Supplementary Material

Thiophene-Fused Phospholo[3,2-*b*]phospholes and Their Dichalcogenides: Synthesis and Structure–Photophysical Properties Relationships

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1. ^{1}H, $^{13}C\{^{1}H\}$, and $^{31}P\{^{1}H\}$ NMR Spectra

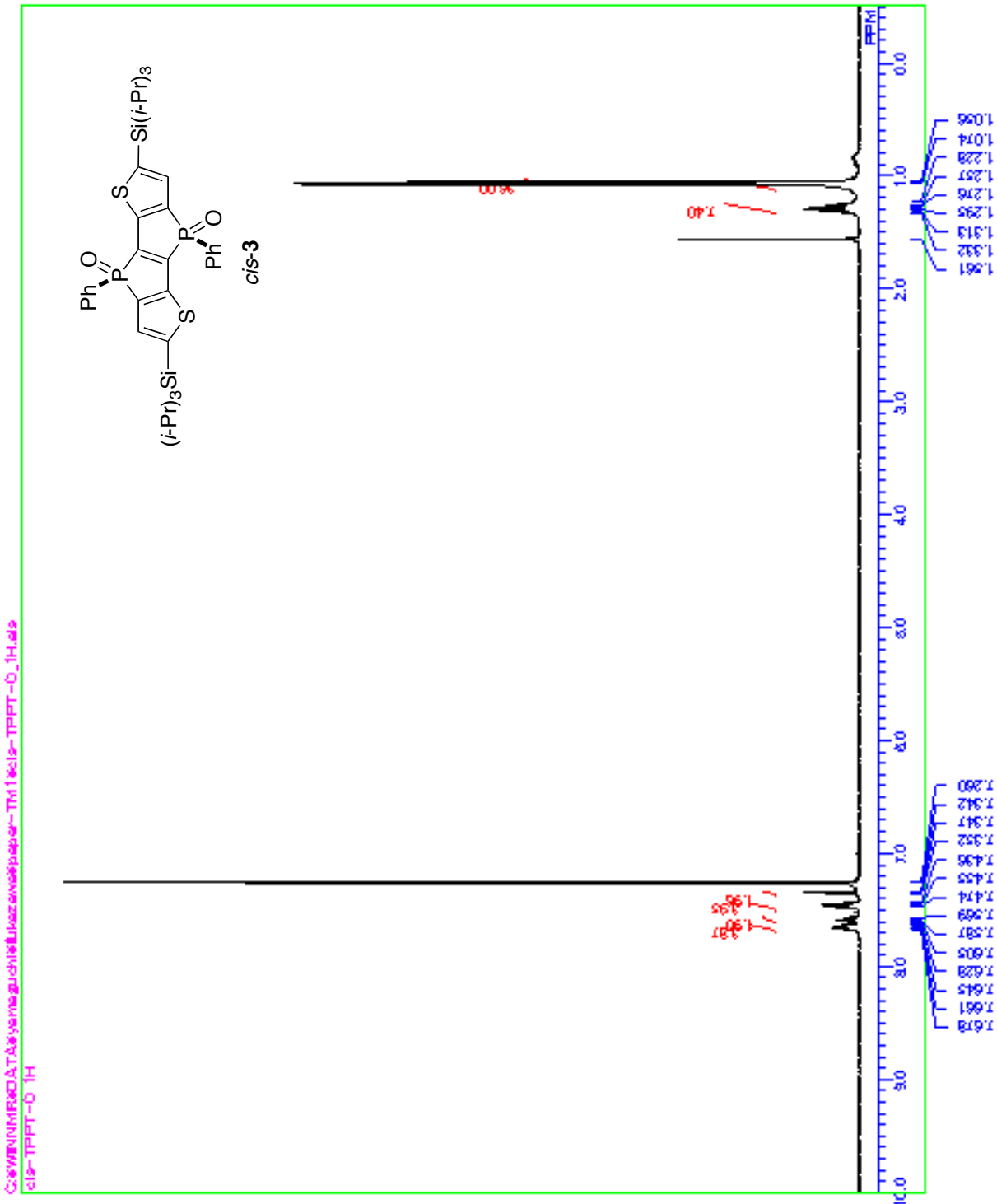

Figure S1. ^{1}H NMR Spectrum of *cis*-**3** ($CDCl_3$, 400 MHz).

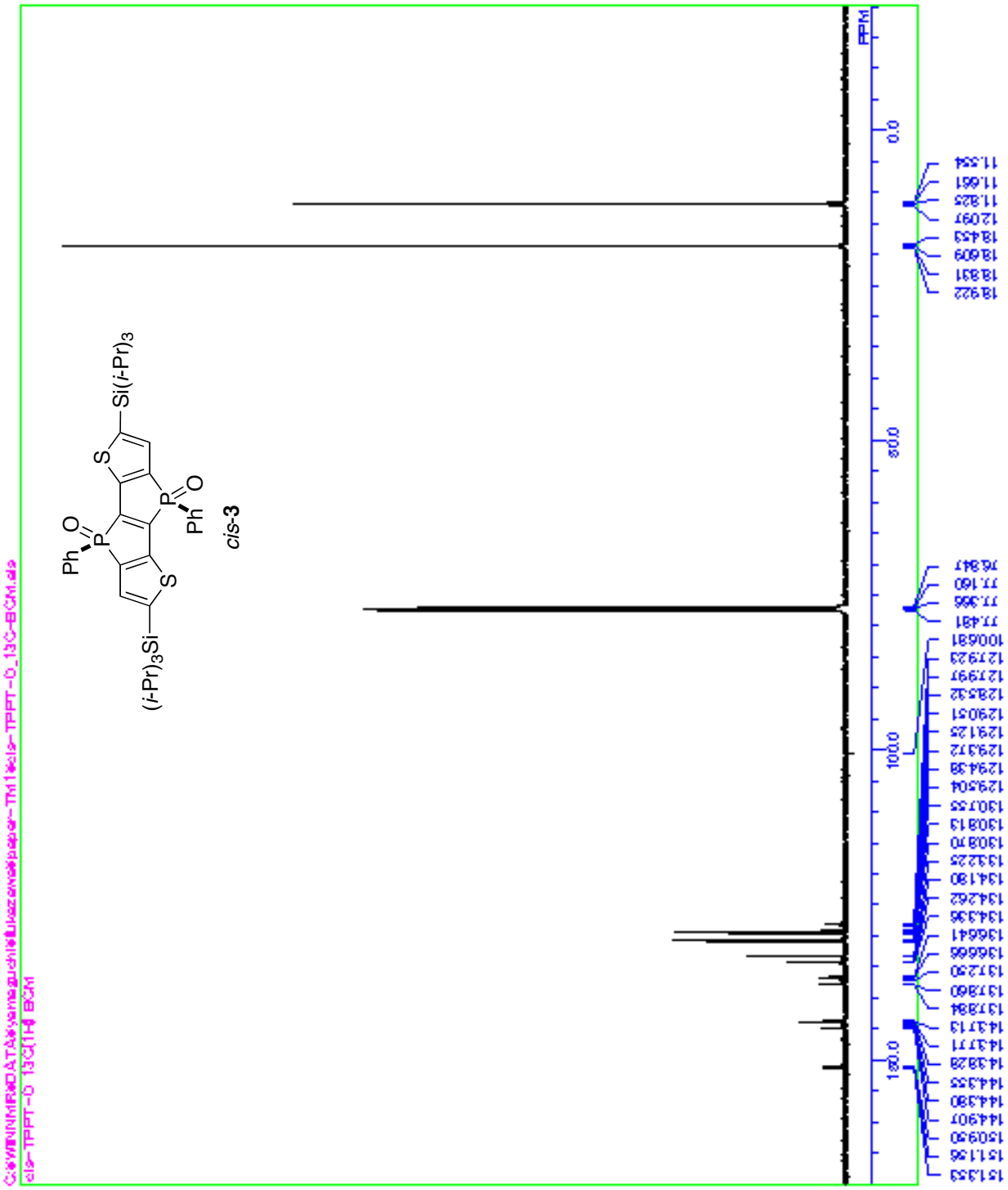

Figure S2. $^{13}C\{^{1}H\}$ NMR Spectrum of *cis*-**3** ($CDCl_3$, 100 MHz).

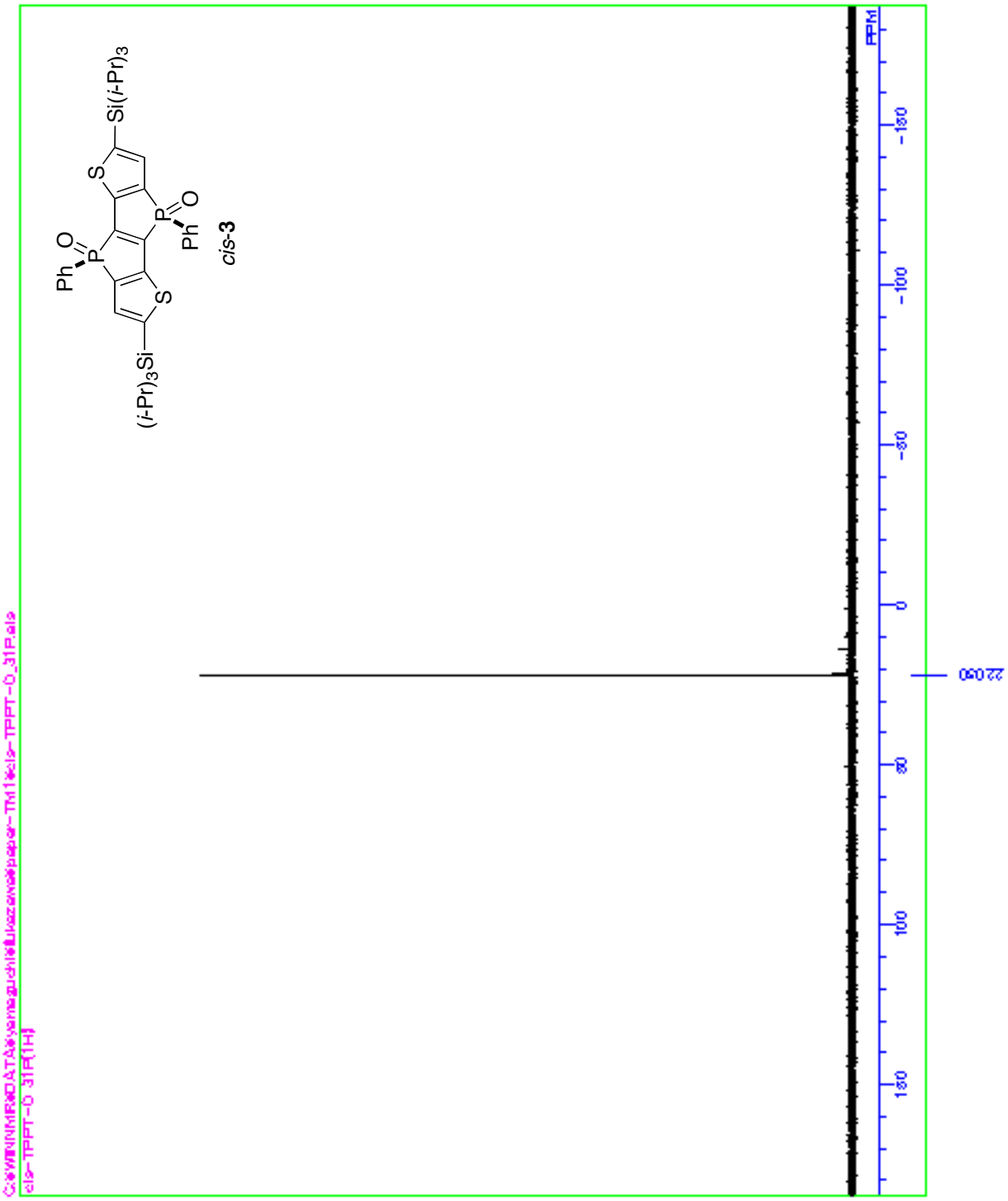

Figure S3. $^{31}P\{^{1}H\}$ NMR Spectrum of *cis*-**3** ($CDCl_3$, 162 MHz).

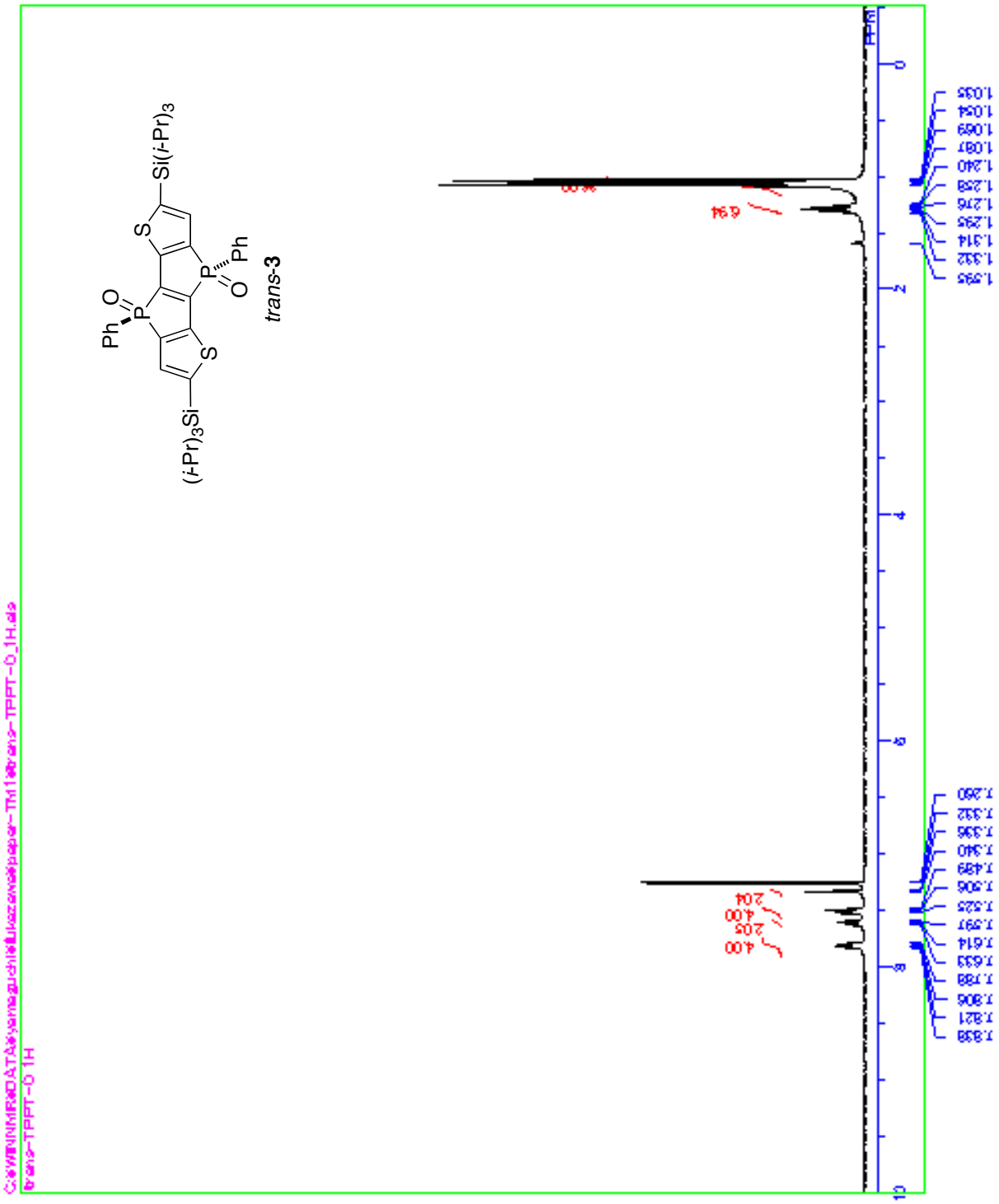

Figure S4. ^{1}H NMR Spectrum of *trans*-**3** ($CDCl_3$, 400 MHz).

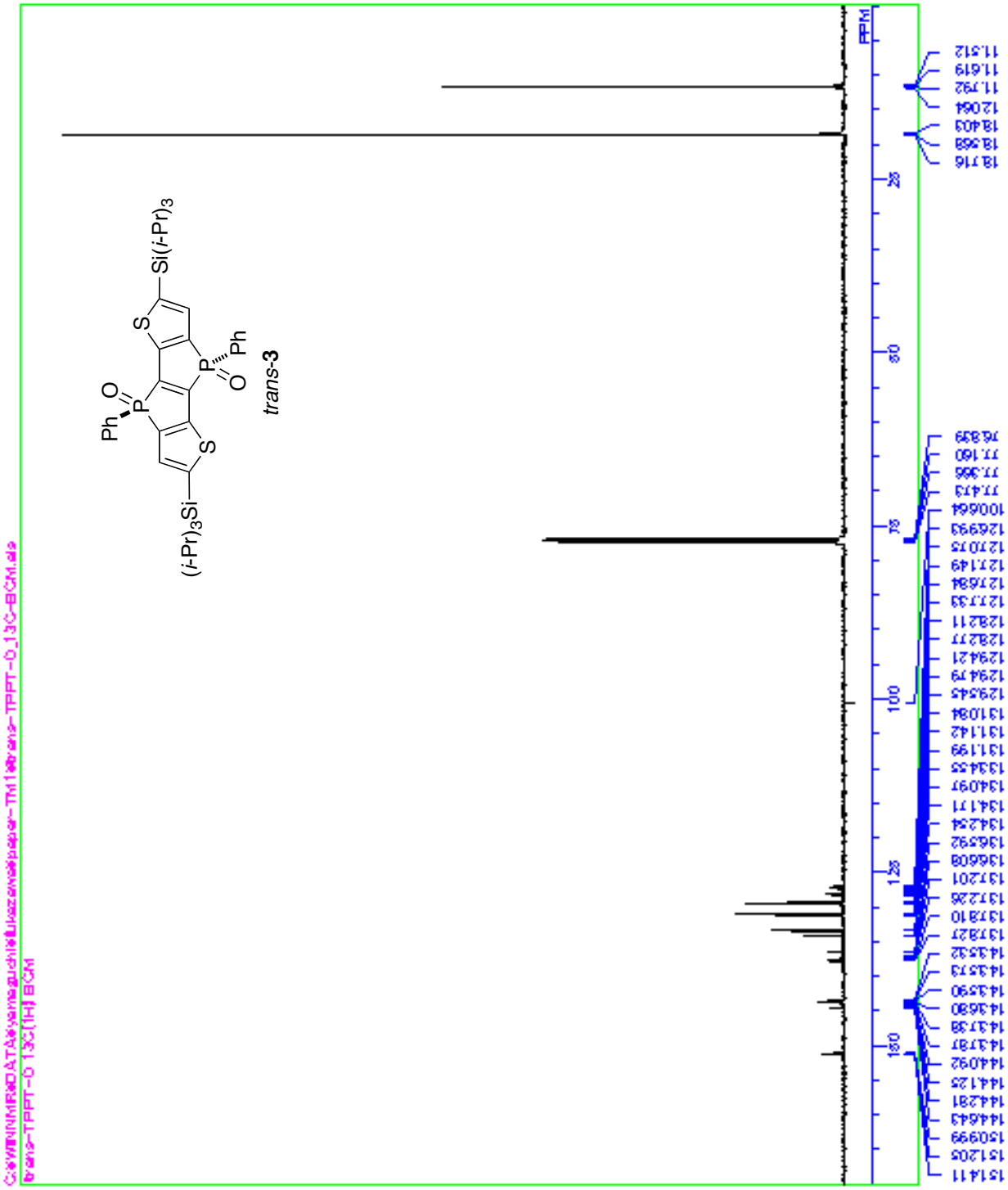

Figure S5. $^{13}C\{^{1}H\}$ NMR Spectrum of *trans*-**3** ($CDCl_3$, 100 MHz).

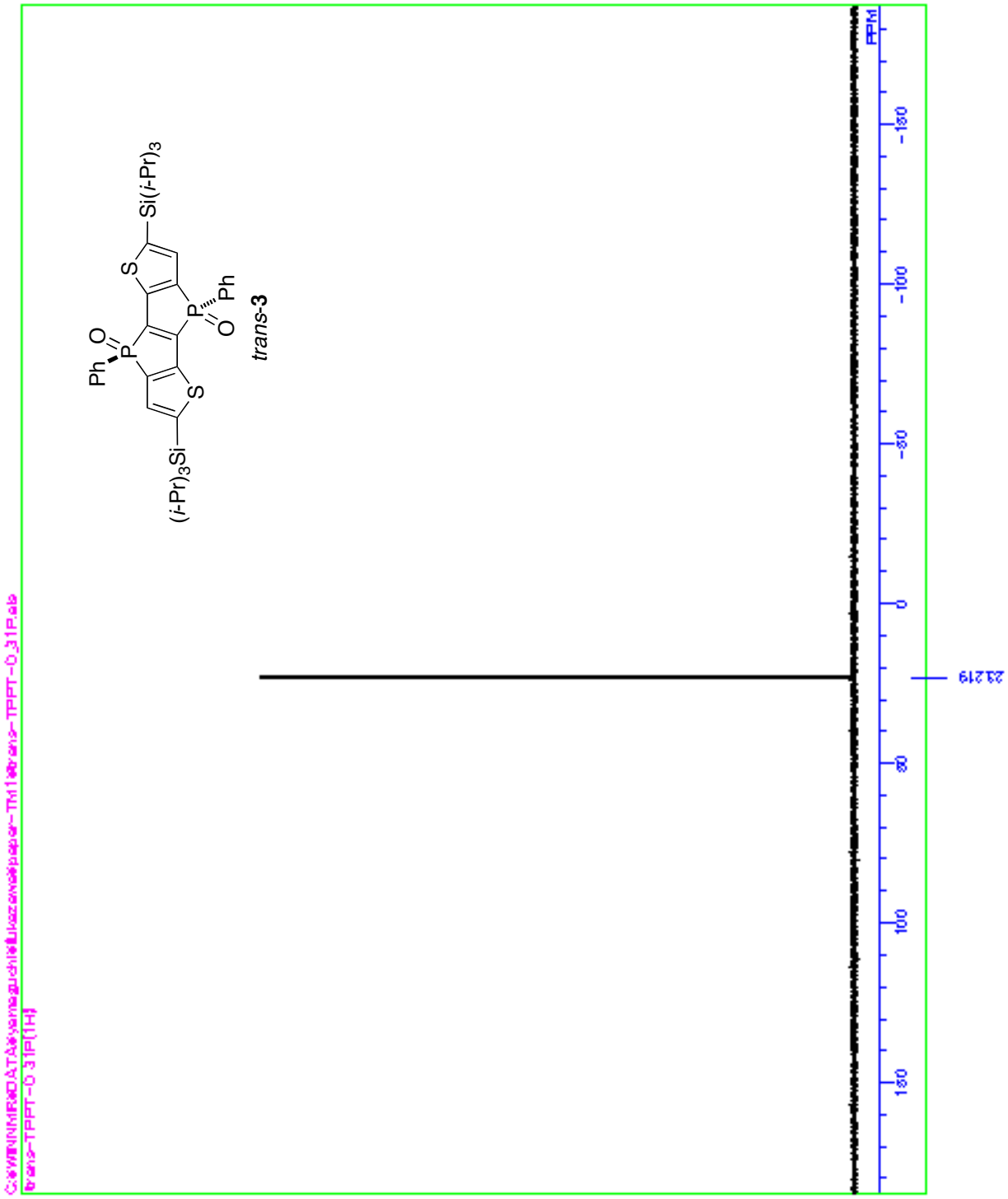

Figure S6. $^{31}P\{^{1}H\}$ NMR Spectrum of *trans*-**3** ($CDCl_3$, 162 MHz).

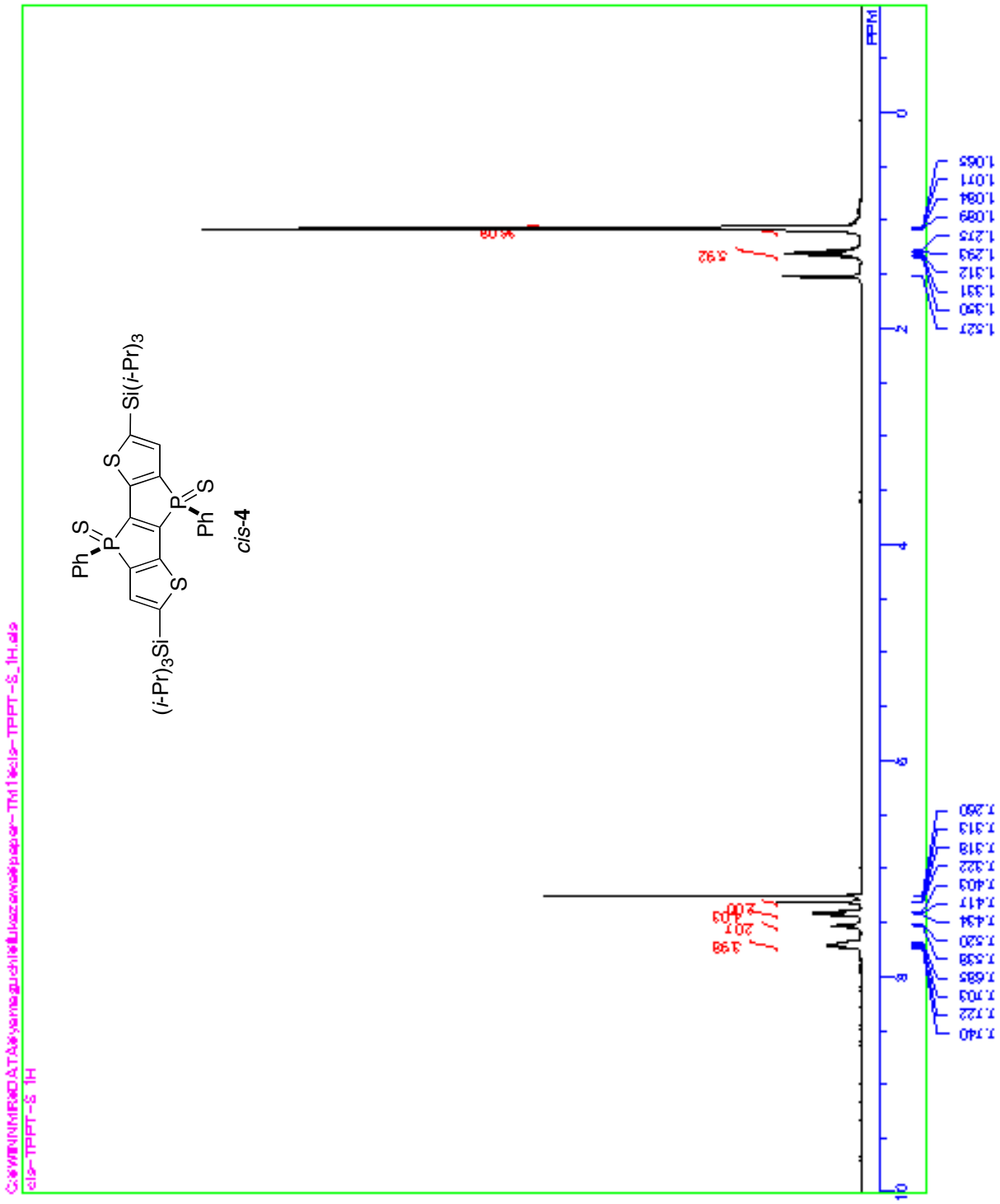

Figure S7. ^{1}H NMR Spectrum of *cis*-**4** ($CDCl_3$, 400 MHz).

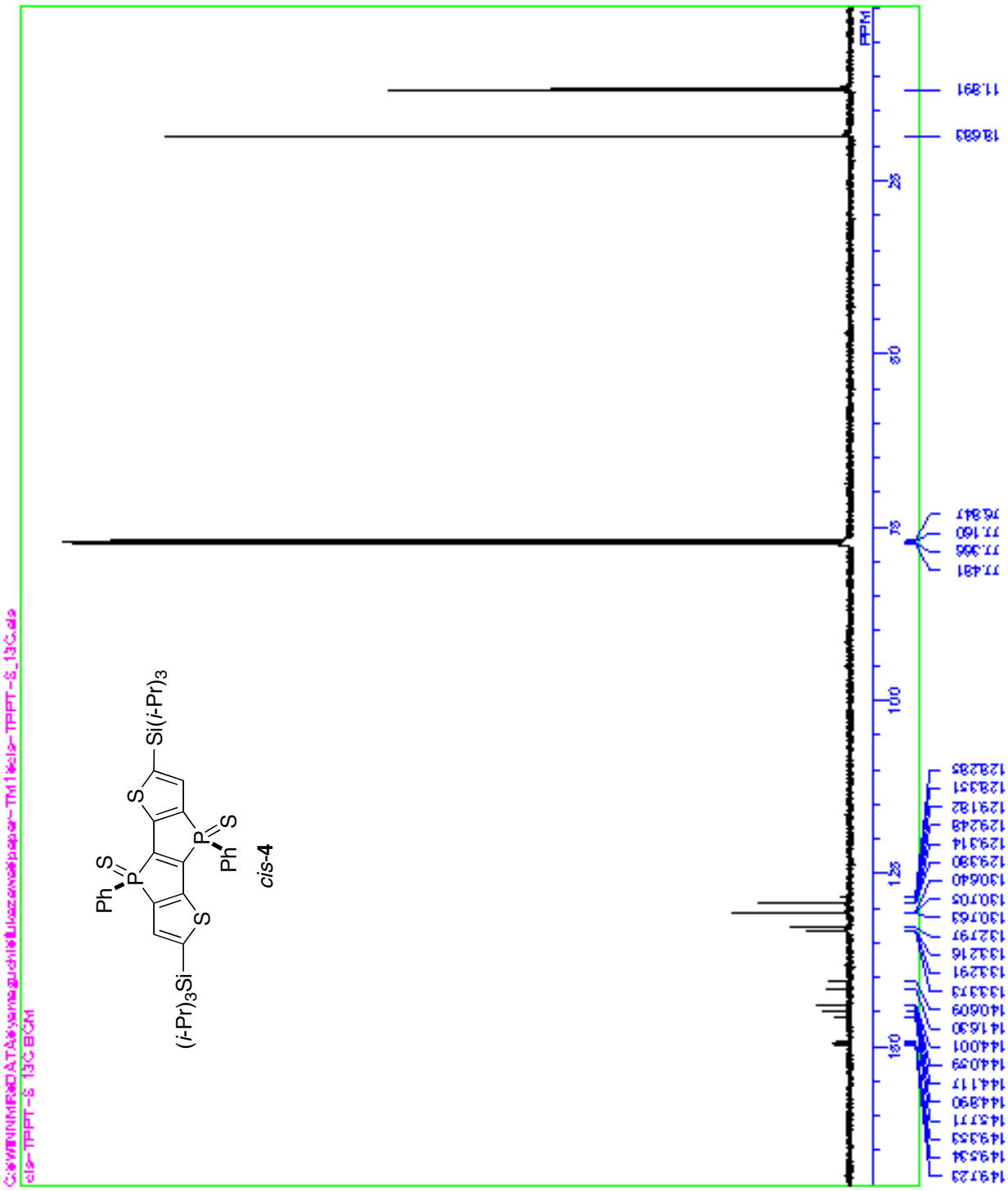

Figure S8. $^{13}C\{^{1}H\}$ NMR Spectrum of *cis*-**4** ($CDCl_3$, 100 MHz).

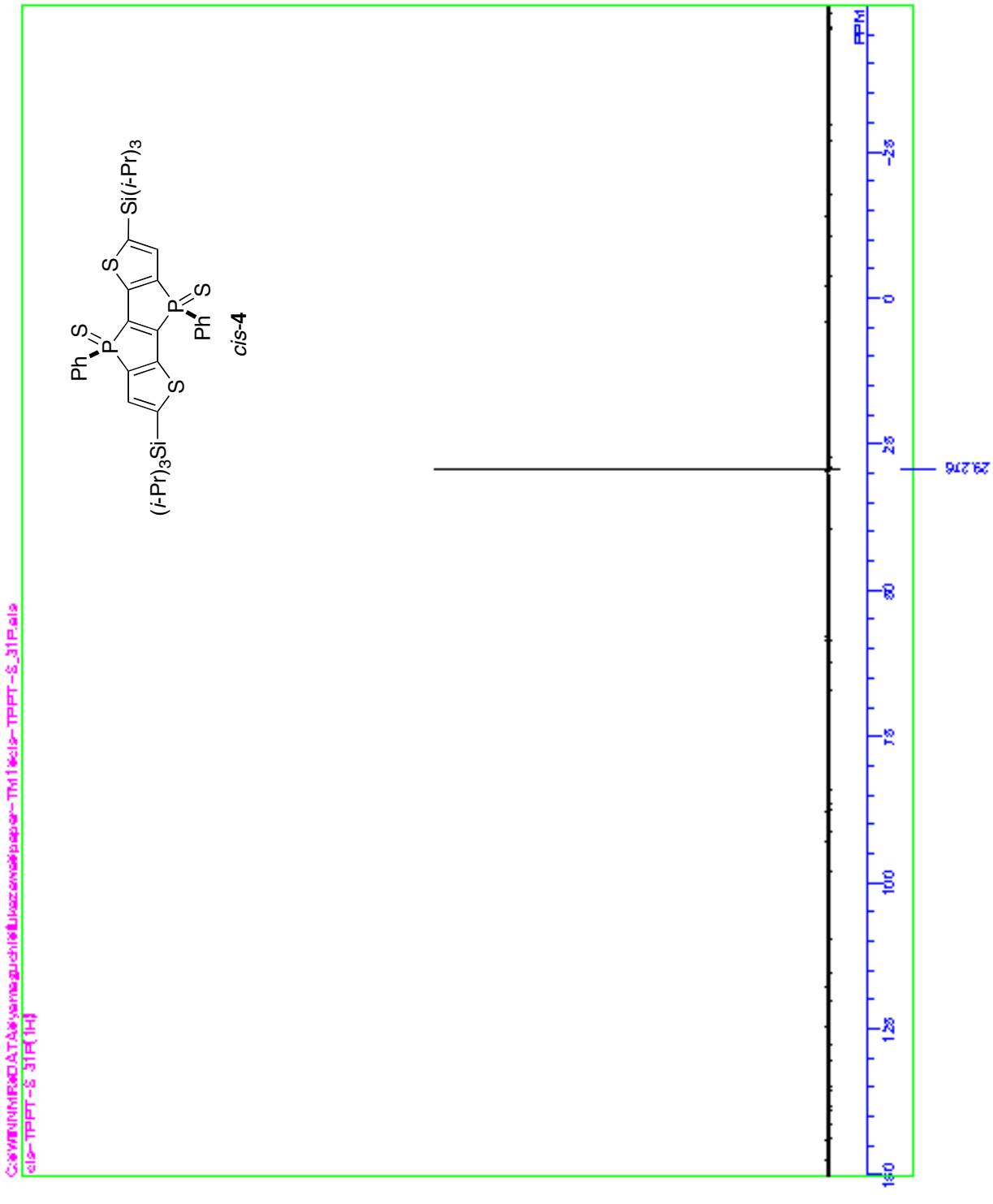

Figure S9. $^{31}P\{^{1}H\}$ NMR Spectrum of *cis*-**4** ($CDCl_3$, 162 MHz).

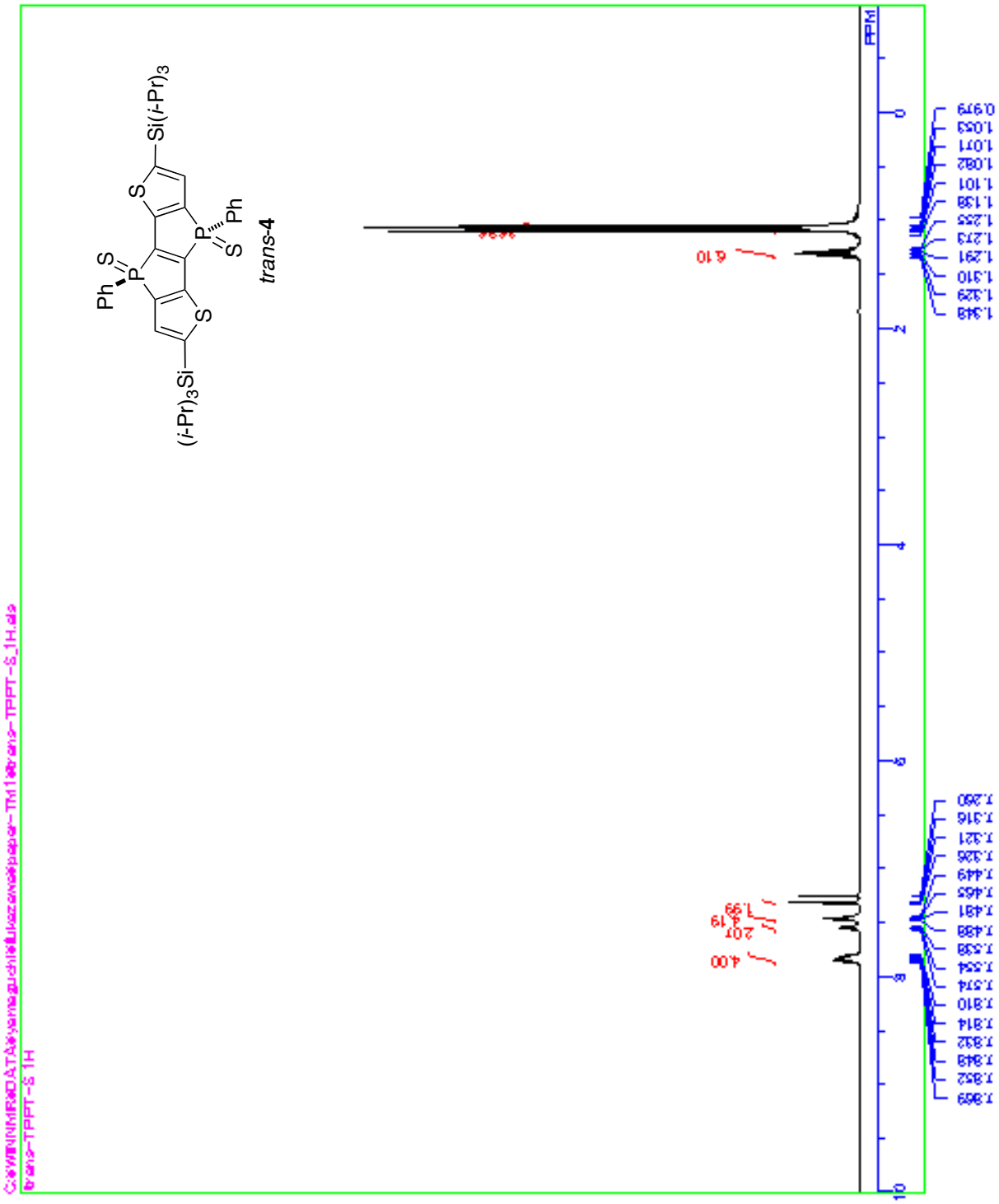

Figure S10. ^{1}H NMR Spectrum of *trans*-**4** ($CDCl_3$, 400 MHz).

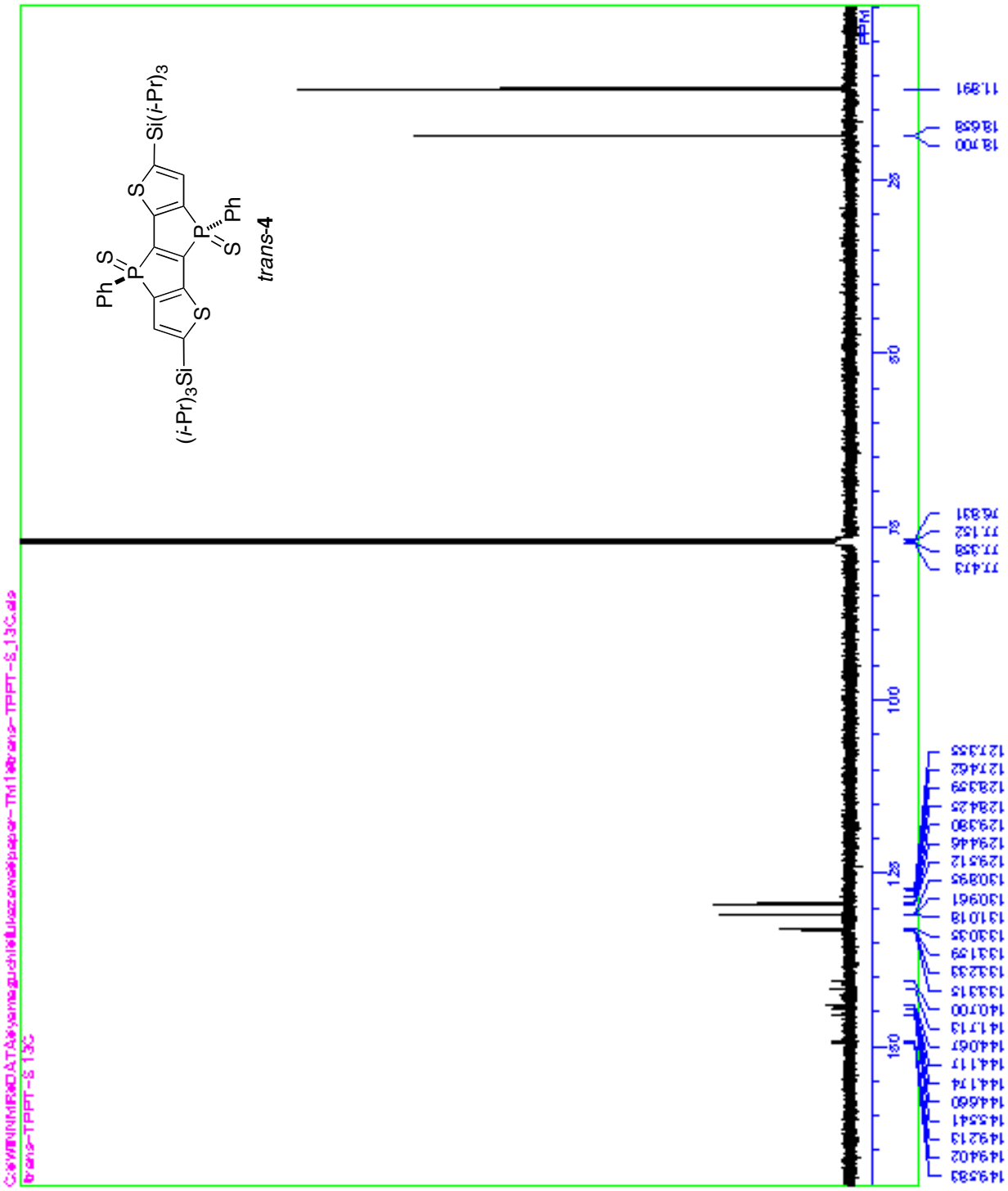

Figure S11. $^{13}C\{^{1}H\}$ NMR Spectrum of *trans*-**4** ($CDCl_3$, 100 MHz).

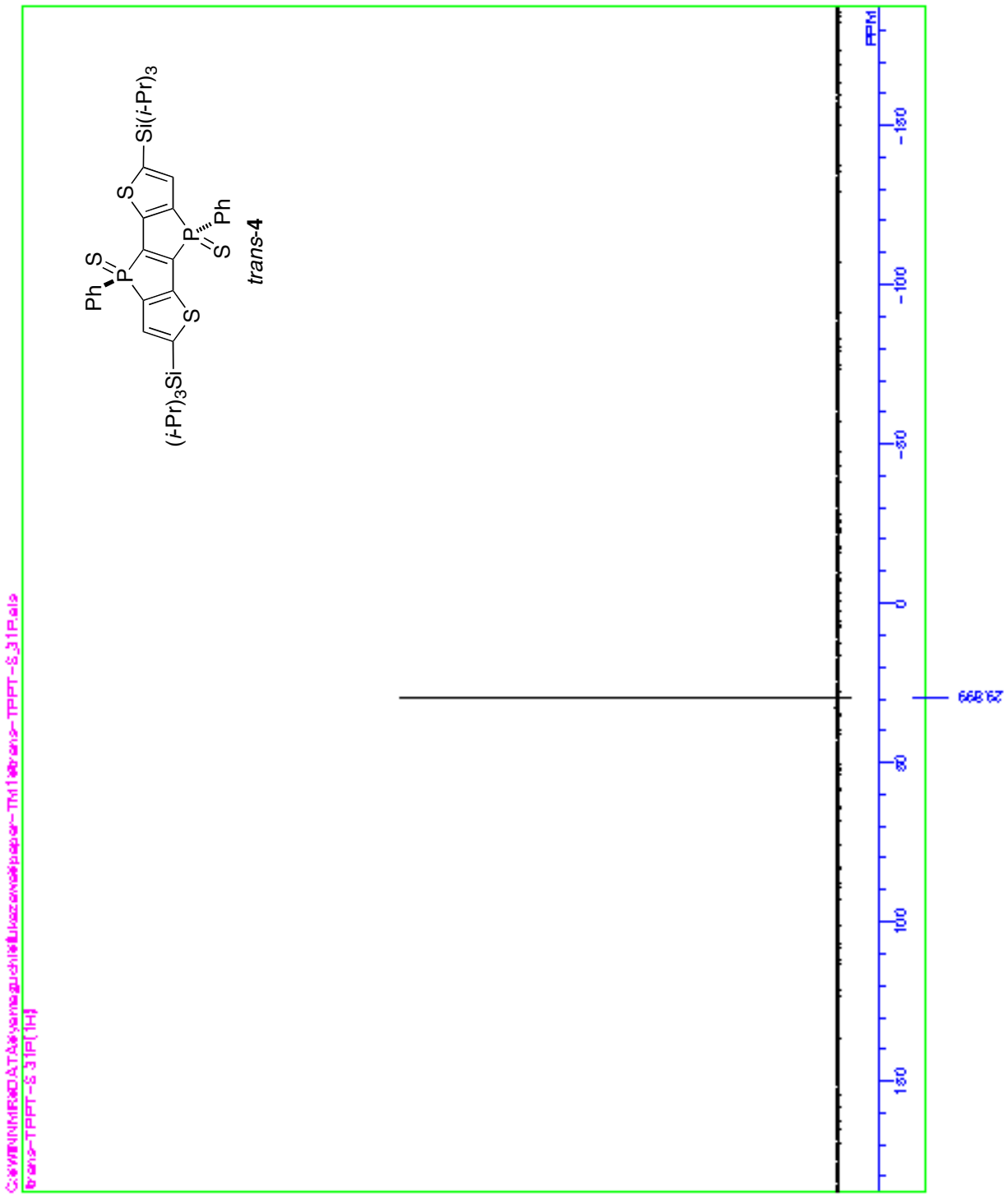

Figure S12. $^{31}P\{^{1}H\}$ NMR Spectrum of *trans*-**4** ($CDCl_3$, 162 MHz).

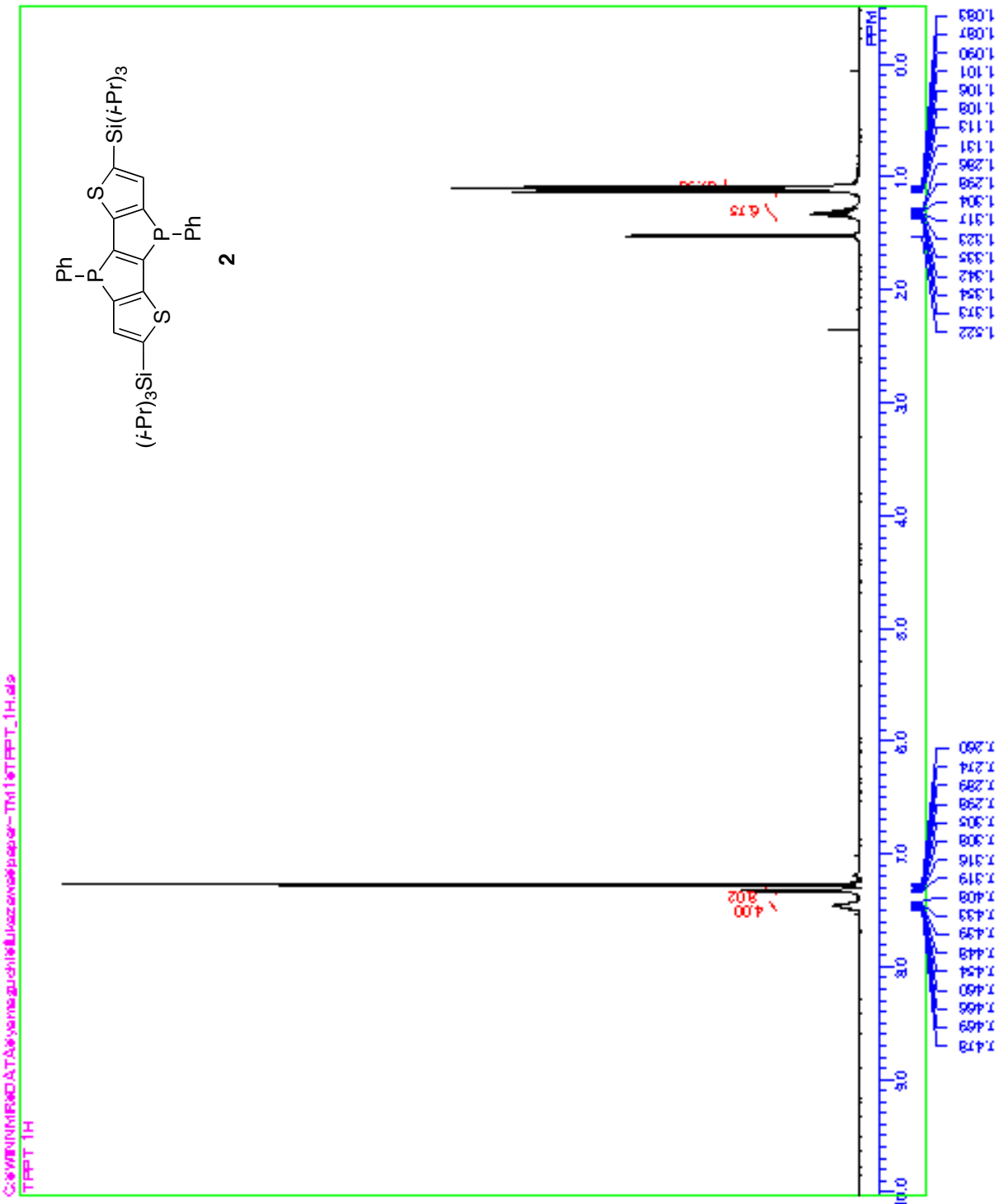

Figure S13. ^{1}H NMR Spectrum of **2** ($CDCl_3$, 400 MHz).

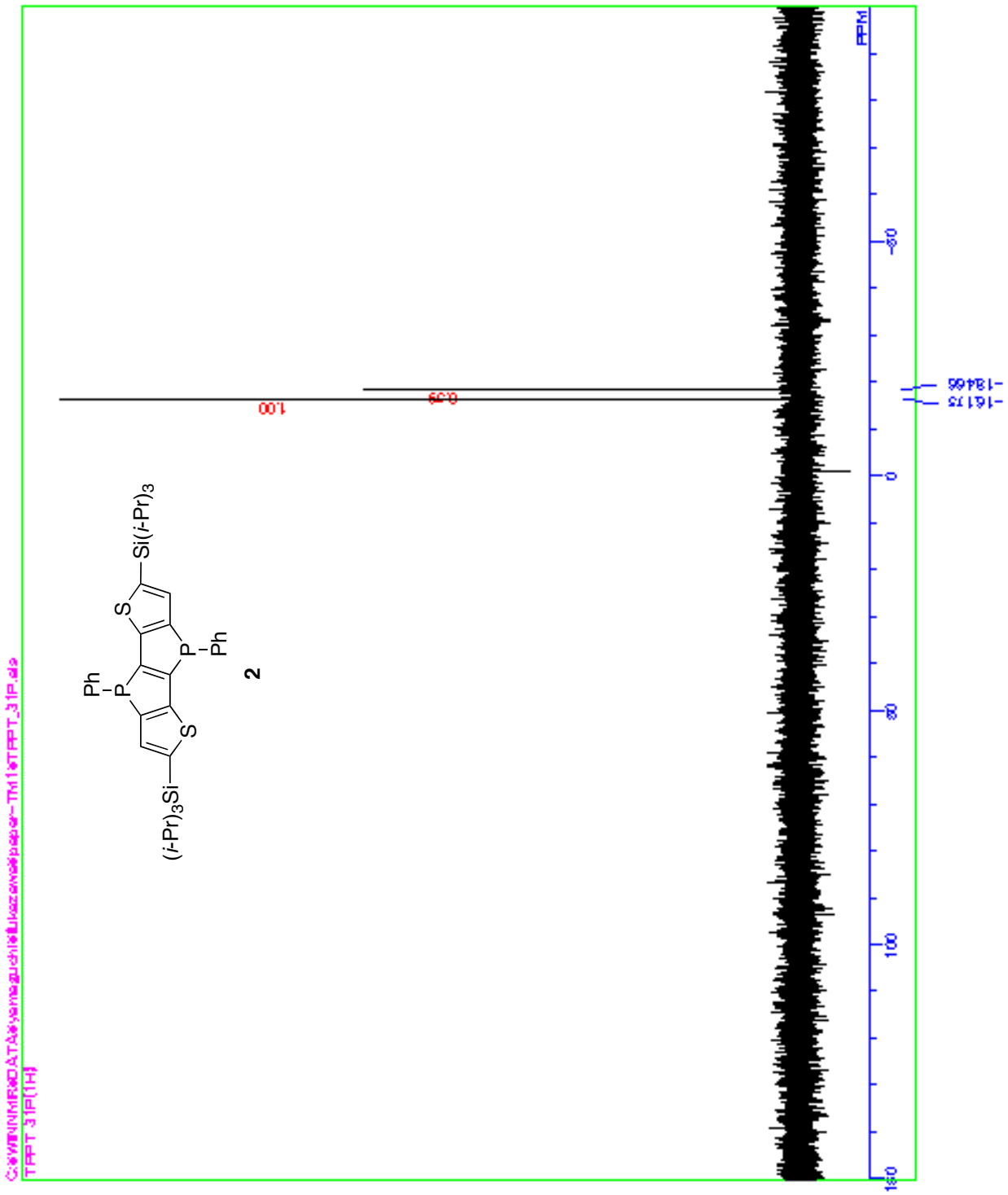

Figure S14. $^{31}P\{^{1}H\}$ NMR Spectrum of **2** ($CDCl_3$, 162 MHz).

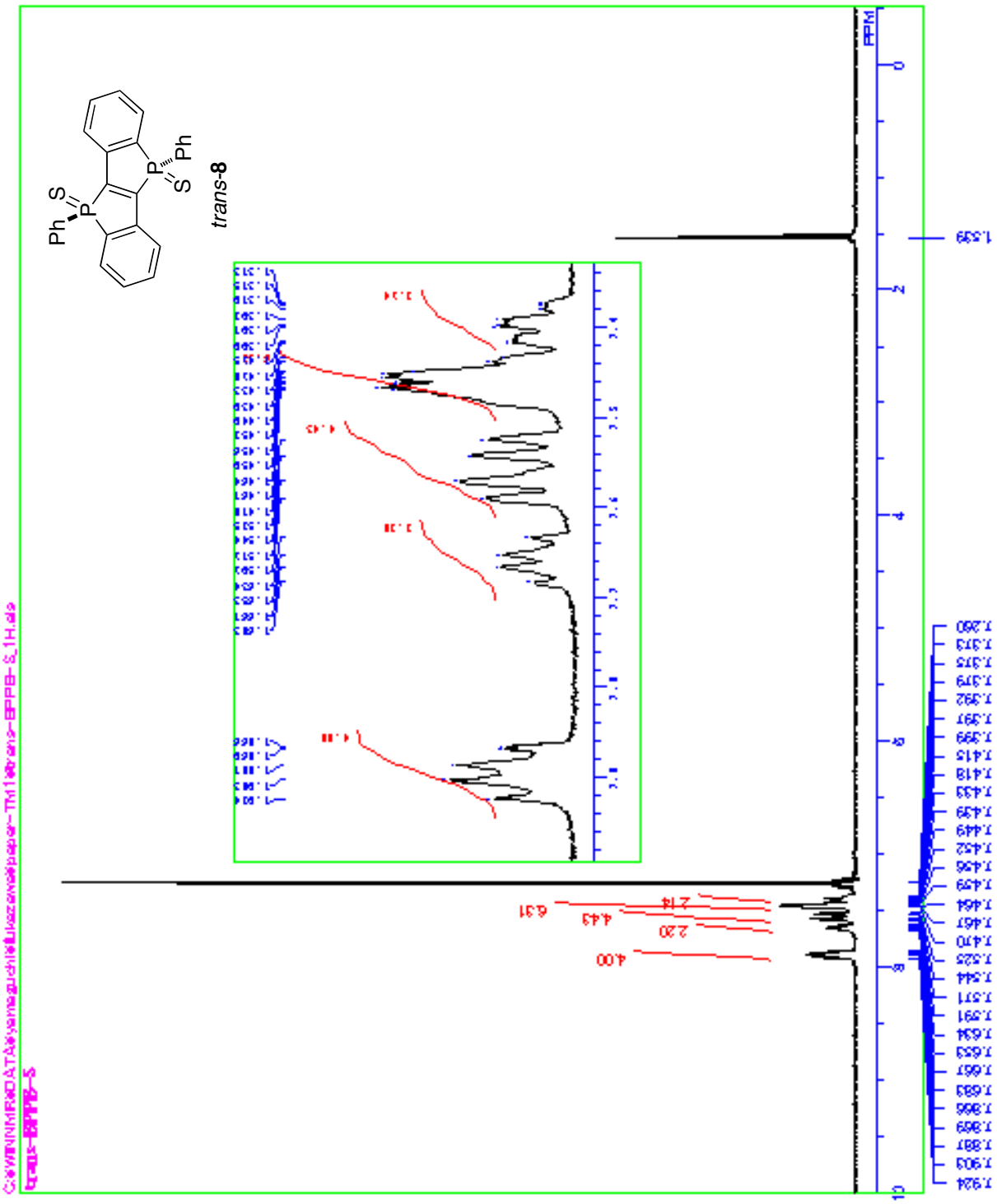

Figure S15. ^{1}H NMR Spectrum of *trans*-**8** ($CDCl_3$, 400 MHz).

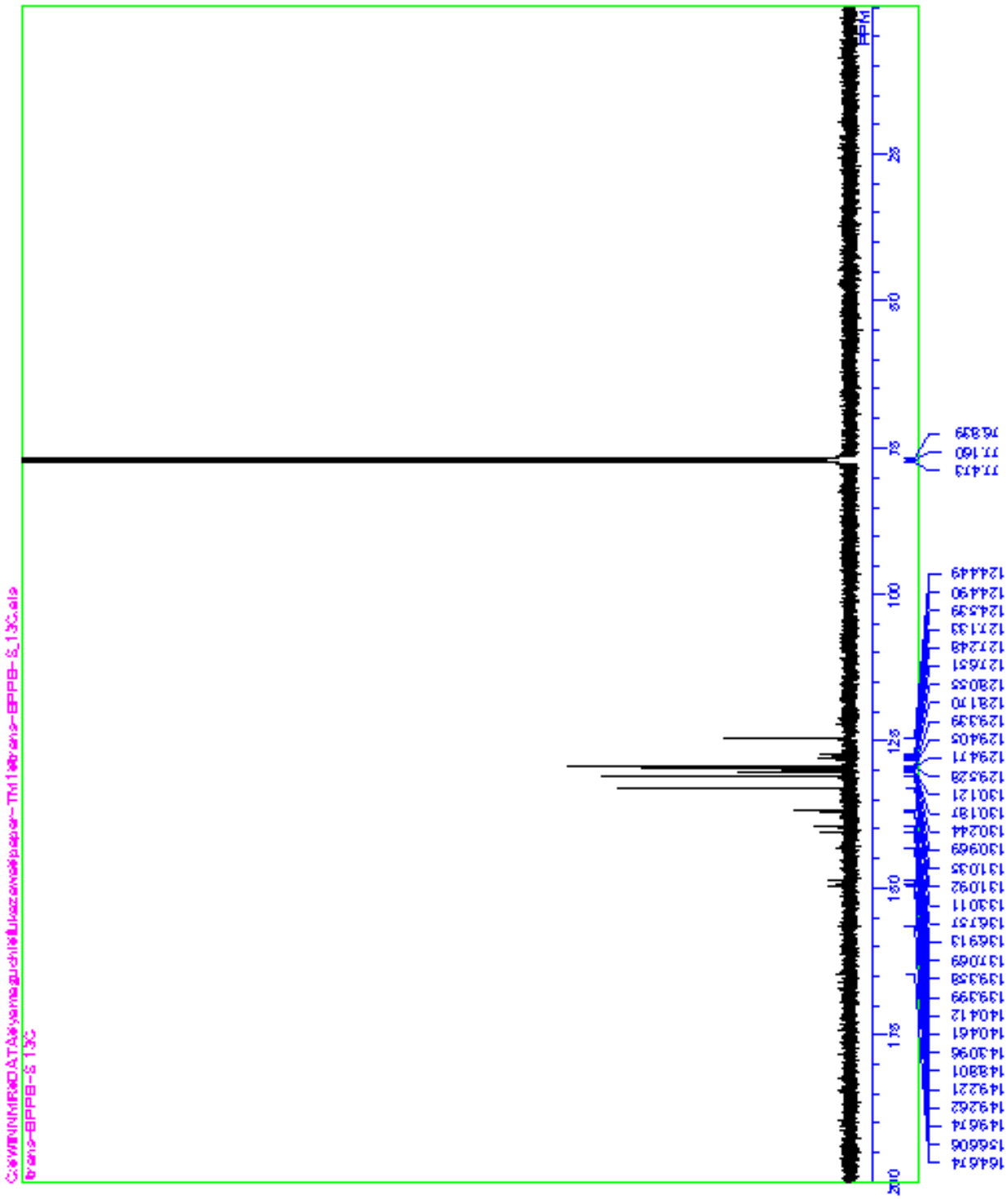

Figure S16. $^{13}C\{^{1}H\}$ NMR Spectrum of *trans*-**8** ($CDCl_3$, 100 MHz).

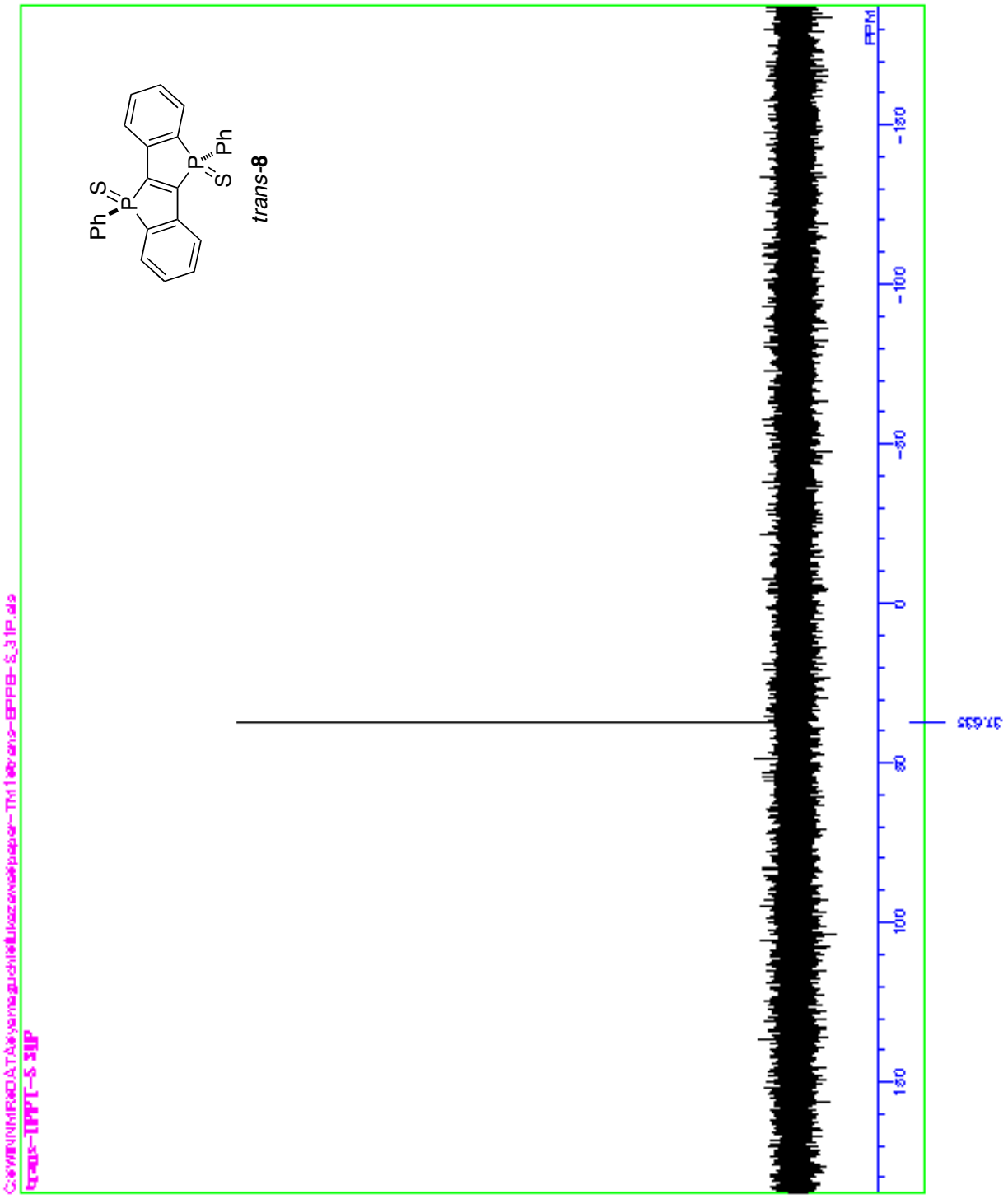

Figure S17. $^{31}P\{^{1}H\}$ NMR Spectrum of *trans*-**8** ($CDCl_3$, 162 MHz).

2. UV/Vis Absorption and Fluorescence Spectra of *cis*-3, *cis*-4, and *trans*-8

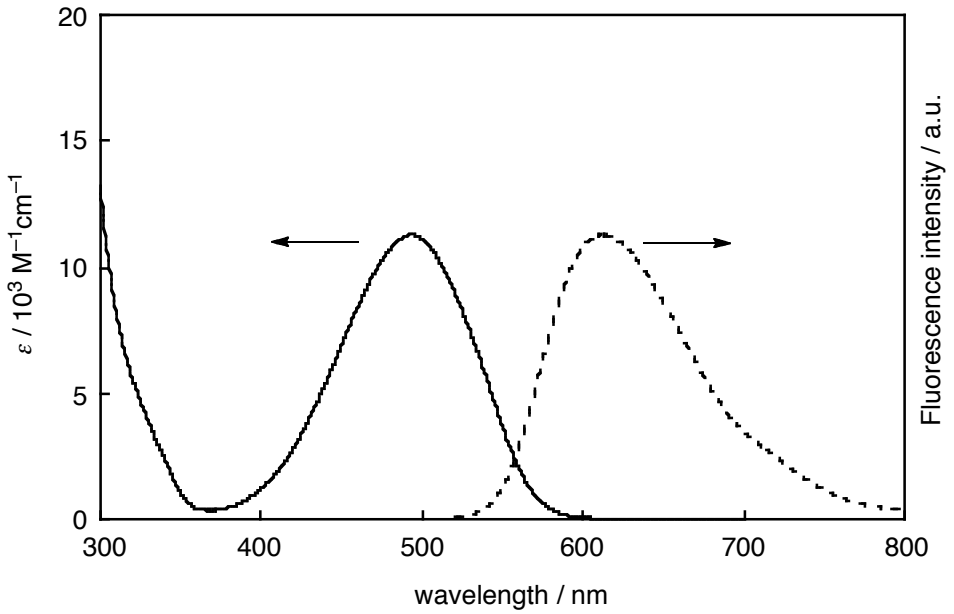

Figure S18. UV/Vis absorption (solid line) and fluorescence spectra (broken line) of *cis*-**3** in CH_2Cl_2.

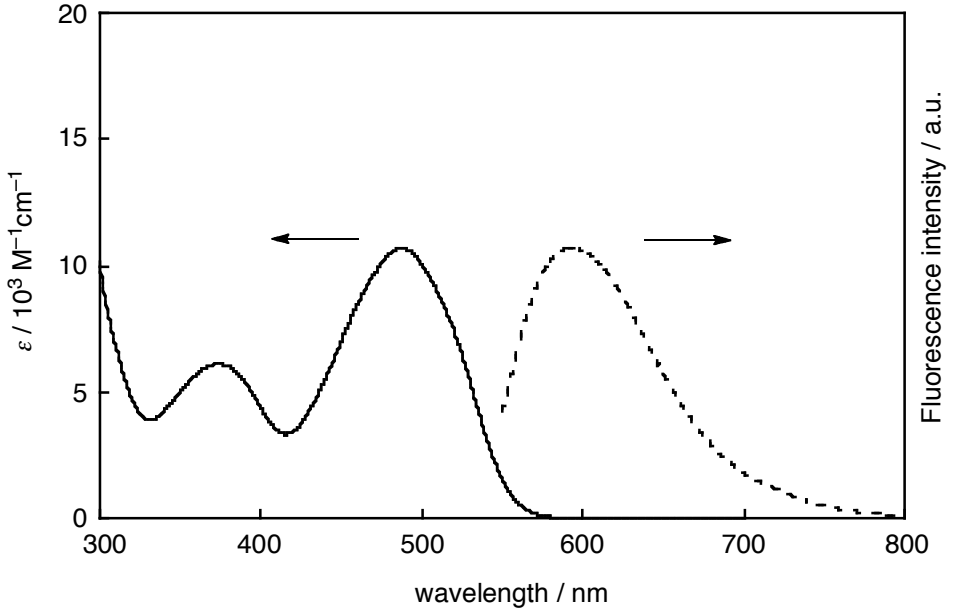

Figure S19. UV/Vis absorption (solid line) and fluorescence spectra (broken line) of *cis*-**4** in CH_2Cl_2.

3. Crystallographic Data

Table S1. Bond Lengths [Å] and Angles [°] for *cis*-**3**

P(1)-O(1)	1.482(3)	C(9)-C(10)	1.375(6)
P(1)-C(1)	1.794(4)	C(11)-C(16)	1.379(6)
P(1)-C(11)	1.796(4)	C(11)-C(12)	1.381(6)
P(1)-C(4)	1.826(4)	C(12)-C(13)	1.383(7)
P(2)-O(2)	1.484(3)	C(13)-C(14)	1.373(7)
P(2)-C(17)	1.790(5)	C(14)-C(15)	1.368(7)
P(2)-C(5)	1.799(4)	C(15)-C(16)	1.392(7)
P(2)-C(3)	1.812(4)	C(17)-C(22)	1.401(6)
S(1)-C(2)	1.714(4)	C(17)-C(18)	1.407(6)
S(1)-C(7)	1.738(4)	C(18)-C(19)	1.386(6)
S(2)-C(6)	1.719(4)	C(19)-C(20)	1.389(7)
S(2)-C(10)	1.744(4)	C(20)-C(21)	1.379(7)
Si(1)-C(23)	1.884(5)	C(21)-C(22)	1.389(6)
Si(1)-C(7)	1.885(4)	C(23)-C(24)	1.530(7)
Si(1)-C(29)	1.896(5)	C(23)-C(25)	1.543(7)
Si(1)-C(26)	1.897(4)	C(26)-C(27)	1.531(6)
Si(2)-C(38)	1.878(5)	C(26)-C(28)	1.543(6)
Si(2)-C(35)	1.881(5)	C(29)-C(30)	1.522(6)
Si(2)-C(10)	1.885(5)	C(29)-C(31)	1.547(7)
Si(2)-C(32)	1.888(5)	C(32)-C(34)	1.535(7)
C(1)-C(2)	1.381(6)	C(32)-C(33)	1.537(7)
C(1)-C(8)	1.397(6)	C(35)-C(36)	1.540(7)
C(2)-C(3)	1.456(6)	C(35)-C(37)	1.553(6)
C(3)-C(4)	1.352(6)	C(38)-C(40)	1.533(7)
C(4)-C(6)	1.462(6)	C(38)-C(39)	1.533(7)
C(5)-C(6)	1.373(6)	C(41)-Cl(1)	1.751(5)
C(5)-C(9)	1.403(6)	C(41)-Cl(3)	1.752(5)
C(7)-C(8)	1.376(6)	C(41)-Cl(2)	1.758(5)
O(1)-P(1)-C(1)	118.08(19)	O(2)-P(2)-C(3)	115.92(19)
O(1)-P(1)-C(11)	114.62(19)	C(17)-P(2)-C(3)	107.0(2)
C(1)-P(1)-C(11)	108.5(2)	C(5)-P(2)-C(3)	92.0(2)
O(1)-P(1)-C(4)	114.66(18)	C(2)-S(1)-C(7)	92.8(2)
C(1)-P(1)-C(4)	90.51(19)	C(6)-S(2)-C(10)	92.4(2)
C(11)-P(1)-C(4)	107.7(2)	C(23)-Si(1)-C(7)	108.9(2)
O(2)-P(2)-C(17)	113.26(19)	C(23)-Si(1)-C(29)	108.6(2)
O(2)-P(2)-C(5)	118.85(19)	C(7)-Si(1)-C(29)	106.4(2)
C(17)-P(2)-C(5)	107.5(2)	C(23)-Si(1)-C(26)	111.3(2)

C(7)-Si(1)-C(26)	110.1(2)	C(12)-C(11)-P(1)	118.9(3)
C(29)-Si(1)-C(26)	111.4(2)	C(11)-C(12)-C(13)	119.8(5)
C(38)-Si(2)-C(35)	117.1(2)	C(14)-C(13)-C(12)	121.2(5)
C(38)-Si(2)-C(10)	107.1(2)	C(15)-C(14)-C(13)	119.4(4)
C(35)-Si(2)-C(10)	106.0(2)	C(14)-C(15)-C(16)	119.6(5)
C(38)-Si(2)-C(32)	109.0(2)	C(11)-C(16)-C(15)	121.1(4)
C(35)-Si(2)-C(32)	108.7(2)	C(22)-C(17)-C(18)	119.5(4)
C(10)-Si(2)-C(32)	108.7(2)	C(22)-C(17)-P(2)	119.9(4)
C(2)-C(1)-C(8)	112.4(4)	C(18)-C(17)-P(2)	120.3(3)
C(2)-C(1)-P(1)	109.8(3)	C(19)-C(18)-C(17)	120.3(4)
C(8)-C(1)-P(1)	137.8(3)	C(18)-C(19)-C(20)	119.8(5)
C(1)-C(2)-C(3)	115.4(4)	C(21)-C(20)-C(19)	120.0(5)
C(1)-C(2)-S(1)	111.0(3)	C(20)-C(21)-C(22)	121.4(5)
C(3)-C(2)-S(1)	133.6(3)	C(21)-C(22)-C(17)	119.0(5)
C(4)-C(3)-C(2)	112.7(4)	C(24)-C(23)-C(25)	109.8(4)
C(4)-C(3)-P(2)	110.5(3)	C(24)-C(23)-Si(1)	111.5(3)
C(2)-C(3)-P(2)	136.4(3)	C(25)-C(23)-Si(1)	114.4(3)
C(3)-C(4)-C(6)	112.9(4)	C(27)-C(26)-C(28)	110.4(4)
C(3)-C(4)-P(1)	111.5(3)	C(27)-C(26)-Si(1)	111.2(3)
C(6)-C(4)-P(1)	134.6(3)	C(28)-C(26)-Si(1)	115.5(3)
C(6)-C(5)-C(9)	112.0(4)	C(30)-C(29)-C(31)	109.9(4)
C(6)-C(5)-P(2)	108.2(3)	C(30)-C(29)-Si(1)	113.8(3)
C(9)-C(5)-P(2)	139.7(3)	C(31)-C(29)-Si(1)	112.4(3)
C(5)-C(6)-C(4)	116.3(4)	C(34)-C(32)-C(33)	111.0(5)
C(5)-C(6)-S(2)	111.5(3)	C(34)-C(32)-Si(2)	111.8(3)
C(4)-C(6)-S(2)	132.1(3)	C(33)-C(32)-Si(2)	114.0(4)
C(8)-C(7)-S(1)	109.1(3)	C(36)-C(35)-C(37)	109.4(4)
C(8)-C(7)-Si(1)	128.5(3)	C(36)-C(35)-Si(2)	115.0(3)
S(1)-C(7)-Si(1)	122.4(2)	C(37)-C(35)-Si(2)	113.5(3)
C(7)-C(8)-C(1)	114.8(4)	C(40)-C(38)-C(39)	111.3(5)
C(10)-C(9)-C(5)	115.1(4)	C(40)-C(38)-Si(2)	112.5(4)
C(9)-C(10)-S(2)	109.0(3)	C(39)-C(38)-Si(2)	115.2(4)
C(9)-C(10)-Si(2)	129.5(3)	Cl(1)-C(41)-Cl(3)	110.4(3)
S(2)-C(10)-Si(2)	121.3(3)	Cl(1)-C(41)-Cl(2)	110.7(3)
C(16)-C(11)-C(12)	118.7(4)	Cl(3)-C(41)-Cl(2)	110.7(3)
C(16)-C(11)-P(1)	122.3(3)		

Table S2. Bond Lengths [Å] and Angles [°] for *trans*-**3**

P(1)-O(1)	1.478(4)	C(6)-C(11)	1.385(6)
P(1)-C(6)	1.793(6)	C(7)-C(8)	1.378(7)
P(1)-C(1)	1.813(10)	C(8)-C(9)	1.378(8)
P(1)-C(5)#1	1.819(6)	C(9)-C(10)	1.368(8)
C(1)-C(4)	1.386(7)	C(10)-C(11)	1.386(7)
C(1)-C(2)	1.402(7)	Si(1)-C(12)	1.878(6)
C(2)-C(3)	1.380(8)	Si(1)-C(14)	1.892(7)
C(3)-S(1)	1.743(6)	Si(1)-C(13)	1.897(7)
C(3)-Si(1)	1.881(9)	C(12)-C(15)	1.526(8)
S(1)-C(4)	1.726(10)	C(12)-C(16)	1.543(8)
C(4)-C(5)	1.452(7)	C(13)-C(17)	1.482(8)
C(5)-C(5)#1	1.366(9)	C(13)-C(18)	1.555(9)
C(5)-P(1)#1	1.819(6)	C(14)-C(19)	1.530(7)
C(6)-C(7)	1.384(7)	C(14)-C(20)	1.552(10)

O(1)-P(1)-C(6)	114.7(3)	C(11)-C(6)-P(1)	120.1(4)
O(1)-P(1)-C(1)	121.4(2)	C(8)-C(7)-C(6)	119.6(5)
C(6)-P(1)-C(1)	107.4(2)	C(9)-C(8)-C(7)	120.5(5)
O(1)-P(1)-C(5)#1	113.7(2)	C(10)-C(9)-C(8)	120.4(5)
C(6)-P(1)-C(5)#1	105.27(19)	C(9)-C(10)-C(11)	119.5(5)
C(1)-P(1)-C(5)#1	91.20(19)	C(6)-C(11)-C(10)	120.4(5)
C(4)-C(1)-C(2)	112.1(4)	C(12)-Si(1)-C(3)	108.2(2)
C(4)-C(1)-P(1)	108.9(3)	C(12)-Si(1)-C(14)	109.9(3)
C(2)-C(1)-P(1)	138.5(4)	C(3)-Si(1)-C(14)	107.7(3)
C(3)-C(2)-C(1)	115.0(5)	C(12)-Si(1)-C(13)	107.0(3)
C(2)-C(3)-S(1)	109.1(4)	C(3)-Si(1)-C(13)	106.1(3)
C(2)-C(3)-Si(1)	127.0(4)	C(14)-Si(1)-C(13)	117.6(3)
S(1)-C(3)-Si(1)	123.8(2)	C(15)-C(12)-C(16)	110.3(5)
C(4)-S(1)-C(3)	92.6(2)	C(15)-C(12)-Si(1)	110.8(4)
C(1)-C(4)-C(5)	115.8(4)	C(16)-C(12)-Si(1)	113.2(4)
C(1)-C(4)-S(1)	111.0(3)	C(17)-C(13)-C(18)	112.1(5)
C(5)-C(4)-S(1)	133.0(4)	C(17)-C(13)-Si(1)	117.2(4)
C(5)#1-C(5)-C(4)	113.3(5)	C(18)-C(13)-Si(1)	111.0(5)
C(5)#1-C(5)-P(1)#1	110.9(4)	C(19)-C(14)-C(20)	109.8(4)
C(4)-C(5)-P(1)#1	135.8(3)	C(19)-C(14)-Si(1)	114.2(4)
C(7)-C(6)-C(11)	119.6(4)	C(20)-C(14)-Si(1)	113.7(4)
C(7)-C(6)-P(1)	120.3(3)		

Symmetry transformations used to generate equivalent atoms: #1 $-x, -y, -z$

Table S3. Bond Lengths [Å] and Angles [°] for *cis*-**4**

S(1)-C(4)	1.719(3)	C(12)-H(7)	1.0000
S(1)-C(1)	1.731(3)	C(13)-H(8)	0.9800
C(1)-C(2)	1.377(4)	C(13)-H(9)	0.9800
C(1)-Si(1)	1.883(3)	C(13)-H(10)	0.9800
C(2)-C(3)	1.375(4)	C(14)-H(11)	0.9800
C(2)-H(1)	0.9500	C(14)-H(12)	0.9800
C(3)-C(4)	1.366(4)	C(14)-H(13)	0.9800
C(3)-P(1)	1.810(3)	C(15)-C(16)	1.532(4)
C(4)-C(5)	1.458(4)	C(15)-C(17)	1.534(4)
C(5)-C(5)#1	1.349(6)	C(15)-H(14)	1.0000
C(5)-P(1)#1	1.811(3)	C(16)-H(15)	0.9800
P(1)-C(6)	1.801(3)	C(16)-H(16)	0.9800
P(1)-C(5)#1	1.811(3)	C(16)-H(17)	0.9800
P(1)-S(2)	1.9480(11)	C(17)-H(18)	0.9800
C(6)-C(7)	1.396(4)	C(17)-H(19)	0.9800
C(6)-C(11)	1.399(4)	C(17)-H(20)	0.9800
C(7)-C(8)	1.386(4)	C(18)-C(19)	1.530(5)
C(7)-H(2)	0.9500	C(18)-C(20)	1.535(4)
C(8)-C(9)	1.380(5)	C(18)-H(21)	1.0000
C(8)-H(3)	0.9500	C(19)-H(22)	0.9800
C(9)-C(10)	1.391(5)	C(19)-H(23)	0.9800
C(9)-H(4)	0.9500	C(19)-H(24)	0.9800
C(10)-C(11)	1.390(4)	C(20)-H(25)	0.9800
C(10)-H(5)	0.9500	C(20)-H(26)	0.9800
C(11)-H(6)	0.9500	C(20)-H(27)	0.9800
Si(1)-C(12)	1.888(3)	C(21)-Cl(1)	1.750(4)
Si(1)-C(15)	1.888(3)	C(21)-Cl(2)	1.756(4)
Si(1)-C(18)	1.891(3)	C(21)-H(28)	0.9900
C(12)-C(13)	1.530(5)	C(21)-H(29)	0.9900
C(12)-C(14)	1.537(5)		

C(4)-S(1)-C(1)	92.40(14)	C(4)-C(3)-P(1)	108.5(2)
C(2)-C(1)-S(1)	108.2(2)	C(2)-C(3)-P(1)	139.7(2)
C(2)-C(1)-Si(1)	132.2(2)	C(3)-C(4)-C(5)	116.5(3)
S(1)-C(1)-Si(1)	119.55(18)	C(3)-C(4)-S(1)	111.4(2)
C(3)-C(2)-C(1)	116.2(3)	C(5)-C(4)-S(1)	132.0(2)
C(3)-C(2)-H(1)	121.9	C(5)#1-C(5)-C(4)	112.3(3)
C(1)-C(2)-H(1)	121.9	C(5)#1-C(5)-P(1)#1	111.6(3)
C(4)-C(3)-C(2)	111.8(3)	C(4)-C(5)-P(1)#1	136.0(2)

C(6)-P(1)-C(3)	109.56(14)	H(8)-C(13)-H(10)	109.5
C(6)-P(1)-C(5)#1	106.62(14)	H(9)-C(13)-H(10)	109.5
C(3)-P(1)-C(5)#1	90.89(14)	C(12)-C(14)-H(11)	109.5
C(6)-P(1)-S(2)	115.13(11)	C(12)-C(14)-H(12)	109.5
C(3)-P(1)-S(2)	119.14(10)	H(11)-C(14)-H(12)	109.5
C(5)#1-P(1)-S(2)	112.40(10)	C(12)-C(14)-H(13)	109.5
C(7)-C(6)-C(11)	120.1(3)	H(11)-C(14)-H(13)	109.5
C(7)-C(6)-P(1)	121.8(2)	H(12)-C(14)-H(13)	109.5
C(11)-C(6)-P(1)	118.1(2)	C(16)-C(15)-C(17)	110.3(3)
C(8)-C(7)-C(6)	119.3(3)	C(16)-C(15)-Si(1)	112.5(2)
C(8)-C(7)-H(2)	120.3	C(17)-C(15)-Si(1)	112.1(2)
C(6)-C(7)-H(2)	120.3	C(16)-C(15)-H(14)	107.2
C(9)-C(8)-C(7)	120.7(3)	C(17)-C(15)-H(14)	107.2
C(9)-C(8)-H(3)	119.7	Si(1)-C(15)-H(14)	107.2
C(7)-C(8)-H(3)	119.7	C(15)-C(16)-H(15)	109.5
C(8)-C(9)-C(10)	120.4(3)	C(15)-C(16)-H(16)	109.5
C(8)-C(9)-H(4)	119.8	H(15)-C(16)-H(16)	109.5
C(10)-C(9)-H(4)	119.8	C(15)-C(16)-H(17)	109.5
C(11)-C(10)-C(9)	119.7(3)	H(15)-C(16)-H(17)	109.5
C(11)-C(10)-H(5)	120.1	H(16)-C(16)-H(17)	109.5
C(9)-C(10)-H(5)	120.1	C(15)-C(17)-H(18)	109.5
C(10)-C(11)-C(6)	119.8(3)	C(15)-C(17)-H(19)	109.5
C(10)-C(11)-H(6)	120.1	H(18)-C(17)-H(19)	109.5
C(6)-C(11)-H(6)	120.1	C(15)-C(17)-H(20)	109.5
C(1)-Si(1)-C(12)	107.15(14)	H(18)-C(17)-H(20)	109.5
C(1)-Si(1)-C(15)	107.75(13)	H(19)-C(17)-H(20)	109.5
C(12)-Si(1)-C(15)	109.32(14)	C(19)-C(18)-C(20)	110.6(3)
C(1)-Si(1)-C(18)	105.89(14)	C(19)-C(18)-Si(1)	114.1(2)
C(12)-Si(1)-C(18)	116.97(14)	C(20)-C(18)-Si(1)	113.8(2)
C(15)-Si(1)-C(18)	109.34(14)	C(19)-C(18)-H(21)	105.8
C(13)-C(12)-C(14)	110.0(3)	C(20)-C(18)-H(21)	105.8
C(13)-C(12)-Si(1)	114.9(2)	Si(1)-C(18)-H(21)	105.8
C(14)-C(12)-Si(1)	112.5(2)	C(18)-C(19)-H(22)	109.5
C(13)-C(12)-H(7)	106.3	C(18)-C(19)-H(23)	109.5
C(14)-C(12)-H(7)	106.3	H(22)-C(19)-H(23)	109.5
Si(1)-C(12)-H(7)	106.3	C(18)-C(19)-H(24)	109.5
C(12)-C(13)-H(8)	109.5	H(22)-C(19)-H(24)	109.5
C(12)-C(13)-H(9)	109.5	H(23)-C(19)-H(24)	109.5
H(8)-C(13)-H(9)	109.5	C(18)-C(20)-H(25)	109.5
C(12)-C(13)-H(10)	109.5	C(18)-C(20)-H(26)	109.5

H(25)-C(20)-H(26)	109.5	Cl(1)-C(21)-H(28)	109.3
C(18)-C(20)-H(27)	109.5	Cl(2)-C(21)-H(28)	109.3
H(25)-C(20)-H(27)	109.5	Cl(1)-C(21)-H(29)	109.3
H(26)-C(20)-H(27)	109.5	Cl(2)-C(21)-H(29)	109.3
Cl(1)-C(21)-Cl(2)	111.8(2)	H(28)-C(21)-H(29)	107.9

Symmetry transformations used to generate equivalent atoms: #1 $-x+2, y, -z+3/2$

4. Theoretical Calculations

Table S4. The Cartesian Coordinates (Å) of the Optimized Structure for *trans*-**2'**

atom	*x*	*y*	*z*
C	-0.485724048706	-0.303519329425	-0.388070847731
C	0.485724048706	0.303519329425	0.388070847731
C	0.819418631782	0.700691420053	-2.125417555251
C	-0.283882924652	-0.081643773567	-1.795694086664
C	0.952205666193	0.895449105412	-3.525796682672
H	1.746676279357	1.480115369590	-3.978669584982
C	-0.017836509818	0.261961335501	-4.279881203409
S	-1.148630978400	-0.579240977051	-3.216489160642
C	-0.819418631782	-0.700691420053	2.125417555251
C	0.283882924652	0.081643773567	1.795694086664
C	-0.952205666193	-0.895449105412	3.525796682672
H	-1.746676279357	-1.480115369590	3.978669584982
C	0.017836509818	-0.261961335501	4.279881203409
S	1.148630978400	0.579240977051	3.216489160642
P	1.616541674452	1.351906426224	-0.610846265825
P	-1.616541674452	-1.351906426224	0.610846265825
Si	0.202135625306	-0.241923792972	6.153792649866
Si	-0.202135625306	0.241923792972	-6.153792649866
C	1.871702168604	-0.992169529125	6.636241807207
H	2.006414028160	-0.986184526430	7.725123877847
H	2.706398943309	-0.433607156279	6.196300861557
H	1.952691442327	-2.030234754452	6.293856466776
C	-0.103633709079	-1.538808365087	-6.787823211506
H	0.860151184375	-1.996147174387	-6.536066890236
H	-0.217704713713	-1.574236856855	-7.878437790317
H	-0.890695745229	-2.165510354513	-6.351882146315
C	1.206727705554	1.270188194390	-6.886227561620
H	2.189129359062	0.859863156517	-6.625468752239
H	1.172996849432	2.309918897508	-6.540740304492
H	1.136428133933	1.284925254834	-7.980763079962
C	-1.206727705554	-1.270188194390	6.886227561620
H	-1.136428133933	-1.284925254834	7.980763079962
H	-1.172996849432	-2.309918897508	6.540740304492
H	-2.189129359062	-0.859863156517	6.625468752239
C	0.103633709079	1.538808365087	6.787823211506
H	0.217704713713	1.574236856855	7.878437790317
H	-0.860151184375	1.996147174387	6.536066890236
H	0.890695745229	2.165510354513	6.351882146315

(continued)

atom	*x*	*y*	*z*
C	-1.871702168604	0.992169529125	-6.636241807207
H	-1.952691442327	2.030234754452	-6.293856466776
H	-2.706398943309	0.433607156279	-6.196300861557
H	-2.006414028160	0.986184526430	-7.725123877847
C	3.246283576781	0.476868467071	-0.517339547042
C	5.769573375721	-0.734935685524	-0.339813040321
C	4.367708731185	1.222986240775	-0.130899869895
C	3.401848903772	-0.886190272211	-0.816000334039
C	4.655761884430	-1.486813421879	-0.727531048245
C	5.624947564851	0.619130521764	-0.041254880764
H	4.257032262884	2.279593013697	0.099488155845
H	2.538932402416	-1.472643081998	-1.118574016717
H	4.766310021583	-2.542805925641	-0.960118218441
H	6.487298687887	1.208037862338	0.259846340716
H	6.746517449867	-1.206388312385	-0.272095801345
C	-3.246283576781	-0.476868467071	0.517339547042
C	-5.769573375721	0.734935685524	0.339813040321
C	-4.367708731185	-1.222986240775	0.130899869895
C	-3.401848903772	0.886190272211	0.816000334039
C	-4.655761884430	1.486813421879	0.727531048245
C	-5.624947564851	-0.619130521764	0.041254880764
H	-4.257032262884	-2.279593013697	-0.099488155845
H	-2.538932402416	1.472643081998	1.118574016717
H	-4.766310021583	2.542805925641	0.960118218441
H	-6.487298687887	-1.208037862338	-0.259846340716
H	-6.746517449867	1.206388312385	0.272095801345

Table S5. The Cartesian Coordinates (Å) of the Optimized Structure for *trans*-**3'**

atom	*x*	*y*	*z*
C	-0.473581797886	-0.310512388892	-0.382662409316
C	0.473581797886	0.310512388892	0.382662409316
C	0.822709950322	0.622526917543	-2.181747244799
C	-0.276709067071	-0.136989009000	-1.809907136953
C	0.948137910330	0.760947395508	-3.585200176425
H	1.740889406816	1.323224300925	-4.067207946939
C	-0.047207052191	0.115781399483	-4.300959548728
S	-1.156267884034	-0.683902202707	-3.193056470361
C	-0.822709950322	-0.622526917543	2.181747244799
C	0.276709067071	0.136989009000	1.809907136953

(continued)

atom	*x*	*y*	*z*
C	-0.948137910330	-0.760947395508	3.585200176425
H	-1.740889406816	-1.323224300925	4.067207946939
C	0.047207052191	-0.115781399483	4.300959548728
S	1.156267884034	0.683902202707	3.193056470361
P	1.708671100766	1.176227229125	-0.684472385161
P	-1.708671100766	-1.176227229125	0.684472385161
Si	0.274954479254	-0.050971313424	6.174901093266
Si	-0.274954479254	0.050971313424	-6.174901093266
C	1.935833678106	-0.831857580308	6.632599230062
H	2.094821305391	-0.806861917824	7.717855598024
H	2.773567996499	-0.302299691000	6.163605469304
H	1.984028964550	-1.878460632221	6.310840576609
C	-0.233462757281	-1.750678871860	-6.749293789557
H	0.723547454347	-2.224168284371	-6.501936341273
H	-0.370098587691	-1.817806667580	-7.835717432399
H	-1.027110949022	-2.343531939342	-6.279288784713
C	1.145590349106	1.024038171163	-6.954785176411
H	2.121353013024	0.590227046740	-6.707553744352
H	1.149012553700	2.070726408873	-6.629447821106
H	1.051674822262	1.020142074259	-8.047551540218
C	-1.145590349106	-1.024038171163	6.954785176411
H	-1.051674822262	-1.020142074259	8.047551540218
H	-1.149012553700	-2.070726408873	6.629447821106
H	-2.121353013024	-0.590227046740	6.707553744352
C	0.233462757281	1.750678871860	6.749293789557
H	0.370098587691	1.817806667580	7.835717432399
H	-0.723547454347	2.224168284371	6.501936341273
H	1.027110949022	2.343531939342	6.279288784713
C	-1.935833678106	0.831857580308	-6.632599230062
H	-1.984028964550	1.878460632221	-6.310840576609
H	-2.773567996499	0.302299691000	-6.163605469304
H	-2.094821305391	0.806861917824	-7.717855598024
C	3.250779733060	0.208785047067	-0.559139168924
C	5.672633136921	-1.164457413853	-0.328717808040
C	4.421514344917	0.902854144077	-0.228696286165
C	3.295830186022	-1.176798914076	-0.774583047981
C	4.504934980770	-1.859458985473	-0.657740628849
C	5.630745490728	0.213838132907	-0.115533141210
H	4.372781802119	1.975621628670	-0.066873984796

(continued)

atom	*x*	*y*	*z*
H	2.391447470203	-1.721653043759	-1.032712575041
H	4.537098706352	-2.932816806225	-0.823283778202
H	6.538178924790	0.754598148706	0.139199578744
H	6.614161850387	-1.699859673284	-0.239155030095
C	-3.250779733060	-0.208785047067	0.559139168924
C	-5.672633136921	1.164457413853	0.328717808040
C	-4.421514344917	-0.902854144077	0.228696286165
C	-3.295830186022	1.176798914076	0.774583047981
C	-4.504934980770	1.859458985473	0.657740628849
C	-5.630745490728	-0.213838132907	0.115533141210
H	-4.372781802119	-1.975621628670	0.066873984796
H	-2.391447470203	1.721653043759	1.032712575041
H	-4.537098706352	2.932816806225	0.823283778202
H	-6.538178924790	-0.754598148706	-0.139199578744
H	-6.614161850387	1.699859673284	0.239155030095
O	1.913232182258	2.643933061122	-0.453129267803
O	-1.913232182258	-2.643933061122	0.453129267803

Table S6. The Cartesian Coordinates (Å) of the Optimized Structure for *trans*-**4'**

atom	*x*	*y*	*z*
C	-0.498666698856	-0.277760954618	-0.377364208372
C	0.498666698856	0.277760954618	0.377364208372
C	0.845233974914	0.535077268844	-2.188810968630
C	-0.304431933763	-0.140540781781	-1.804927087920
C	0.971604956754	0.667767302465	-3.592203916105
H	1.798045042740	1.174939232821	-4.078293086830
C	-0.072844755310	0.094187052121	-4.297339885492
S	-1.231044783312	-0.622095837287	-3.181934146544
C	-0.845233974914	-0.535077268844	2.188810968630
C	0.304431933763	0.140540781781	1.804927087920
C	-0.971604956754	-0.667767302465	3.592203916105
H	-1.798045042740	-1.174939232821	4.078293086830
C	0.072844755310	-0.094187052121	4.297339885492
S	1.231044783312	0.622095837287	3.181934146544
P	1.775259101795	1.053053982335	-0.704844944959
P	-1.775259101795	-1.053053982335	0.704844944959
Si	0.311319771827	-0.034633149875	6.171022242419
Si	-0.311319771827	0.034633149875	-6.171022242419

(continued)

atom	*x*	*y*	*z*
C	1.975000886666	-0.818544517075	6.611559510525
H	2.142131382518	-0.798222326988	7.695643547596
H	2.809941853492	-0.287481304350	6.139192353352
H	2.019990841521	-1.863771406553	6.284998760631
C	-0.274003580392	-1.764699694585	-6.752638516546
H	0.684012538532	-2.239548144776	-6.511852025154
H	-0.415797318800	-1.827098645827	-7.838704478112
H	-1.065617208350	-2.358649522116	-6.280768959844
C	1.106153172504	1.008881368464	-6.954473677192
H	2.082597229035	0.570450733825	-6.718079838828
H	1.115099584263	2.052993384129	-6.621283669581
H	1.004392418729	1.012490916879	-8.046529345244
C	-1.106153172504	-1.008881368464	6.954473677192
H	-1.004392418729	-1.012490916879	8.046529345244
H	-1.115099584263	-2.052993384129	6.621283669581
H	-2.082597229035	-0.570450733825	6.718079838828
C	0.274003580392	1.764699694585	6.752638516546
H	0.415797318800	1.827098645827	7.838704478112
H	-0.684012538532	2.239548144776	6.511852025154
H	1.065617208350	2.358649522116	6.280768959844
C	-1.975000886666	0.818544517075	-6.611559510525
H	-2.019990841521	1.863771406553	-6.284998760631
H	-2.809941853492	0.287481304350	-6.139192353352
H	-2.142131382518	0.798222326988	-7.695643547596
C	3.254544009152	-0.028339663272	-0.580027346780
C	5.516135630667	-1.654927501850	-0.384609726766
C	4.507523186326	0.543420704749	-0.337897573890
C	3.133371387783	-1.419473407675	-0.724542501253
C	4.263778064118	-2.227702813712	-0.624887341108
C	5.636697280836	-0.272441427988	-0.242168847115
H	4.588744976076	1.620804340783	-0.226069326865
H	2.163297790864	-1.871486124404	-0.911960185126
H	4.166715068557	-3.304262527648	-0.733847061664
H	6.608847000034	0.175171800124	-0.054920395161
H	6.395817457275	-2.288357716477	-0.307871456991
C	-3.254544009152	0.028339663272	0.580027346780
C	-5.516135630667	1.654927501850	0.384609726766
C	-4.507523186326	-0.543420704749	0.337897573890
C	-3.133371387783	1.419473407675	0.724542501253

(continued)

atom	*x*	*y*	*z*
C	-4.263778064118	2.227702813712	0.624887341108
C	-5.636697280836	0.272441427988	0.242168847115
H	-4.588744976076	-1.620804340783	0.226069326865
H	-2.163297790864	1.871486124404	0.911960185126
H	-4.166715068557	3.304262527648	0.733847061664
H	-6.608847000034	-0.175171800124	0.054920395161
H	-6.395817457275	2.288357716477	0.307871456991
S	2.101093646021	2.975857680875	-0.431361257765
S	-2.101093646021	-2.975857680875	0.431361257765