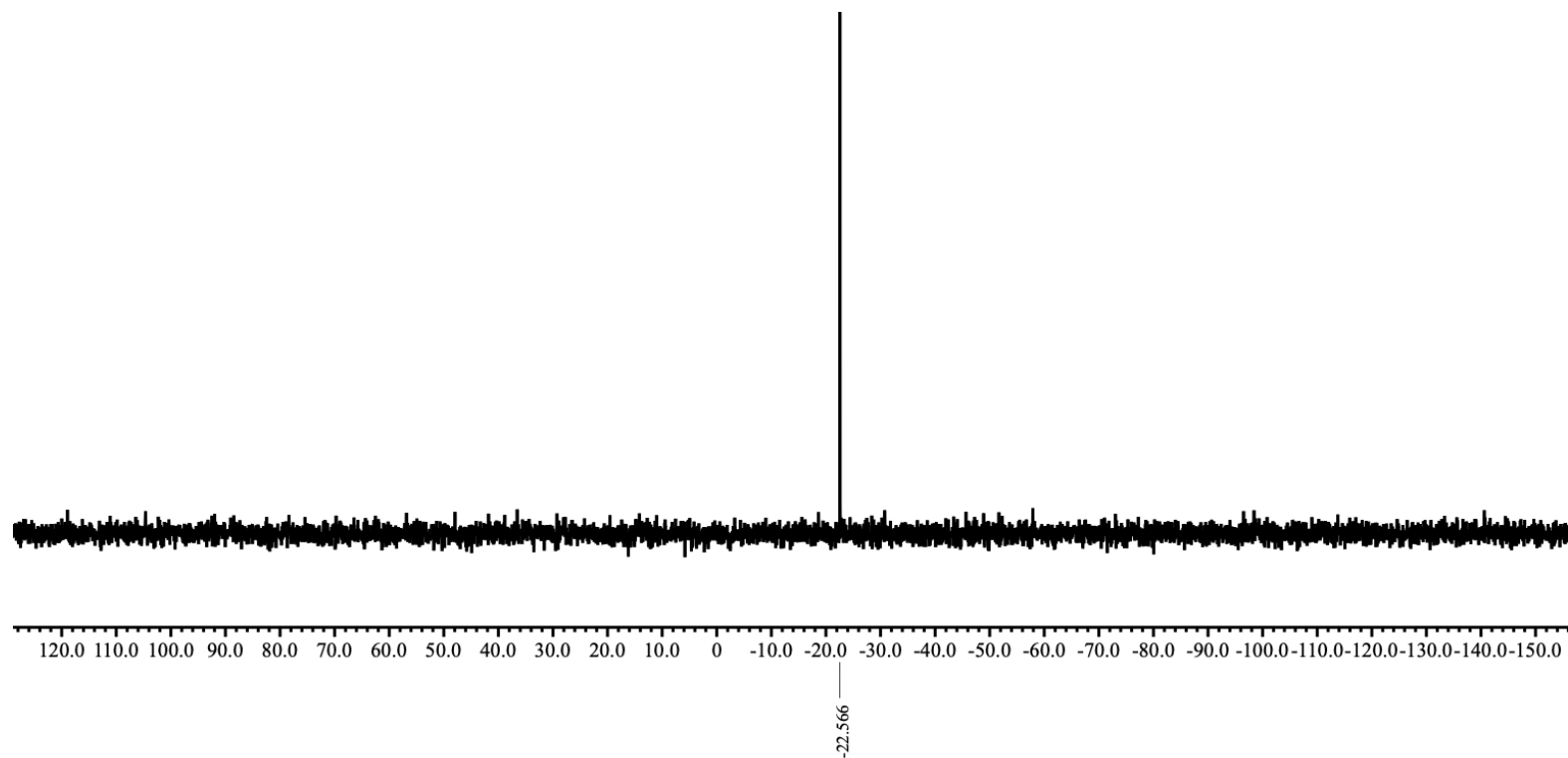
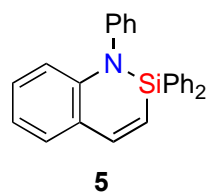


Figure S5. $^{29}\text{Si}\{^1\text{H}\}$ DEPT NMR (119 MHz, CDCl_3) spectrum of **5**.

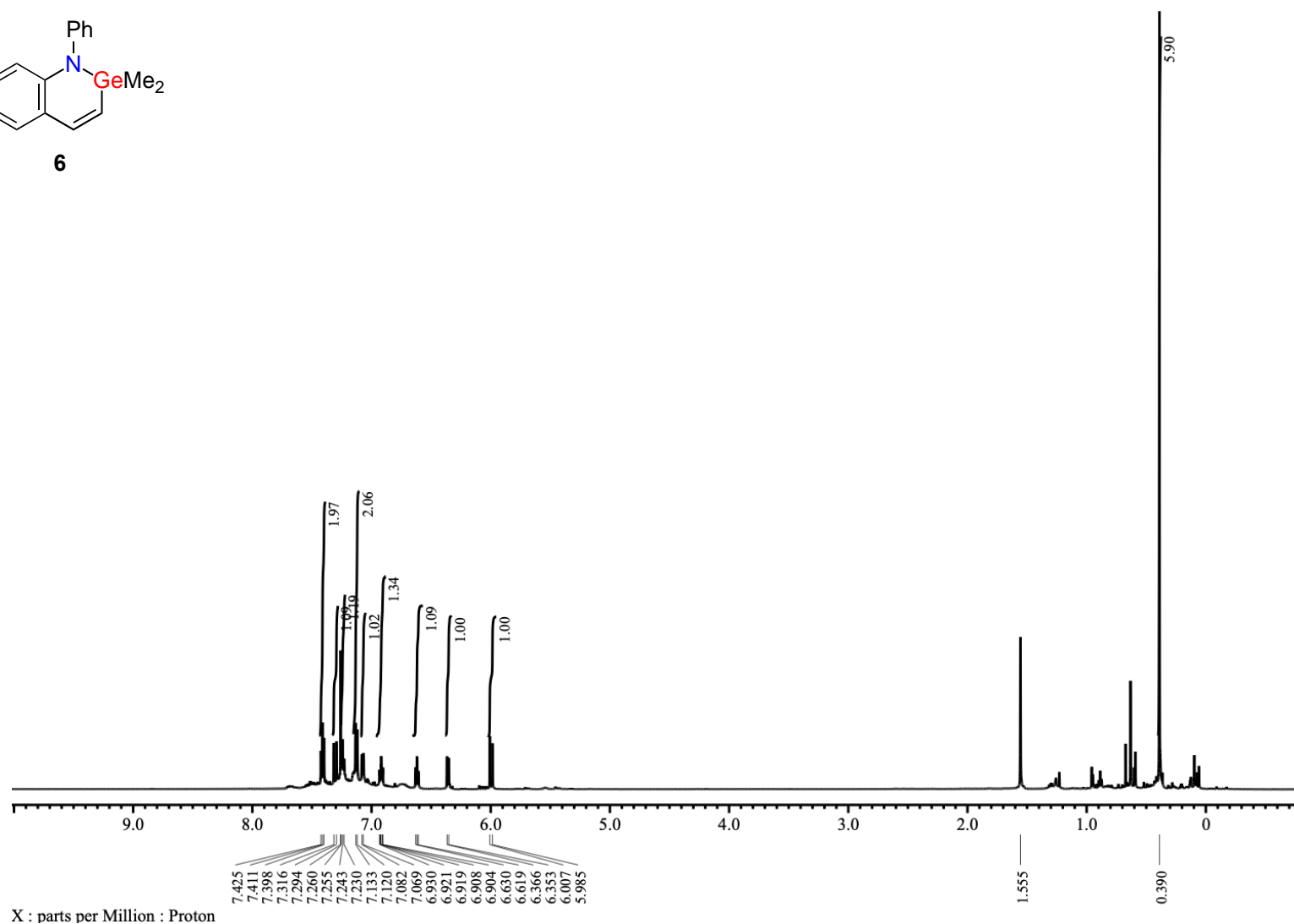
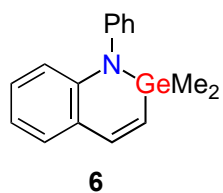


Figure S6. ^1H NMR (600 MHz, CDCl_3) spectrum of **6**.

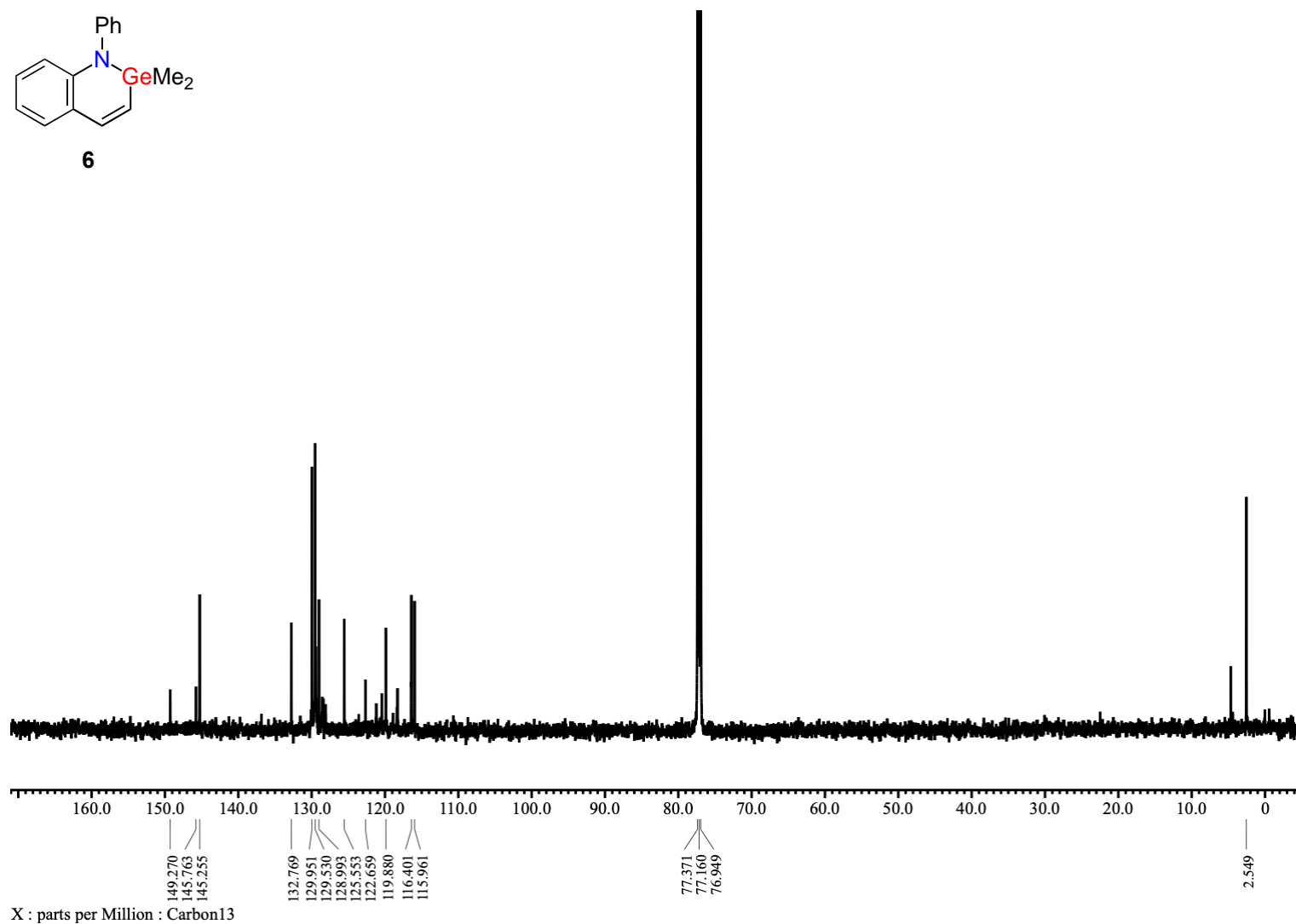
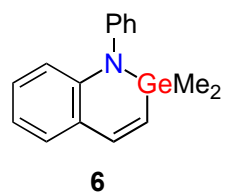


Figure S7. ^{13}C NMR (151 MHz, CDCl_3) spectrum of **6**.