

[4+2] versus [2+2] dimerisation in P(V) derivatives of 2,4-disubstituted phospholes

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² NIMBE, CEA, CNRS, Université Paris-Saclay, CEA Saclay 91191 Gif-sur-Yvette cedex, France

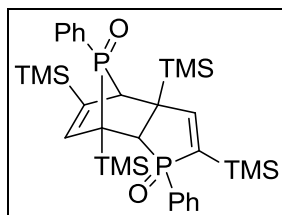
Correspondence should be addressed to Florian Jaroschik;
florian.jaroschik@enscm.fr

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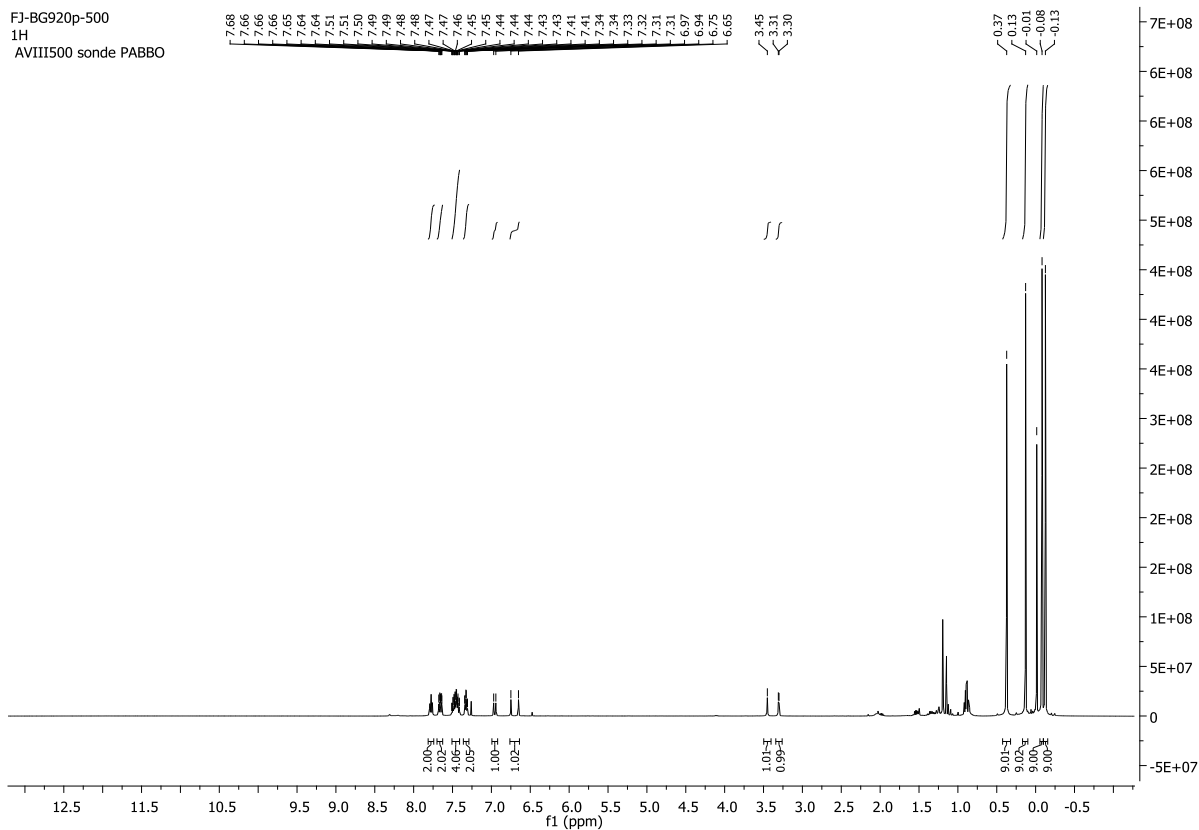
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III. Details on DFT calculations	S31

I. NMR spectra

Dimer of 1-phenyl-2,4-bis(trimethylsilyl)-oxophosphole (3b)

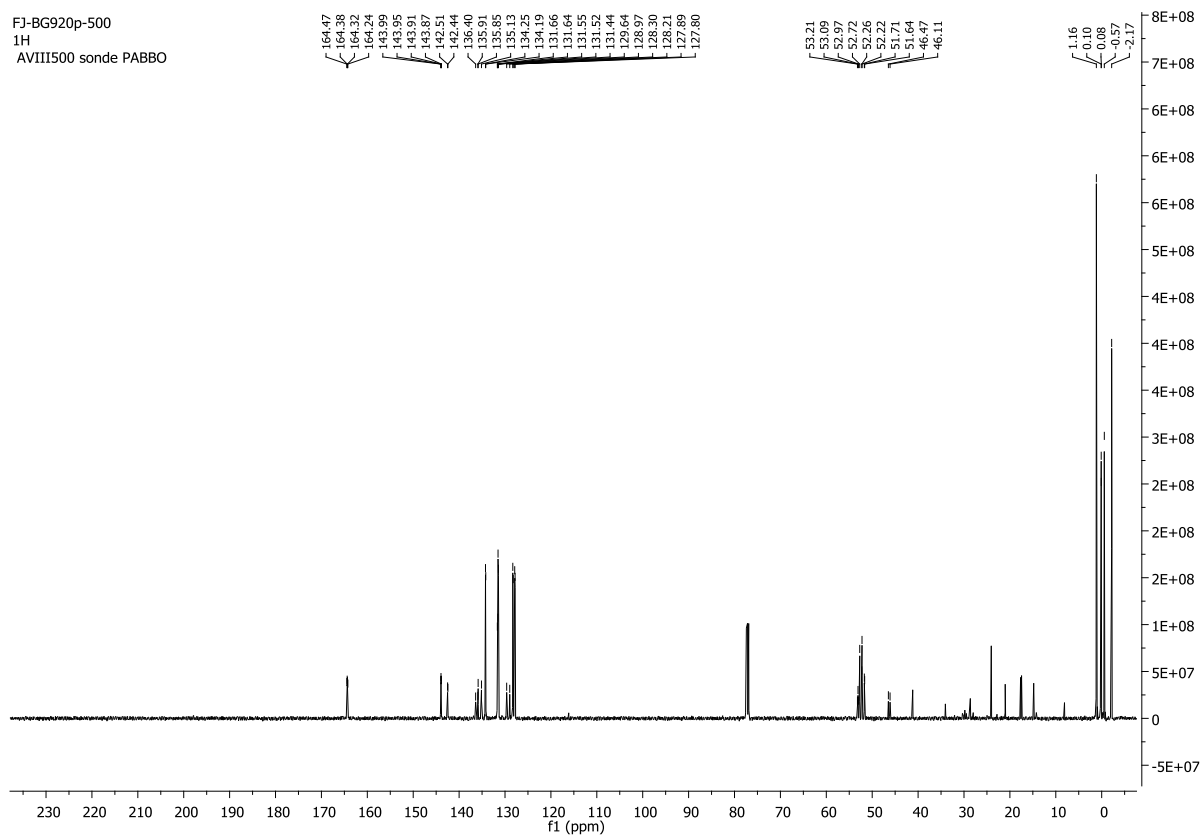


^1H (500 MHz, CDCl_3)



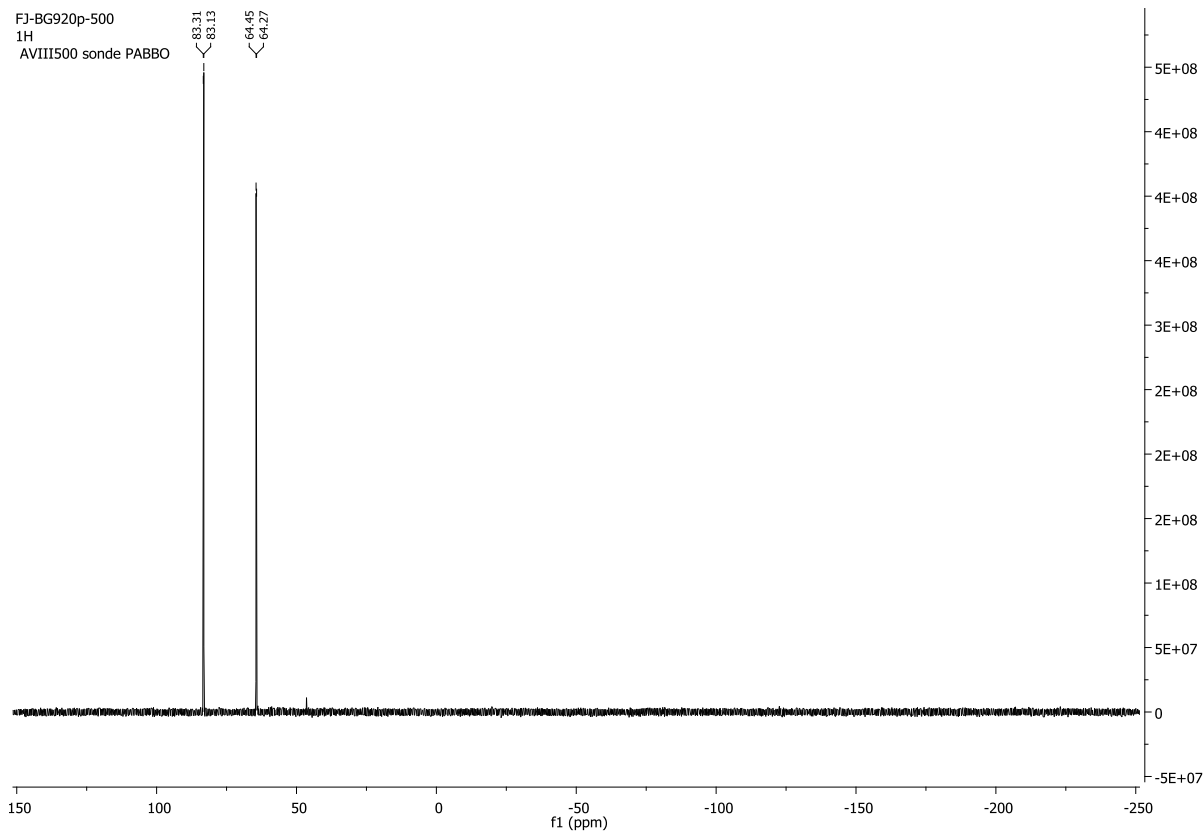
^{13}C (125 MHz, CDCl_3)

FJ-BG920p-500
1H
AVIII500 sonde PABBO



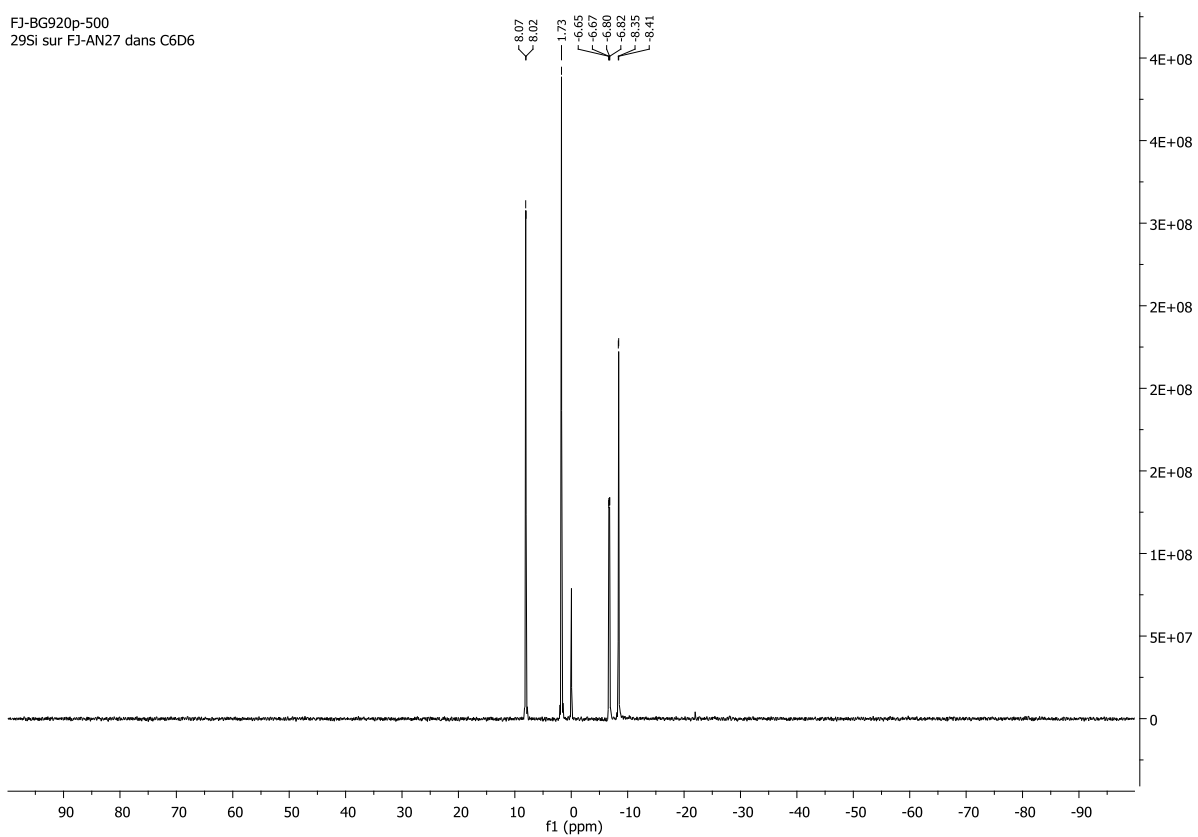
^{31}P (200 MHz, CDCl_3)

FJ-BG920p-500
1H
AVIII500 sonde PABBO

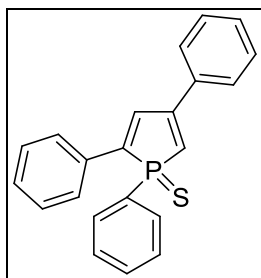


^{29}Si (100 MHz, CDCl_3)

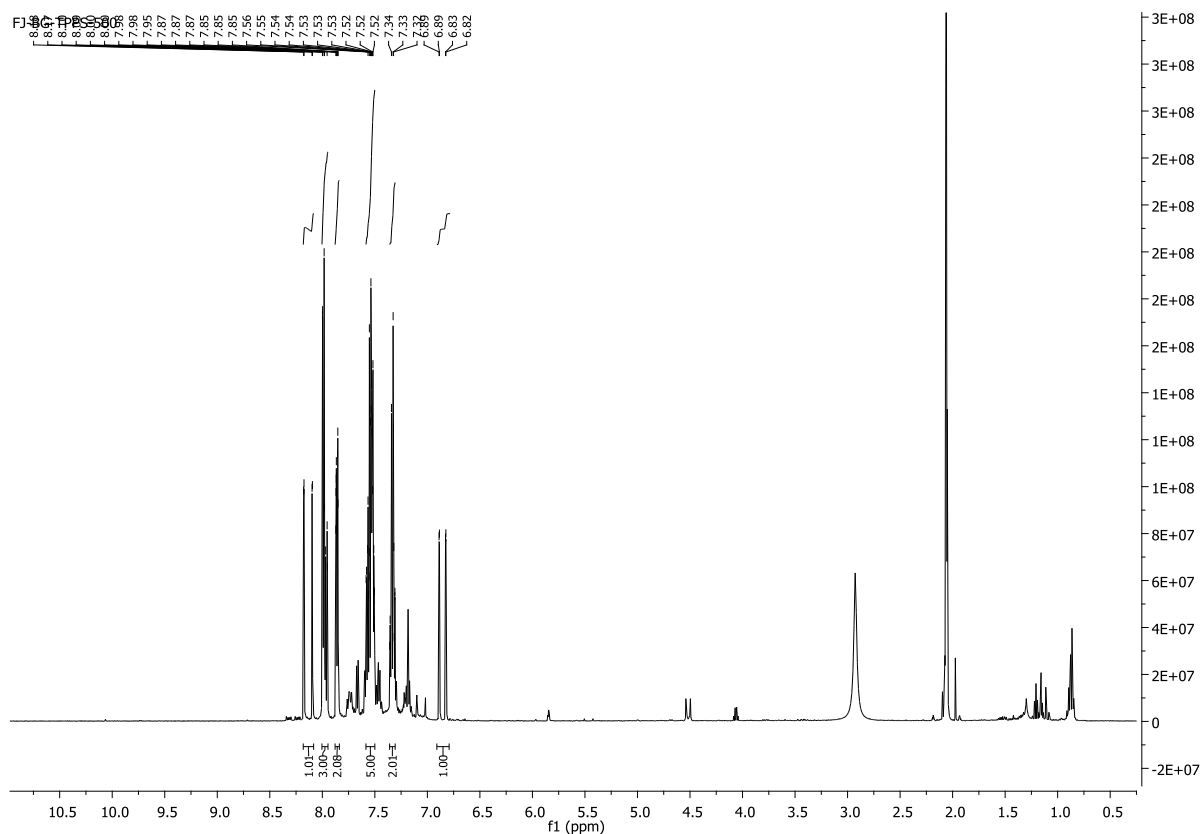
FJ-BG920p-500
29Si sur FJ-AN27 dans C_6D_6



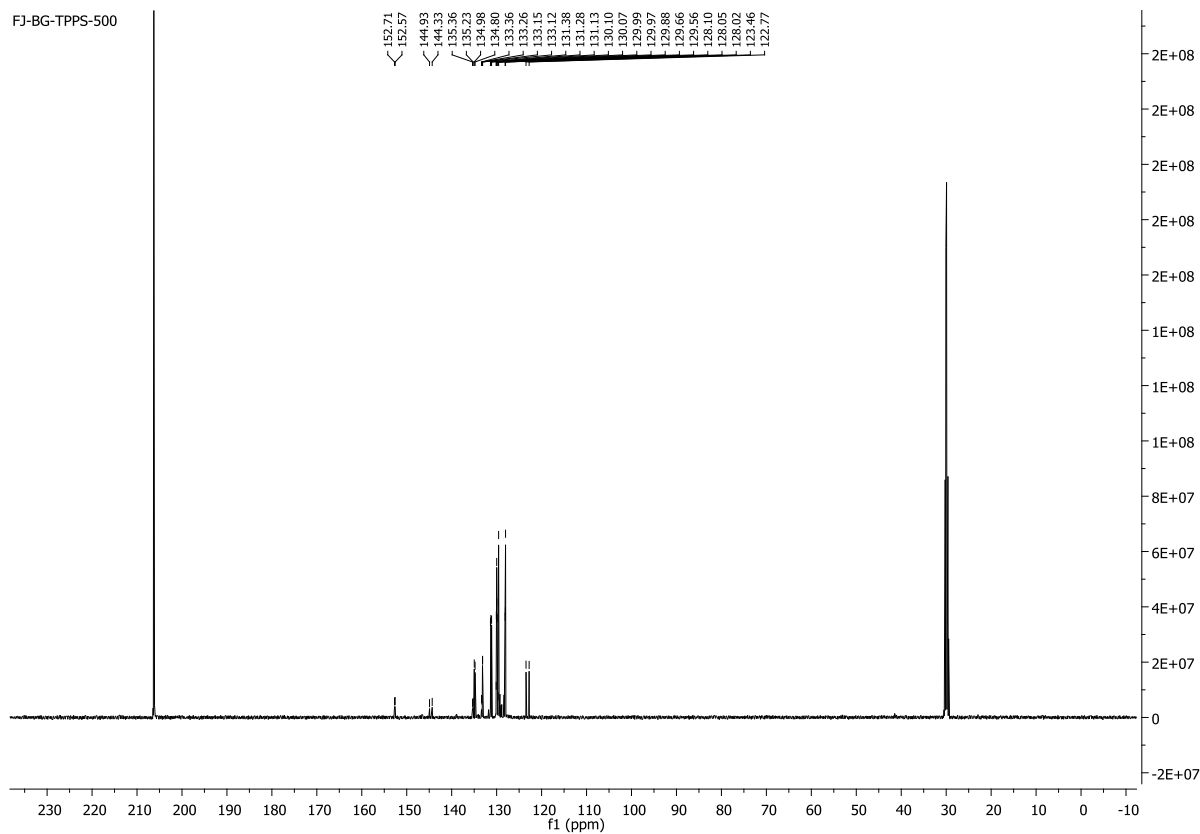
1,2,4-triphenyl-thiooxophosphole (4a)



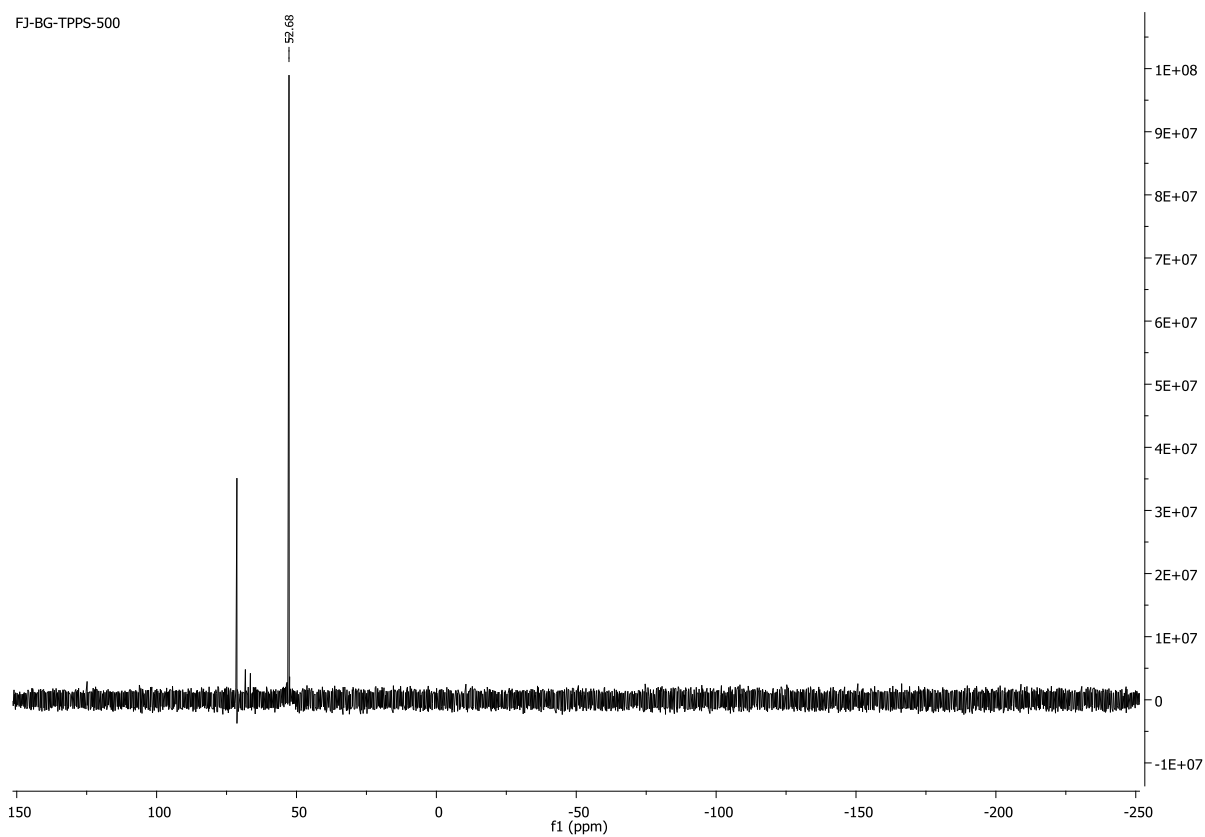
¹H (500 MHz, CDCl₃)



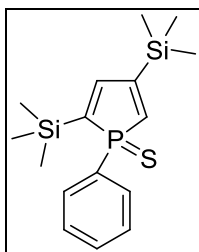
¹³C (125 MHz, CDCl₃)



^{31}P (200 MHz, CDCl_3)

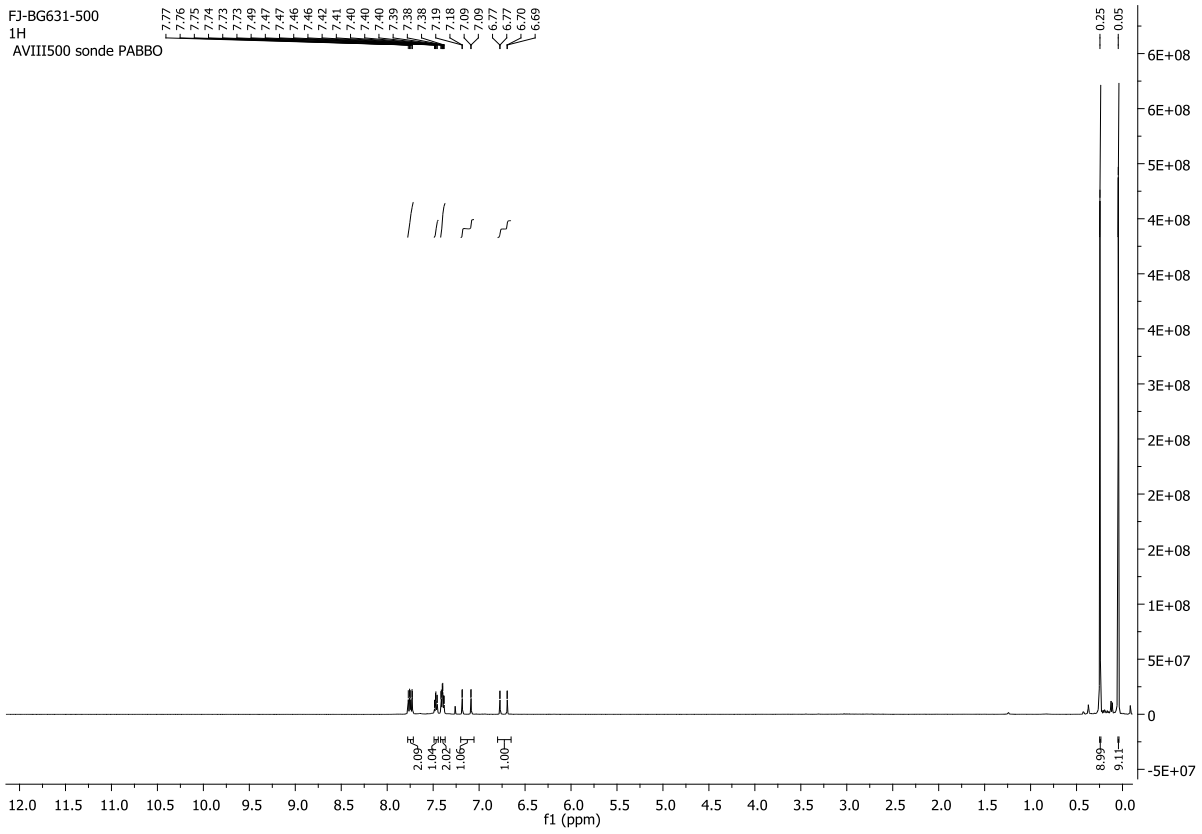


1-phenyl-2,4-bis(trimethylsilyl)-thioxophosphole (4b)



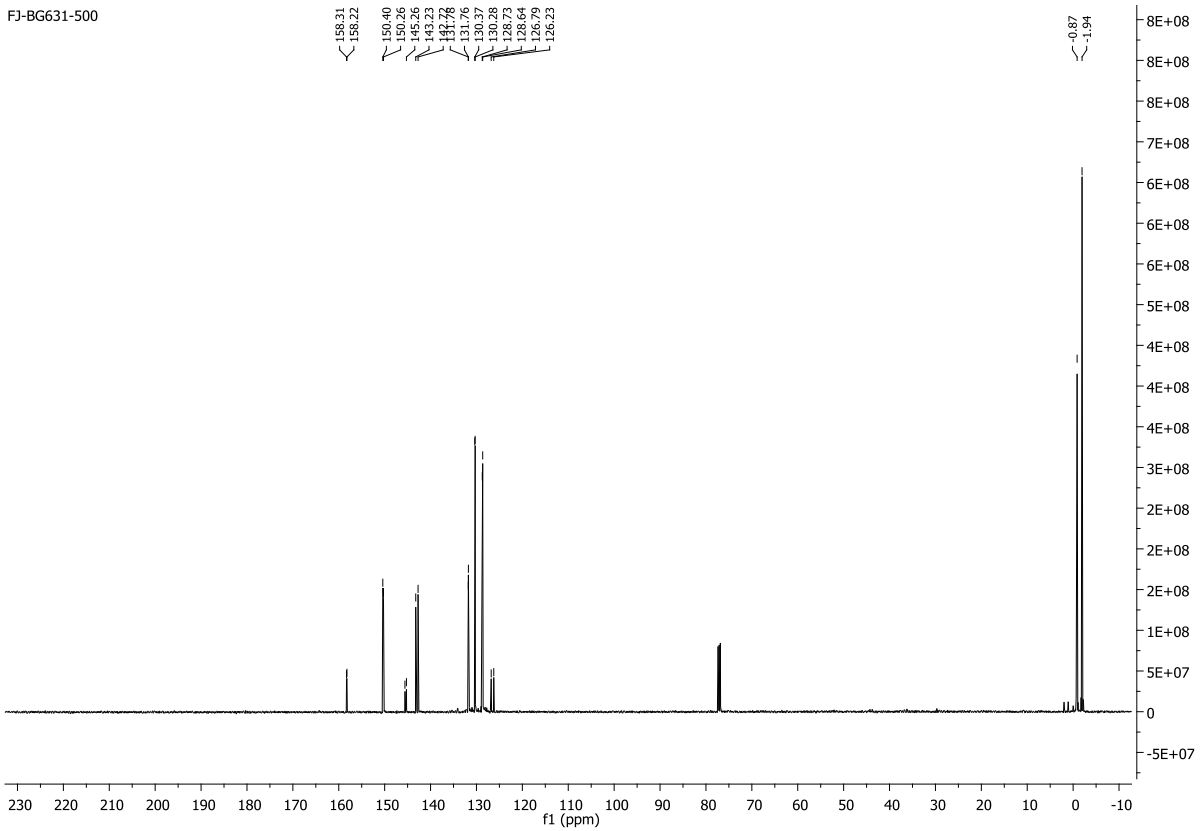
¹H (500 MHz, CDCl₃)

FJ-BG631-500
1H
AVIII500 sonde PABBO



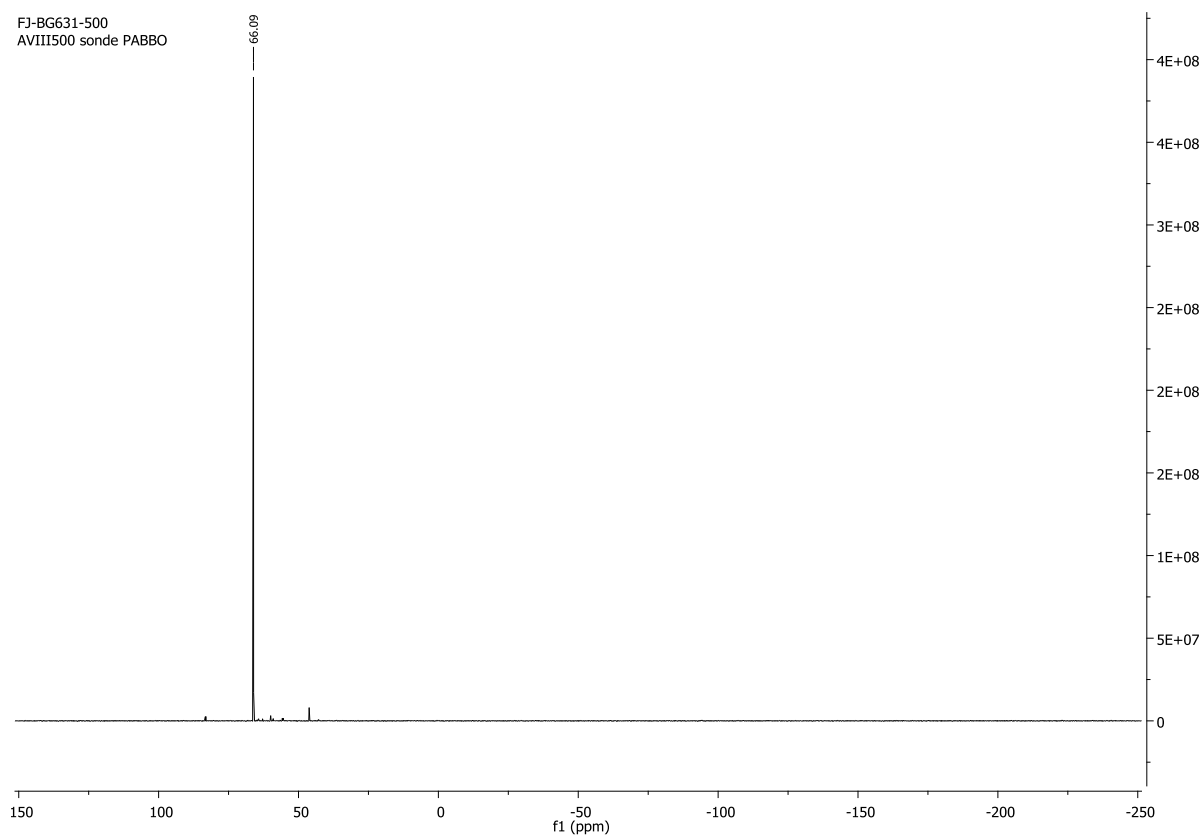
¹³C (125 MHz, CDCl₃)

FJ-BG631-500



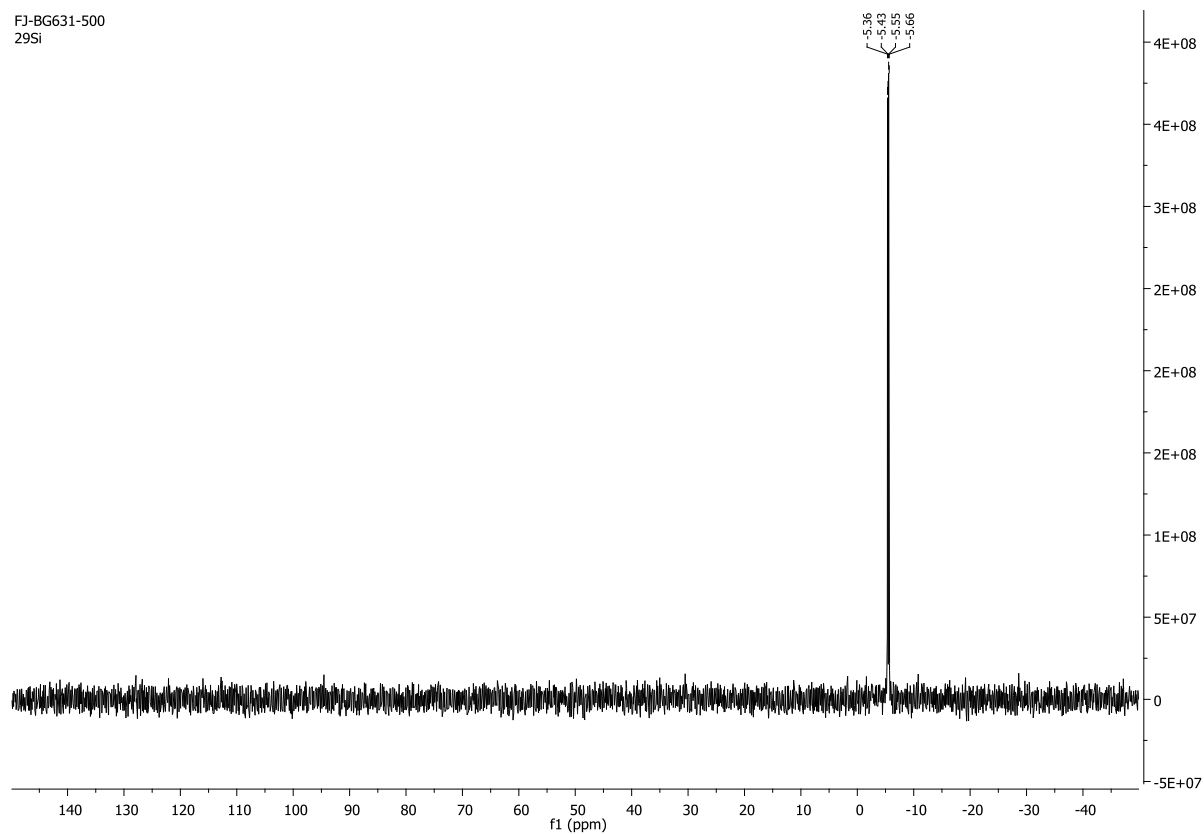
^{31}P (200 MHz, CDCl_3)

FJ-BG631-500
AVIII500 sonde PABBO

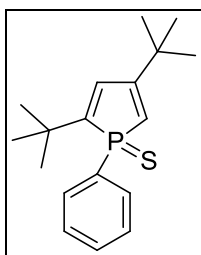


^{29}Si (100 MHz, CDCl_3)

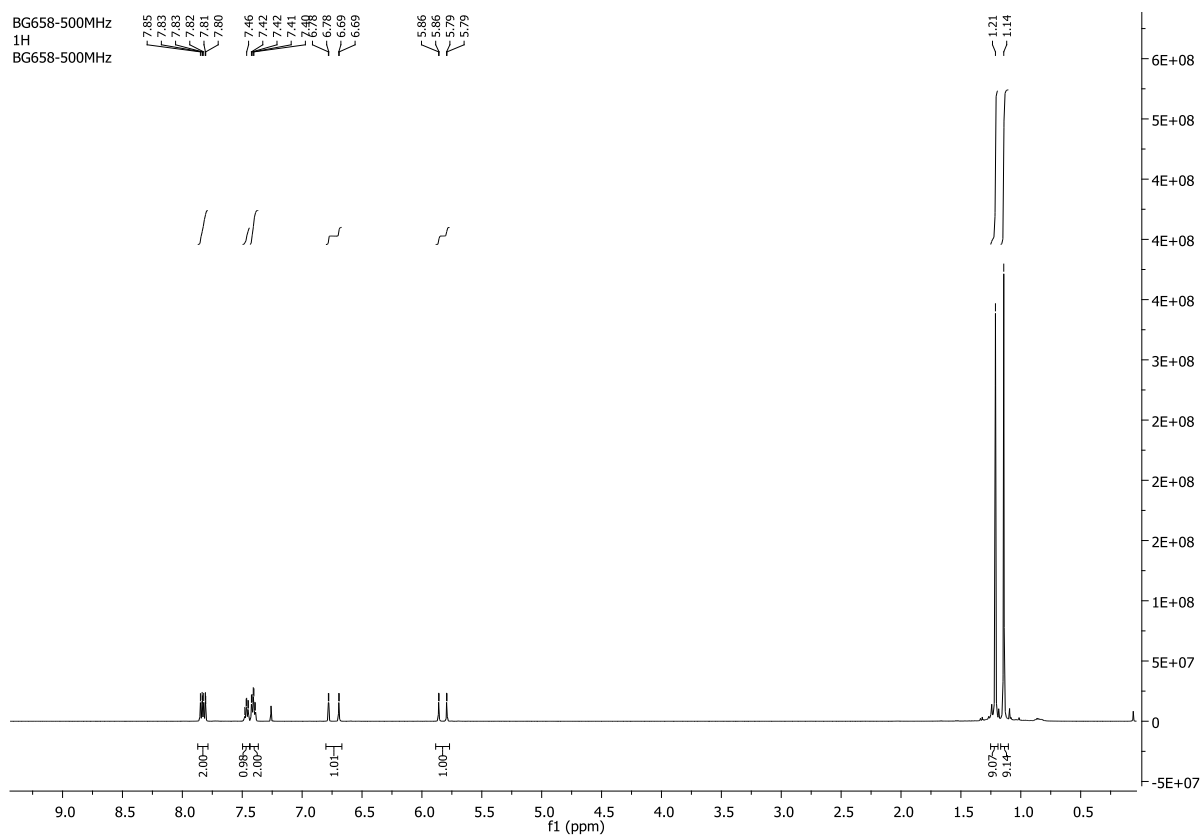
FJ-BG631-500
 ^{29}Si



2,4-bis(tert-butyl)-1-phenyl-thioxophosphole (4c)

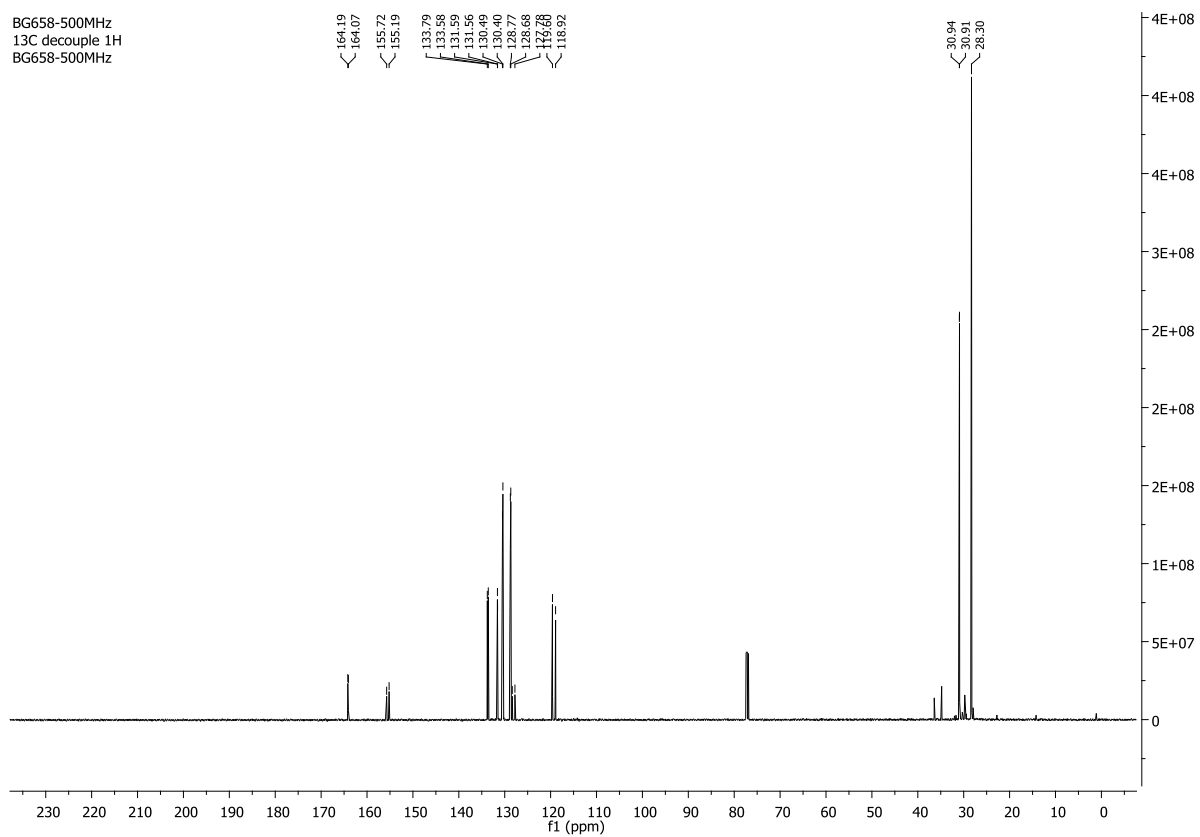


^1H (500 MHz, CDCl_3)



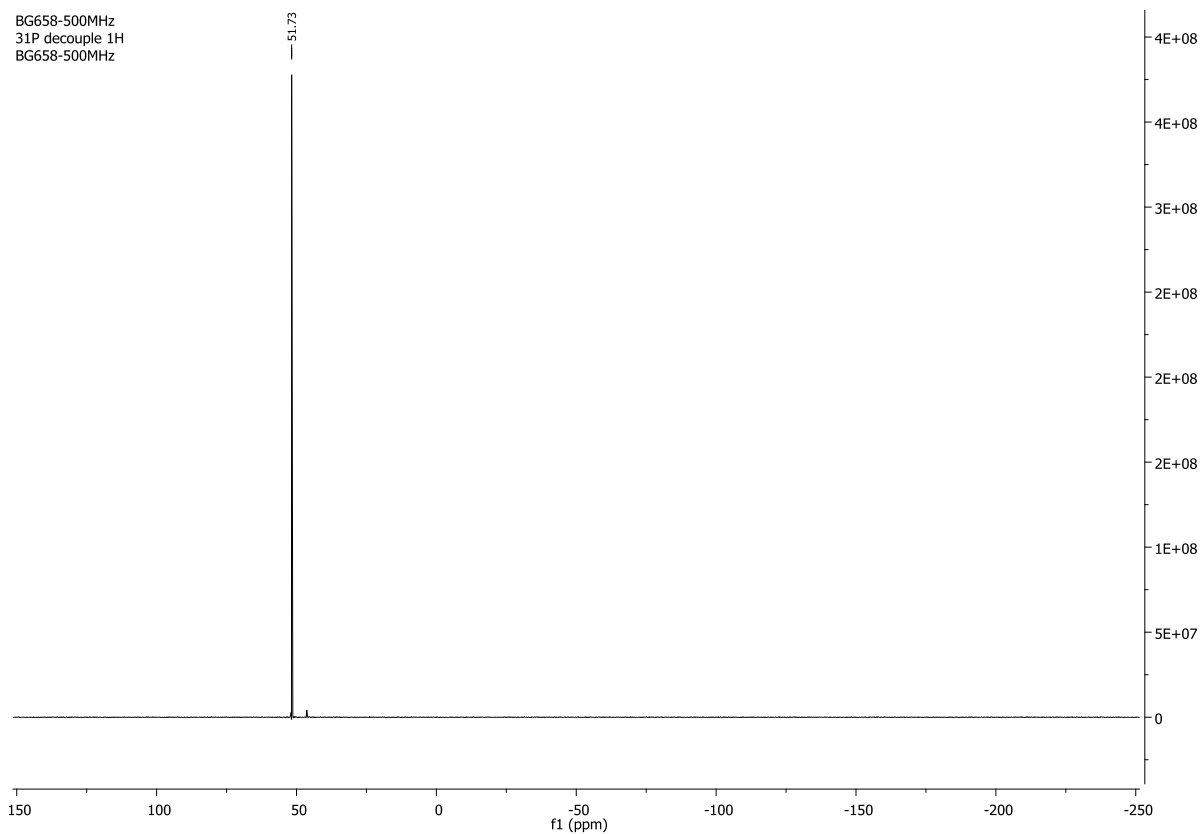
¹³C (125 MHz, CDCl₃)

BG658-500MHz
13C decouple 1H
BG658-500MHz

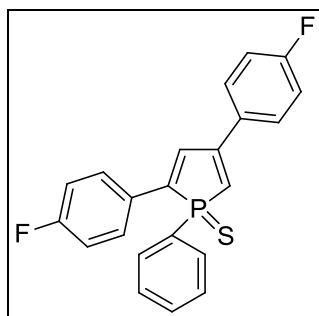


³¹P (200 MHz, CDCl₃)

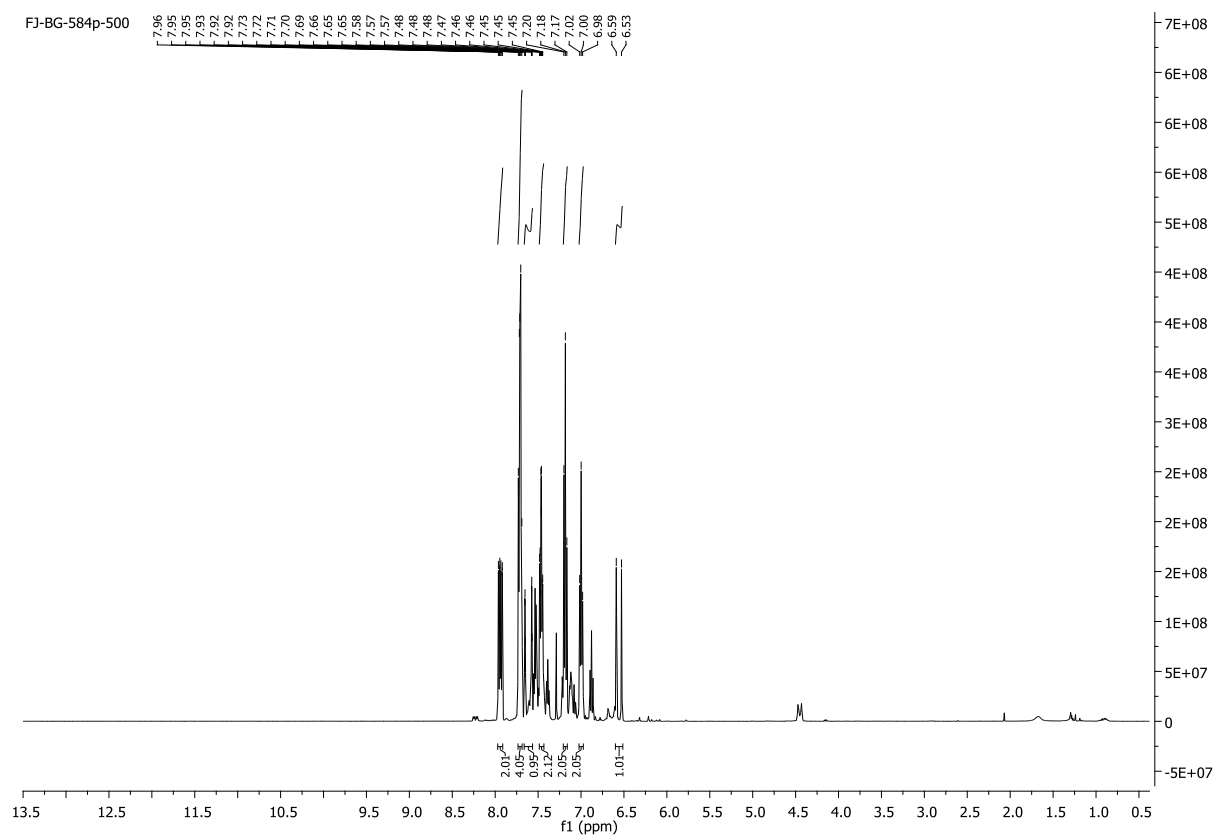
BG658-500MHz
31P decouple 1H
BG658-500MHz



2,4-bis(4-fluorophenyl)-1-phenyl-thioxophosphole (4d)

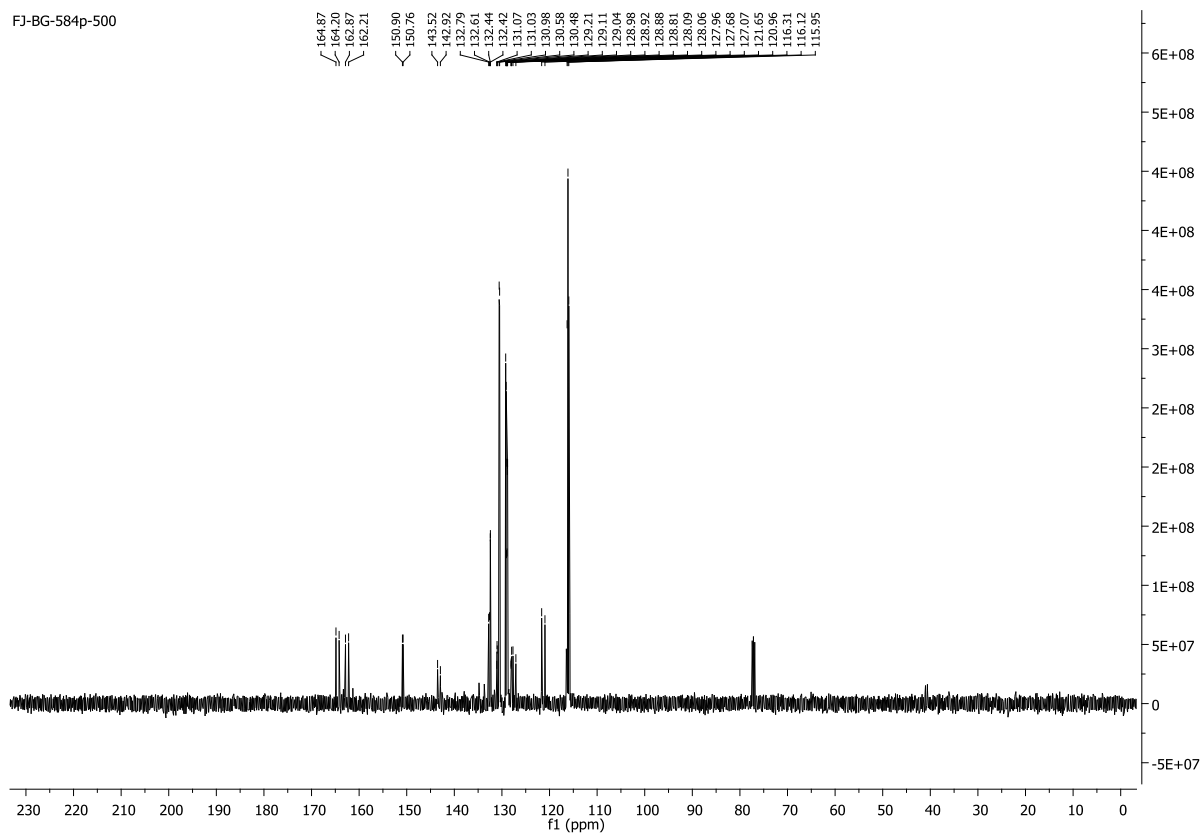


^1H (500 MHz, CDCl_3)



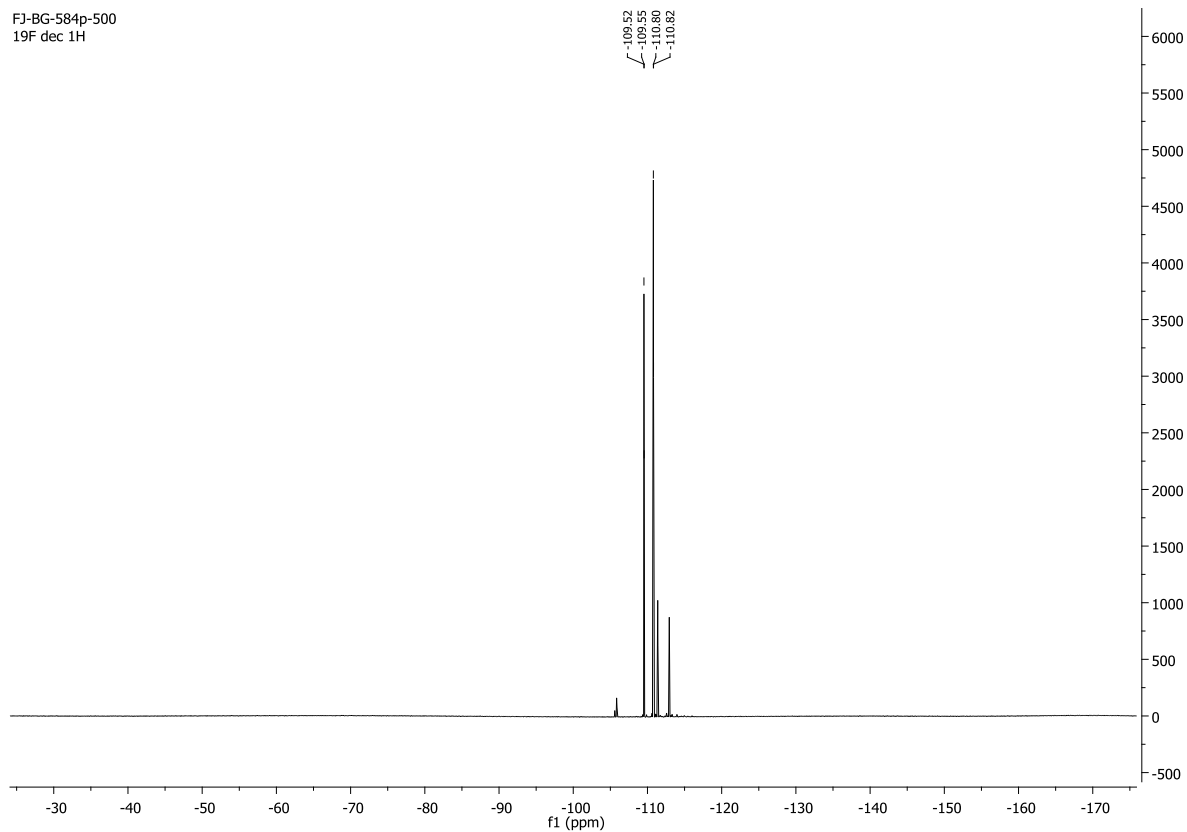
¹³C (125 MHz, CDCl₃)

FJ-BG-584p-500



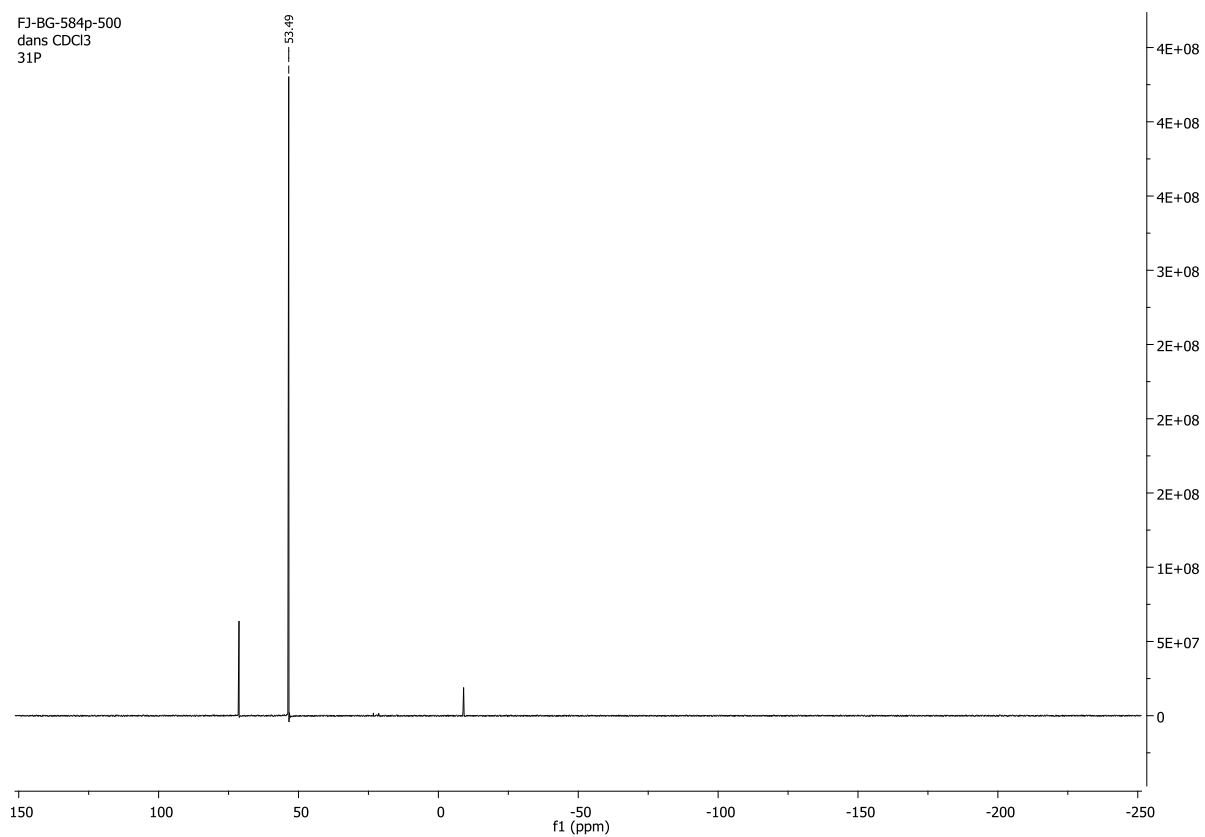
¹⁹F (470 MHz, CDCl₃)

FJ-BG-584p-500
19F dec 1H

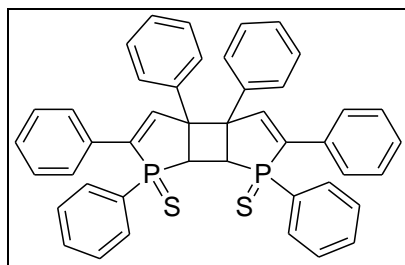


^{31}P (200 MHz, CDCl_3)

FJ-BG-584p-500
dans CDCl_3
 ^{31}P

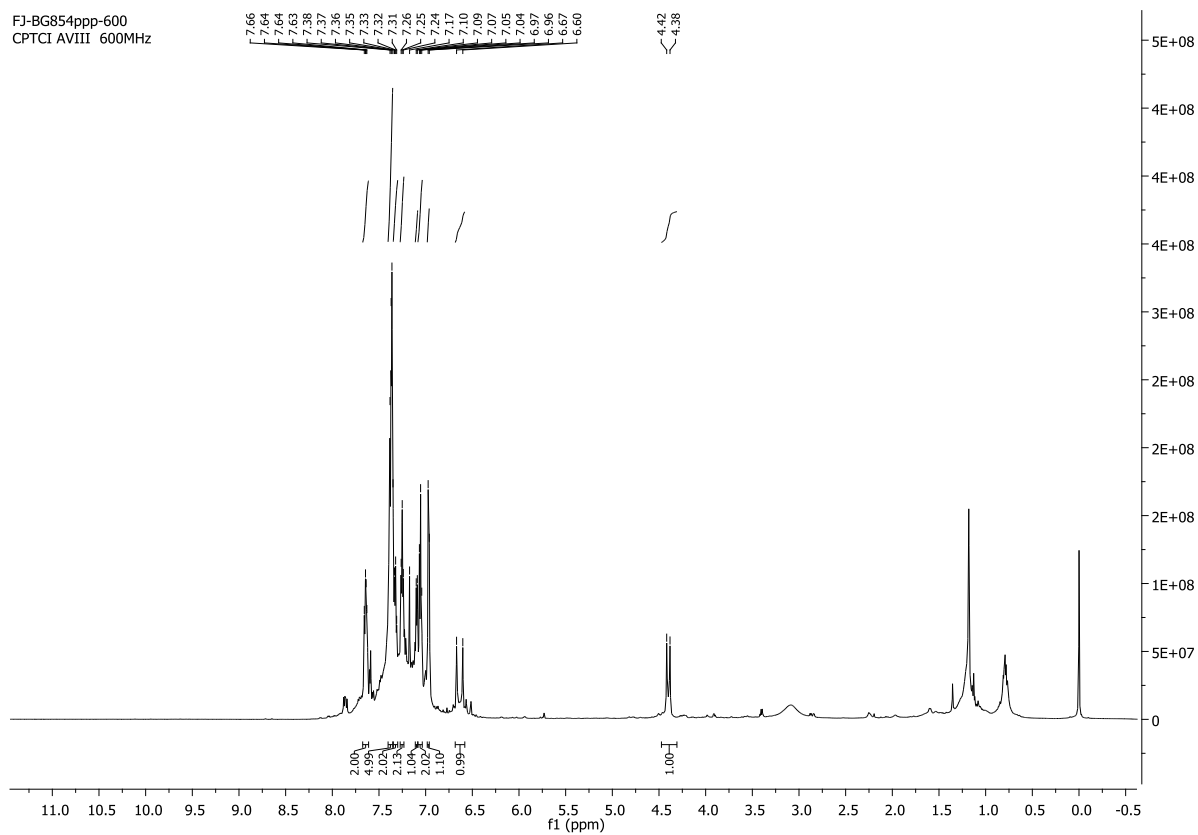


Dimer of 1,2,4-triphenyl-thiooxophosphole (5a)



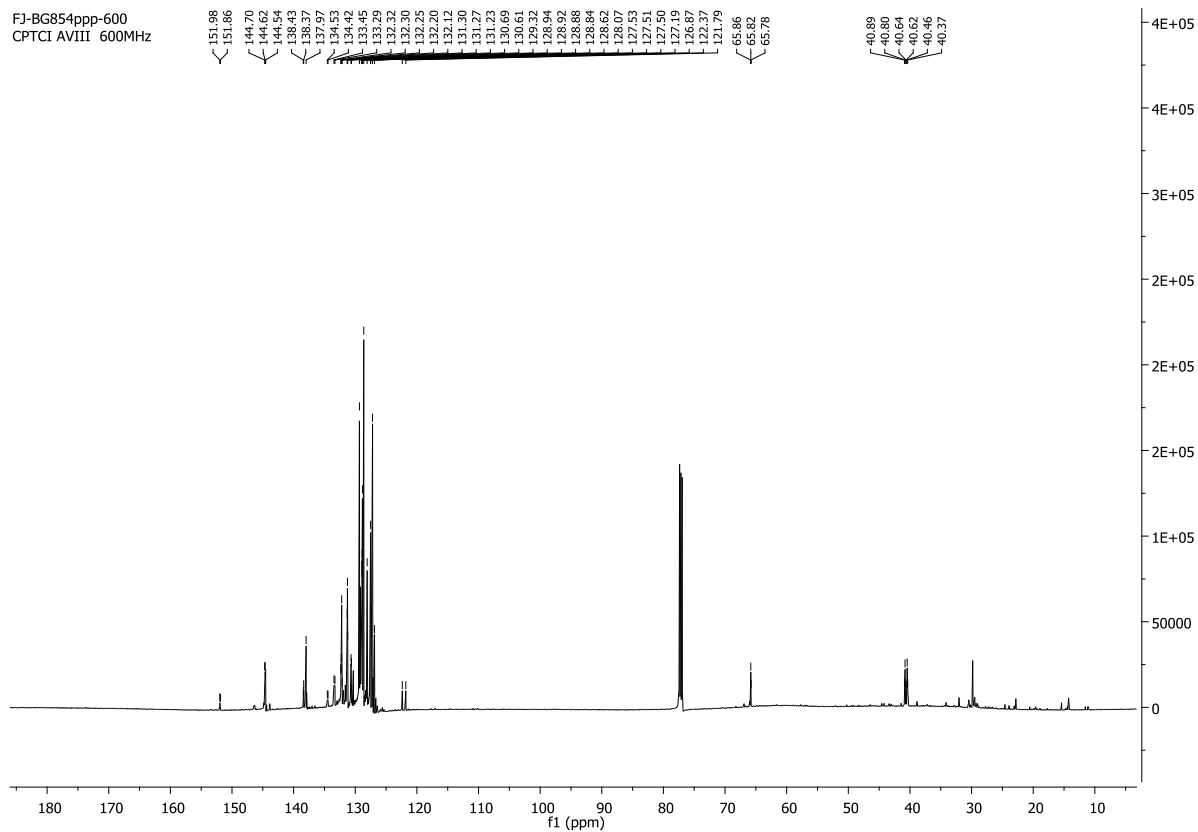
¹H (600 MHz, CDCl₃)

FJ-BG854ppp-600
CPTCI AVIII 600MHz



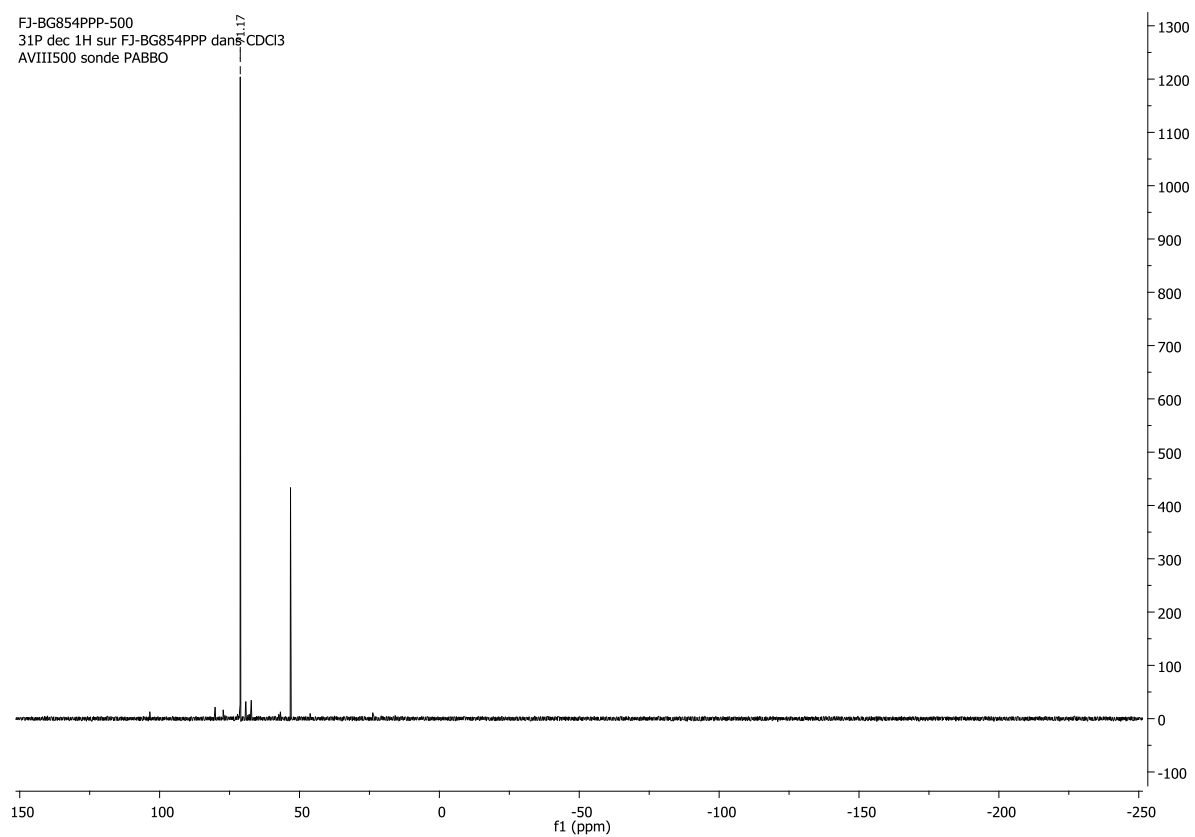
¹³C (150 MHz, CDCl₃)

FJ-BG854ppp-600
CPTCI AVIII 600MHz

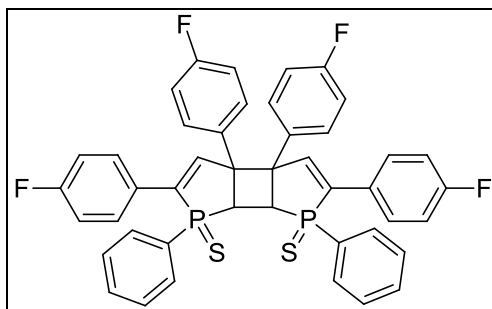


^{31}P (200 MHz, CDCl_3)

FJ-BG854PPP-500
31P dec 1H sur FJ-BG854PPP dans CDCl_3
AVIII500 sonde PABBO

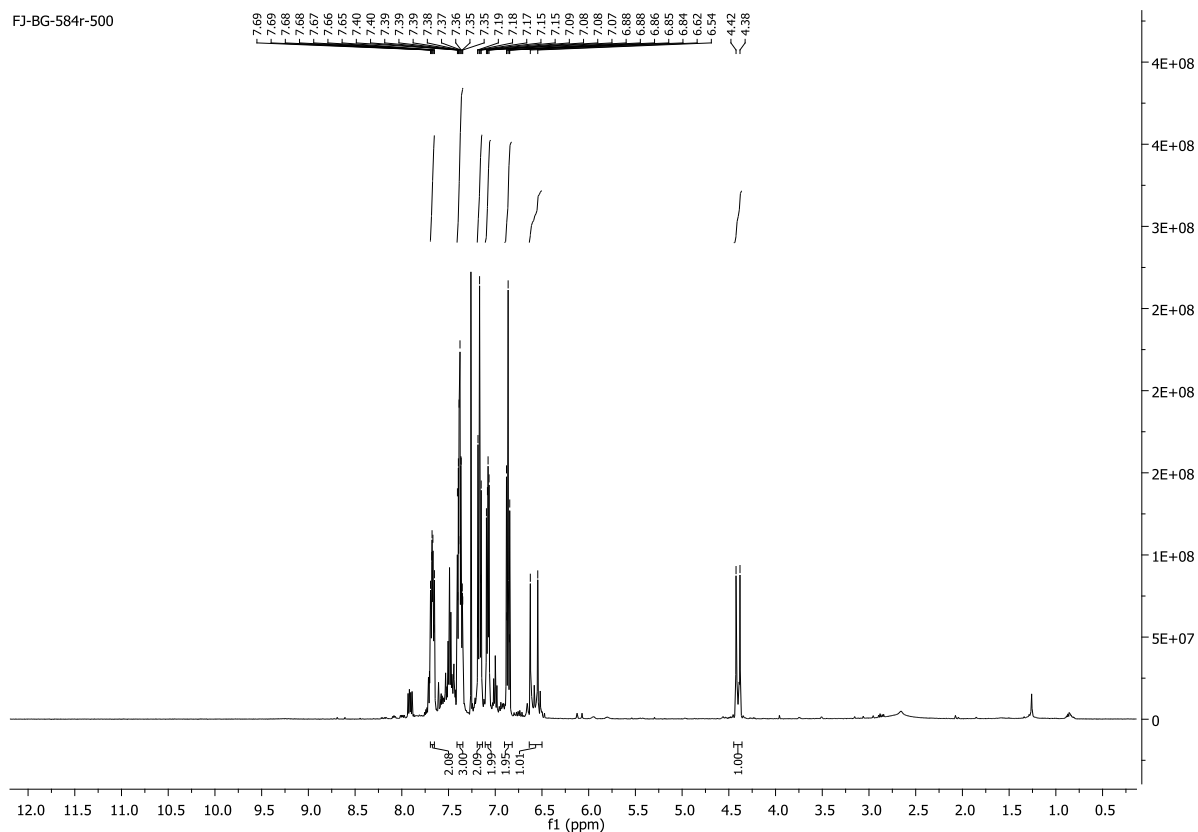


Dimer of 2,4-bis(4-fluorophenyl)-1-phenyl-thiooxophosphole (5d)



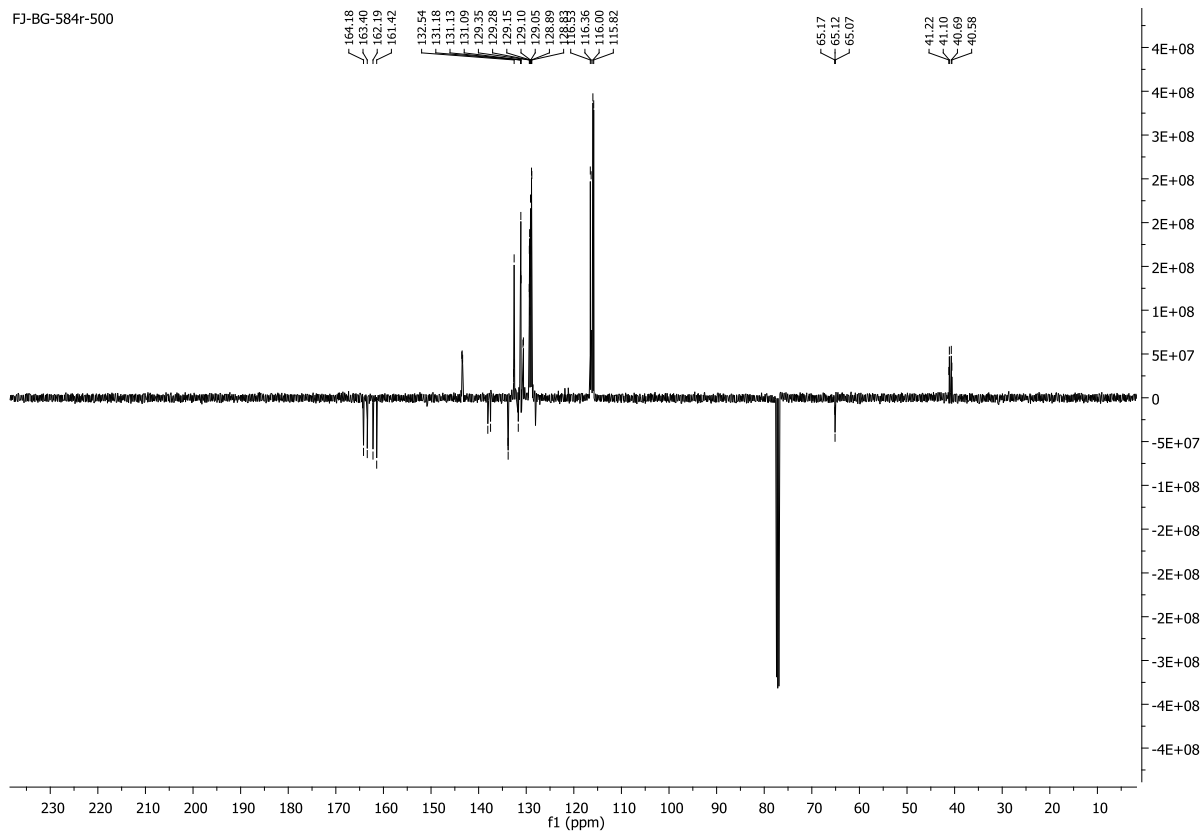
¹H (500 MHz, CDCl₃)

FJ-BG-584r-500



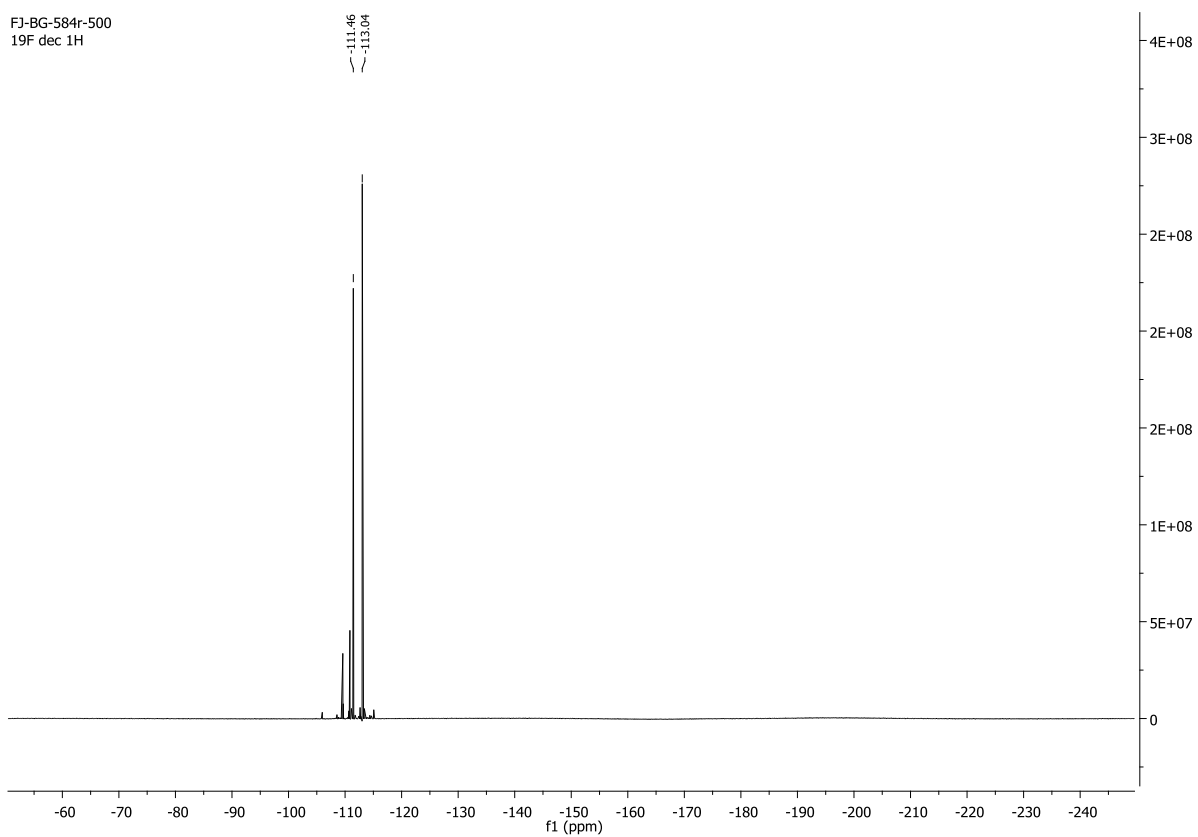
¹³C jmod (125 MHz, CDCl₃)

FJ-BG-584r-500



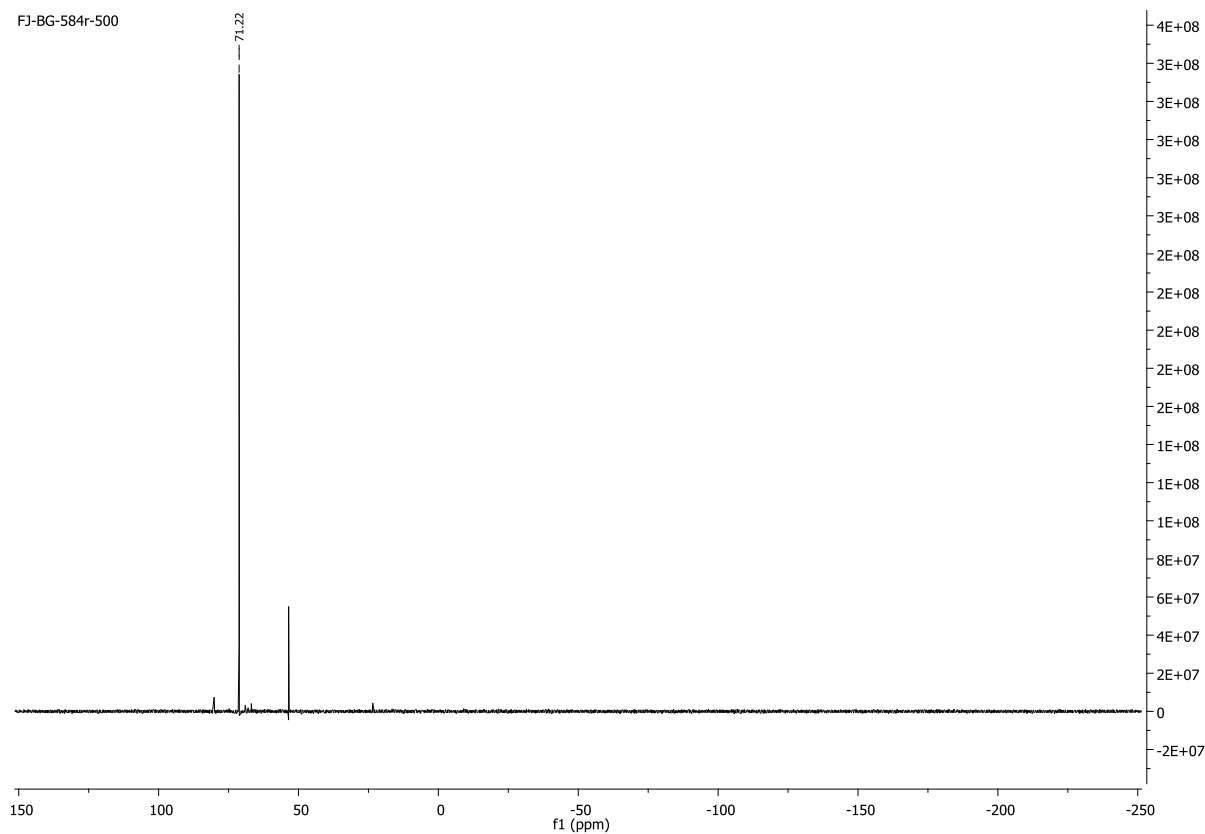
^{19}F (470 MHz, CDCl_3)

FJ-BG-584r-500
19F dec 1H

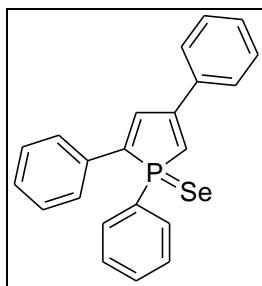


^{31}P (200 MHz, CDCl_3)

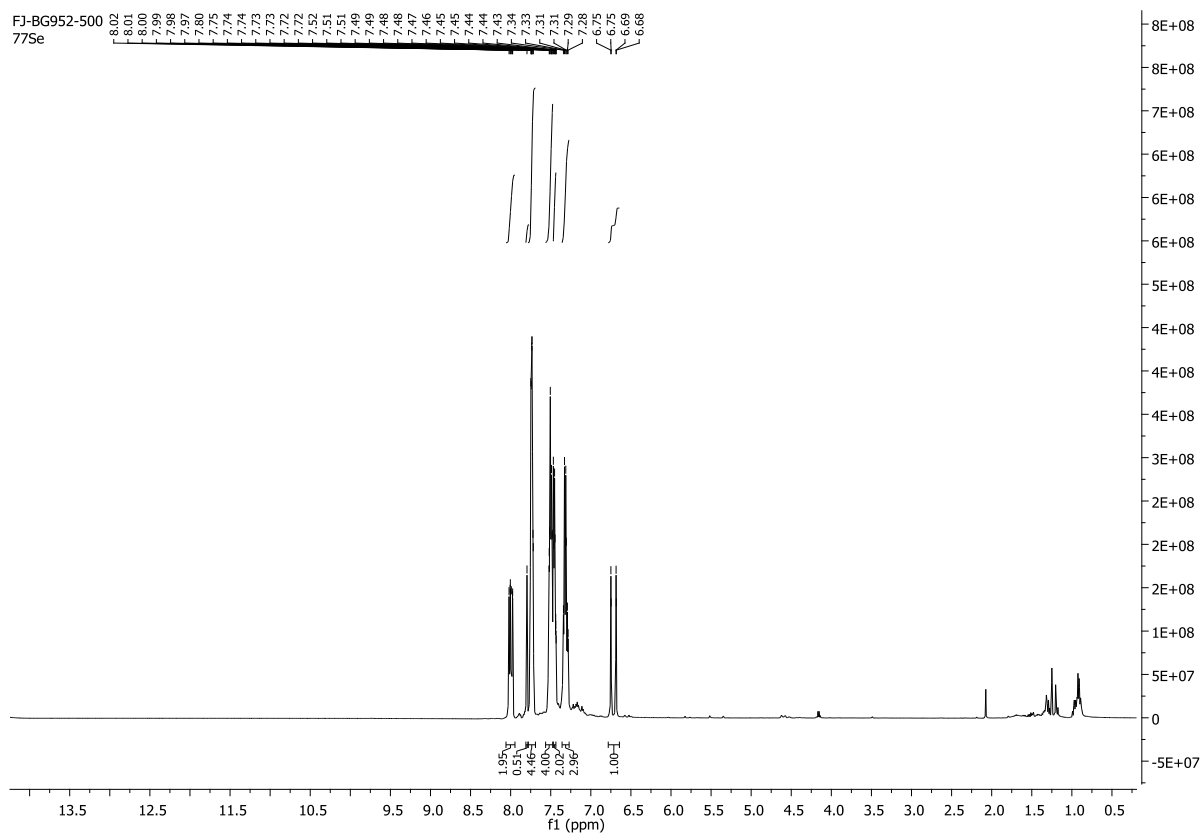
FJ-BG-584r-500



1,2,4-triphenyl-selenooxophosphole (6a)

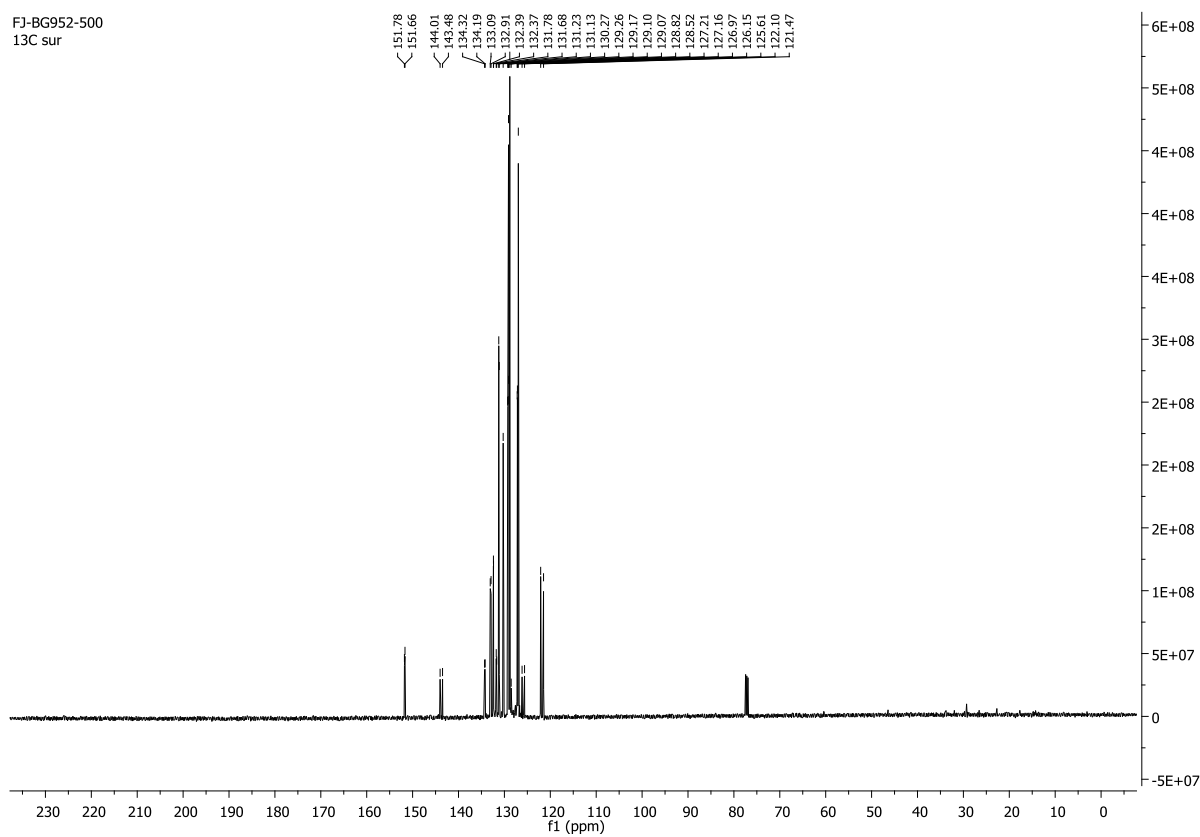


^1H (500 MHz, CDCl_3)



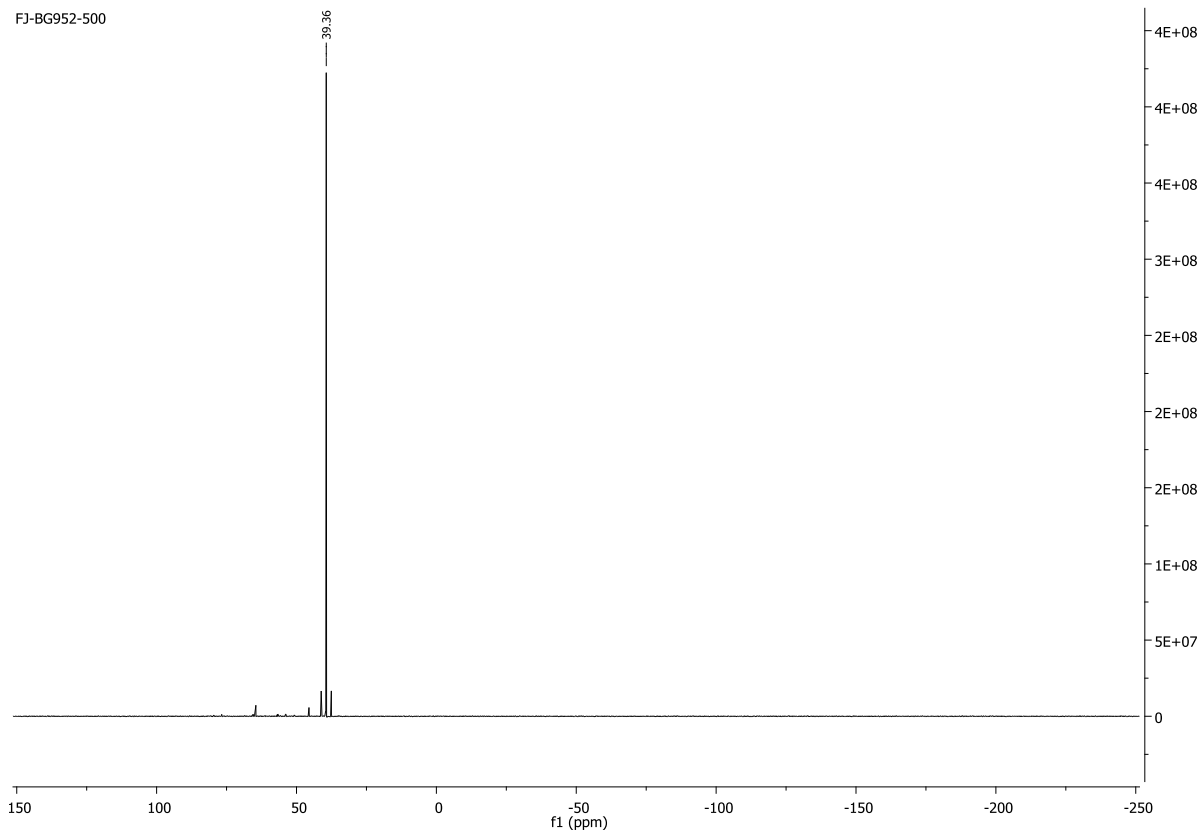
^{13}C (125 MHz, CDCl_3)

FJ-BG952-500
13C sur



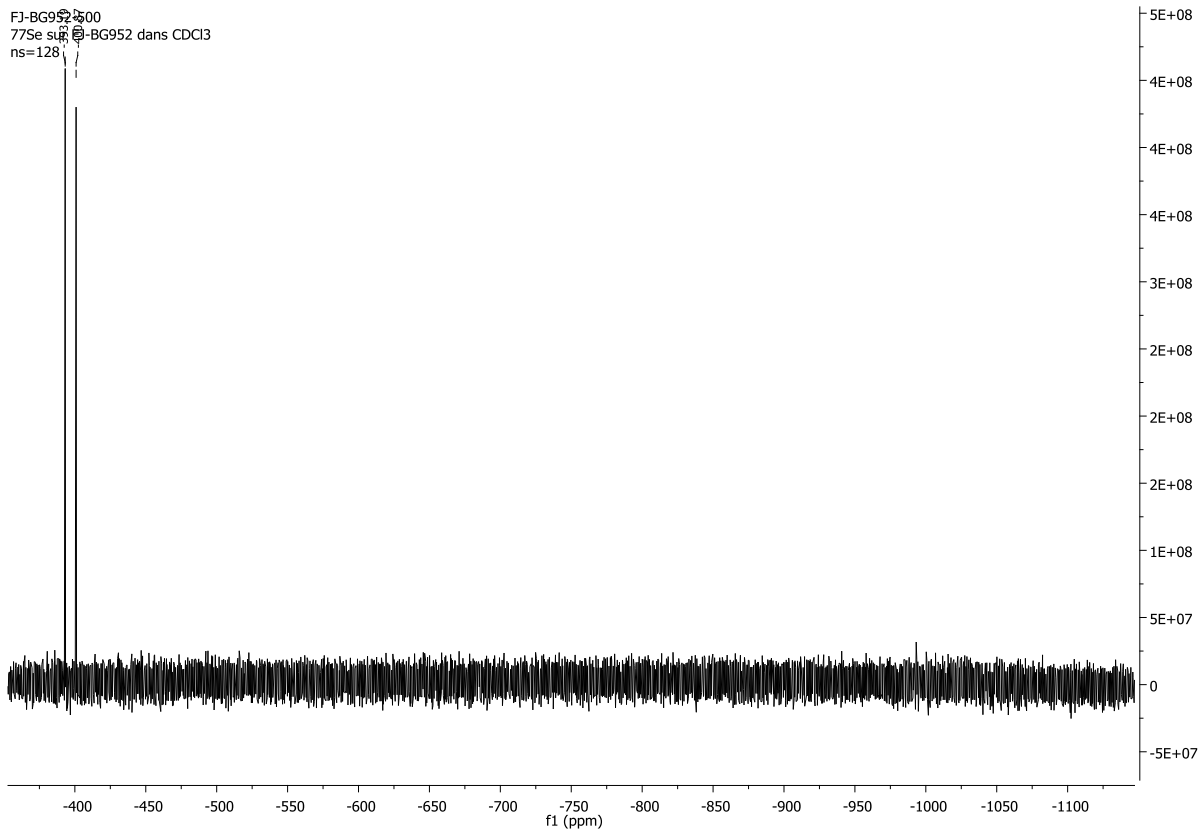
^{31}P (200 MHz, CDCl_3)

FJ-BG952-500

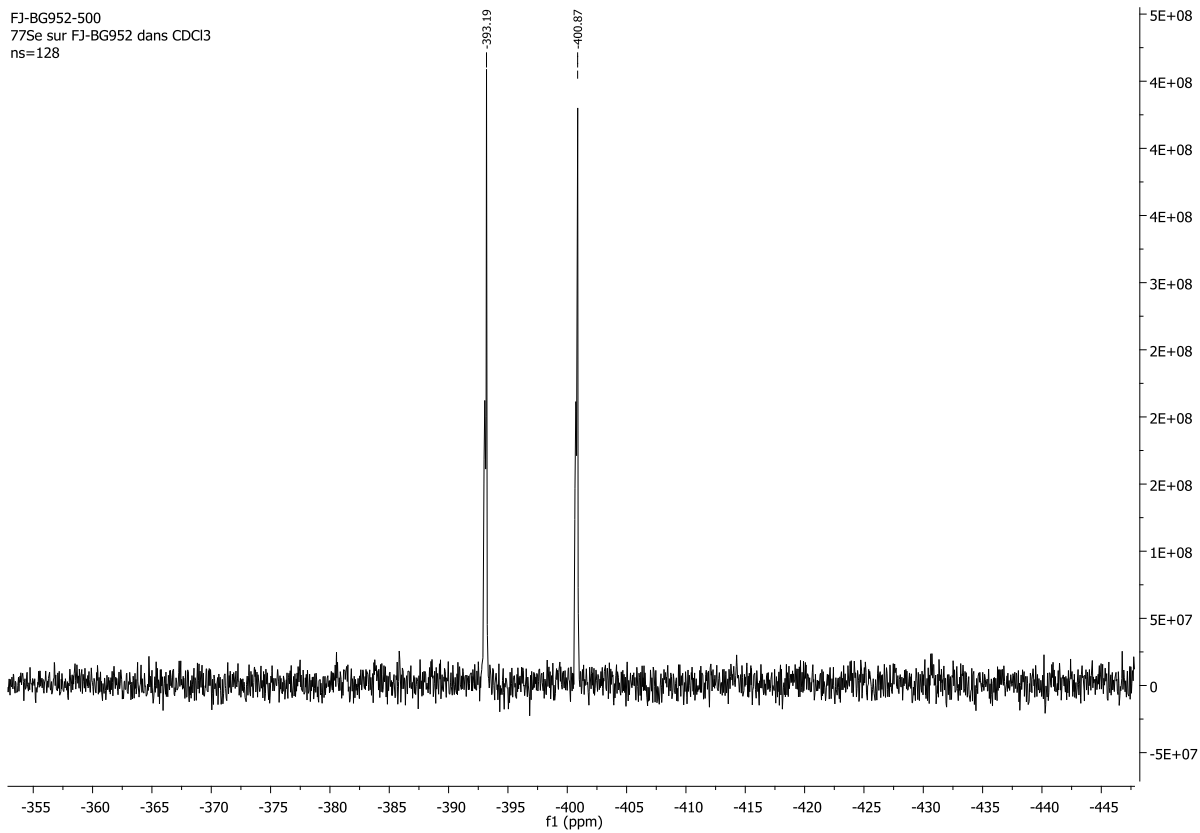


^{77}Se (96 MHz, CDCl_3)

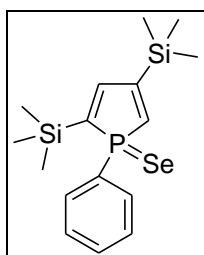
FJ-BG952-500
 ^{77}Se sur FJ-BG952 dans CDCl_3
ns=128



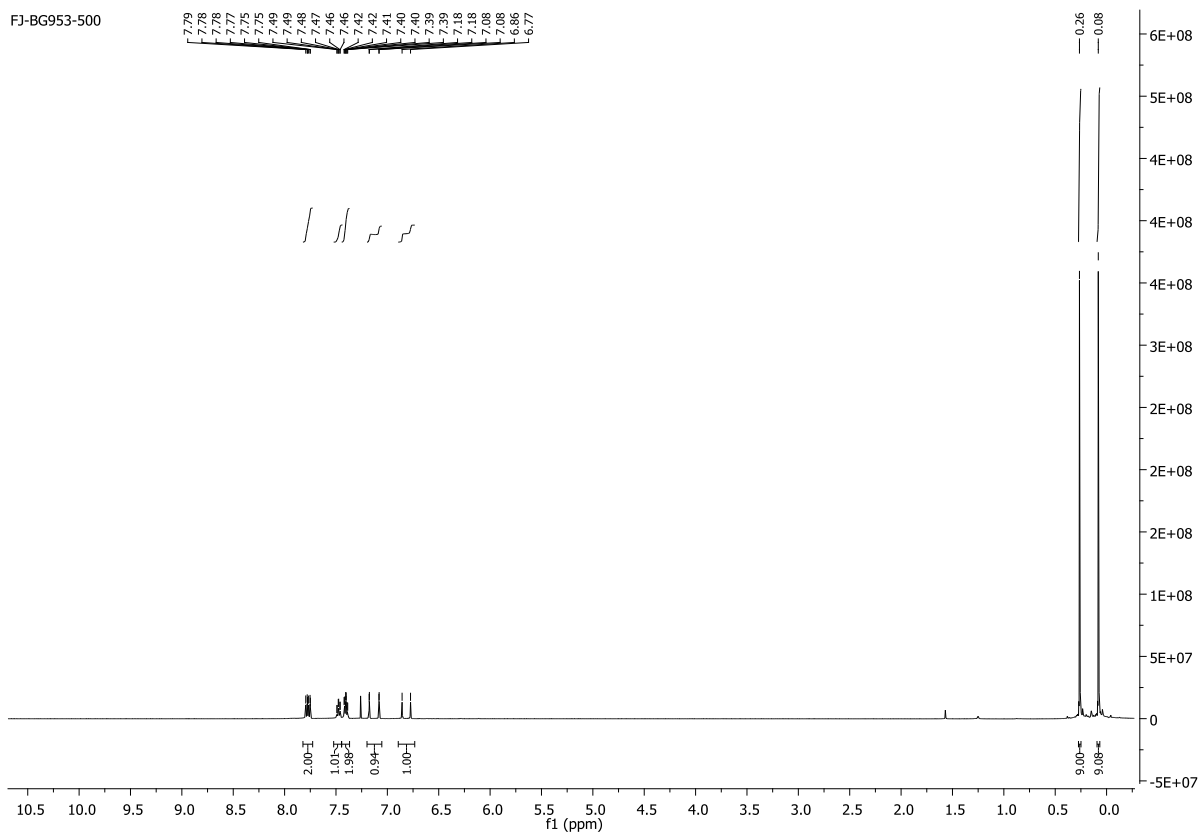
FJ-BG952-500
 ^{77}Se sur FJ-BG952 dans CDCl_3
ns=128



1-phenyl-2,4-bis(trimethylsilyl)-selenooxophosphole (6b)

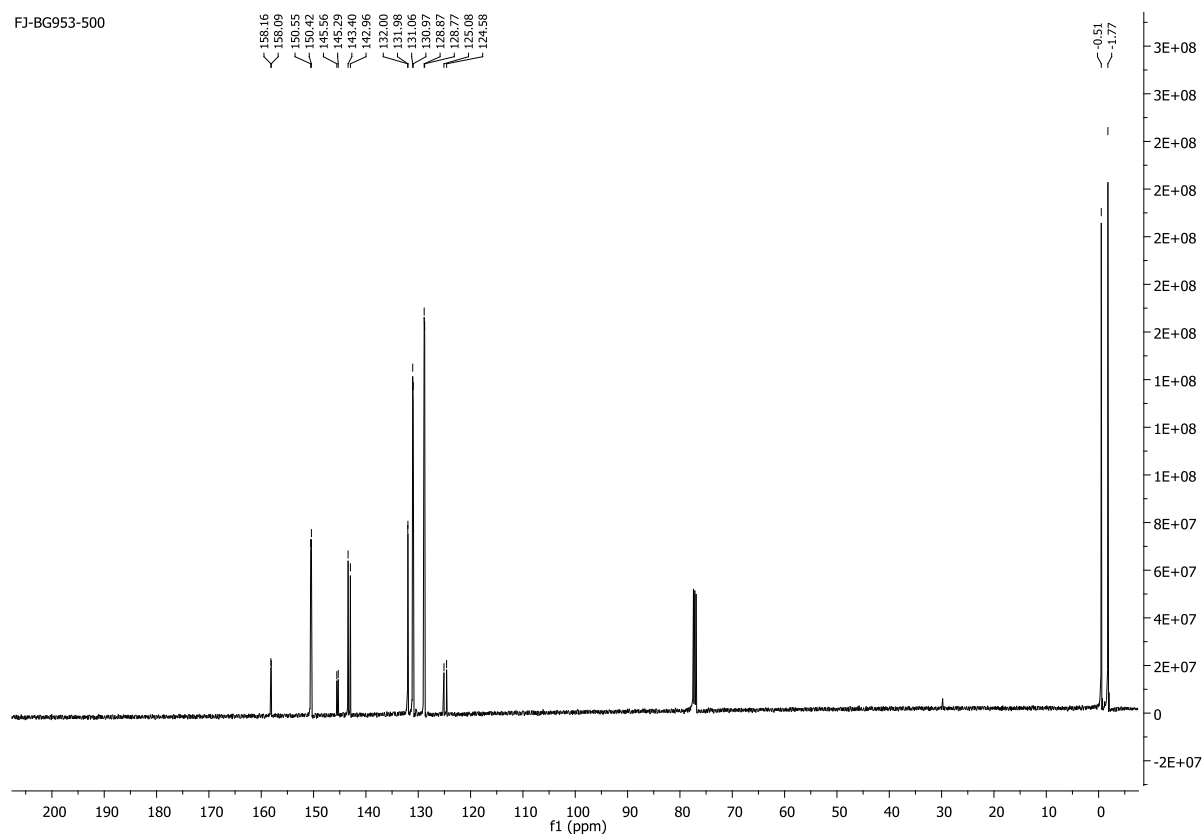


^1H (500 MHz, CDCl_3)



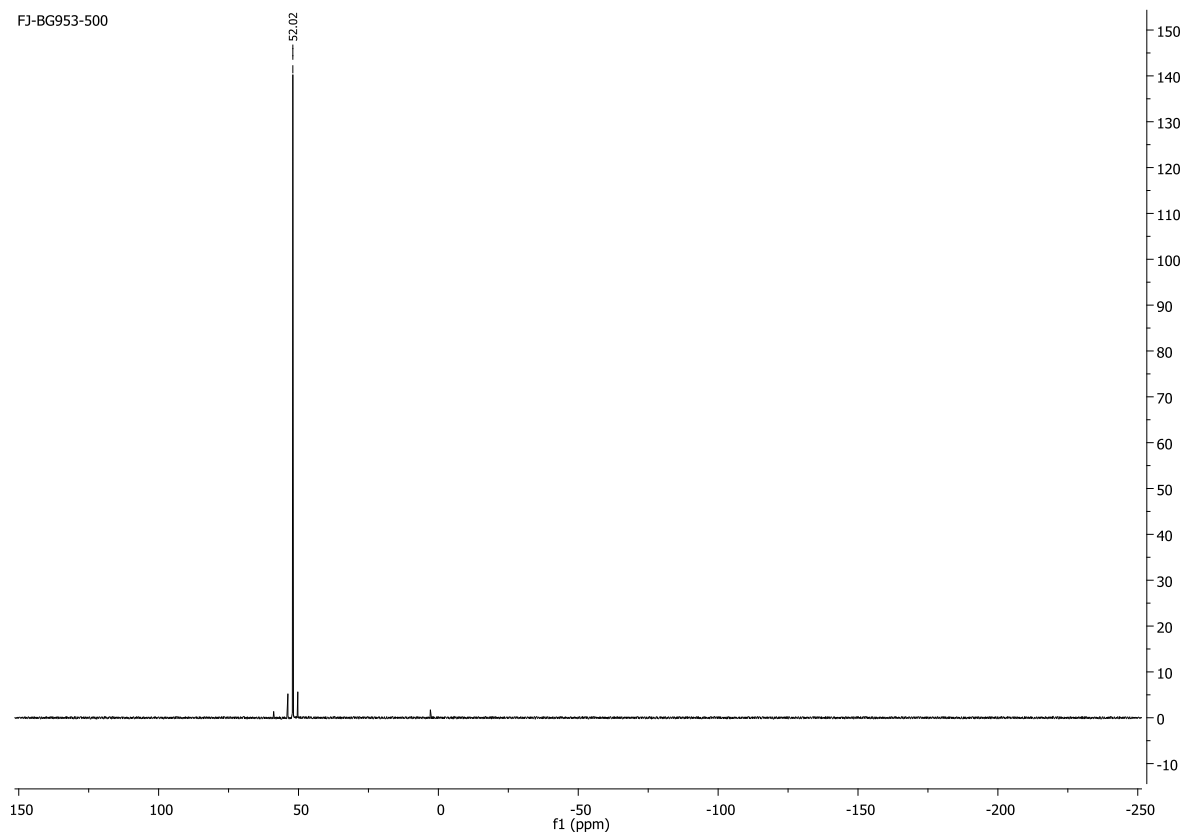
^{13}C (125 MHz, CDCl_3)

FJ-BG953-500



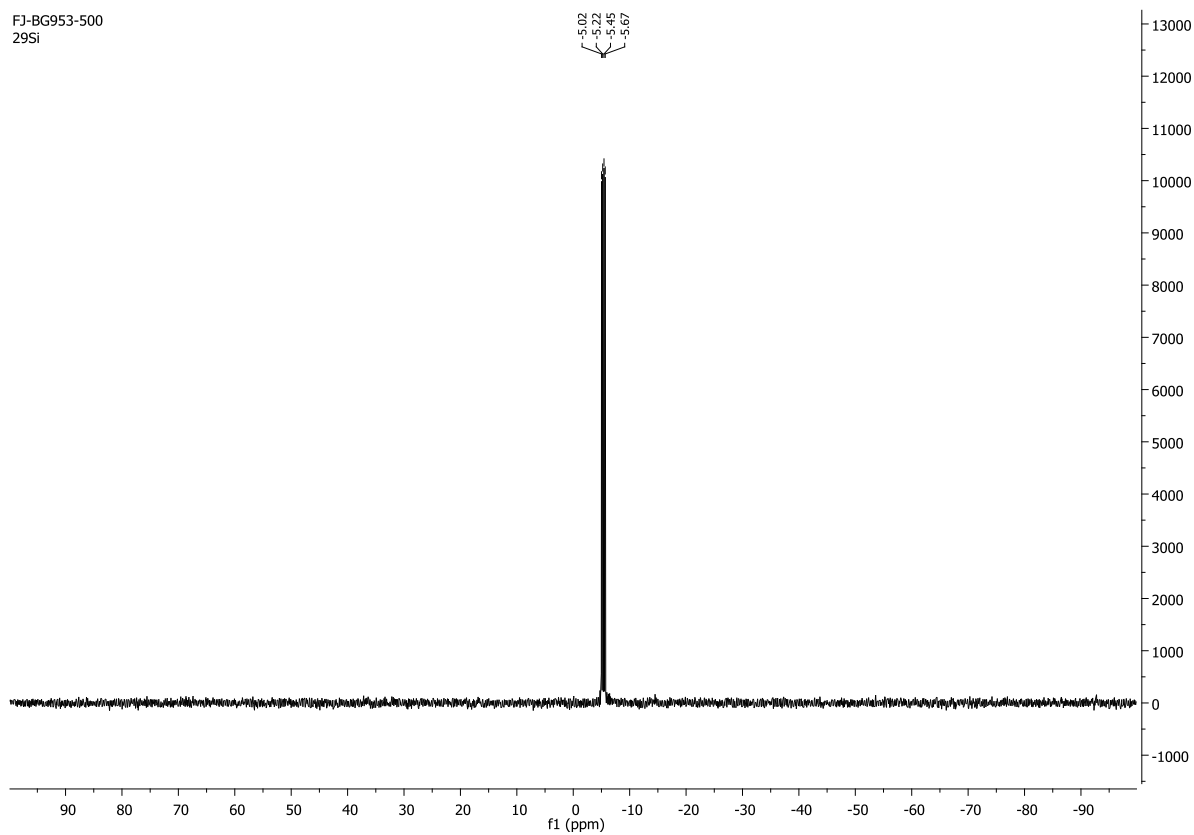
^{31}P (200 MHz, CDCl_3)

FJ-BG953-500



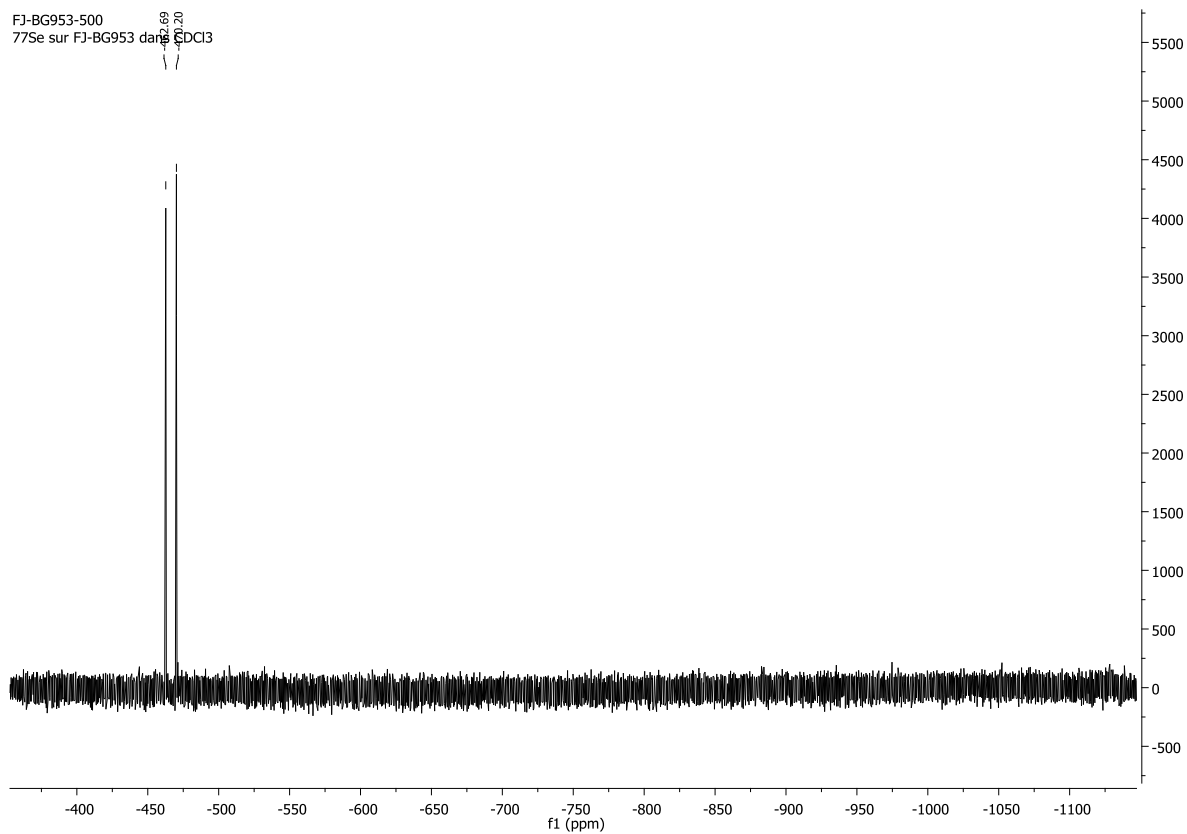
^{29}Si (100 MHz, CDCl_3)

FJ-BG953-500
29Si

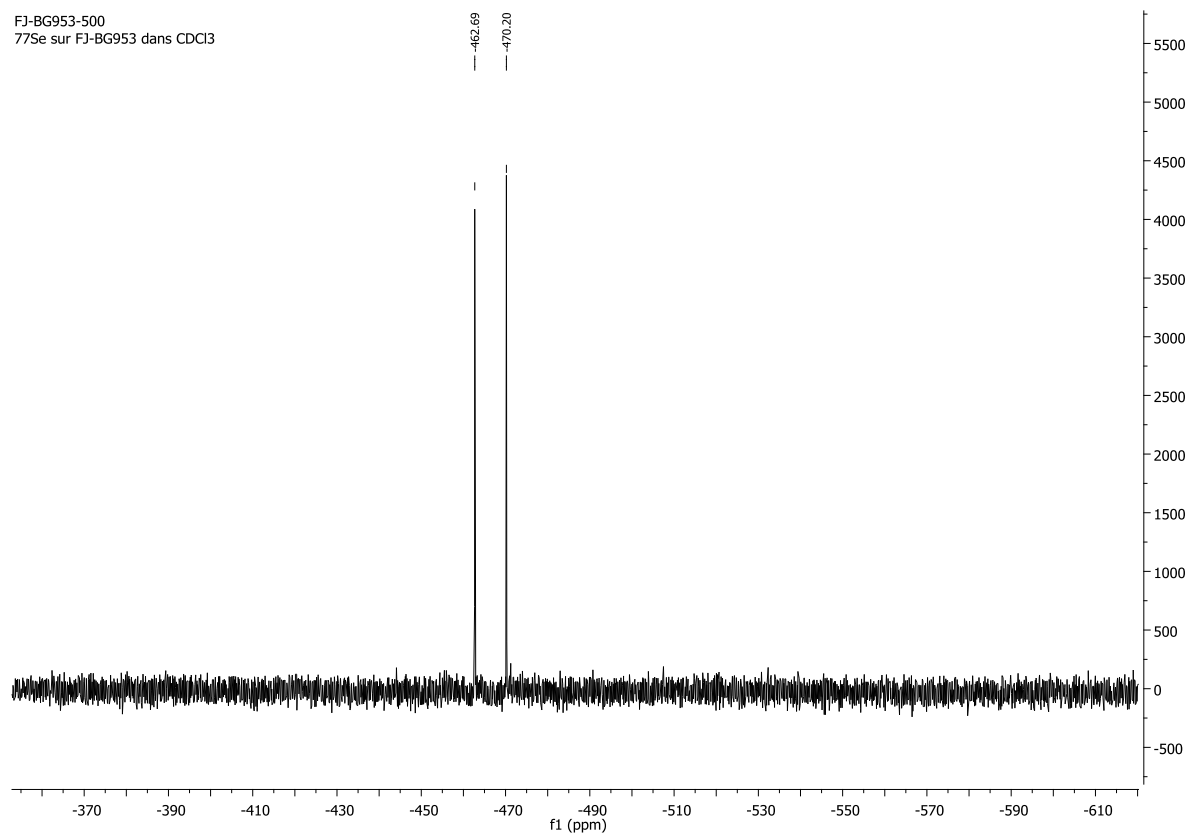


^{77}Se (96 MHz, CDCl_3)

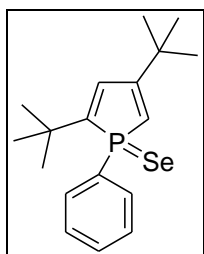
FJ-BG953-500
77Se sur FJ-BG953 dans CDCl_3



FJ-BG953-500
77Se sur FJ-BG953 dans CDCl3

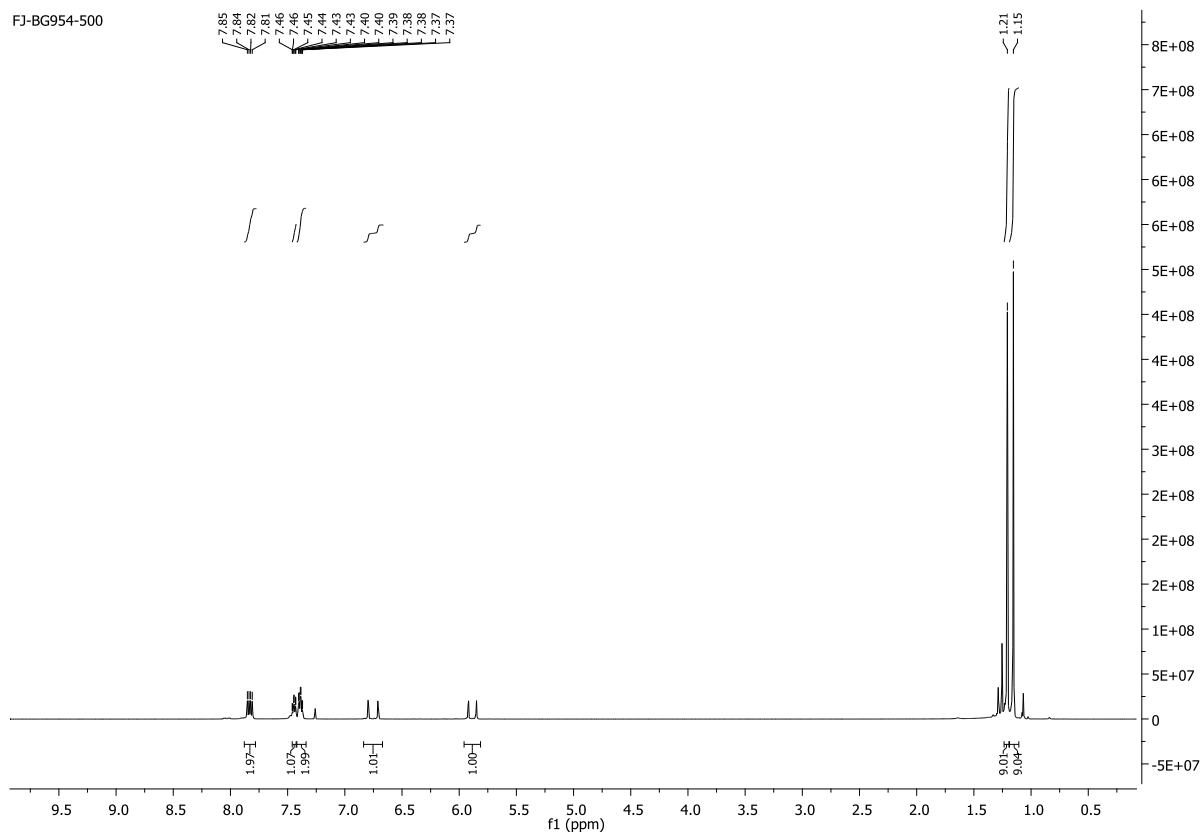


2,4-bis(tert-butyl)-1-phenyl-selenooxophosphole (6c)



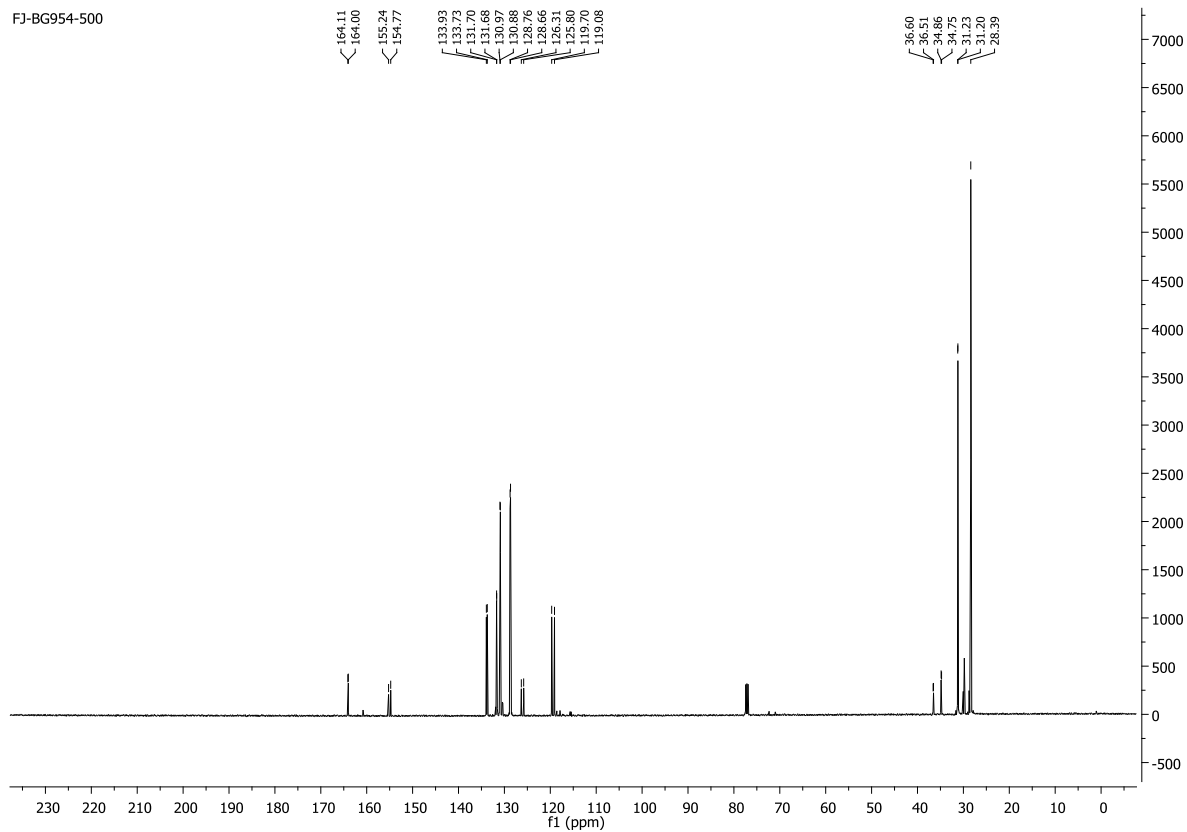
¹H (500 MHz, CDCl₃)

FJ-BG954-500



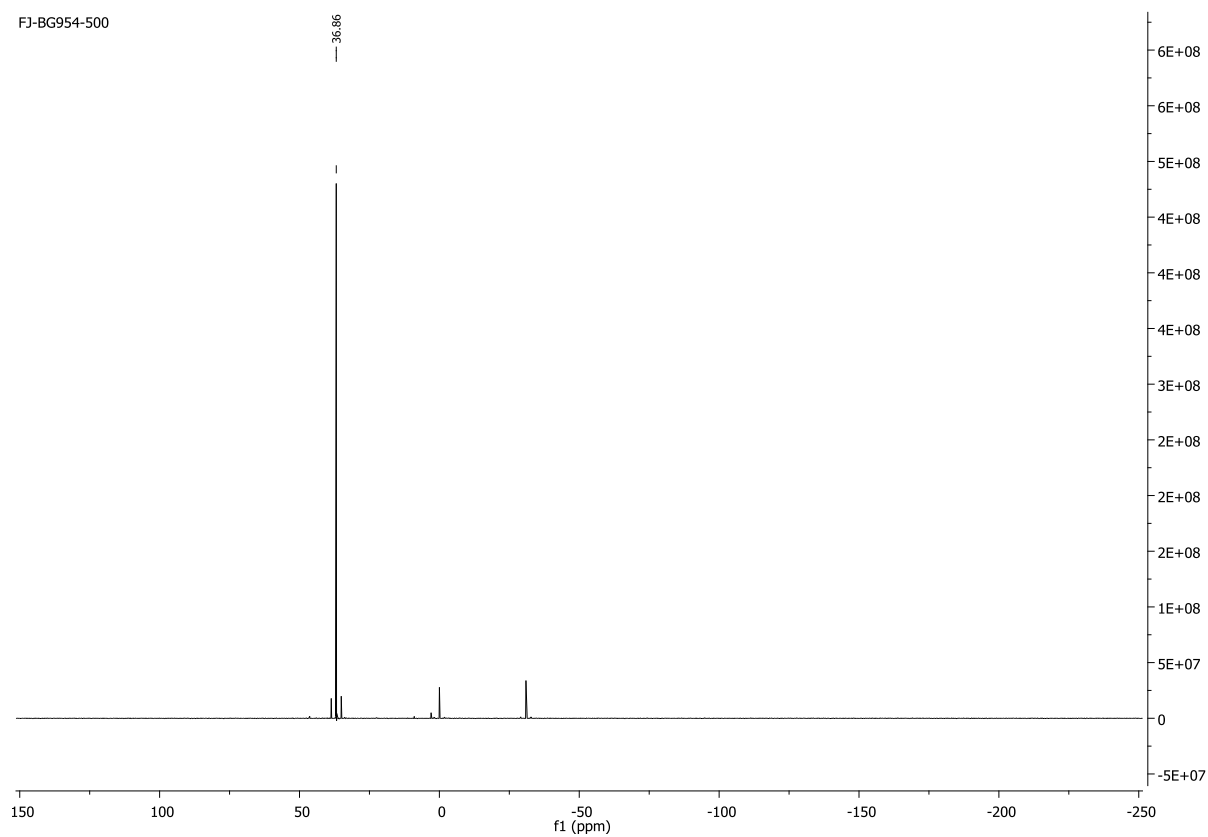
¹³C (125 MHz, CDCl₃)

FJ-BG954-500



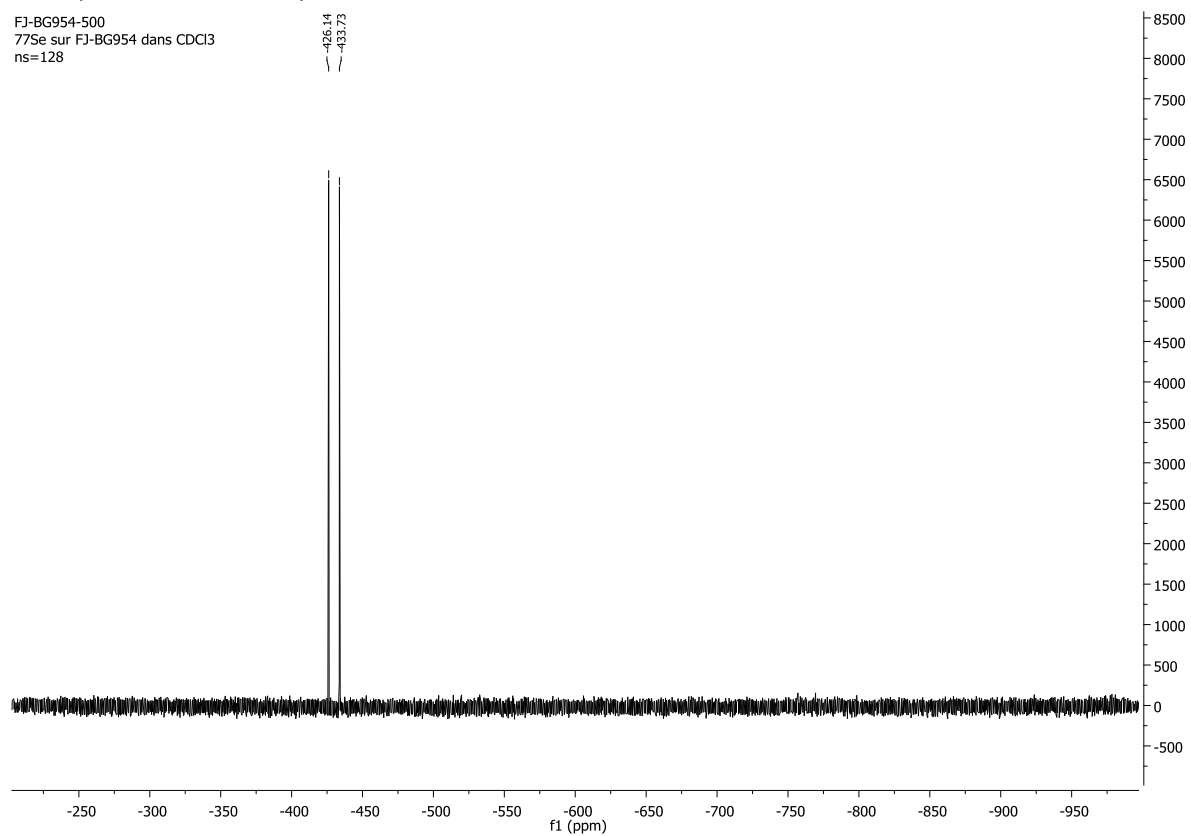
^{31}P (200 MHz, CDCl_3)

FJ-BG954-500

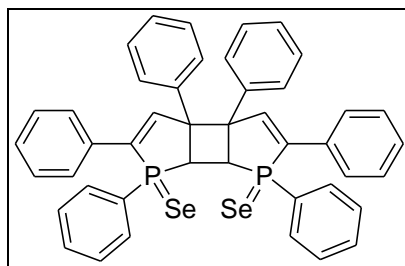


^{77}Se (96 MHz, CDCl_3)

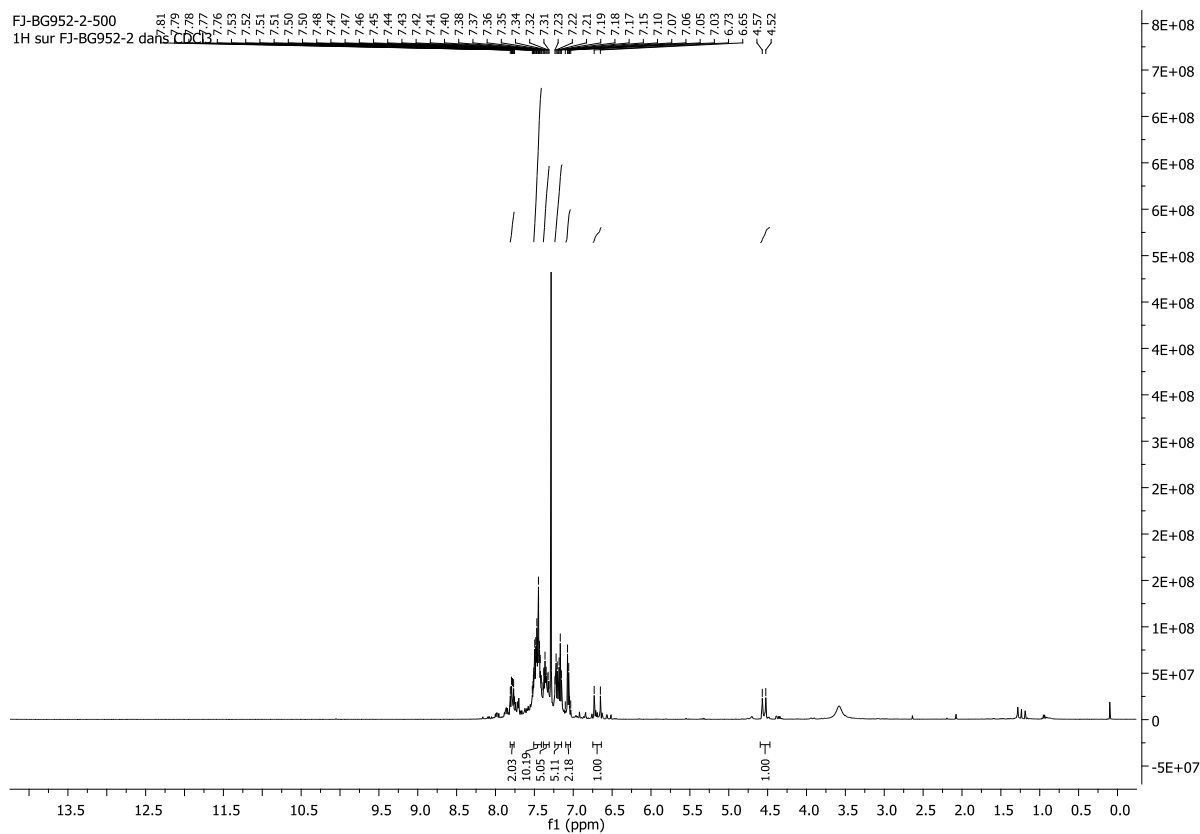
FJ-BG954-500
77Se sur FJ-BG954 dans CDCl_3
ns=128



Dimer of 1,2,4-triphenyl-selenooxophosphole (7a)

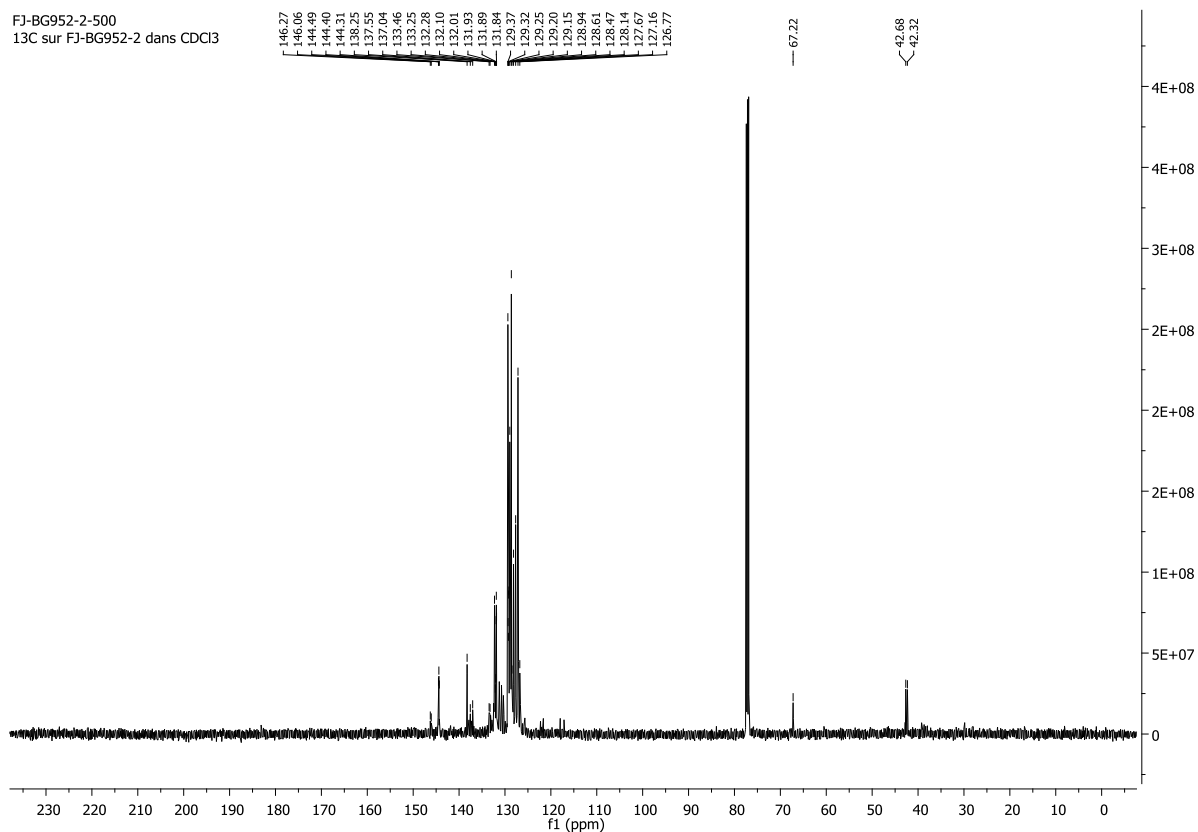


^1H (500 MHz, CDCl_3)



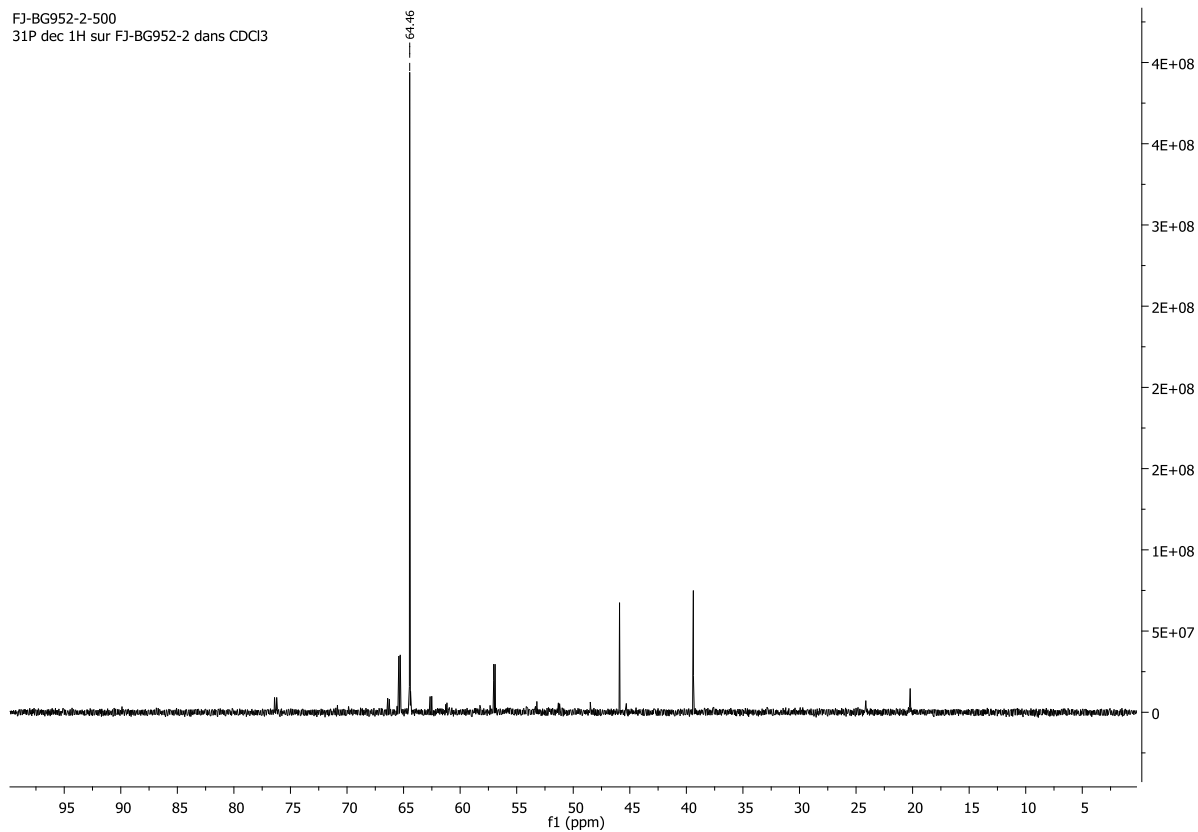
^{13}C (125 MHz, CDCl_3)

FJ-BG952-2-500
13C sur FJ-BG952-2 dans CDCl_3



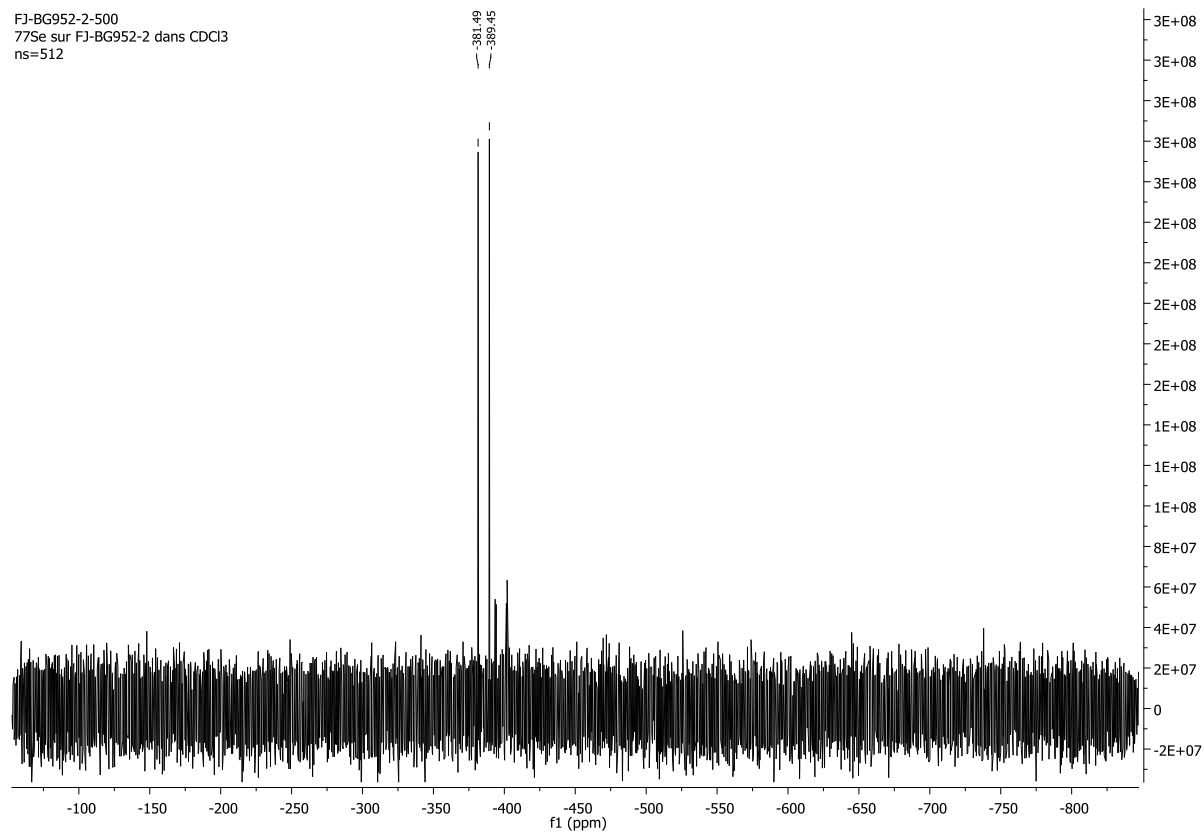
^{31}P (200 MHz, CDCl_3)

FJ-BG952-2-500
31P dec 1H sur FJ-BG952-2 dans CDCl_3



^{77}Se (96 MHz, CDCl_3)

FJ-BG952-2-500
77Se sur FJ-BG952-2 dans CDCl_3
ns=512



II. Crystallographic data for 5d

CCDC 1882024	
Molecular formula	C ₄₆ H ₃₂ Cl ₆ F ₄ P ₂ S ₂
Molecular weight	999.48
Crystal habit	Colourless prismatic
Crystal dimensions(mm)	0.2x0.2x0.1
Crystal system	monoclinic
Space group	C2/c
a(Å)	22.047(5)
b(Å)	8.630(5)
c(Å)	23.537(5)
α(°)	90.00
β(°)	92.993(5)
γ(°)	90.00
V(Å ³)	4472(3)
Z	4
d(g-cm ⁻³)	1.484
F(000)	2032
μ(cm ⁻¹)	0.600
Absorption corrections	none
Diffractometer	Brucker APEX-II CCD
X-ray source	MoK α
λ(Å)	0.71073
Monochromator	graphite
T (K)	100.0(2)
Scan mode	phi and omega scans
Maximum θ	29.91
HKL ranges	-32 32 ; -12 12 ; -34 34
Reflections measured	45860
Unique data	7461
Rint	0.0489
Reflections used	5166
Criterion	I > 2σ(I)
Refinement type	Fsqd
Hydrogen atoms	geom
Parameters refined	307
Reflections / parameter	24
wR2	0.0898
R1	0.0434
Weights a, b	0.0448 ; 3.6083
GoF	1.014

III. DFT Calculations

All computations were performed with Gaussian16, Rev B.01.¹ The functional used is B3LYP-D3², and the basis set 6-31G*³ has been used for all atoms (P, C, H, O, S, Se).

1a

Element	X	Y	Z
C	-1.19836700	-1.06777799	-1.01661897
C	-1.80169702	0.00706200	-0.42782599
C	-0.86173803	1.08630300	-0.11621800
C	0.43460900	0.85643500	-0.46754700
H	-1.71092606	-1.97771800	-1.30694497
H	-1.20076895	2.02374291	0.31677201
C	1.50998294	-1.81314802	-0.28287101
C	2.65605807	-2.44475794	-0.78184301
C	1.14794195	-2.00767994	1.05991495
C	3.43272901	-3.25890803	0.04812200
H	2.94274712	-2.30008197	-1.82035995
C	1.92146206	-2.82048297	1.88561499
H	0.26087001	-1.51546800	1.44926798
C	3.06600189	-3.44758797	1.38045597
H	4.32091808	-3.74394298	-0.34805900
H	1.63529003	-2.96520400	2.92420602
H	3.66838789	-4.08086014	2.02645612
C	1.57933700	1.73870802	-0.22353300
C	2.70642900	1.72958195	-1.06696200
C	1.59281301	2.60309005	0.88921899
C	3.79725194	2.55984902	-0.81510299
H	2.71486998	1.07973695	-1.93782604
C	2.68014407	3.43736410	1.13528705
H	0.75137800	2.59650612	1.57625902
C	3.78912807	3.42071891	0.28435001
H	4.65389109	2.53775096	-1.48363900
H	2.66831112	4.09393597	2.00148392
H	4.63978481	4.06765890	0.48050100
C	-3.24444103	0.10450000	-0.12070900
C	-3.69367790	0.81875902	1.00385702
C	-4.20152283	-0.52802598	-0.93313098
C	-5.05195808	0.88901699	1.31123698
H	-2.97150302	1.30235100	1.65578496
C	-5.55909777	-0.45778900	-0.62633401
H	-3.87417603	-1.05705202	-1.82360899
C	-5.99093580	0.25103599	0.49776101
H	-5.37692785	1.44036901	2.18969202
H	-6.28263903	-0.94886202	-1.27177501
H	-7.04980898	0.30935699	0.73460603
P	0.52983999	-0.71998698	-1.40437102

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	1	2	3
	A	A	A
Frequencies --	20.1722	29.2887	32.9932
Red. masses --	3.8155	5.4582	5.2177
Frc consts --	0.0009	0.0028	0.0033
IR Inten --	0.0352	0.1545	0.1298

Sum of electronic and zero-point Energies=	-1189.611369
Sum of electronic and thermal Energies=	-1189.592674
Sum of electronic and thermal Enthalpies=	-1189.591730
Sum of electronic and thermal Free Energies=	-1189.661500

HF = -1189.93185902

1b

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=====
Element          X           Y           Z
=====
C          1.07831097   -1.07506502   -1.03136802
C          1.85015595   -0.21311601   -0.30782101
C          1.09191597   0.97967303    0.10710700
C         -0.21213700    1.05369306   -0.28738701
H          1.42338395   -2.01605201   -1.44882905
H          1.56458902    1.75519395    0.71019799
P         -0.54008597   -0.34821200   -1.41324604
C         -1.76815295   -1.37243295   -0.48354501
C         -2.98948312   -1.69300497   -1.08999300
C         -1.52760398   -1.79142106    0.83525503
C         -3.96083403   -2.41428089   -0.38820800
H         -3.18420005   -1.37371099   -2.11068606
C         -2.49373794   -2.51370811    1.53227496
H         -0.58341599   -1.53744602    1.30962002
C         -3.71420598   -2.82426810    0.92199099
H         -4.90664721   -2.65430403   -0.86676401
H         -2.29987502   -2.83177710    2.55350995
H         -4.46839619   -3.38439298    1.46844494
C         -2.10816097    3.20092106   -1.41720402
C         -2.87388897    1.63773096    1.12938404
C         -0.55502599    3.69163203    1.22605395
H         -1.30473995    3.66965294   -1.99742699
H         -2.58798504    2.45358992   -2.06063008
H         -2.85311294    3.97235298   -1.18532205
H         -2.51754808    1.14247406    2.03995299
H         -3.60155106    2.40520406    1.42183495
H         -3.39726400    0.88141900    0.53374499
H         -1.24568796    4.49216890    1.51782095
H         -0.15629400    3.24640298    2.14545298
H          0.28058299    4.15308905    0.68643397
C          3.84685206   -0.37977800    2.01144195
C          4.18854284   -2.20519900   -0.47620001
C          4.72012711    0.84456402   -0.68647301
H          3.49702001    0.58972102    2.38664603
H          3.26400995   -1.16008902    2.51503301
H          4.89499712   -0.49445200    2.31416202
H          4.09107018   -2.29115009   -1.56493497
H          5.23636389   -2.40355396   -0.22029200
H          3.57931805   -2.99545908   -0.02169500
H          5.77903414    0.72656602   -0.42465001
H          4.63644409    0.80269200   -1.77879202
H          4.40748405    1.84639704   -0.36804700
Si         -1.43759096    2.40001392    0.16062200
Si          3.66027999   -0.49479899    0.13023899
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	1	2	3
	A	A	A
Frequencies --	15.2919	17.4310	30.6660
Red. masses --	3.2255	2.9836	4.2233
Frc consts --	0.0004	0.0005	0.0023
IR Inten --	0.0254	0.0175	0.1146

Sum of electronic and zero-point Energies=	-1544.817016
Sum of electronic and thermal Energies=	-1544.791607
Sum of electronic and thermal Enthalpies=	-1544.790663

Sum of electronic and thermal Free Energies= -1544.874272

HF = -1545.17896838

1c

Element	X	Y	Z
C	0.97071803	-1.04614604	-1.07538497
C	1.88162005	-0.45272800	-0.26330999
C	1.41334701	0.84413499	0.25446400
C	0.17554000	1.24023902	-0.13457200
H	1.09553301	-2.00360394	-1.56602705
H	2.04531407	1.43844295	0.90757000
P	-0.45997000	0.02714300	-1.37315798
C	-1.81922603	-0.85232198	-0.46883801
C	-3.07121491	-0.98686999	-1.08168304
C	-1.63019502	-1.37340796	0.82137799
C	-4.12211895	-1.62550998	-0.41521099
H	-3.22674990	-0.58779299	-2.08094501
C	-2.67706800	-2.00874996	1.48580098
H	-0.65855402	-1.27139401	1.29762602
C	-3.92685008	-2.13487911	0.86831897
H	-5.08998299	-1.72301900	-0.90005398
H	-2.52216911	-2.40610290	2.48581290
H	-4.74282312	-2.63012004	1.38813102
C	-0.61836702	3.44246507	-1.02925301
C	-1.94756997	2.26618910	0.75525600
C	0.26287800	3.30555701	1.31553495
H	0.37818000	3.66489100	-1.42722905
H	-1.19610202	2.95479202	-1.82158005
H	-1.11094797	4.39148092	-0.78249401
H	-1.92405605	1.60808694	1.63046205
H	-2.43336797	3.20699096	1.04177701
H	-2.57287788	1.78313398	-0.00206700
H	-0.26862299	4.22503519	1.58628905
H	0.37509999	2.69989705	2.22214293
H	1.26206303	3.59015608	0.96666700
C	3.32644105	-1.14573300	1.65794897
C	3.50773597	-2.37728810	-0.51842999
C	4.34747410	-0.01938400	-0.35712299
H	3.17205811	-0.18728900	2.16527891
H	2.56376505	-1.84492397	2.01983500
H	4.31030416	-1.52738905	1.95711994
H	3.48348808	-2.31996489	-1.61246502
H	4.49434614	-2.75249195	-0.22310001
H	2.75903893	-3.11071205	-0.19789900
H	5.34113216	-0.39462799	-0.08264000
H	4.31482792	0.09997100	-1.44593596
H	4.22772598	0.97182798	0.09359300
C	-0.52117699	2.54542089	0.22826700
C	3.25185299	-1.00138998	0.11975100

	1 A	2 A	3 A
Frequencies --	17.3731	35.1313	40.0969
Red. masses --	2.8844	3.5880	3.6234
Frc consts --	0.0005	0.0026	0.0034
IR Inten --	0.0379	0.1202	0.0624

Sum of electronic and zero-point Energies= -1041.959153
Sum of electronic and thermal Energies= -1041.939037
Sum of electronic and thermal Enthalpies= -1041.938092
Sum of electronic and thermal Free Energies= -1042.008019

HF = -1042.34446406

1d

Element	X	Y	Z
C	-1.20490694	1.18843997	1.04675698

C	-1.70044100	0.03842000	0.50107902
C	-0.65836602	-0.94983900	0.21261799
C	0.61059701	-0.57652700	0.53952003
H	-1.80455506	2.05059004	1.31532097
H	-0.90403998	-1.93166900	-0.18378200
C	1.40821302	2.17835903	0.25258499
C	2.49532509	2.93137908	0.71384799
C	1.01178503	2.29437900	-1.08956397
C	3.18046904	3.78790307	-0.15321299
H	2.80738211	2.84885693	1.75186002
C	1.69392204	3.14961600	-1.95210898
H	0.17026301	1.70857203	-1.44936001
C	2.78031898	3.89781308	-1.48476005
H	4.02345991	4.36738110	0.21359301
H	1.38185203	3.23336601	-2.98990512
H	3.31147695	4.56393909	-2.15947604
C	1.83790600	-1.34278595	0.30812201
C	2.96791291	-1.18893194	1.13444698
C	1.93137801	-2.23760200	-0.77691901
C	4.13984489	-1.90468299	0.90088600
H	2.92050791	-0.51400298	1.98408699
C	3.09308290	-2.96480799	-1.01830399
H	1.08847499	-2.34378791	-1.45309305
C	4.18365479	-2.78668499	-0.17253800
H	5.01087809	-1.79418004	1.53817105
H	3.17243290	-3.65143895	-1.85466695
C	-3.12820792	-0.21820199	0.21956000
C	-3.51608109	-1.01599896	-0.87178802
C	-4.13733006	0.34198901	1.02306998
C	-4.86022615	-1.24117696	-1.16223705
H	-2.75817490	-1.44821501	-1.51839304
C	-5.48519802	0.12705600	0.74640000
H	-3.85912204	0.93478799	1.88915002
C	-5.82632303	-0.66351098	-0.34611699
H	-5.16765785	-1.84867096	-2.00692797
H	-6.26930714	0.54884499	1.36636806
P	0.55359399	1.03257704	1.42262805
F	5.31531811	-3.48419309	-0.40568700
F	-7.12995911	-0.88032299	-0.61769402

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	1	2	3
	A	A	A
Frequencies --	20.8332	26.9623	27.2431
Red. masses --	4.0947	5.8937	7.9409
Frc consts --	0.0010	0.0025	0.0035
IR Inten --	0.0336	0.1686	0.1845

Sum of electronic and zero-point Energies= -1388.094390
Sum of electronic and thermal Energies= -1388.073991
Sum of electronic and thermal Enthalpies= -1388.073047
Sum of electronic and thermal Free Energies= -1388.147005

HF = -1388.39842578

2a

=====

Element	X	Y	Z
C	1.24009299	-0.92295301	1.12064803
C	1.80014002	0.09862200	0.42777300
C	0.82749701	1.14249897	0.00026300
C	-0.46070799	0.93664700	0.35203701
H	1.76638806	-1.79510498	1.48806798
H	1.17429602	2.03527403	-0.51266199
C	-1.32702100	-1.82760000	0.07341700
C	-2.44394493	-2.54770088	0.51246101
C	-0.85758299	-1.99254596	-1.23778498
C	-3.08803892	-3.43130112	-0.35711801
H	-2.79422498	-2.40752006	1.53092098
C	-1.50372100	-2.87392092	-2.10227299
H	0.00931700	-1.43192601	-1.57807696
C	-2.61951089	-3.59408689	-1.66182005
H	-3.95468903	-3.99056602	-0.01507300

H	-1.13960803	-3.00123692	-3.11823893
H	-3.12178707	-4.28107405	-2.33781409
C	-1.62447500	1.78033495	0.07212400
C	-2.76686692	1.70905995	0.89319402
C	-1.63290298	2.67090392	-1.01890004
C	-3.87304711	2.51720691	0.63555002
H	-2.76972604	1.03150403	1.74197495
C	-2.73984909	3.47609711	-1.27116203
H	-0.77366602	2.71225095	-1.68266702
C	-3.86496496	3.40346193	-0.44363499
H	-4.74401999	2.45453000	1.28227997
H	-2.73082304	4.15428591	-2.12037492
H	-4.73065519	4.02878714	-0.64455402
C	3.23445392	0.21600001	0.09999200
C	3.65414190	0.84547299	-1.08481896
C	4.21309185	-0.31230199	0.96091199
C	5.00873804	0.93104500	-1.40576804
H	2.91615605	1.24706697	-1.77329099
C	5.56569099	-0.22106300	0.64271402
H	3.90585399	-0.77203602	1.89570606
C	5.96921682	0.39967901	-0.54321003
H	5.31313610	1.41258097	-2.33106899
H	6.30762005	-0.62671602	1.32508099
H	7.02489901	0.47274801	-0.78949702
P	-0.54809302	-0.67326099	1.25465798
O	-1.21245503	-0.69565803	2.60398102

=====

	1	2	3
	A	A	A
Frequencies --	26.5957	27.7491	34.6945
Red. masses --	4.3020	4.9264	5.5426
Frc consts --	0.0018	0.0022	0.0039
IR Inten --	0.1101	0.2733	0.2168

Sum of electronic and zero-point Energies= -1264.849763
Sum of electronic and thermal Energies= -1264.830140
Sum of electronic and thermal Enthalpies= -1264.829196
Sum of electronic and thermal Free Energies= -1264.900444

HF = -1265.17498537

2b

Element	X	Y	Z
C	-1.13712299	-0.86589402	1.17266095
C	-1.85738206	-0.11138500	0.31371900
C	-1.05714703	1.02224505	-0.26363200
C	0.23281400	1.13875103	0.11822700
H	-1.49804997	-1.73888505	1.70593905
H	-1.53041995	1.71336699	-0.96131998
P	0.57863402	-0.24273400	1.26982296
C	1.58946598	-1.42115796	0.29899600
C	2.77978206	-1.87913895	0.87518603
C	1.23317206	-1.83483100	-0.99268198
C	3.61150694	-2.74573708	0.16092500
H	3.04269505	-1.54535496	1.87494504
C	2.06501889	-2.69937611	-1.70188200
H	0.31136301	-1.47379398	-1.44201696
C	3.25592089	-3.15455008	-1.12544894
H	4.53637981	-3.09893203	0.60907501
H	1.78871596	-3.01754808	-2.70370007
H	3.90454412	-3.82660699	-1.68114305
C	2.03305101	3.32403398	1.21000397
C	2.98553109	1.54592502	-1.13977802
C	0.71447802	3.61653304	-1.61272001
H	1.22291505	3.95099497	1.60064602
H	2.28097701	2.58704090	1.98283303
H	2.90756011	3.96418405	1.04091799
H	2.69029903	0.96550900	-2.02143788
H	3.75517201	2.26496506	-1.44658399
H	3.43955803	0.84733897	-0.42793700
H	1.42338705	4.39868689	-1.91033494

H	0.40033501	3.09012294	-2.52211308
H	-0.16655099	4.11290216	-1.18839395
C	-3.72188592	-0.77940899	-2.01435208
C	-4.31233120	-1.89152300	0.82928097
C	-4.65234804	1.14389300	0.22524901
H	-3.30055904	0.05055800	-2.59450293
H	-3.15143609	-1.68253005	-2.26174903
H	-4.75399780	-0.93112898	-2.35328603
H	-4.26210880	-1.70211899	1.90790796
H	-5.35909891	-2.09767890	0.57572800
H	-3.73523092	-2.80004001	0.62030298
H	-5.70169592	1.02659297	-0.07192600
H	-4.62958813	1.37511206	1.29646695
H	-4.25076723	2.01214600	-0.31108600
Si	1.50463700	2.43279099	-0.36714199
Si	-3.66030192	-0.42038199	-0.15671200
O	1.19503498	0.07151500	2.60585690

=====

	1	2	3
	A	A	A
Frequencies --	19.4589	25.4024	28.7994
Red. masses --	3.0432	3.2175	4.2890
Frc consts --	0.0007	0.0012	0.0021
IR Inten --	0.0468	0.0777	0.2518

Sum of electronic and zero-point Energies=	-1620.055505
Sum of electronic and thermal Energies=	-1620.029121
Sum of electronic and thermal Enthalpies=	-1620.028177
Sum of electronic and thermal Free Energies=	-1620.113270

HF = -1620.42197728

2c

Element	X	Y	Z
C	-1.03289497	-0.92155498	1.16513801
C	-1.90232003	-0.43483901	0.25676000
C	-1.42572498	0.81693703	-0.41338599
C	-0.21598400	1.27964997	-0.04784900
H	-1.16020596	-1.81943405	1.75551796
H	-2.05563092	1.31331396	-1.14508498
P	0.46903500	0.09444500	1.19066799
C	1.72261095	-0.89329302	0.29244500
C	2.97995996	-1.04199600	0.88833302
C	1.46683300	-1.47924900	-0.95572901
C	3.97837400	-1.77104998	0.23703200
H	3.16215205	-0.57962602	1.85426795
C	2.46586299	-2.20346308	-1.60376501
H	0.49003199	-1.36246896	-1.41833103
C	3.72318792	-2.34947300	-1.00741696
H	4.95430613	-1.88508296	0.70130801
H	2.26716495	-2.65422392	-2.57257199
H	4.50108290	-2.91424298	-1.51446998
C	0.53816801	3.51667190	0.72230399
C	1.92537796	2.23651290	-0.94746500
C	-0.27503800	3.22708988	-1.64582896
H	-0.47291499	3.79678893	1.03900301
H	1.04209805	3.05134010	1.57459295
H	1.07848895	4.43100691	0.44692400
H	1.93364096	1.51472199	-1.77154803
H	2.41550899	3.15607500	-1.28831995
H	2.52541494	1.82043099	-0.13206901
H	0.24707900	4.14072418	-1.95160997
H	-0.34232599	2.56693602	-2.51881695
H	-1.29151905	3.51026297	-1.34897304
C	-3.23331189	-1.38785195	-1.62835705
C	-3.54949999	-2.30606198	0.68615299
C	-4.36139488	0.00789100	0.15162000
H	-3.04619908	-0.50895602	-2.25476003
H	-2.45588803	-2.12978292	-1.84467804
H	-4.20029593	-1.81017995	-1.92630398
H	-3.57721400	-2.09774804	1.76146901

H	-4.52454805	-2.71391392	0.39696699
H	-2.79479599	-3.07992196	0.50616097
H	-5.33802414	-0.40504801	-0.12751199
H	-4.39234114	0.27371100	1.21396101
H	-4.21383905	0.92870200	-0.42267299
C	0.48265201	2.55179501	-0.48907501
C	-3.24977899	-1.03280401	-0.12237400
O	0.99884701	0.64380902	2.48703599

	1	2	3
	A	A	A
Frequencies --	33.1787	37.2974	40.2453
Red. masses --	3.7301	3.0668	3.5841
Frc consts --	0.0024	0.0025	0.0034
IR Inten --	0.2345	0.1156	0.0989

Sum of electronic and zero-point Energies= -1117.200432
Sum of electronic and thermal Energies= -1117.179376
Sum of electronic and thermal Enthalpies= -1117.178431
Sum of electronic and thermal Free Energies= -1117.249607

HF = -1117.59040394

4a

Element	X	Y	Z
C	-1.27657700	1.07670200	0.79926002
C	-1.87209797	-0.02468900	0.28009200
C	-0.92842501	-1.13569403	0.00590600
C	0.36828199	-0.92399901	0.32918200
H	-1.76828694	2.00093699	1.07441401
H	-1.29036903	-2.07976794	-0.39117301
C	1.38560295	1.73560596	-0.24793500
C	2.50312996	2.50175905	0.09510900
C	0.95519298	1.67910397	-1.58262599
C	3.18946695	3.21037412	-0.89424598
H	2.82700896	2.53838396	1.13130403
C	1.64287806	2.38806891	-2.56499290
H	0.08751900	1.08154404	-1.84901905
C	2.76151991	3.15447092	-2.22121000
H	4.05809784	3.80502200	-0.62517297
H	1.30841100	2.34348893	-3.59789109
H	3.29712605	3.70610595	-2.98919702
C	1.50155497	-1.82355201	0.08991500
C	2.65780711	-1.77768505	0.89142299
C	1.45755005	-2.74907708	-0.97174400
C	3.72318411	-2.64266801	0.64644599
H	2.70981097	-1.07635903	1.71762502
C	2.52236009	-3.61333799	-1.20998800
H	0.59153599	-2.76929903	-1.62732506
C	3.66095304	-3.56469989	-0.40026900
H	4.60469294	-2.59636998	1.28007305
H	2.47019005	-4.31681013	-2.03672791
H	4.49489689	-4.23496389	-0.59003299
C	-3.31618690	-0.15690300	0.00530600
C	-3.77698207	-0.94448501	-1.06401205
C	-4.26211596	0.51419801	0.80050099
C	-5.14050817	-1.04664505	-1.33814001
H	-3.06429505	-1.45949996	-1.70188105
C	-5.62389421	0.40720701	0.52911502
H	-3.92301798	1.09861004	1.65079200
C	-6.06876421	-0.37245601	-0.54250097
H	-5.47725677	-1.65276694	-2.17474389
H	-6.34053421	0.92525798	1.16048396
H	-7.13149500	-0.45761400	-0.75172299
P	0.49160799	0.78196001	1.04097605
S	1.17426705	1.00406897	2.88112712

	1	2	3
	A	A	A
Frequencies --	22.5820	26.0088	28.4931

Red. masses --	3.7843	4.7370	4.5216
Frc consts --	0.0011	0.0019	0.0022
IR Inten --	0.0806	0.3962	0.1782

Sum of electronic and zero-point Energies=	-1587.821055
Sum of electronic and thermal Energies=	-1587.800926
Sum of electronic and thermal Enthalpies=	-1587.799982
Sum of electronic and thermal Free Energies=	-1587.872953

HF = -1588.14432363

4b

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=====
Element          X          Y          Z
=====
C          -1.15084803   -0.90724301    1.03486097
C          -1.90503895   -0.14442800    0.21264599
C          -1.12784898    0.98467398   -0.38665700
C           0.17460801    1.11048496   -0.04413700
H          -1.48134696   -1.77397203    1.59619904
H          -1.61916006    1.67496502   -1.07211900
P           0.55513197   -0.26039499    1.11278605
C           1.58068597   -1.43243599    0.13028599
C           2.77429795   -1.93105805    0.65899003
C           1.17943001   -1.80056405   -1.16316903
C           3.56780100   -2.79129410   -0.10466000
H           3.07650805   -1.63807905    1.66057205
C           1.97415197   -2.65847993   -1.92093205
H           0.25322101   -1.40969503   -1.57591295
C           3.17108297   -3.15362191   -1.39240897
H           4.49656677   -3.17496610    0.30865401
H           1.66274405   -2.93984199   -2.92335391
H           3.79109001   -3.82032895   -1.98574305
C           1.77943206    3.57582307    0.82364702
C           2.98914409    1.52597499   -1.15792000
C           0.63437301    3.34570599   -2.06309199
H           0.88329297    4.13167000    1.12301099
H           2.12069511    3.00309396    1.69300401
H           2.55711794    4.30192709    0.55560499
H           2.79056406    0.79870403   -1.95323896
H           3.73030806    2.24491191   -1.52815795
H           3.43850207    0.97981501   -0.32084301
H           1.31533396    4.12295914   -2.43068600
H           0.41163099    2.67434812   -2.90092611
H           -0.29936299    3.84001493   -1.76853597
C           -3.89728904   -0.75372702   -2.02324390
C           -4.32872677   -1.93344200    0.82284701
C           -4.69693422    1.11582398    0.31171000
H           -3.50690293    0.08941100   -2.60609198
H           -3.34424090   -1.65152705   -2.32366395
H           -4.94708109   -0.89557898   -2.30774808
H           -4.21742201   -1.76864398    1.90094495
H           -5.38843822   -2.13390398    0.62463701
H           -3.76545596   -2.83685994    0.56074601
H           -5.76236582    1.00607002    0.07502300
H           -4.60940886    1.32194304    1.38466501
H           -4.32593489    1.99589396   -0.22734800
Si           1.41129601    2.41114092   -0.61315203
Si           -3.73296595   -0.43965101   -0.16404200
S           1.28787696    0.20309800    2.88735199
=====

```

	1	2	3
	A	A	A
Frequencies --	19.5107	21.6817	28.6386
Red. masses --	3.0371	3.0816	4.6537
Frc consts --	0.0007	0.0009	0.0022
IR Inten --	0.0641	0.0895	0.4065

Sum of electronic and zero-point Energies=	-1943.029063
Sum of electronic and thermal Energies=	-1943.002277
Sum of electronic and thermal Enthalpies=	-1943.001332
Sum of electronic and thermal Free Energies=	-1943.087494

HF = -1943.39374981

4c

```
=====
Element          X           Y           Z
=====
C          -1.06270695    -0.88637203    1.09356296
C          -1.95878506    -0.43397900    0.19338500
C          -1.46954894     0.73995697   -0.58543801
C          -0.23768499     1.20361495   -0.29602799
H          -1.18675303    -1.71585500    1.77649498
H          -2.10277796     1.19087398   -1.34302998
P           0.45030200     0.10947600    1.02905798
C           1.68587601    -0.95510399    0.17144200
C           2.96388197    -1.11985397    0.71171898
C           1.34727502    -1.59203303   -1.03240001
C           3.90277410    -1.91476500    0.04898800
H           3.21609902    -0.62234199    1.64396000
C           2.28749490    -2.38203692   -1.69087994
H           0.35375699    -1.46350098   -1.45328295
C           3.56783605    -2.54353404   -1.15076399
H           4.89579201    -2.03959608    0.47208601
H           2.02358103    -2.87147403   -2.62459898
H           4.30019999    -3.15931511   -1.66596103
C           0.34098101    3.59533405    0.09616300
C           1.96822095     2.10344005   -1.11841595
C          -0.16719700     2.80250192   -2.23841095
H          -0.71253502     3.84881496    0.25910199
H           0.78671497     3.35353088    1.06476498
H           0.84924001     4.47714901   -0.31377700
H           2.10613108     1.25764298   -1.80032694
H           2.46227503     2.98024988   -1.55268002
H           2.47543311     1.86706197   -0.17732300
H           0.37614900     3.64904308   -2.67301798
H          -0.13384300     1.97177804   -2.95292211
H          -1.21167397     3.11174393   -2.11759496
C          -3.42703295    -1.47235501   -1.53880095
C          -3.64743590    -2.19605303    0.85487998
C          -4.40047503     0.10245500    0.18249300
H          -3.24185801    -0.65290302   -2.24177289
H          -2.69203305    -2.26118207   -1.73642302
H          -4.42464018    -1.87449002   -1.75123203
H          -3.60983801    -1.90394497    1.91016698
H          -4.65061617    -2.58564806    0.64902103
H          -2.93198109    -3.01135111    0.69872397
H          -5.40648079    -0.28939900   -0.00882100
H          -4.35973692     0.45230201    1.21978295
H          -4.25081015     0.96797401   -0.47182500
C           0.47092700     2.40895796   -0.89202201
C          -3.34660506    -1.00233603   -0.06687900
S           1.08805704     0.93335497    2.70619011
=====
```

	1	2	3
	A	A	A
Frequencies --	33.7211	36.8282	39.3973
Red. masses --	4.2309	3.3342	2.9938
Frc consts --	0.0028	0.0027	0.0027
IR Inten --	0.3793	0.1462	0.1123

Sum of electronic and zero-point Energies= -1440.172350
Sum of electronic and thermal Energies= -1440.150845
Sum of electronic and thermal Enthalpies= -1440.149900
Sum of electronic and thermal Free Energies= -1440.222235

HF = -1440.56044073

4d

```
=====
Element          X           Y           Z
=====
C          -1.28135204     1.19661200    0.80483001
=====
```

C	-1.76899004	0.01568000	0.35124499
C	-0.72251499	-1.00932300	0.11930900
C	0.54970402	-0.65260398	0.41158399
H	-1.85949600	2.08069491	1.04110205
H	-0.99271500	-2.00507307	-0.22075699
C	1.29234397	2.06119704	-0.31297800
C	2.33722901	2.94416404	-0.02590300
C	0.85272098	1.89893198	-1.63601601
C	2.94193602	3.66358089	-1.05969000
H	2.66866994	3.06282091	1.00171900
C	1.45893300	2.61916804	-2.66280890
H	0.04121300	1.21131504	-1.85868800
C	2.50499010	3.50229812	-2.37505889
H	3.75403094	4.34921885	-0.83424997
H	1.11738205	2.49290705	-3.68655705
H	2.97711992	4.06268120	-3.17751288
C	1.76541400	-1.44393396	0.20416901
C	2.92272806	-1.23177898	0.97897297
C	1.80565202	-2.43259907	-0.79978400
C	4.07184505	-1.99059403	0.77210802
H	2.91469693	-0.48084301	1.76182103
C	2.94657612	-3.19904304	-1.01280904
H	0.93993598	-2.58469892	-1.43733597
C	4.06593323	-2.96559405	-0.21890301
H	4.96533012	-1.83932102	1.36842895
H	2.98896694	-3.95731997	-1.78750205
C	-3.19473195	-0.27528000	0.10987200
C	-3.58942509	-1.16742802	-0.90306902
C	-4.19526815	0.34507599	0.88064200
C	-4.93574905	-1.42489100	-1.15298402
H	-2.83947110	-1.64850605	-1.52358401
C	-5.54361010	0.09430900	0.64627302
H	-3.90944409	1.01027298	1.68955600
C	-5.89355707	-0.78827798	-0.37173599
H	-5.25100899	-2.10365200	-1.93820095
H	-6.32216311	0.55841398	1.24223900
P	0.50902301	1.09223199	1.03437996
S	1.18803406	1.46786404	2.85067701
F	5.17683601	-3.70010209	-0.42577901
F	-7.19703102	-1.03725696	-0.60206300

=====

	1	2	3
	A	A	A
Frequencies --	21.6926	24.3093	26.3740
Red. masses --	4.0689	5.5211	4.3641
Frc consts --	0.0011	0.0019	0.0018
IR Inten --	0.0988	0.4999	0.0506

Sum of electronic and zero-point Energies= -1786.304088
Sum of electronic and thermal Energies= -1786.282253
Sum of electronic and thermal Enthalpies= -1786.281309
Sum of electronic and thermal Free Energies= -1786.358526

HF = -1786.61087673

6a

Element	X	Y	Z
C	-1.33053195	-1.13660300	-0.29100001
C	-1.98643398	0.03554300	-0.10246700
C	-1.09228206	1.21667504	-0.08132600
C	0.22632800	0.98347199	-0.28095701
H	-1.77807701	-2.12047100	-0.34654400
H	-1.50090098	2.21563911	0.04109700
C	1.30598199	-1.40160406	0.98628998
C	2.46144390	-2.18124795	0.88802898
C	0.81333297	-1.02813494	2.24630809
C	3.12427497	-2.58775592	2.04871202
H	2.83144903	-2.46368504	-0.09377100
C	1.47802305	-1.43719101	3.40019798
H	-0.08397200	-0.41971999	2.32085991

C	2.63491511	-2.21751690	3.30197501
H	4.02277899	-3.19363999	1.97056496
H	1.09587097	-1.14803505	4.37542391
H	3.15240788	-2.53482008	4.20336294
C	1.31894505	1.96036696	-0.22591799
C	2.51648808	1.76686502	-0.93980497
C	1.19138598	3.11623001	0.56992799
C	3.54116797	2.70928693	-0.87038201
H	2.63207507	0.88670999	-1.56398499
C	2.21588492	4.05655813	0.63240999
H	0.29192799	3.26075506	1.16177201
C	3.39653802	3.85756111	-0.08916000
H	4.45577478	2.54513788	-1.43365395
H	2.09915400	4.93925714	1.25556004
H	4.19900417	4.58825684	-0.03550500
C	-3.44740009	0.17160800	0.05594100
C	-3.99321508	1.18594599	0.86174703
C	-4.32484484	-0.72023100	-0.58610702
C	-5.37296486	1.29654896	1.03120697
H	-3.33451891	1.87677801	1.38034594
C	-5.70287609	-0.60569000	-0.42019400
H	-3.91927004	-1.48738301	-1.23920095
C	-6.23274279	0.40229401	0.39052299
H	-5.77602720	2.08152699	1.66528404
H	-6.36563778	-1.29804206	-0.93203902
H	-7.30803299	0.49265501	0.51704901
P	0.43563700	-0.83854198	-0.52950799
Se	1.24420404	-1.53825498	-2.36646199

=====

	1	2	3
	A	A	A
Frequencies --	23.3945	25.5277	29.0279
Red. masses --	3.8115	6.1785	3.9073
Frc consts --	0.0012	0.0024	0.0019
IR Inten --	0.0727	0.4053	0.0541

Sum of electronic and zero-point Energies= -3588.564784
Sum of electronic and thermal Energies= -3588.544333
Sum of electronic and thermal Enthalpies= -3588.543389
Sum of electronic and thermal Free Energies= -3588.617648

HF = -3588.88737204

6b

Element	X	Y	Z
C	-1.20858204	-0.83846599	0.93999898
C	-2.03017092	-0.14119899	0.12272000
C	-1.30245805	0.90819800	-0.65318000
C	0.02904500	1.03864801	-0.44888401
H	-1.49229205	-1.63898504	1.61369205
H	-1.84946096	1.54371905	-1.34930801
P	0.50196499	-0.22036000	0.79450297
C	1.42622304	-1.50354600	-0.15054300
C	2.64837694	-1.98577201	0.32445800
C	0.91019499	-1.97559297	-1.36733103
C	3.35632801	-2.93512702	-0.41715401
H	3.03901291	-1.60931695	1.26607502
C	1.62075806	-2.92153811	-2.10366511
H	-0.03845600	-1.59699905	-1.73833799
C	2.84628391	-3.40144897	-1.62936902
H	4.30783796	-3.30633998	-0.04640800
H	1.22135496	-3.28335309	-3.04735303
H	3.40034199	-4.13714790	-2.20619297
C	1.59984505	3.62920499	0.02083400
C	2.80466390	1.34467304	-1.68967295
C	0.38608399	2.97722006	-2.77159190
H	0.69996703	4.20799398	0.25978100
H	1.96832204	3.18531299	0.95225197
H	2.35913801	4.32221794	-0.36266801
H	2.60278797	0.50677001	-2.36644197

H	3.51898098	2.01714110	-2.18036699
H	3.28760409	0.93607801	-0.79474199
H	1.03710198	3.71116400	-3.26200700
H	0.15909301	2.19143891	-3.50179505
H	-0.55231899	3.48709297	-2.52145910
C	-4.24484921	-0.91377503	-1.83671498
C	-4.40320110	-1.80992496	1.13816500
C	-4.78129816	1.18474996	0.37601700
H	-3.90202498	-0.13942300	-2.53374410
H	-3.73826504	-1.84928298	-2.10191607
H	-5.31988478	-1.05593896	-2.00168490
H	-4.18022299	-1.54751503	2.17897797
H	-5.48037577	-2.00263000	1.06728601
H	-3.88267708	-2.74719906	0.90856999
H	-5.86644697	1.07758904	0.25684801
H	-4.58399487	1.48819995	1.41060805
H	-4.45436716	2.00193906	-0.27823099
Si	1.22304296	2.26869607	-1.22974503
Si	-3.89028907	-0.42966199	-0.04177300
Se	1.45905197	0.46642900	2.56287503

	1	2	3
	A	A	A
Frequencies --	17.4286	21.6667	27.1667
Red. masses --	3.0253	3.2255	4.6868
Frc consts --	0.0005	0.0009	0.0020
IR Inten --	0.0468	0.1126	0.3128

Sum of electronic and zero-point Energies= -3943.773140
Sum of electronic and thermal Energies= -3943.746033
Sum of electronic and thermal Enthalpies= -3943.745089
Sum of electronic and thermal Free Energies= -3943.832758

HF = -3944.13713086

6c

Element	X	Y	Z
C	-1.13578498	-0.55997598	1.18253899
C	-2.09895205	-0.35098001	0.26135099
C	-1.63099694	0.44532800	-0.90755701
C	-0.34841701	0.86134702	-0.89872402
H	-1.23077905	-1.09721196	2.11626410
H	-2.31663799	0.67858100	-1.71615005
P	0.41438499	0.21569601	0.65738100
C	1.49313796	-1.17916906	0.11843600
C	2.80740595	-1.27477705	0.58200097
C	0.99097002	-2.14219499	-0.77041900
C	3.62019396	-2.32824492	0.15538099
H	3.18509007	-0.52245098	1.26917696
C	1.80621803	-3.18961692	-1.19464505
H	-0.03098800	-2.06670094	-1.13176405
C	3.12326503	-3.28325105	-0.73232698
H	4.64226007	-2.39902806	0.51737797
H	1.41630697	-3.93238211	-1.88550997
H	3.75801396	-4.10026407	-1.06483305
C	0.32907799	3.20027494	-1.42205405
C	1.82658195	1.29173696	-2.10193992
C	-0.35746700	1.65294194	-3.28694010
H	-0.70336300	3.55036402	-1.31097198
H	0.82706499	3.29343009	-0.45301700
H	0.83909100	3.85041189	-2.14404702
H	1.89422297	0.25349501	-2.44373703
H	2.31717992	1.93118894	-2.84476399
H	2.38525891	1.38034904	-1.16434002
H	0.18270200	2.25593805	-4.02549314
H	-0.39960900	0.62044901	-3.65268612
H	-1.38066995	2.04187107	-3.23369002
C	-3.81368589	-1.76236200	-0.87943399
C	-3.80360699	-1.62483203	1.62725496
C	-4.49002123	0.37946799	0.28052101

H	-3.66037011	-1.24454701	-1.83251202
H	-3.15444493	-2.63786793	-0.85949701
H	-4.85128403	-2.11574793	-0.85537201
H	-3.63022304	-1.00298297	2.51247096
H	-4.84477091	-1.96510196	1.65365601
H	-3.15953112	-2.50871301	1.69709599
H	-5.53278780	0.04317600	0.32275400
H	-4.31050491	1.04912198	1.12867403
H	-4.36469793	0.95954102	-0.64006102
C	0.35755500	1.73447704	-1.92395699
C	-3.53891206	-0.83963197	0.33171099
Se	1.32612705	1.59607100	1.98979604

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	1	2	3
	A	A	A
Frequencies --	31.9650	36.2136	42.7590
Red. masses --	4.3296	3.5761	2.8251
Frc consts --	0.0026	0.0028	0.0030
IR Inten --	0.2787	0.1532	0.0617

Sum of electronic and zero-point Energies=	-3440.916016
Sum of electronic and thermal Energies=	-3440.894177
Sum of electronic and thermal Enthalpies=	-3440.893233
Sum of electronic and thermal Free Energies=	-3440.966958

HF = -3441.30338031