3,5-Diphenyl-2-phosphafuran: Synthesis, Structure, and Thermally Reversible [4+2] Cycloaddition Chemistry

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Supporting Information

Table of Contents

S.1 NMR Spectra of New Compounds

S.1.1 2-Ethoxy-3,5-diphenyl-3-hydro-1,2-oxaphosphole (2)

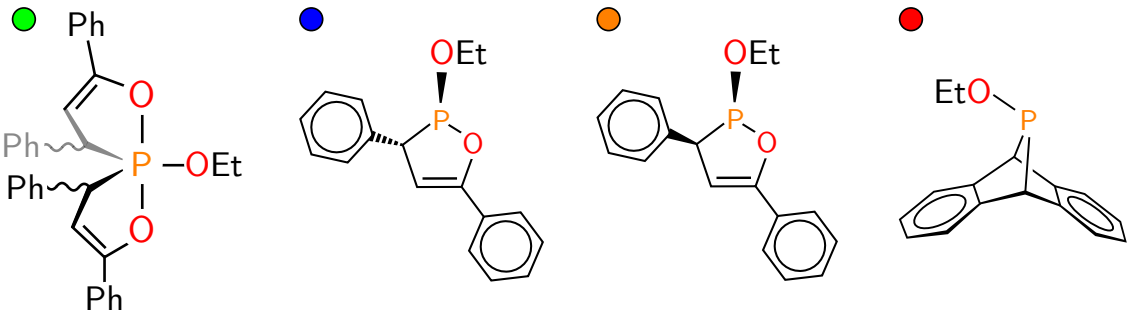

Figure S.1: Labeling scheme for **2** mixture.

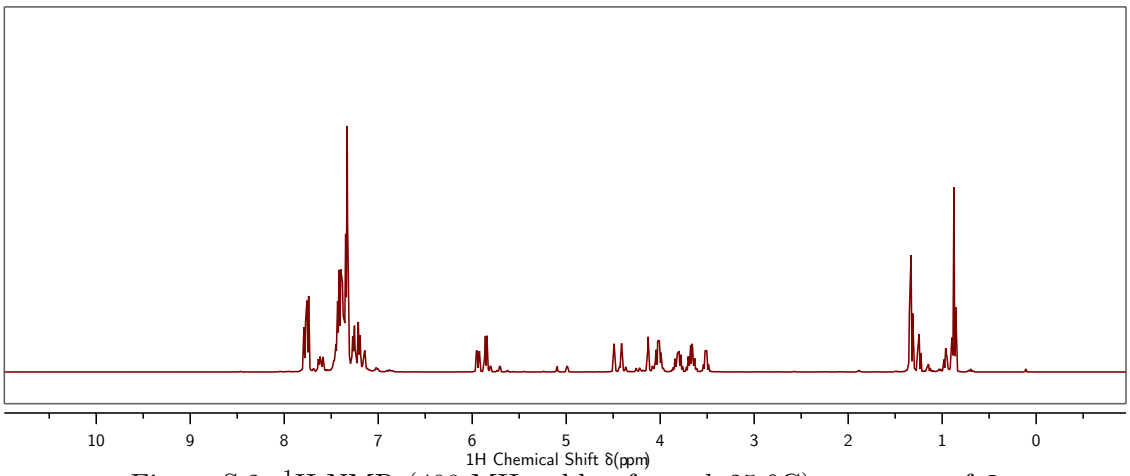

Figure S.2: ^{1}H NMR (400 MHz, chloroform-*d*, 25 °C) spectrum of **2**.

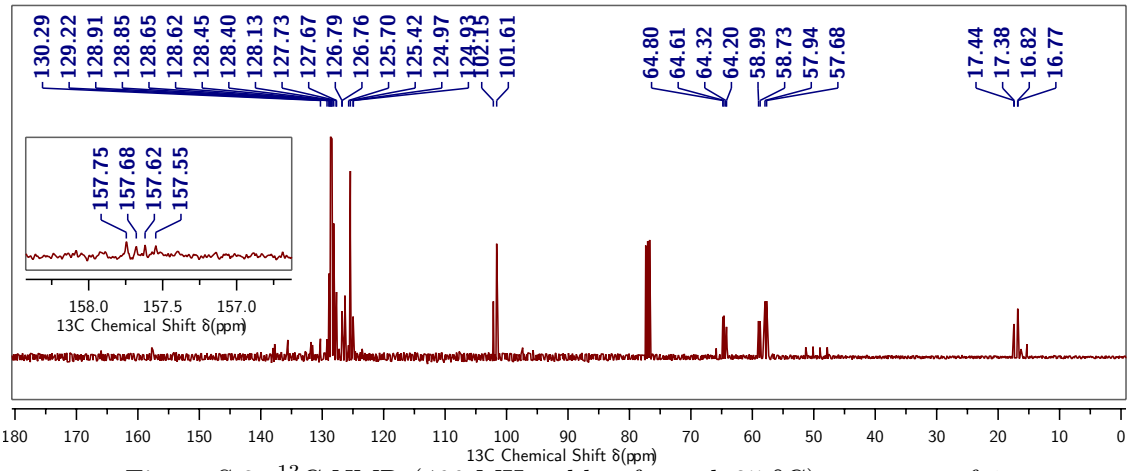

Figure S.3: ^{13}C NMR (400 MHz, chloroform-*d*, 25 °C) spectrum of **2**.

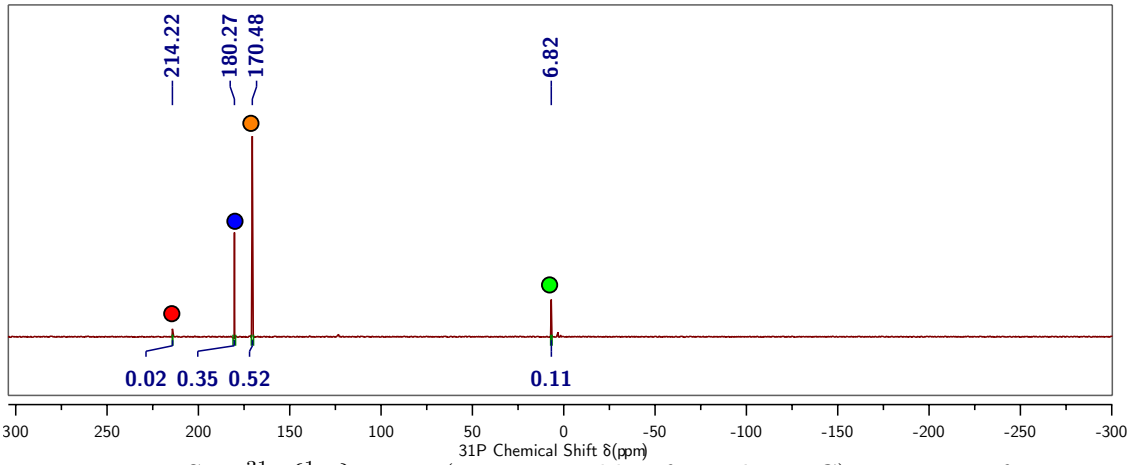

Figure S.4: ^{31}P{^{1}H} NMR (400 MHz, chloroform-*d*, 25 °C) spectrum of **2**.

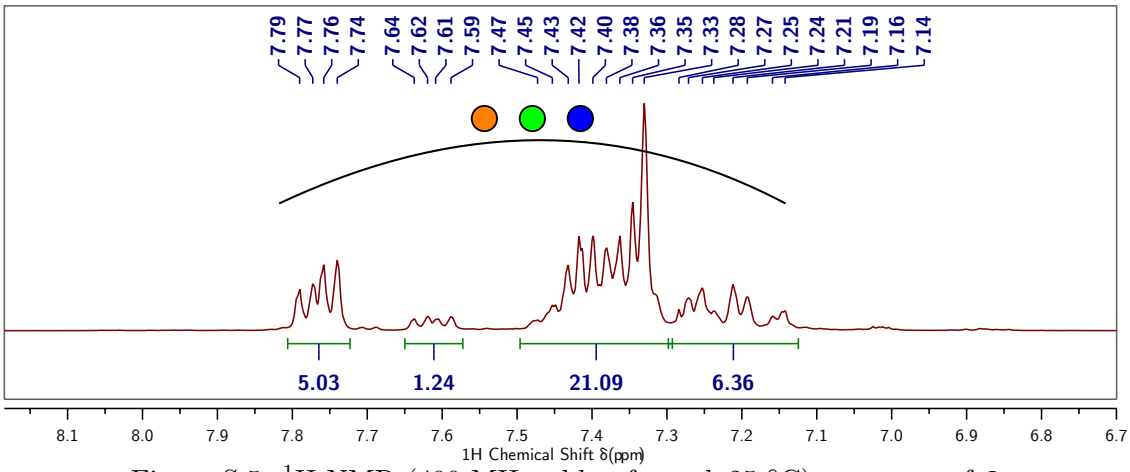

Figure S.5: ^{1}H NMR (400 MHz, chloroform-*d*, 25 °C) spectrum of **2**.

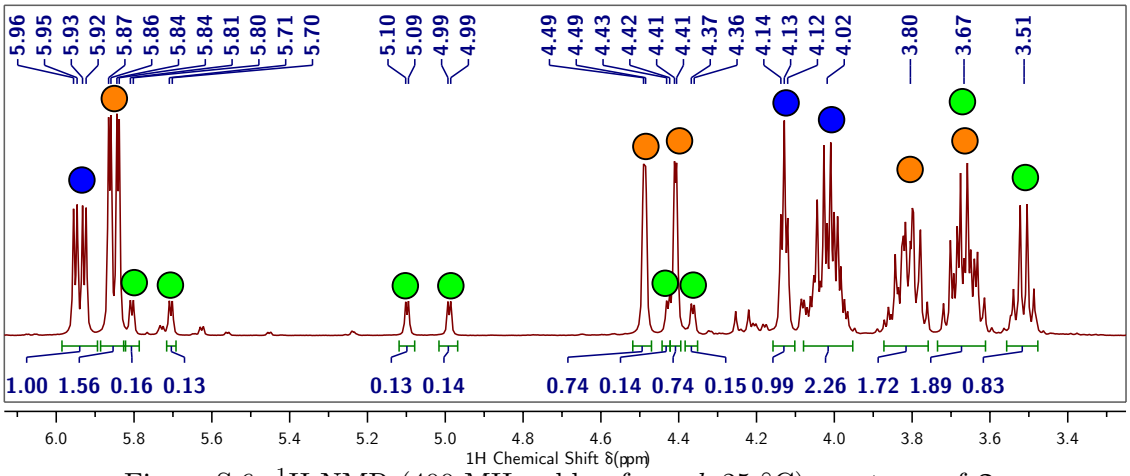

Figure S.6: ^{1}H NMR (400 MHz, chloroform-*d*, 25 °C) spectrum of **2**.

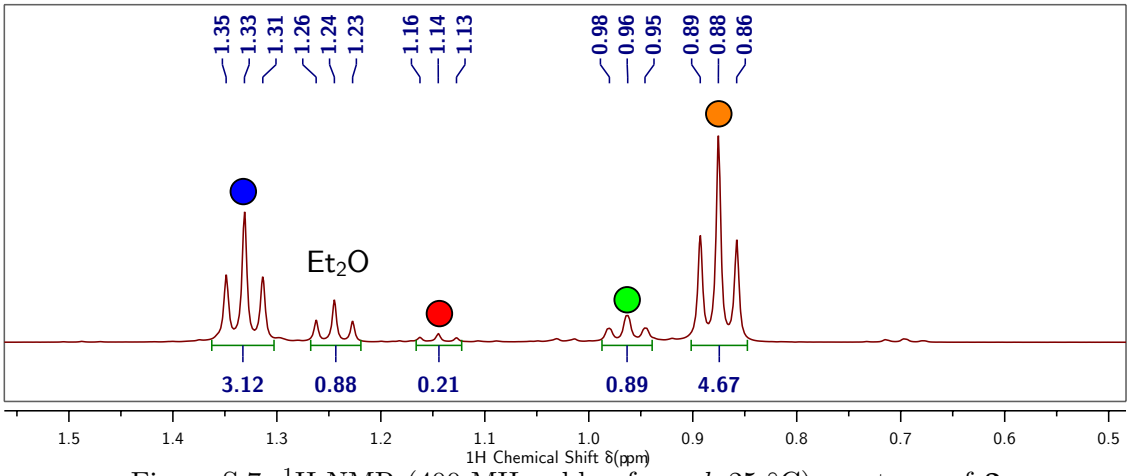

Figure S.7: ^{1}H NMR (400 MHz, chloroform-*d*, 25 °C) spectrum of **2**.

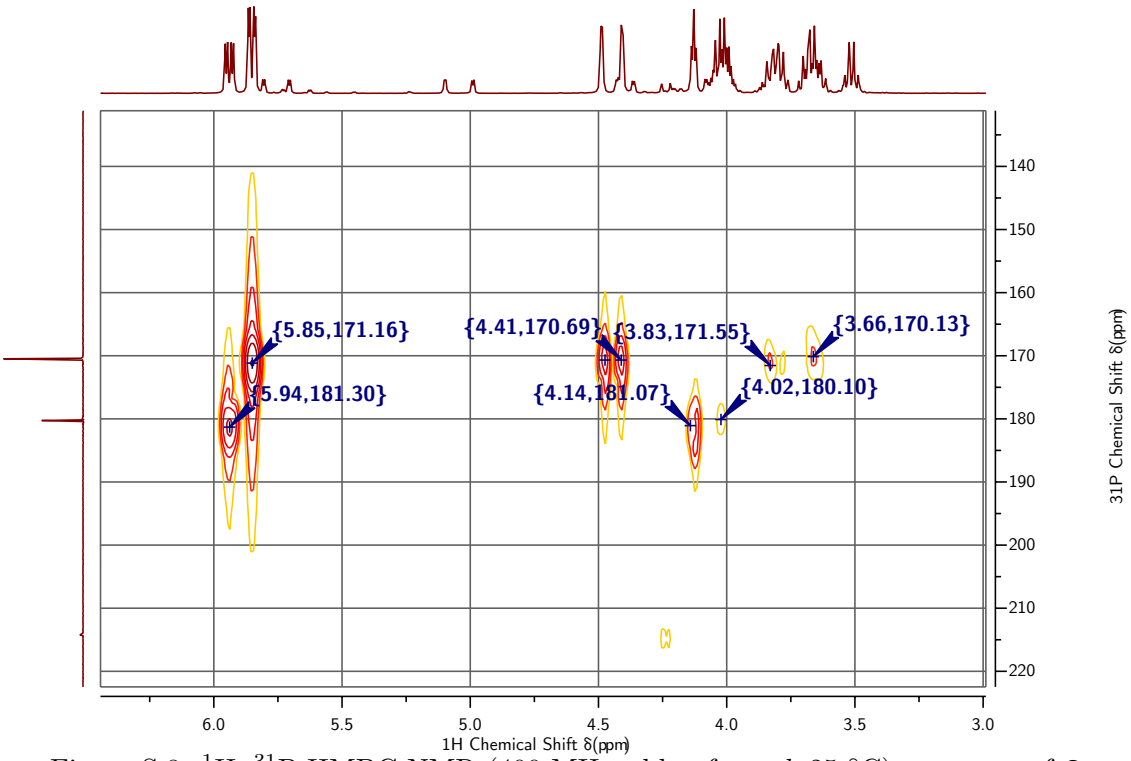

Figure S.8: ^{1}H, ^{31}P-HMBC NMR (400 MHz, chloroform-*d*, 25 °C) spectrum of **2**.

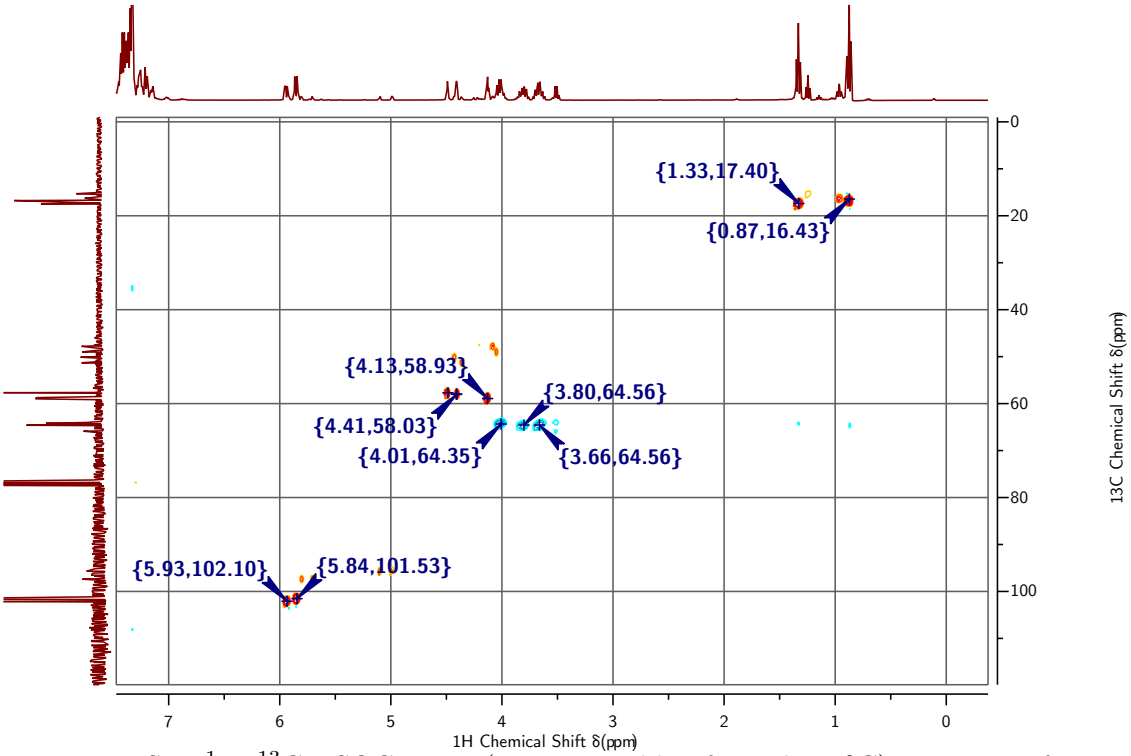

Figure S.9: ^{1}H, ^{13}C-HSQC NMR (400 MHz, chloroform-*d*, 25 °C) spectrum of **2**.

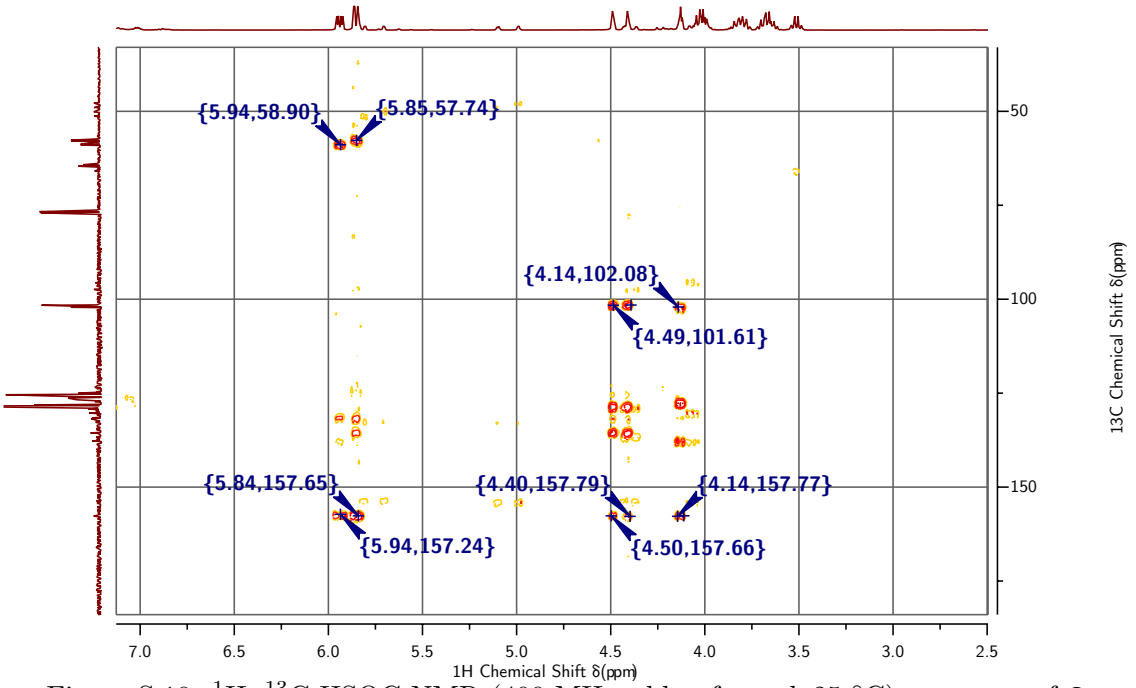

Figure S.10: ^{1}H, ^{13}C-HSQC NMR (400 MHz, chloroform-*d*, 25 °C) spectrum of **2**.

S.1.2 3,5-Diphenyl-2-phosphafuran (DPF)

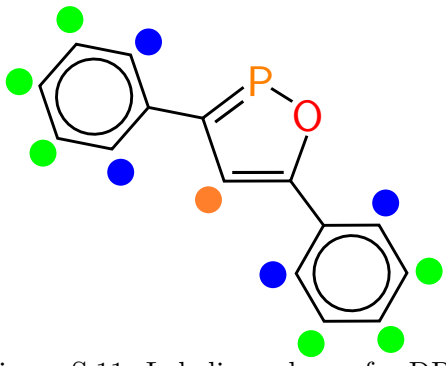

Figure S.11: Labeling scheme for DPF.

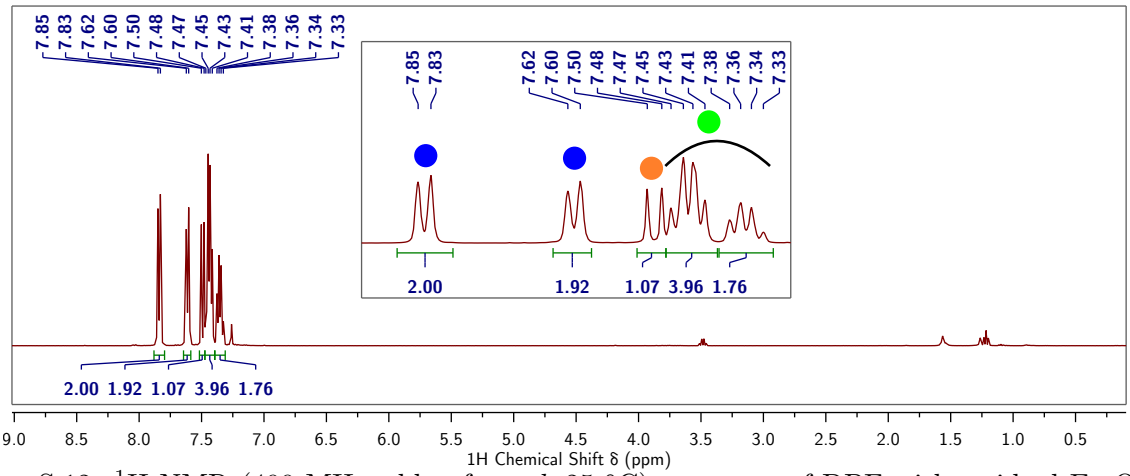

Figure S.12: ^{1}H NMR (400 MHz, chloroform-*d*, 25 °C) spectrum of DPF with residual Et_2O and pentane.

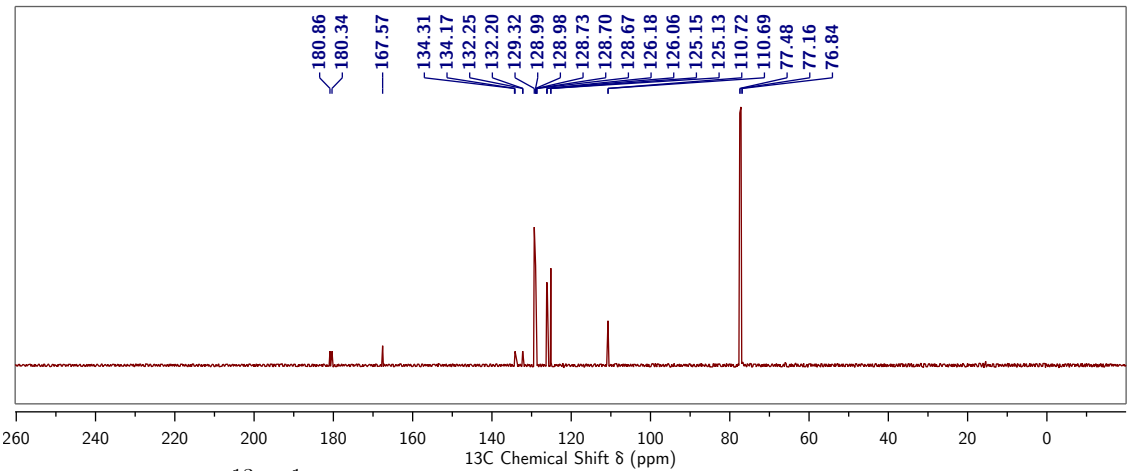

Figure S.13: ^{13}C{^{1}H} NMR (101 MHz, chloroform-*d*, 25 °C) spectrum of DPF.

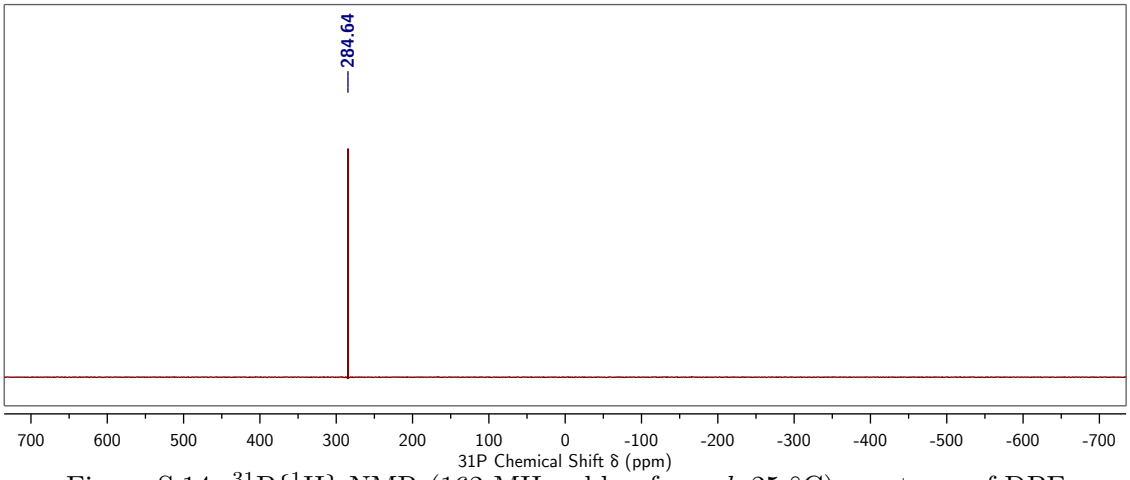

Figure S.14: $^{31}P\{^{1}H\}$ NMR (162 MHz, chloroform-*d*, 25 °C) spectrum of DPF.

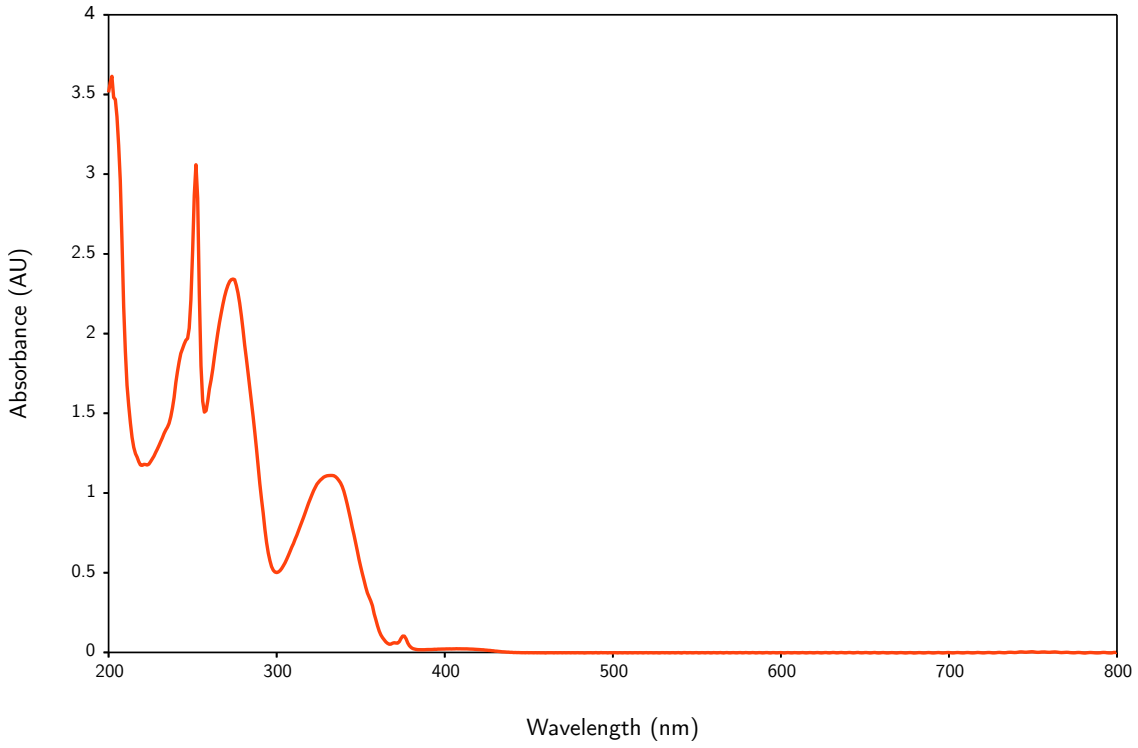

Figure S.15: UV-vis spectrum of DPF in hexanes (20 μM).

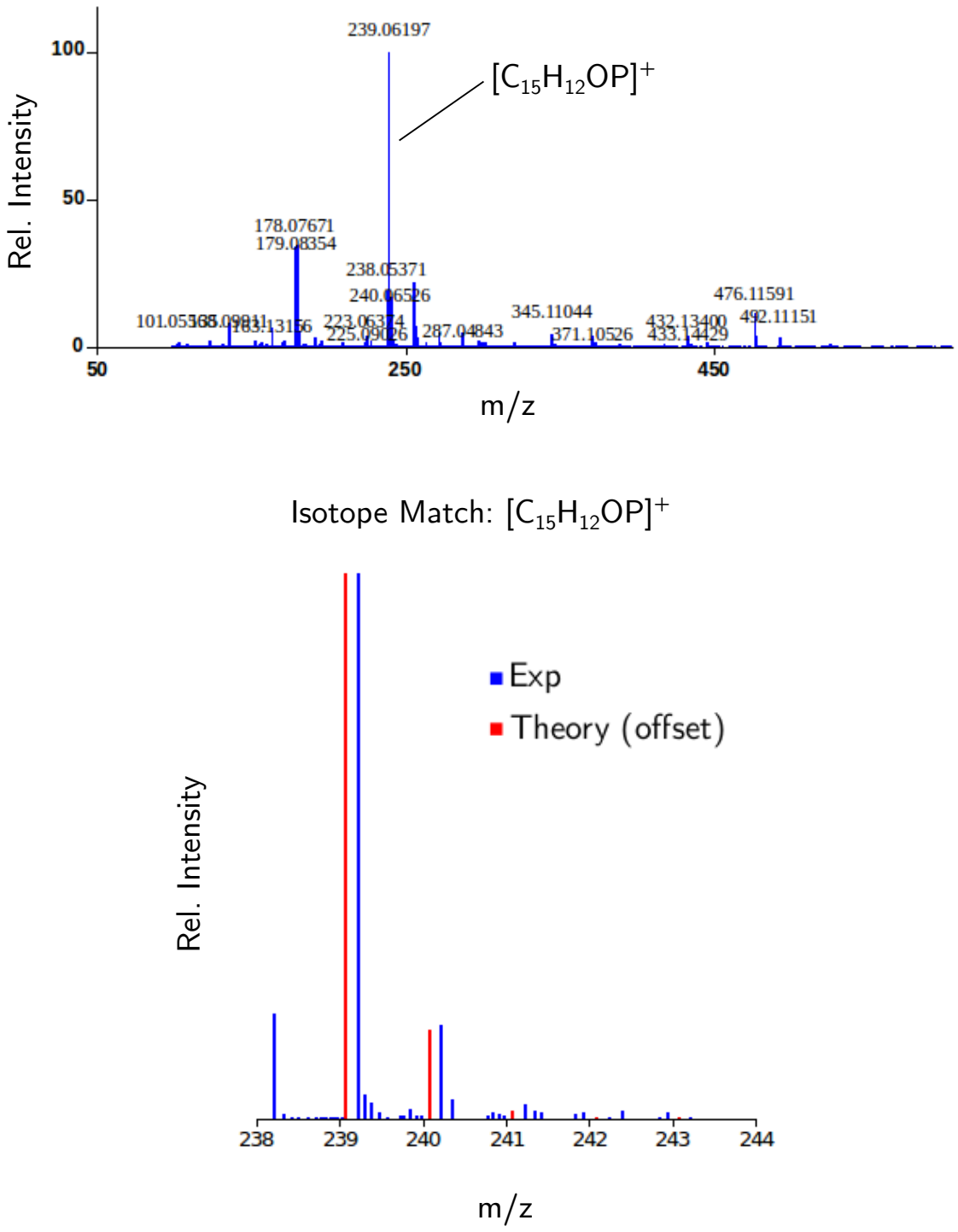

Figure S.16: DART HRMS(Q-TOF) data corresponding to $[C_{15}H_{12}O_1P]^+$.

S.1.3 Dimethyl 4,6-Diphenyl-7-oxa-1-phosphabicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxylate (DPF·DMAD)

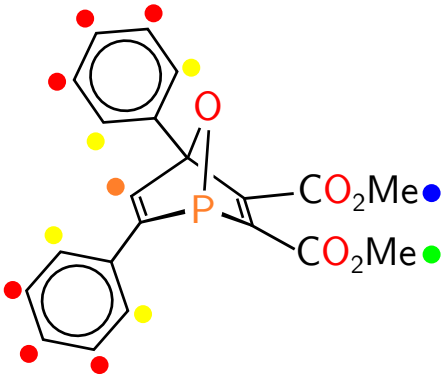

Figure S.17: Labeling scheme for DPF·DMAD.

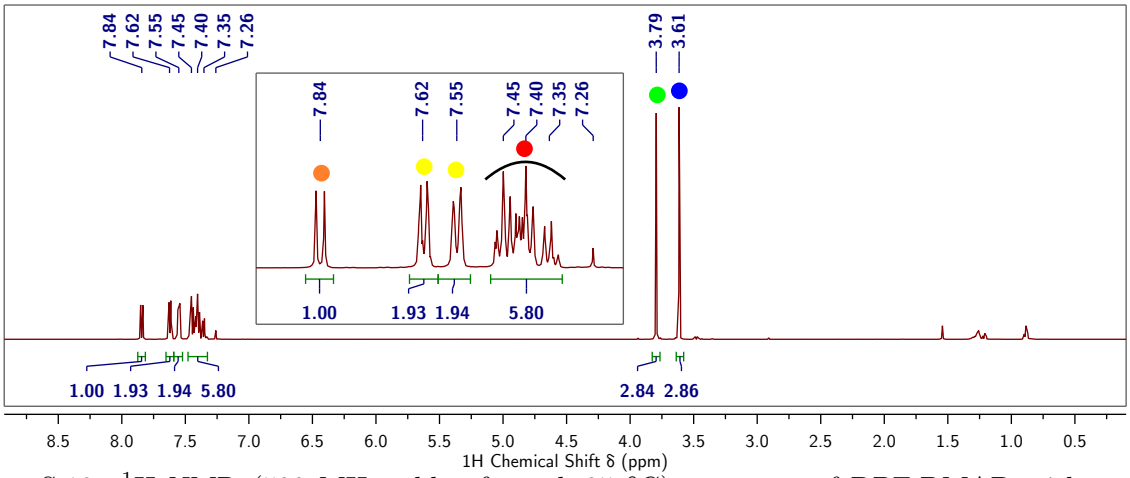

Figure S.18: ^{1}H NMR (500 MHz, chloroform-*d*, 25 °C) spectrum of DPF·DMAD with residual pentane.

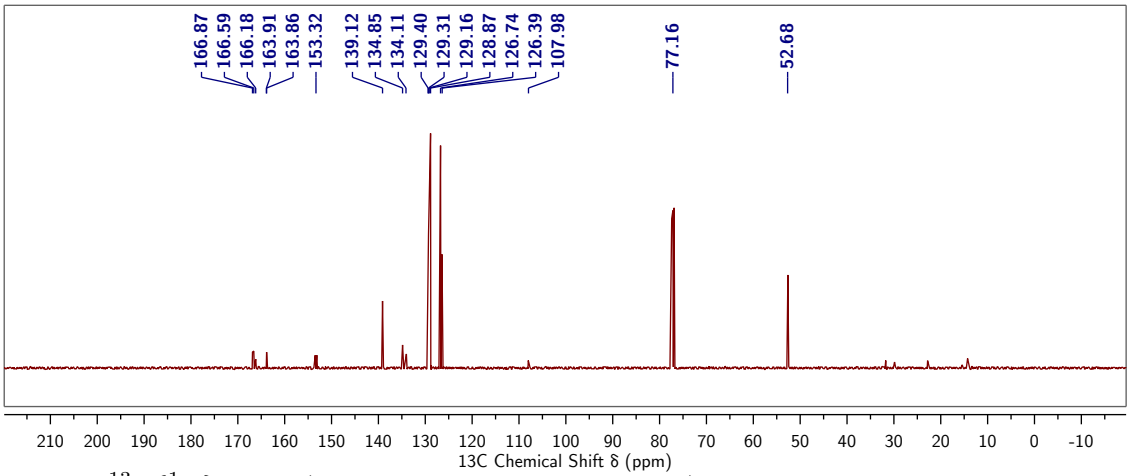

Figure S.19: $^{13}C\{^{1}H\}$ NMR (126 MHz, chloroform-*d*, 25 °C) spectrum of DPF·DMAD with residual pentane.

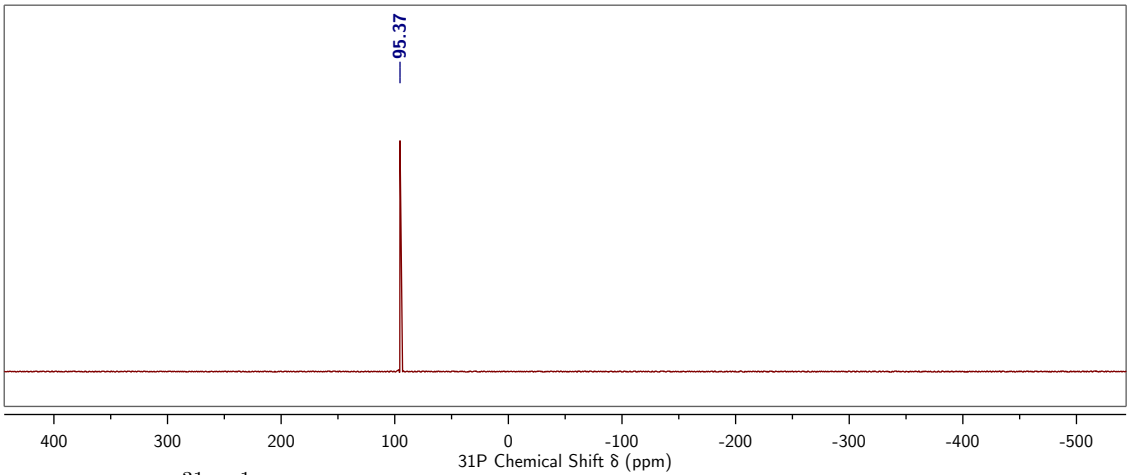

Figure S.20: $^{31}P\{^{1}H\}$ NMR (202 MHz, chloroform-*d*, 25 °C) spectrum of DPF·DMAD.

S.1.4 2,4-Diphenyl-7-oxa-1-phosphabicyclo[2.2.1]hept-2-ene (DPF·C_2H_4)

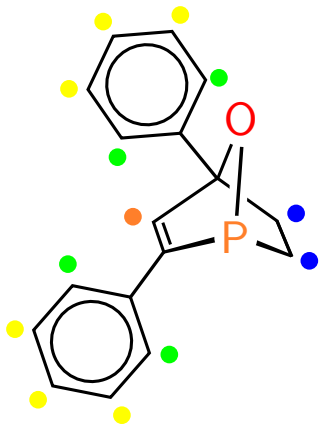

Figure S.21: Labeling scheme for DPF·C_2H_4.

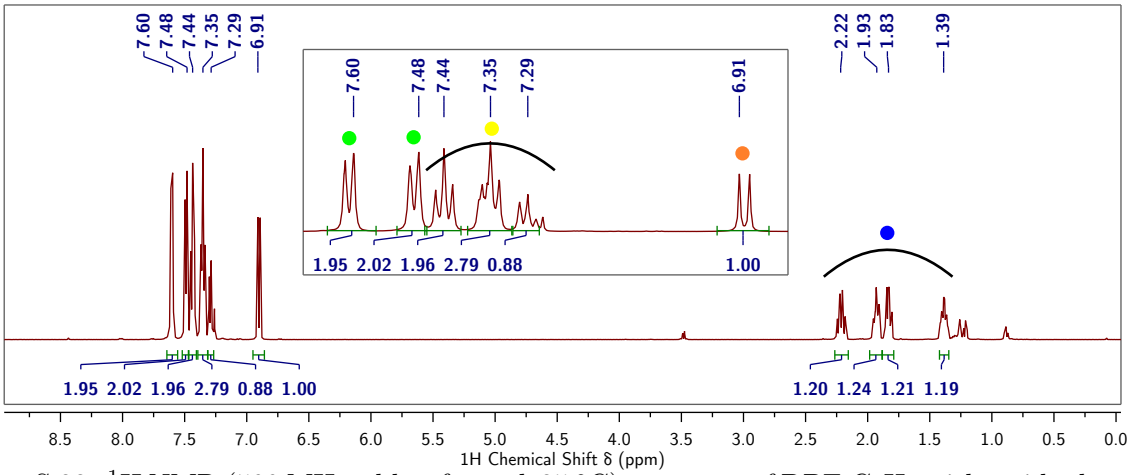

Figure S.22: ^{1}H NMR (500 MHz, chloroform-*d*, 25 °C) spectrum of DPF·C_2H_4 with residual pentane and diethyl ether.

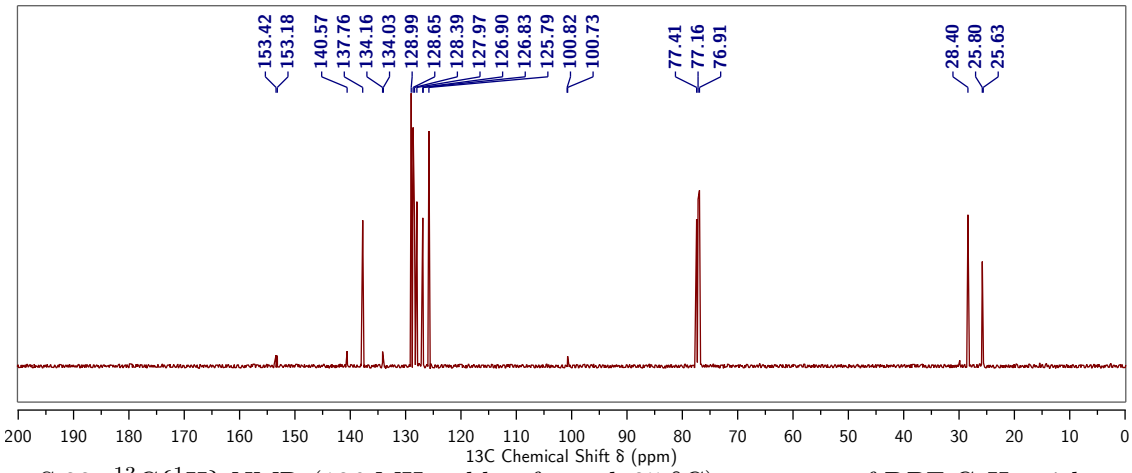

Figure S.23: $^{13}C\{^{1}H\}$ NMR (126 MHz, chloroform-*d*, 25 °C) spectrum of DPF·C_2H_4 with residual pentane.

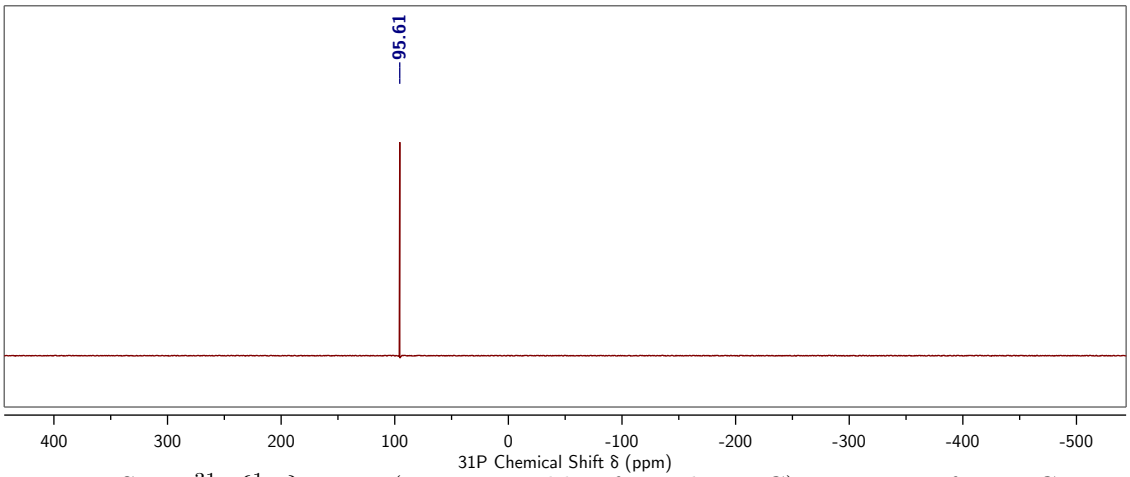

Figure S.24: $^{31}P\{^{1}H\}$ NMR (202 MHz, chloroform-*d*, 25 °C) spectrum of DPF·C_2H_4.

S.1.5 (±)-(1*R*,2*R*,3*S*,6*R*,7*R*,8*S*)-8,10-Diphenyl-11-oxa-1-phosphatetracyclo-[6.2.1.1^{3,6}.0^{2}, 7]dodec-9-ene (DPF·norbornene)

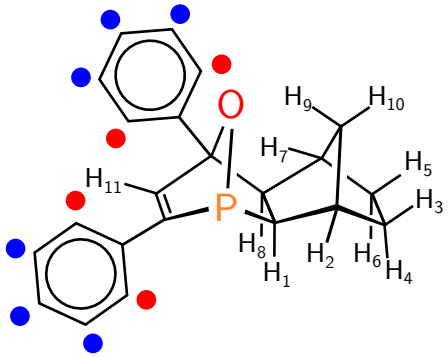

Figure S.25: Labeling scheme for DPF·norbornene.

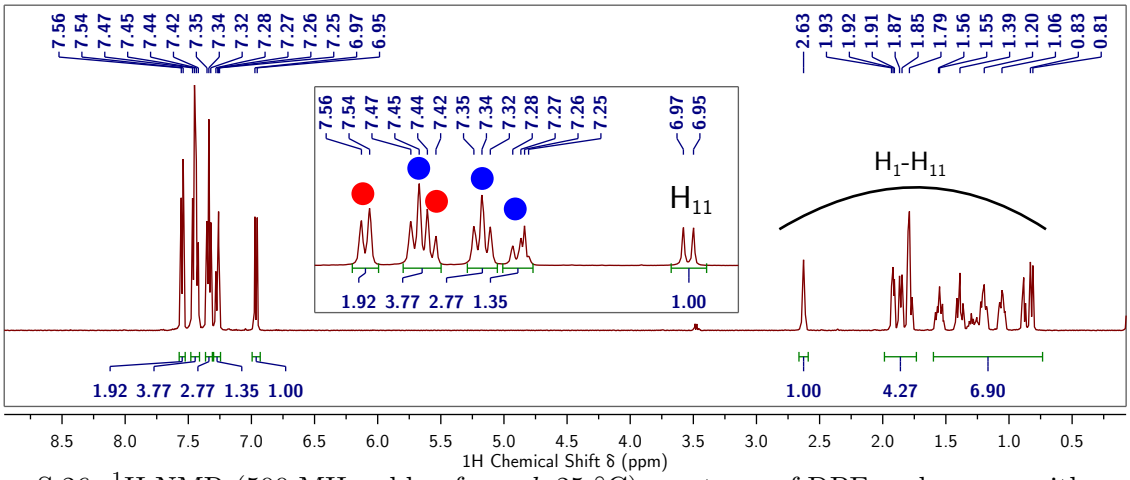

Figure S.26: ^{1}H NMR (500 MHz, chloroform-*d*, 25 °C) spectrum of DPF·norbornene with residual pentane.

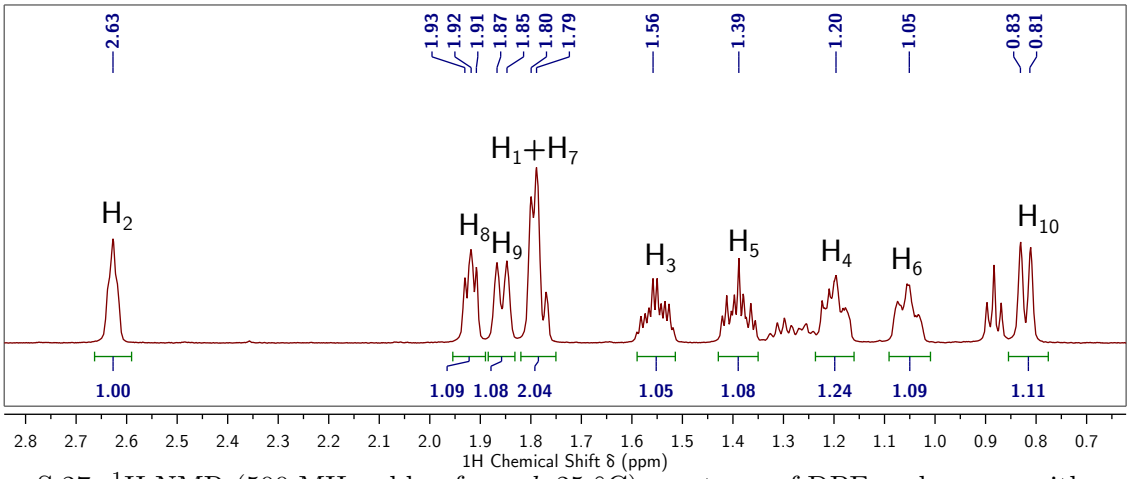

Figure S.27: ^{1}H NMR (500 MHz, chloroform-*d*, 25 °C) spectrum of DPF·norbornene with residual pentane.

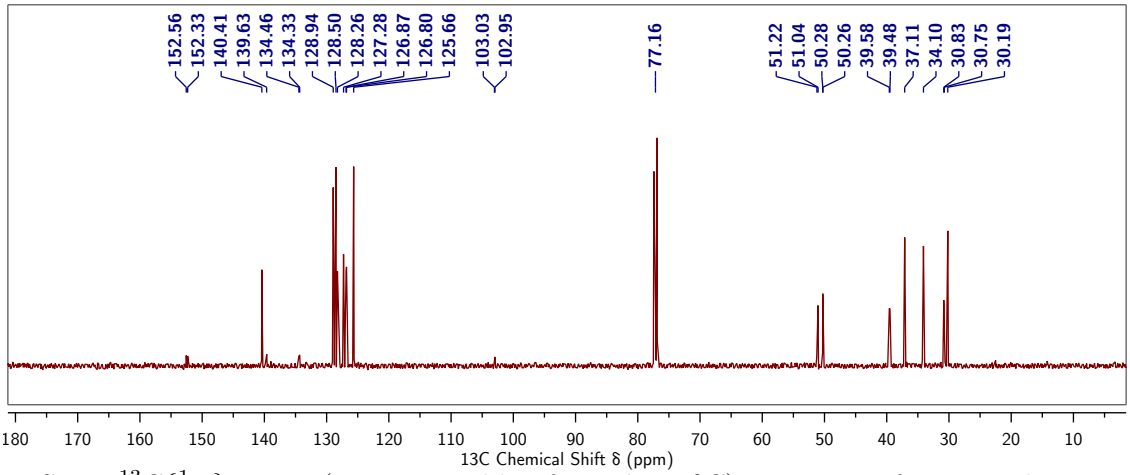

Figure S.28: ^{13}C{^{1}H} NMR (126 MHz, chloroform-*d*, 25 °C) spectrum of DPF·norbornene with residual pentane.

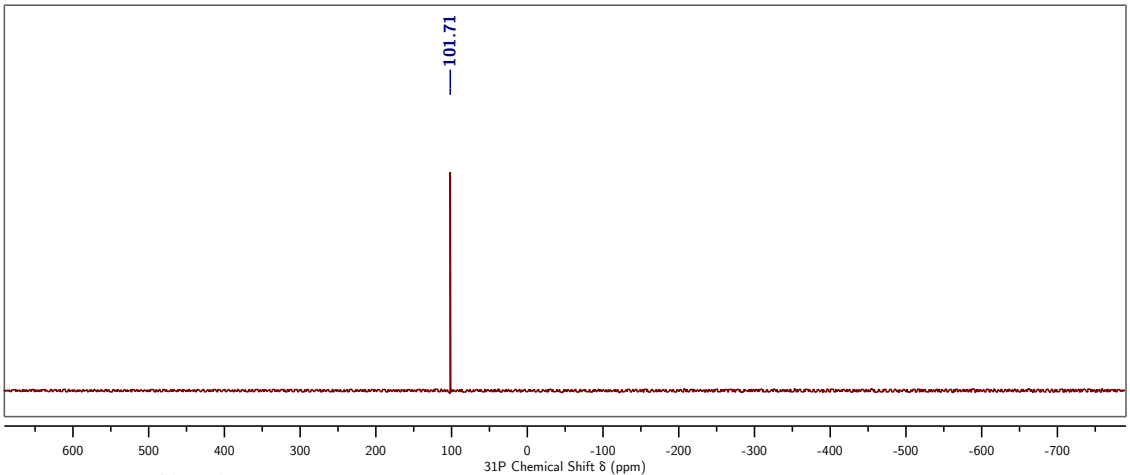

Figure S.29: ^{31}P{^{1}H} NMR (202 MHz, chloroform-*d*, 25 °C) spectrum of DPF·norbornene.

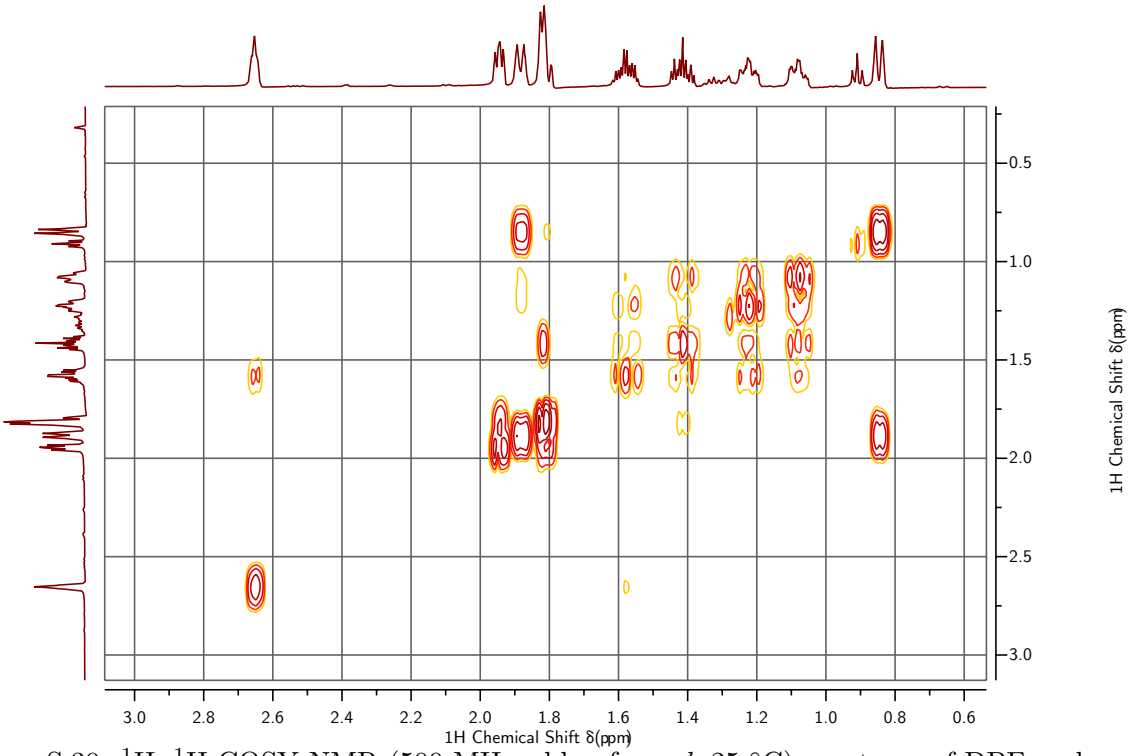

Figure S.30: ^{1}H, ^{1}H-COSY NMR (500 MHz, chloroform-*d*, 25 °C) spectrum of DPF·norbornene.

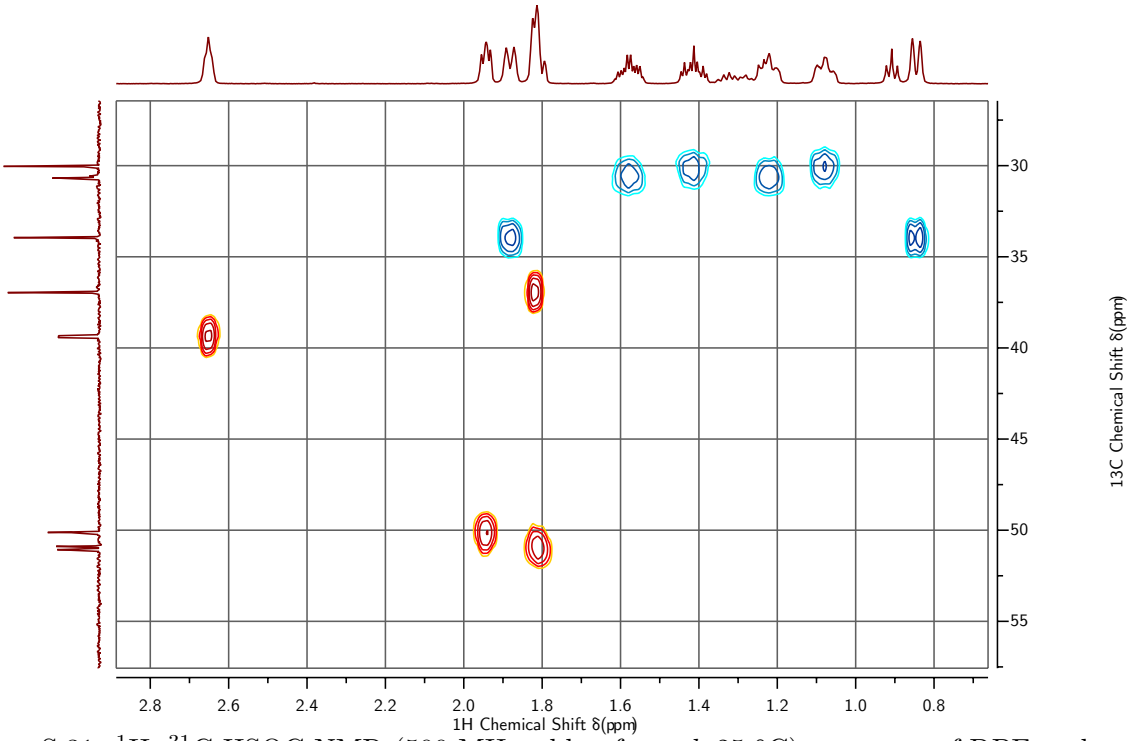

Figure S.31: ^{1}H, ^{31}C-HSQC NMR (500 MHz, chloroform-*d*, 25 °C) spectrum of DPF·norbornene.

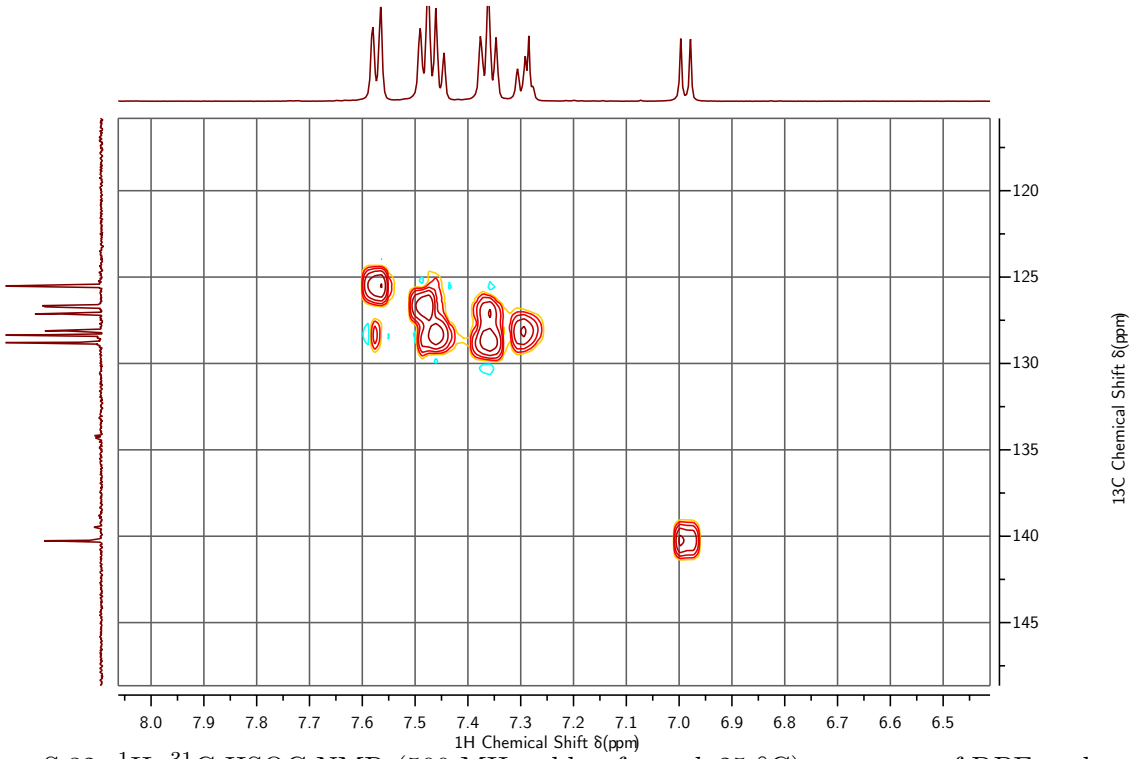

Figure S.32: ^{1}H, ^{31}C-HSQC NMR (500 MHz, chloroform-*d*, 25 °C) spectrum of DPF·norbornene.

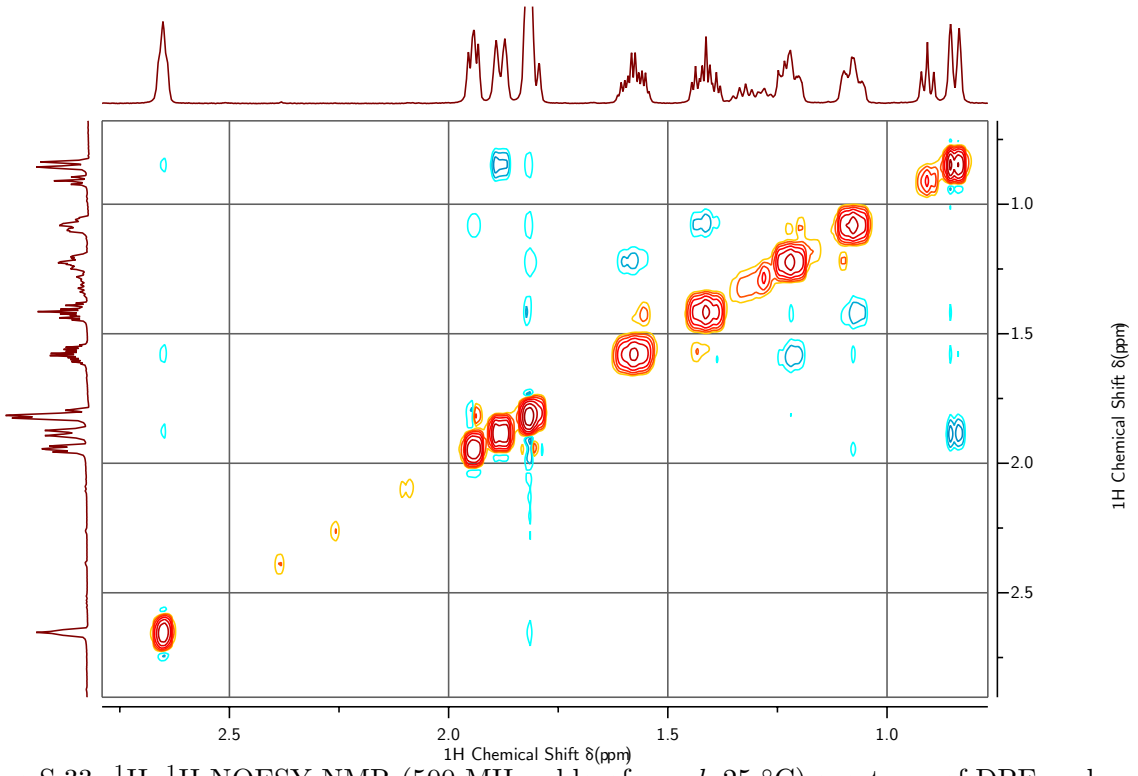

Figure S.33: ^{1}H, ^{1}H-NOESY NMR (500 MHz, chloroform-*d*, 25 °C) spectrum of DPF·norbornene.

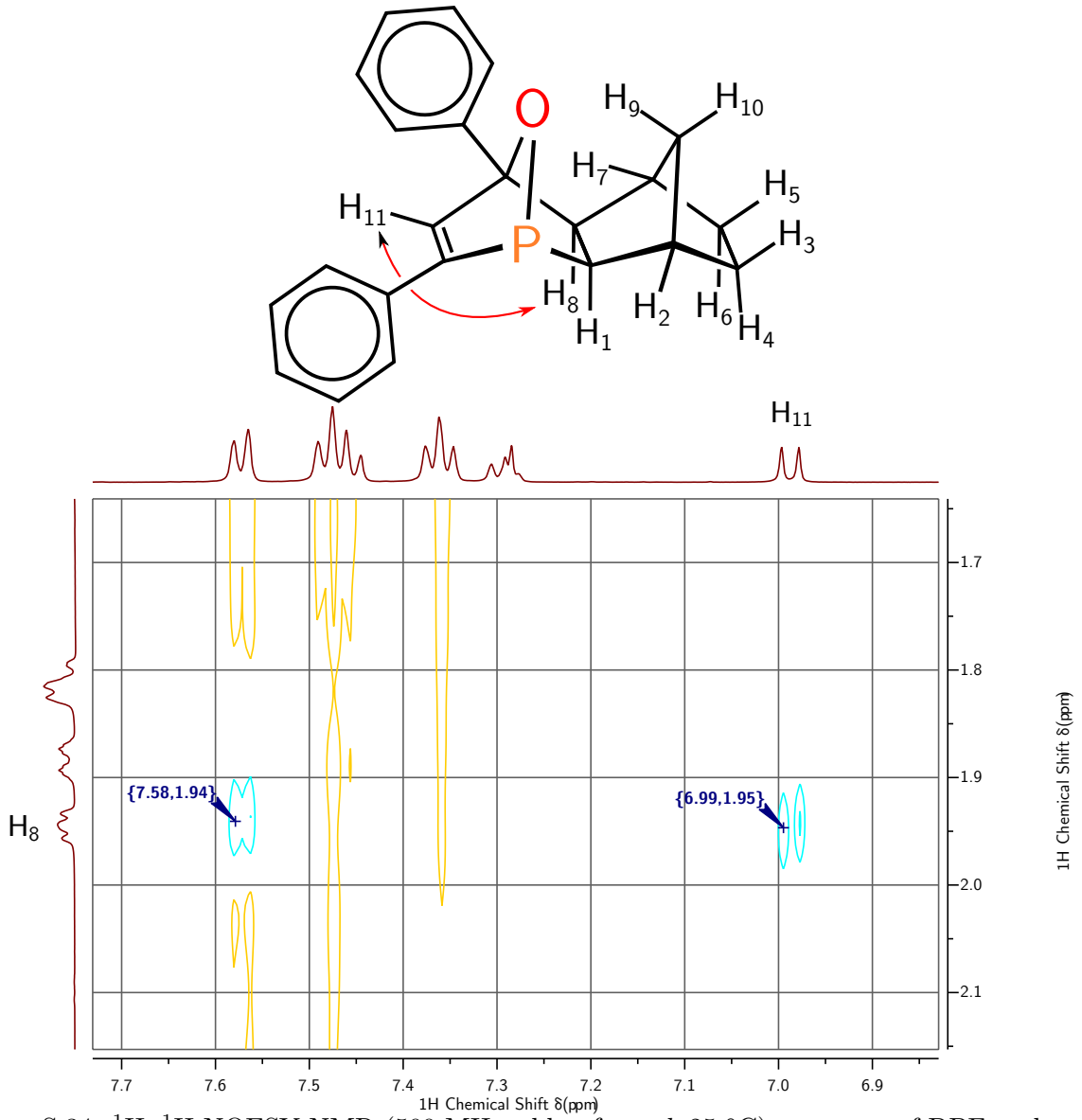

Figure S.34: ^{1}H, ^{1}H-NOESY NMR (500 MHz, chloroform-*d*, 25 °C) spectrum of DPF·norbornene.

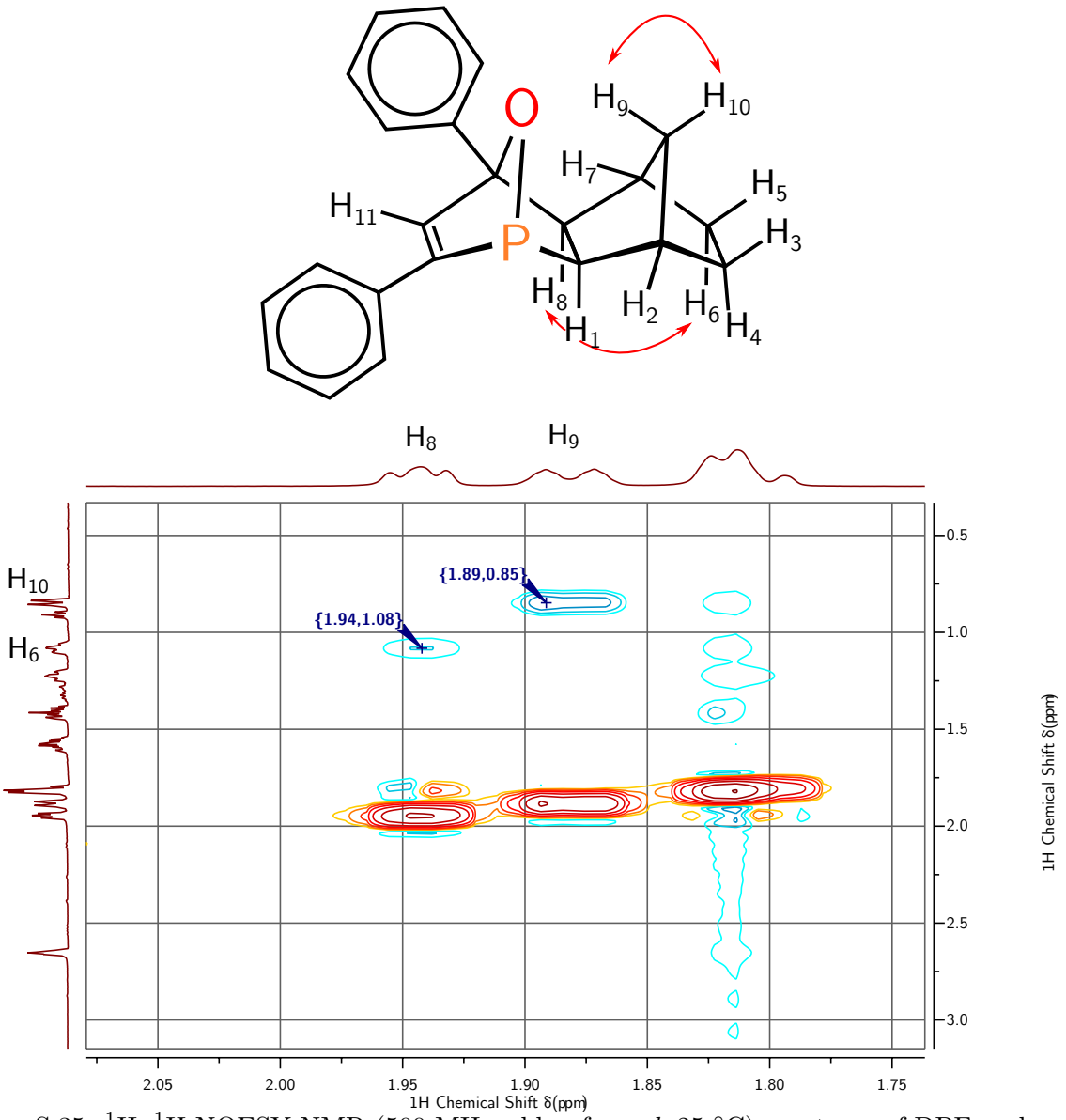

Figure S.35: ^{1}H, ^{1}H-NOESY NMR (500 MHz, chloroform-*d*, 25 °C) spectrum of DPF·norbornene.

S.2 NMR Characterization of Reactivity Studies

S.2.1 Air stability of DPF

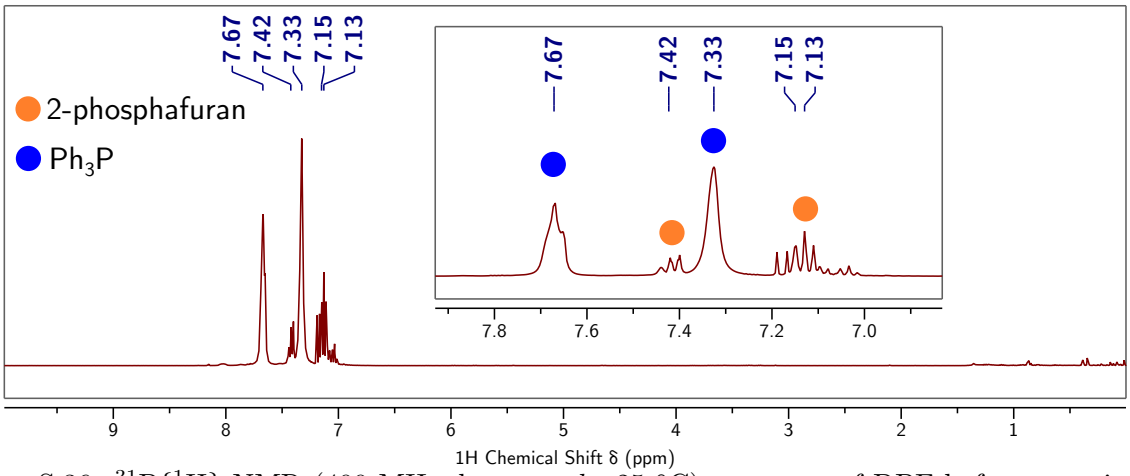

Figure S.36: $^{31}P\{^{1}H\}$ NMR (400 MHz, benzene-d_6, 25 °C) spectrum of DPF before exposing the solution to air.

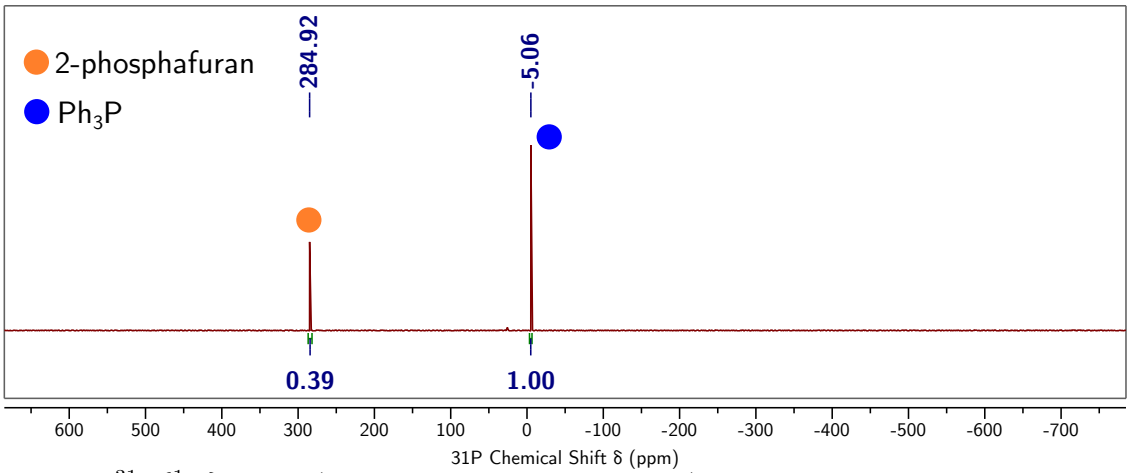

Figure S.37: $^{31}P\{^{1}H\}$ NMR (162 MHz, benzene-d_6, 25 °C) spectrum of DPF before exposing the solution to air.

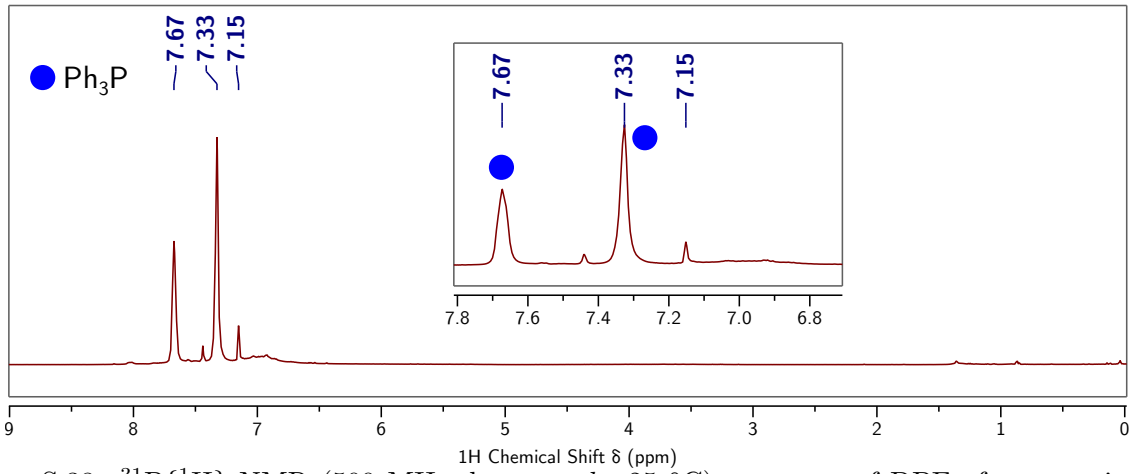

Figure S.38: $^{31}P\{^{1}H\}$ NMR (500 MHz, benzene-d_6, 25 °C) spectrum of DPF after exposing the solution to air for 1 h.

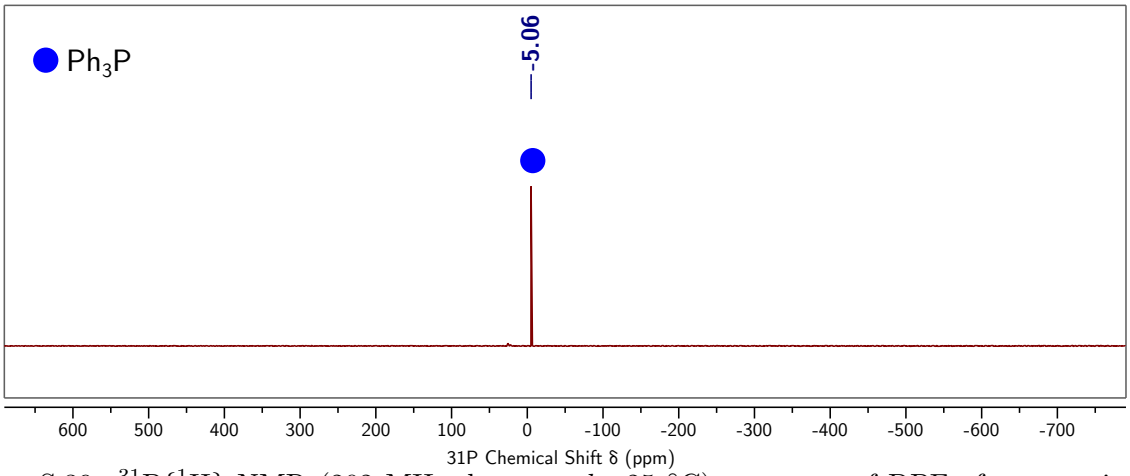

Figure S.39: $^{31}P\{^{1}H\}$ NMR (202 MHz, benzene-d_6, 25 °C) spectrum of DPF after exposing the solution to air for 1 h.

S.2.2 Thermal stability of DPF·C_2H_4

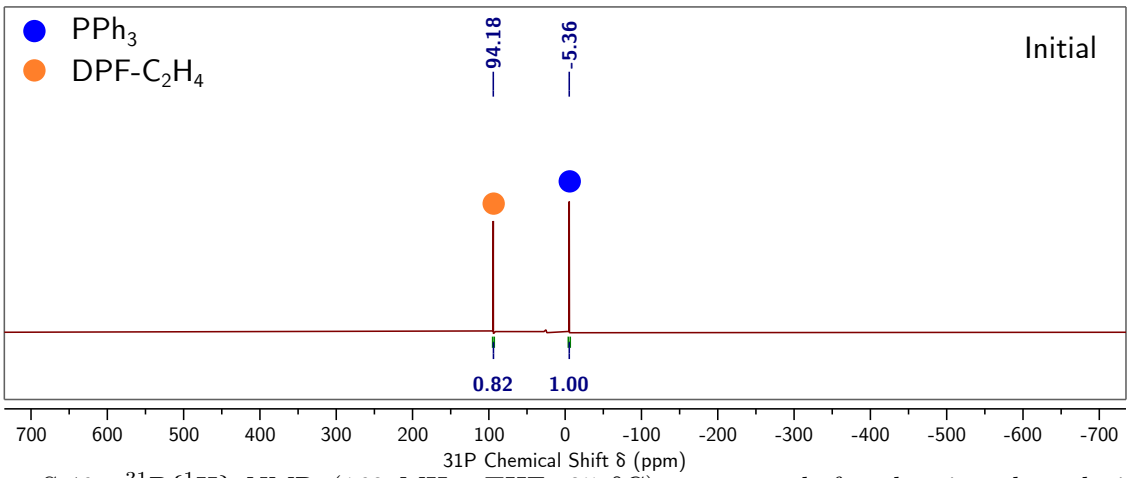

Figure S.40: $^{31}P\{^1H\}$ NMR (162 MHz, THF, 25 °C) spectrum before heating the solution of DPF·C_2H_4.

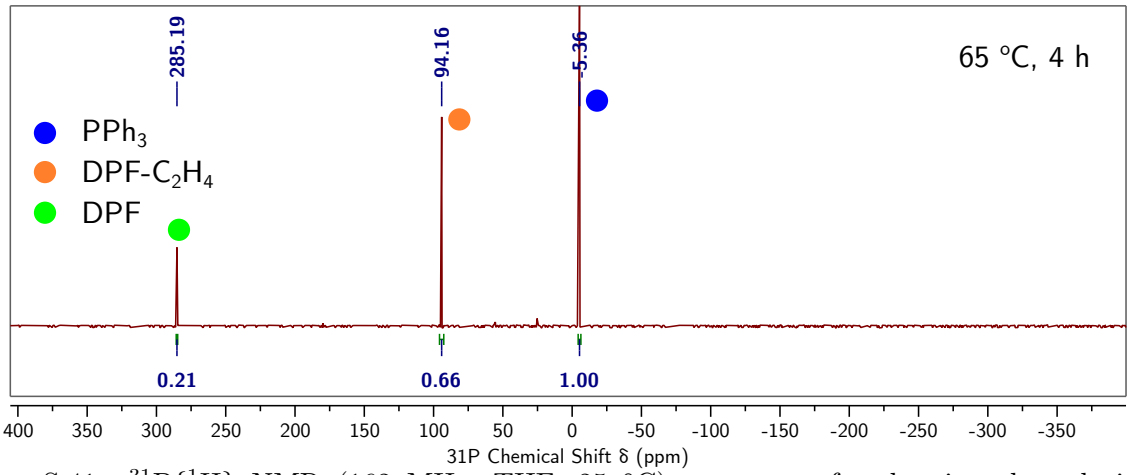

Figure S.41: $^{31}P\{^1H\}$ NMR (162 MHz, THF, 25 °C) spectrum after heating the solution of DPF·C_2H_4 to 65 °C for 4 h.

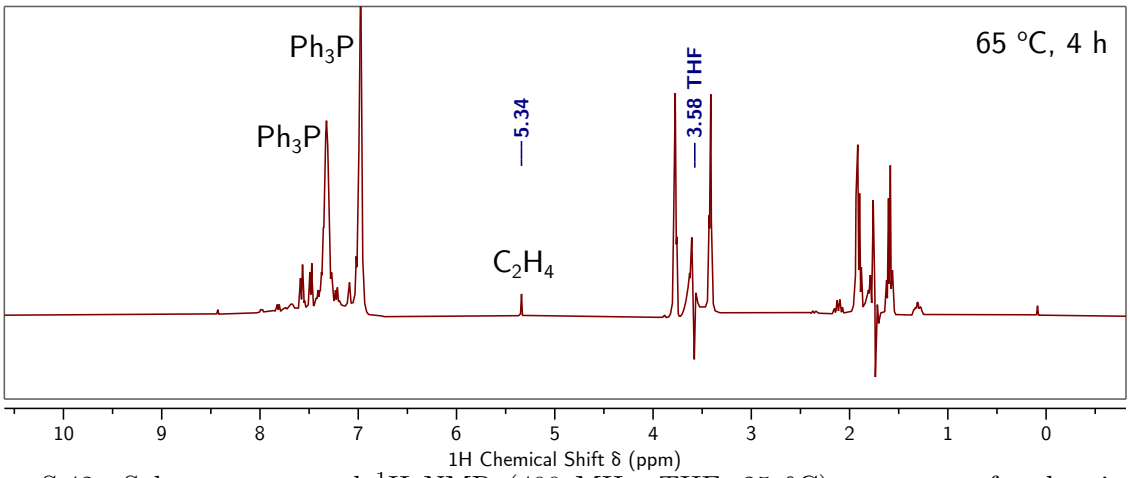

Figure S.42: Solvent-suppressed ^{1}H NMR (400 MHz, THF, 25 °C) spectrum after heating the solution of DPF·C_2H_4 to 65 °C for 4 h.

S.2.3 Thermolysis of DPF·C_2H_4 in the presence of norbornene

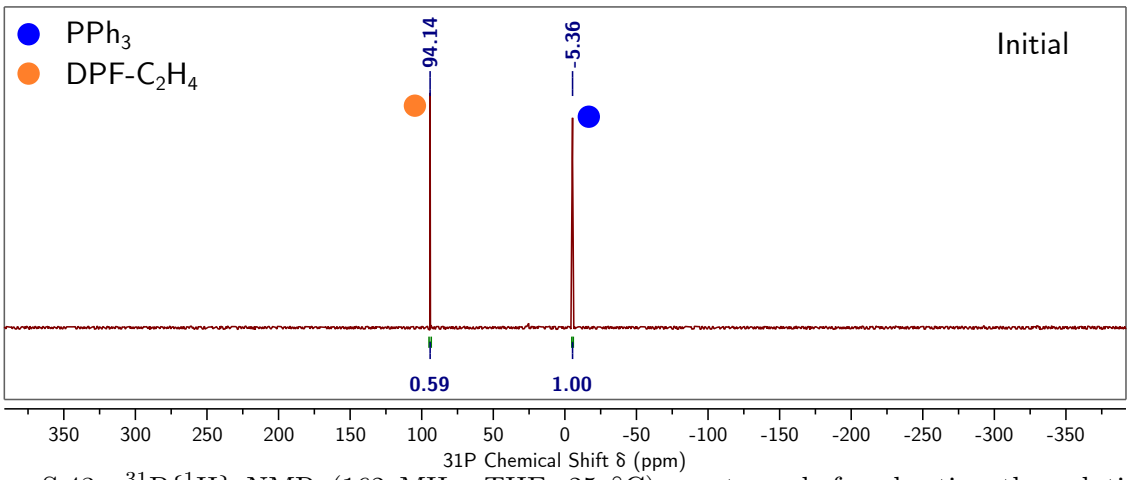

Figure S.43: $^{31}P\{^1H\}$ NMR (162 MHz, THF, 25 °C) spectrum before heating the solution of DPF·C_2H_4 and norbornene.

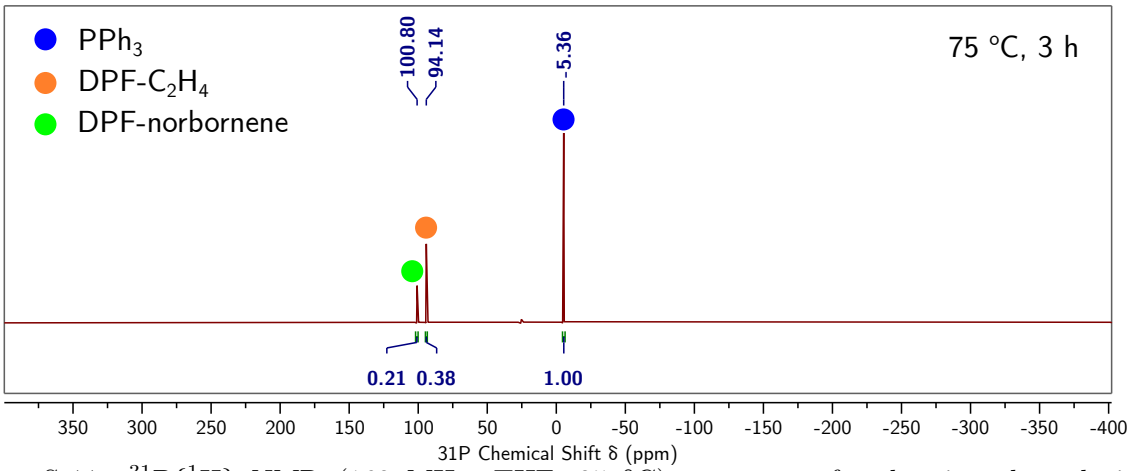

Figure S.44: $^{31}P\{^1H\}$ NMR (162 MHz, THF, 25 °C) spectrum after heating the solution of DPF·C_2H_4 and norbornene to 75 °C for 3 h.

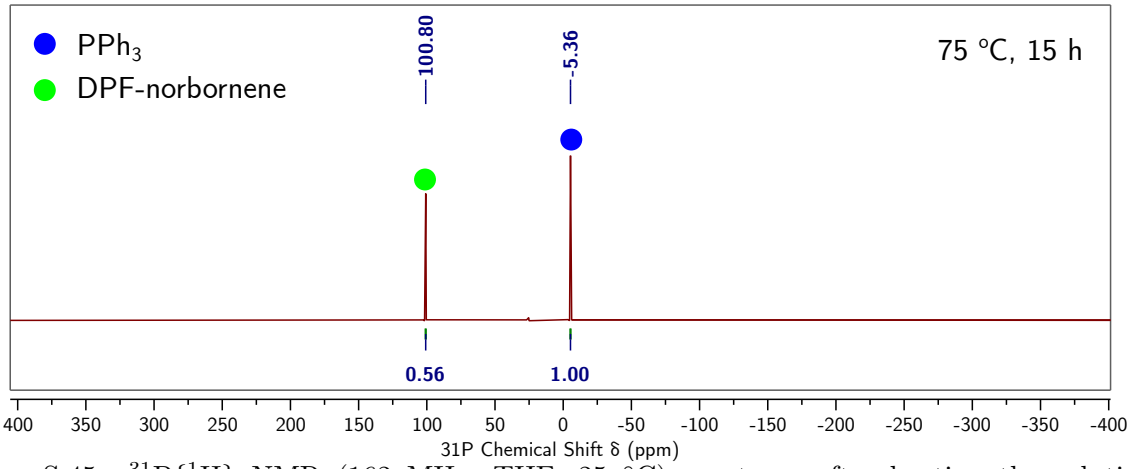

Figure S.45: $^{31}P\{^{1}H\}$ NMR (162 MHz, THF, 25 °C) spectrum after heating the solution of DPF·C_2H_4 and norbornene to 75 °C for 15 h.

S.2.4 Treatment of DPF with 1-hexene

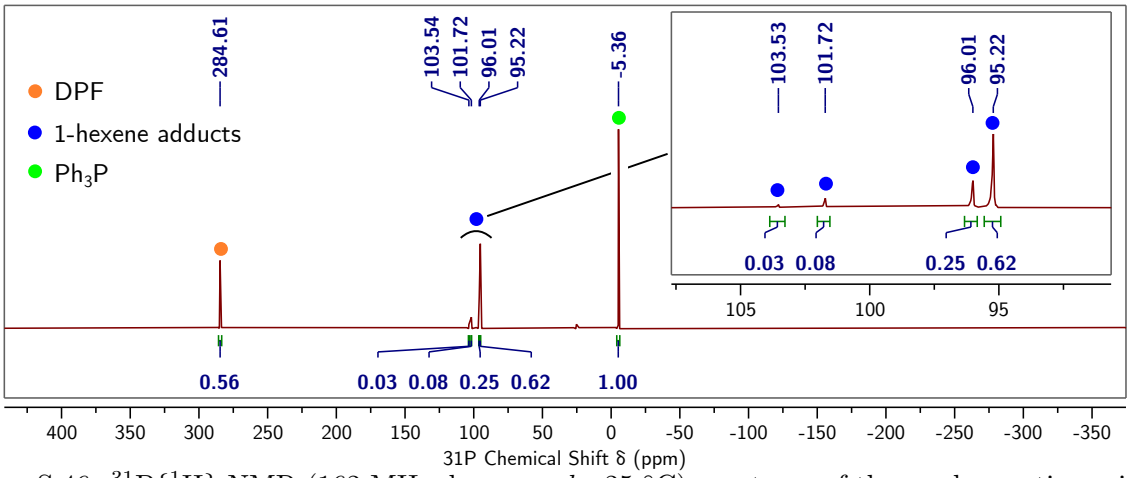

Figure S.46: $^{31}P\{^{1}H\}$ NMR (162 MHz, benzene-d_6, 25 °C) spectrum of the crude reaction mixture 12 h after treating DPF with 1-hexene (10 equiv).

S.3 Crystallographic Details

Table S.1: Crystallographic Data for DPF

	DPF
Reciprocal Net code / CCDC	P8_19019 / CCDC 1913045
Empirical formula, FW (g/mol)	$C_{15}H_{11}OP$, 238.21
Color / Morphology	Orange / Plate
Crystal size (mm^3)	$0.45 \times 0.14 \times 0.10$
Temperature (K)	100(2)
Wavelength (Å)	0.71073
Crystal system, Space group	Orthorhombic, $Pnma$
Unit cell dimensions (Å, °)	$a = 6.2455(2)$, $\alpha = 90$
	$b = 26.0429(10)$, $\beta = 90$
	$c = 7.1575(3)$, $\gamma = 90$
Volume ($Å^3$)	1164.17(8)
Z	4
Density (calc., g/cm^3)	1.359
Absorption coefficient (mm^{-1})	0.214
$F(000)$	496
Theta range for data collection (°)	2.951 to 32.139
Index ranges	$-9 \leq h \leq 9$, $-38 \leq k \leq 38$,
	$-10 \leq l \leq 10$
Reflections collected	159293
Independent reflections, R_{int}	2085, 0.0710
Completeness to $\theta_{\max}$ (%)	99.6
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / Restraints / Parameters	2085 / 299 / 154
Goodness-of-fit[a]	1.058
Final R indices[b] $[I > 2\sigma(I)]$	$R_1 = 0.0335$, $wR_2 = 0.0823$
R indices[b] (all data)	$R_1 = 0.0470$, $wR_2 = 0.1245$
Largest diff. peak and hole ($e \cdot Å^{-3}$)	0.163 and −0.240

[a] GooF $= \sqrt{\frac{\Sigma[w(F_o^2 - F_c^2)^2]}{(n-p)}}$ [b] $R_1 = \frac{\Sigma||F_o| - |F_c||}{\Sigma|F_o|}$; $wR_2 = \sqrt{\frac{\Sigma[w(F_o^2 - F_c^2)^2}{\Sigma[w(F_o^2)^2]}}$; $w = \frac{1}{\sigma^2(F_o^2) + (aP)^2 + bP}$; $P = \frac{2F_c^2 + \max(F_o^2, 0)}{3}$

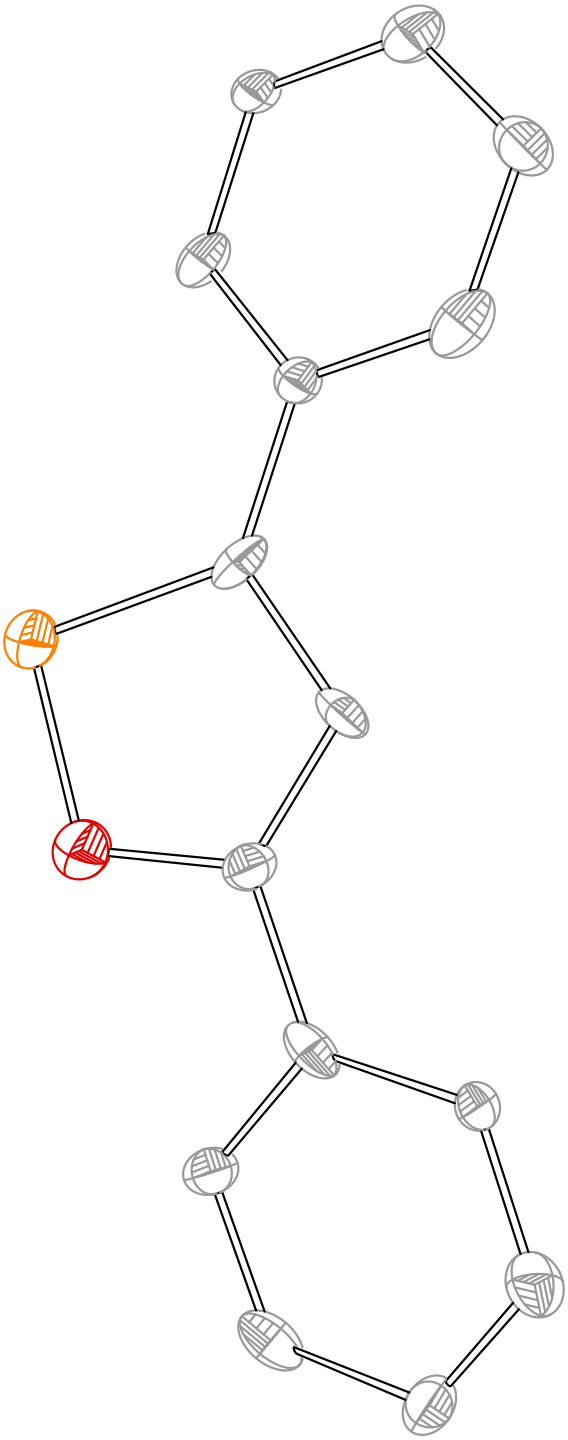

Figure S.47: Molecular structure of DPF shown with 50% probability thermal ellipsoids. Hydrogen atoms are omitted for clarity. P (orange), O (red), C (gray).

Table S.2: Crystallographic Data for DPF·DMAD and DPF·C_2H_4

	DPF·DMAD	DPF·C_2H_4
Reciprocal Net code / CCDC	X8_19016 / CCDC 1912975	P8_19036 / CCDC 1912977
Empirical formula, FW (g/mol)	$C_{21}H_{17}O_5P$, 380.34	$C_{17}H_{15}OP$, 226.26
Color / Morphology	Colourless / Needle	Colourless / Needle
Crystal size (mm^3)	$0.45 \times 0.05 \times 0.05$	$0.15 \times 0.03 \times 0.03$
Temperature (K)	100(2)	100(2)
Wavelength (Å)	0.71073	0.71073
Crystal system, Space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$
Unit cell dimensions (Å, °)	$a = 16.489(6)$, $\alpha = 90$	$a = 9.3363(8)$, $\alpha = 90$
	$b = 6.505(2)$, $\beta = 101.069(10)$	$b = 6.1033(5)$, $\beta = 92.134(4)$
	$c = 17.146(6)$, $\gamma = 90$	$c = 24.037(2)$, $\gamma = 90$
Volume ($Å^3$)	1804.8(11)	1368.7(2)
Z	4	4
Density (calc., g/cm^3)	1.400	1.292
Absorption coefficient (mm^{-1})	0.183	0.189
$F(000)$	728	560
Theta range for data collection (°)	2.421 to 27.462	1.696 to 33.727
Index ranges	$-21 \leq h \leq 21$, $-8 \leq k \leq 8$,	$-14 \leq h \leq 14$, $-9 \leq k \leq 9$,
	$-20 \leq l \leq 20$	$-37 \leq l \leq 37$
Reflections collected	70122	92311
Independent reflections, R_{int}	3734, 0.1627	5462, 0.0779
Completeness to θ_{max} (%)	100.0	99.8
Absorption correction	None	None
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / Restraints / Parameters	3734 / 395 / 246	5462 / 288 / 172
Goodness-of-fit[a]	1.031	1.042
Final R indices[b] $[I > 2\sigma(I)]$	$R_1 = 0.0415$, $wR_2 = 0.0876$	$R_1 = 0.0399$, $wR_2 = 0.1004$
R indices[b] (all data)	$R_1 = 0.0847$, $wR_2 = 0.1319$	$R_1 = 0.595$, $wR_2 = 0.1104$
Largest diff. peak and hole ($e \cdot Å^{-3}$)	0.540 and −0.499	0.425 and −0.340

[a] GooF $= \sqrt{\frac{\Sigma[w(F_o^2 - F_c^2)^2]}{(n-p)}}$ [b] $R_1 = \frac{\Sigma||F_o|-|F_c||}{\Sigma|F_o|}$; $wR_2 = \sqrt{\frac{\Sigma[w(F_o^2-F_c^2)^2}{\Sigma[w(F_o^2)^2]}}$; $w = \frac{1}{\sigma^2(F_o^2)+(aP)^2+bP}$; $P = \frac{2F_c^2+\max(F_o^2,0)}{3}$

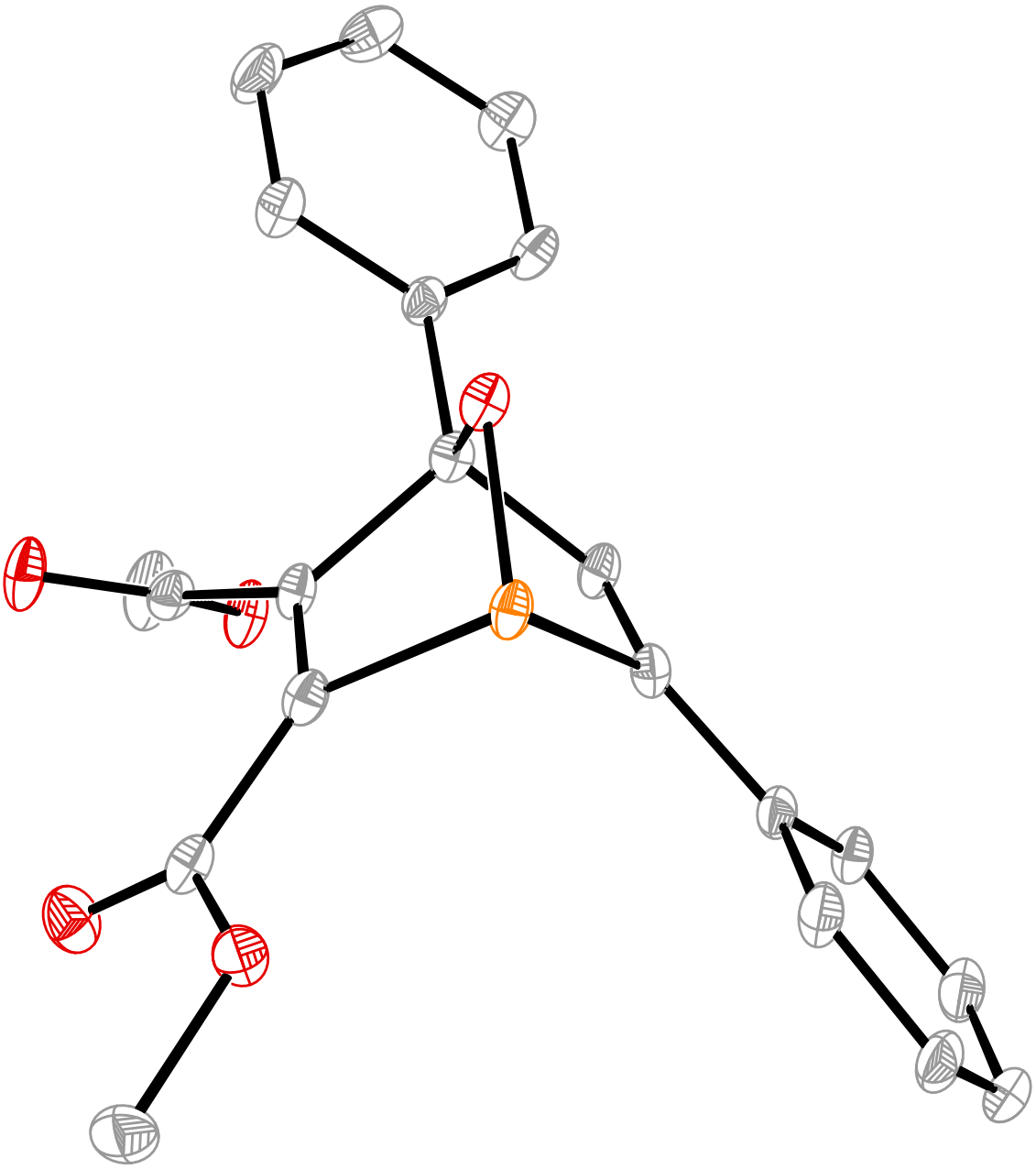

Figure S.48: Molecular structure of DPF·DMAD shown with 50% probability thermal ellipsoids. Hydrogen atoms are omitted for clarity. P (orange), O (red), C (gray).

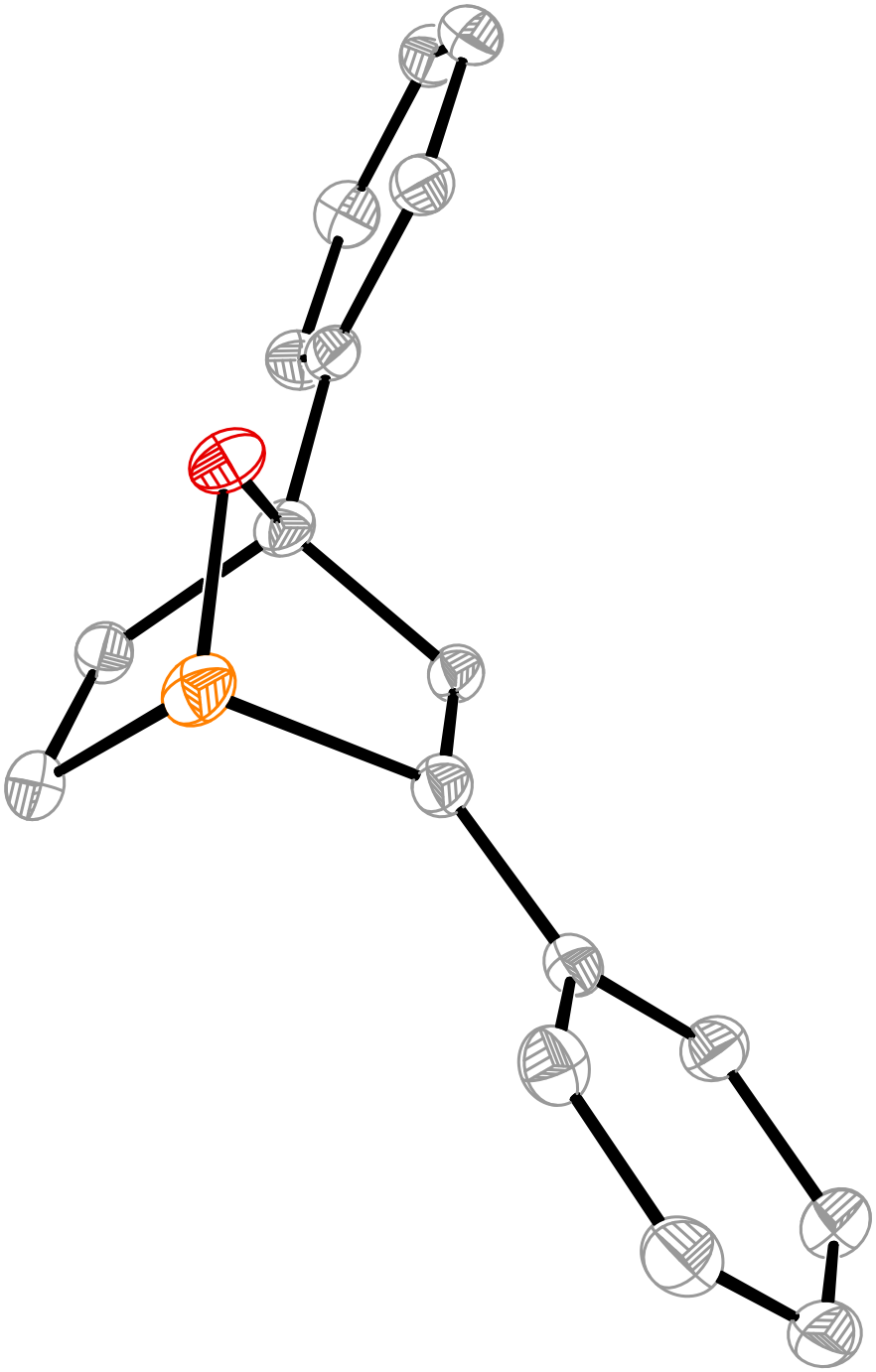

Figure S.49: Molecular structure of DPF·C_2H_4 shown with 50% probability thermal ellipsoids. Hydrogen atoms are omitted for clarity. P (orange), O (red), C (gray).

S.4 Total Energy, Imaginary Frequencies, and Coordinates (xyz) of Calculated Structures

S.4.1 EtOPA

Final Gibbs Free Enthalpy: 1034.96276680 Eh

Total Enthalpy: 1034.90760813 Eh

Number of Imaginary Frequencies: 0

C	-0.88349708345181	2.94404834579470	-0.31777207443451
C	-0.45835915214999	2.36749304087286	0.89141316518362
C	-2.32556824537840	3.39842920107353	-0.19234563096059
C	-1.58870589202856	2.38580149443627	1.89433560308038
P	-2.12680912969851	4.20848957117394	1.52335631381269
C	-3.17695227895026	2.18530040117747	0.12107855851281
H	-2.68619979205580	4.04160356802807	-0.98921028035781
C	-2.74474072263461	1.59842694124844	1.32074488787386
H	-1.30601274684368	2.14936129247152	2.91599334210938
O	-3.69991772034266	4.29985682536651	1.98099330525828
C	-4.09986650886271	5.12156700387206	3.08420860099416
C	-4.66780298714908	4.25441419581815	4.19080047947929
H	-4.85475260290879	5.81389757390800	2.70688452338690
H	-3.25243256069402	5.71416160966542	3.44356565799264
H	-5.46484290792968	3.62255887098381	3.79991931808269
H	-5.07502797877974	4.87466714702187	4.99169936974496
H	-3.89739518358332	3.60732738547137	4.61291010896387
C	-0.01743805045685	3.03720569472302	-1.39411217472252
C	0.83998218418633	1.90452570202379	1.03163589524105
C	1.28196341410353	2.55120850305179	-1.25692491590097
C	1.70762138271126	1.99387890065547	-0.05494977741197
H	-0.34216149516313	3.48108246039340	-2.32626887437911
H	1.96736901553146	2.60932863325874	-2.09181373438376
H	1.17421738757437	1.47062348307316	1.96546524202789
H	2.72030774058681	1.62390806207026	0.03643280892933

C	-4.24931849449028	1.66073258067923	-0.57086980944528
C	-4.89799564541690	0.53111405978609	-0.05791551272102
C	-4.46531934927886	-0.05489616364077	1.12329807831958
C	-3.37573783789206	0.47820574579986	1.82233873932116
H	-4.59363167298140	2.12147225650022	-1.48817876386998
H	-5.74575521290530	0.11509104625462	-0.58589967579545
H	-4.97704958642636	-0.92530501965576	1.51194910474855
H	-3.03727028624099	0.02180958664291	2.74420812131989

S.4.2 *Trans*-chalcone

Final Gibbs Free Enthalpy: 653.75258848 Eh

Total Enthalpy: 653.69999690 Eh

Number of Imaginary Frequencies: 0

C	-9.04103168140876	4.87864672701036	1.10544432718074
C	-8.84823662103394	3.91663565373057	0.19100579384205
C	-7.92662744334394	5.31868699964736	1.97629632139908
H	-9.99905052094622	5.36775012534668	1.20255890310536
C	-9.79939999621117	3.38947973751379	-0.77942122240457
H	-7.85587262244197	3.47838516201772	0.16064968528613
C	-9.36954635544671	2.37303947058937	-1.64374451376735
C	-11.11871303599070	3.85058670349854	-0.90657092529124
C	-11.96422240845721	3.31791855389902	-1.86565101864310
C	-11.51933892194525	2.30649110932839	-2.71614602025662
C	-10.21739192011393	1.83585008911224	-2.60196991875510
H	-9.86201823407633	1.05286670127066	-3.25785059137631
H	-8.35470236882154	2.00693270480635	-1.55659706570014
H	-11.48338447533550	4.63224486717883	-0.25448815237412
H	-12.97576725827585	3.69131000618236	-1.95676539976285
H	-12.18526739062327	1.89173481378773	-3.46059665842355
O	-6.78573351190550	4.91729974215698	1.80116292757576
C	-8.20798457274250	6.29924277375643	3.07408246438888
C	-9.49508883841974	6.64560615349185	3.49379489486843
C	-7.10962287743597	6.88290915398881	3.71449742033344

C	-7.29065084039685	7.79846238793968	4.73747665219604
C	-8.57705475999637	8.14101978364773	5.14474037220954
C	-9.67760935220435	7.56100947907102	4.52420848995538
H	-10.67723499745083	7.82107229417868	4.84700077231716
H	-10.36189503251907	6.19253175639247	3.03533201379281
H	-6.12058147892499	6.59771030039180	3.38659163457941
H	-6.43233274407913	8.24559067566464	5.22078659024010
H	-8.72004973945239	8.85417607439992	5.94516222348465

S.4.3 EtOPA + *trans*-chalcone (TS1)

Final Gibbs Free Enthalpy: 1688.67598899 Eh

Total Enthalpy: 1688.59328220 Eh

Number of Imaginary Frequencies: 1

C	-0.37254147941197	1.33686971412874	0.07202659305537
C	-0.08688056955038	2.07584273273114	1.23263421543815
C	-1.73046453665987	1.72058595483094	-0.46287869920477
C	-1.23616445341949	3.00242372112983	1.56628952381125
P	-1.51251076121152	3.62031732097483	-0.23997631290091
C	-2.76389666301954	1.42946314011073	0.60325373751728
H	-1.96543065726693	1.36786043706630	-1.46217397114866
C	-2.47593450432442	2.16289031807383	1.76677881321481
H	-1.02777769157039	3.75406300658731	2.31886588417045
O	-3.03868215596500	4.02917858435324	-0.55421121933748
C	-3.70173321516606	5.29564863044989	-0.33488086249761
C	-4.10061368525896	5.45149608568097	1.11723119486171
H	-4.57741286469245	5.25384905439658	-0.98141220314015
H	-3.05361235362576	6.10255731370718	-0.65920393200646
H	-4.70034182121279	4.60462523764868	1.44977786222017
H	-4.68538924328050	6.36391018479730	1.24608120165386
H	-3.21416525888545	5.52772602878832	1.74350889409125
C	0.56387874968519	0.46389287346215	-0.45776836301015
C	1.13983843622589	1.94376211161728	1.86247454628089
C	1.79349240083180	0.32445592243169	0.18332487929873

C	2.07650817005475	1.05622949190097	1.33492726479951
H	0.34526977423362	-0.09678127741666	-1.35756190313756
H	2.53496420728817	-0.35268978992531	-0.21893324756643
H	1.37242404018453	2.52830769841494	2.74288774134287
H	3.03539042025078	0.93730406842253	1.82178577504372
C	-3.88125934005212	0.61748251592971	0.54437083229709
C	-4.70994728433058	0.52787918984380	1.66668045958952
C	-4.41968572220085	1.24641461929548	2.81965064288276
C	-3.29573894186670	2.07588963531058	2.87509650600384
H	-4.11842739107216	0.06604207562900	-0.35633852461948
H	-5.58884734273226	-0.10150921116335	1.63376667675260
H	-5.06907159688253	1.16548835899255	3.68090960413308
H	-3.07658111932065	2.64557765913455	3.76891409341481
C	0.69753401761844	4.35269766757459	-0.96020892470852
C	1.05478050812804	5.07105284887790	0.19418723964830
C	0.29555910304206	4.91445166187585	-2.26602795420344
H	1.20240255084278	3.39769643214672	-1.07187756782923
C	0.13882826001534	5.94061812390670	0.81191913679178
H	1.86478962594083	4.68100104758496	0.79363479693444
O	-1.04743576444265	6.02723389458484	0.38372463239975
C	0.48298170820173	6.64900661207021	2.07717832235928
C	1.79787509502697	6.97707005974142	2.41538928818235
C	-0.55055012309004	7.04076967388951	2.93140067637312
C	2.07262915174948	7.66328873332100	3.59193979324214
C	-0.27710838737076	7.72235738674755	4.10773769020668
C	1.03666701923418	8.03511886084669	4.44247849311775
H	-1.08794820772327	8.02080779916135	4.75914582191573
H	1.25057752933348	8.57501255221974	5.35506140664017
H	2.60303965472862	6.71808795324959	1.74141528032053
H	3.09325041515322	7.92234882901142	3.84196082522715
H	-1.56568913517945	6.80882953629216	2.64518650390247
C	0.26522018218385	4.06215030511044	-3.37593778214933
C	-0.03724903708870	4.54306218423134	-4.64194425509859

C	-0.31545678584471	5.89312743292058	-4.82217896617805
H	0.49721787963284	3.01246570264808	-3.23963056684569
H	-0.04614907281382	3.86745918471004	-5.48695243417373
C	-0.28415567755510	6.75047025610172	-3.72619010159266
H	-0.54720991121244	6.27616156987434	-5.80703928601706
C	0.01958833590060	6.26975628459519	-2.46080081033535
H	-0.49433922950888	7.80362451948614	-3.85902746567241
H	0.04410474932196	6.94241947988416	-1.61894149576164

S.4.4 EtOPA + *trans*-chalcone (I1)

Final Gibbs Free Enthalpy: 1688.72024149 Eh

Total Enthalpy: 1688.63984866 Eh

Number of Imaginary Frequencies: 0

C	-0.41718666412221	1.54815451847297	0.29657300119200
C	0.00288714259992	2.05208484531085	1.54027015848177
C	-1.69363104074939	2.19624507460555	-0.12262917032116
C	-0.99159726013509	3.04130633251912	2.07411640371099
P	-1.27742639415005	4.06947665152706	0.45717375072876
C	-2.74824088817510	1.91968995496870	0.90963403711228
H	-1.99795863148482	2.03774205887214	-1.15210612092465
C	-2.34548621264354	2.39388019950382	2.16935681098881
H	-0.67383160578268	3.61631760205924	2.93607034841471
O	-2.67508055428725	4.54445084543275	-0.16573863801723
C	-3.39562787718020	5.77999823368741	0.00989028427478
C	-4.19332357605211	5.75666117893832	1.29681170445669
H	-4.05027647803518	5.83070327341562	-0.85951518647343
H	-2.70568757387172	6.61888231156837	-0.02458616965336
H	-4.81302136976133	4.86122255437369	1.34435629974226
H	-4.84428050857271	6.63103474406562	1.35167275963142
H	-3.52769112052898	5.76323510062856	2.15844135252035
C	0.39270703079978	0.66800780884163	-0.40835385033673
C	1.23618527562804	1.69912833521111	2.06615553788502
C	1.61535285306895	0.28722351715877	0.13776005075790

C	2.03781871653905	0.80433900149109	1.36133306626605
H	0.07582969760848	0.28440186540949	-1.37026570903180
H	2.24854651792387	-0.40622445767760	-0.39910804454756
H	1.57365621397898	2.12054233316180	3.00471489171492
H	2.99427938778167	0.50449812757279	1.76870486175654
C	-4.00400541485903	1.35489184585461	0.74991797229169
C	-4.84239377934147	1.24592626505249	1.85849989730948
C	-4.43414033498680	1.70492697651732	3.10798533058669
C	-3.17967249221568	2.29037984893959	3.26995718017152
H	-4.33180038287635	1.00540416209448	-0.22090750468643
H	-5.82250807777144	0.80108903350588	1.74675568352804
H	-5.09569801021942	1.60763829858125	3.95838718957239
H	-2.86386535063379	2.66311725017372	4.23601790077909
C	0.28834102258586	4.45030620616146	-0.49890458073664
C	0.98900258150746	5.46131360526396	0.35949608106534
C	-0.05716691894274	4.89958234626710	-1.90189607826978
H	0.84894270027102	3.51975810120917	-0.56058140397827
C	0.21145966315104	6.01342992727486	1.30507629675165
H	2.01936682511778	5.73075430108994	0.19107503923525
O	-1.08012168672710	5.58991340982747	1.33142464329737
C	0.55013453260721	7.02673468286806	2.31375318839223
C	1.87612206094622	7.35079277211785	2.62241775945485
C	-0.47782058163785	7.68668011824014	2.99544558387707
C	2.16227191173356	8.31482095975617	3.57850218754992
C	-0.18870172805289	8.65133206352939	3.95119290250560
C	1.13055820680957	8.97024049737271	4.24614791738066
H	-0.99707349758007	9.15178379516605	4.46743984026737
H	1.35595221584016	9.71744986747806	4.99448139362704
H	2.68374693928436	6.82929532733677	2.12765288315606
H	3.19116363871846	8.55278218629354	3.81513175651725
H	-1.50174573477373	7.43307634370806	2.76643591180460
C	-0.13063915155174	3.96732667472601	-2.93639111448124
C	-0.47364094671487	4.36345742644760	-4.22330092629452

C	-0.75351515882968	5.69794297161159	-4.49383653382900
H	0.09467887728862	2.92865008012000	-2.73094864898535
H	-0.51785949590980	3.62999361821944	-5.01741124705090
C	-0.68736287211018	6.63304047383946	-3.46649814535114
H	-1.01955909014157	6.00732717376798	-5.49571108117961
C	-0.34124286676228	6.23518608770862	-2.18158218375526
H	-0.90388557638476	7.67443058185381	-3.66592107400084
H	-0.27644710723444	6.96500270890644	-1.38621644685151

S.4.5 I1 to 2 (TS2)

Final Gibbs Free Enthalpy: 1688.71024658 Eh

Total Enthalpy: 1688.62779702 Eh

Number of Imaginary Frequencies: 1

C	-0.36981008444553	1.50637705857036	0.08888165267591
C	-0.06705520206462	1.85015035666758	1.43270252198004
C	-1.65874364186606	1.92669161469087	-0.38543730985776
C	-1.10806698104547	2.57440886314620	2.12137155707034
P	-1.15984802932065	4.23159518145986	0.45531622012192
C	-2.76869012393548	1.86888887519857	0.52481151949674
H	-1.86937934507236	1.82988335705315	-1.44375597623256
C	-2.47541845582234	2.18635265781761	1.87580545712306
H	-0.86956553104826	3.01041292124725	3.08471378187753
O	-2.53532440594092	4.84778506646428	-0.09960214674072
C	-3.11609976281935	6.13140865036907	0.20708505720681
C	-3.94302451435483	6.04181867604687	1.47301984413135
H	-3.73133210661739	6.37669008384370	-0.65758390200804
H	-2.33213450807602	6.88302558295213	0.29099471267894
H	-4.70181999105523	5.26616553268224	1.37593658568525
H	-4.43896850520965	6.99449072105606	1.67020271628689
H	-3.30959478226039	5.79478328885097	2.32399205026137
C	0.62862249687103	0.91331817766820	-0.70285751304168
C	1.21795736603060	1.61285092349021	1.94192367740260
C	1.87868861349115	0.66033811002164	-0.17440085998607

C	2.17709732362886	1.01185887086760	1.15108208188547
H	0.40365611519661	0.64286546685028	-1.72689775161302
H	2.63584708049543	0.18902585855115	-0.78662270618823
H	1.44856064074059	1.90380824215874	2.95917948017034
H	3.16109883827115	0.80988015042301	1.55260229760897
C	-4.10365424082880	1.64678197374204	0.15047303234446
C	-5.10689761845102	1.69182489775015	1.09717008356611
C	-4.81043576374782	1.98787496515460	2.43632240685081
C	-3.51027708573866	2.25230885951702	2.81872363451056
H	-4.33507267169033	1.42954879951268	-0.88450955901428
H	-6.13068084437027	1.49754104691481	0.80583757468325
H	-5.60567772308215	2.01469063306174	3.16887080970667
H	-3.27929704421258	2.50566612395710	3.84572834531733
C	0.27269429308327	4.75624271789207	-0.68691027534886
C	0.82992142259802	5.97410705350803	-0.01352775842537
C	-0.19478098520211	4.91946755505240	-2.10589645834395
H	0.97680658071266	3.92050275821142	-0.63807138296521
C	0.27432226054434	6.26783406529554	1.16630000626076
H	1.59965833470253	6.57858008115653	-0.46866722132713
O	-0.73929098447292	5.43032393023160	1.58606615259953
C	0.56857340007846	7.37486284513511	2.08278984402376
C	1.86899777587731	7.86237319641360	2.24027181416757
C	-0.46832569169997	7.96375294431444	2.81282622107623
C	2.12146060699670	8.92035292898962	3.10422677664296
C	-0.21507299391577	9.02861049307940	3.66498796103659
C	1.08057924980133	9.51120054687430	3.81313474483730
H	-1.02895671568800	9.48173366045587	4.21509524922075
H	1.27966692824423	10.33759243318764	4.48170478591920
H	2.68130326484230	7.38954688664849	1.70513289350602
H	3.13286728498005	9.28374978146005	3.23101010754208
H	-1.47146865509054	7.57813927920468	2.70505246581543
C	-0.15374891074214	3.83558527741514	-2.98275324003775
C	-0.63968138016304	3.94945258724697	-4.27857998930642

C	-1.17081691314494	5.15464934190431	-4.72153234085910
H	0.27039427733727	2.90078589938547	-2.64307276282829
H	-0.60071292689374	3.09724703513877	-4.94424322167462
C	-1.21141005510139	6.24374911676871	-3.85789989232736
H	-1.54778781171934	5.24689823558065	-5.73134300868272
C	-0.73426235123106	6.12394611930981	-2.55935214200160
H	-1.62160865886079	7.18648547776500	-4.19630931592421
H	-0.77471015752194	6.97219616461665	-1.88934938855595

S.4.6 2

Final Gibbs Free Enthalpy: 1149.48820995 Eh

Total Enthalpy: 1149.42587685 Eh

Number of Imaginary Frequencies: 0

P	-0.67298247063520	5.10054683335824	1.41973135666850
O	-1.62575664824670	5.93959724475713	0.39480232069306
C	-2.90887718842079	5.40819744367181	0.02411036364582
C	-2.82227210776011	4.65999936296031	-1.29317881653221
H	-3.57781913948225	6.26563572876171	-0.04828199929546
H	-3.27852806957232	4.75703693000213	0.82131940512478
H	-2.45518096395967	5.31371660292646	-2.08346689815757
H	-3.80410386336861	4.27615505404916	-1.57818805943438
H	-2.13477178371033	3.81782057600571	-1.21456442413339
C	0.97655149526577	5.16539502135246	0.47778582952646
C	1.59179164455093	6.43837599394832	0.98164295970121
C	0.83751850006453	5.04092203996424	-1.01352150891478
H	1.54194001706293	4.30269348000615	0.85022095266390
C	0.95165031592264	7.00723360529318	2.00784460944600
H	2.48796325815325	6.84129030501668	0.53800673868669
O	-0.18372792452757	6.33008292978199	2.43934962898515
C	1.27740191445505	8.22387402121681	2.75501893294215
C	2.34211770948102	9.04476268237329	2.35870496829065
C	0.53029290906953	8.59005992296956	3.87913466405483
C	2.65427167186347	10.18979209696786	3.07175665485718

C	0.84664502308518	9.74112999859323	4.59213108219298
C	1.91186300221069	10.54043979812837	4.19757891323296
H	0.25996744801174	10.01218491467727	5.45990847764898
H	2.16277409966168	11.43231919572687	4.75604901201022
H	2.92230851359206	8.78934815638944	1.48355140412994
H	3.47777019654023	10.81231614579090	2.74836879756265
H	-0.29616489389666	7.96762490267162	4.18691867145697
C	0.90419973975884	3.79228477335658	-1.63199166996101
C	0.74414802966142	3.66766767768326	-3.00700558682814
C	0.52347872625818	4.79484230805311	-3.78977006900535
H	1.08781272627959	2.90982282070234	-1.03144369050682
H	0.80142950922200	2.69068060250064	-3.46868192422654
C	0.45419285526833	6.04415596597340	-3.18299455485315
H	0.40789531908244	4.70101756216828	-4.86124104335140
C	0.60315653201371	6.16415447823256	-1.80812358372504
H	0.27988059608107	6.92846749074052	-3.78198567094182
H	0.53221330096394	7.13535533322833	-1.33883624365402

S.4.7 Anthracene

Final Gibbs Free Enthalpy: 539.27491664 Eh

Total Enthalpy: 539.23106085 Eh

Number of Imaginary Frequencies: 0

C	-0.84376010372539	2.67743680982163	-0.31230803538463
C	-0.37870968350266	1.72054041070766	0.65846972555852
C	-2.20275544363487	2.72137519791805	-0.62422228116487
C	-1.29791738937641	0.86263182438677	1.26110337058642
C	-3.12196352820715	1.86347318715339	-0.02157355984904
C	-2.65691403316068	0.90659023077014	0.94921046278799
C	0.10600280670152	3.54869097150293	-0.91990542342153
C	1.01182545039898	1.68420794947663	0.96817779544598
C	1.42911653824147	3.48016665493852	-0.59577004134358
C	1.88814066802613	2.53422384258683	0.36188958200848
H	-0.24537406442829	4.26938719238385	-1.64693039592139

H	2.13902835759796	4.14684685212045	-1.06632734904582
H	1.36083694572132	0.96406018585692	1.69683140689659
H	2.94036611888931	2.49400769627593	0.61053905876870
C	-4.51249461677727	1.89978019744073	-0.33128721965557
C	-5.38880070744151	1.04976484535879	0.27501576446979
C	-4.92977940712723	0.10382774158665	1.23267978430505
C	-3.60666563681247	0.03533325425929	1.55682834549571
H	-4.86150654189056	2.61991707707598	-1.05995302063309
H	-6.44102560433793	1.08996296317567	0.02636298609769
H	-5.63969457183261	-0.56284556484359	1.70324231374986
H	-3.25527560976416	-0.68534987439702	2.28386112272881
H	-2.55432675480902	3.44225225476514	-1.35214182393763
H	-0.94634318874849	0.14174809967866	1.98901743145755

S.4.8 DPF

Final Gibbs Free Enthalpy: 994.67615455 Eh

Total Enthalpy: 994.62442672 Eh

Number of Imaginary Frequencies: 0

C	-2.99902323423460	-0.31037723969745	0.00050484039162
C	-2.41749457589881	-1.54098960004349	0.00079678343963
C	-0.99660042080492	-1.46465719417034	0.00043746972659
O	-2.10658956494417	0.68972890094680	0.00002377931436
P	-0.53073171548270	0.17160302741992	-0.00075258560961
H	-2.98320394516669	-2.45844188441336	0.00113727650376
C	-4.41132950981739	0.08292186543315	0.00039327076738
C	-4.75436168144071	1.43437196209736	0.00119273830149
C	-5.42888977170830	-0.87064119078762	-0.00081310492744
C	-6.75556362258005	-0.47735795373382	-0.00144371403083
C	-7.08951784356672	0.87015756693151	-0.00069590426597
C	-6.08330755712276	1.82387224665327	0.00074275254946
H	-3.97034216347087	2.17819385248507	0.00215417098137
H	-6.33405080910144	2.87720759471312	0.00136105987440
H	-5.18576984158304	-1.92526568162770	-0.00155700735888

H	-7.53598993018388	-1.22702008994296	-0.00256385182818
H	-8.12866046221783	1.17422958594449	-0.00117083934872
C	-0.07608871646041	-2.61393671397544	0.00037298457795
C	-0.54724627253107	-3.92412752440444	0.00131906360136
C	0.33044121990812	-4.99716736001179	0.00109738232189
C	1.30763365651210	-2.41174848842225	-0.00082138067997
C	2.18473634946413	-3.48024046714657	-0.00126029101155
C	1.69865587339657	-4.78069361181355	-0.00029392386043
H	3.25198865612357	-3.29727915697899	-0.00225966901445
H	2.38461216777892	-5.61741254850429	-0.00054331910224
H	1.70680395175660	-1.40265615941151	-0.00151214280359
H	-1.61197761490604	-4.11564522515942	0.00227489567308
H	-0.06116262171757	-6.00657851237973	0.00187926581752

S.4.9 Ethylene

Final Gibbs Free Enthalpy: 78.56292502 Eh

Total Enthalpy: 78.53782487 Eh

Number of Imaginary Frequencies: 0

C	-4.82874880679000	1.23339311225681	-0.00266666794915
C	-3.61455416608628	0.71353806164619	0.00266850457248
H	-5.63510161636383	0.79511233693894	0.57262273910744
H	-5.06485408696995	2.12494507179518	-0.57205033301341
H	-3.37843920373853	-0.17801001337043	0.57205171189652
H	-2.80820212005142	1.15182143073330	-0.57262595461388

S.4.10 DPF + ethylene (TS)

Final Gibbs Free Enthalpy: 1073.19688909 Eh

Total Enthalpy: 1073.14038534 Eh

Number of Imaginary Frequencies: 1

P	5.51410705609232	1.04974177038882	15.50761915907294
O	4.08591265722524	1.79400211445477	15.16542484041289
C	6.18412952331360	2.51279841263198	16.19738819567353
C	5.37274404100874	3.55513022869603	15.81907521527582

C	4.27087868925190	3.12868952335443	15.05664872292571
C	5.47359518450125	2.87064276566710	13.14445821198786
C	6.04530606197968	1.62035957239362	13.33829925162658
C	7.45977177472906	2.68740851950603	16.91497447498026
C	8.65402619416332	2.21830396279085	16.37383661877477
H	8.63990801413001	1.69774698127391	15.42435819986740
C	9.86176956704629	2.44532125915733	17.01433263972118
H	10.77981904295466	2.08318857996026	16.56715542574005
C	9.89313108408558	3.13889242128562	18.21413959048986
H	10.83491704944532	3.32693919013483	18.71498531618430
C	8.70792640216839	3.59267939895131	18.77336206383345
H	8.72299279025476	4.11976066362880	19.71938302806902
C	7.50057031371912	3.37008458676398	18.13046559074461
C	3.10471480413624	3.91377095974069	14.63512041010845
C	1.85851560007976	3.30453266146802	14.52068903827600
H	1.75207319184811	2.26529659520827	14.80276525041170
C	0.76875631111398	4.02499338847807	14.05984906762065
H	-0.19443206281919	3.53801441506883	13.96956872835905
C	0.91135900039842	5.35868463387288	13.70920254909850
H	0.06110426072064	5.91852119875118	13.34145049174531
C	2.15080592034674	5.97292458910268	13.82982798923165
H	2.27136439551462	7.01085802905072	13.54504033637014
C	3.24232280279508	5.25642181587208	14.28758111940982
H	4.21165010345770	5.73601708467371	14.36017255415291
H	6.08415234882942	3.76277454885556	13.17346479038071
H	4.53742466395010	2.97041153535390	12.61456882400292
H	7.12290578138540	1.51581010593537	13.38780299741118
H	5.54042635778525	0.75910887658683	12.91746894735527
H	5.58658019726669	4.59732353869555	16.01743027995250
H	6.57531087712178	3.71679607224595	18.57607008073303

S.4.11 DPF·C_2H_4

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Final Gibbs Free Enthalpy: 1073.24673771 Eh
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Total Enthalpy: 1073.19111283 Eh

Number of Imaginary Frequencies: 0

P	5.97776247686058	1.40274406684000	14.70320351257084
O	4.44664223159924	2.02462017255168	14.61350080197420
C	6.50318185074702	2.85686475675842	15.72921181088896
C	5.66041748936388	3.83584248329585	15.41754106622355
H	5.69400692739311	4.84368989083622	15.81548711645467
C	4.66846529526604	3.41605153504901	14.35177783163927
C	5.42501329204438	3.39553503320234	12.98541540183117
H	4.68657723370474	3.23682983157681	12.20020608629680
H	5.92242704152711	4.34634426245669	12.79778788305706
C	6.39732653303561	2.20828574384460	13.06247509853736
H	7.44676692252349	2.49504054283554	13.00069028325188
H	6.19471313323345	1.48123363308787	12.27742492703845
C	7.58350673491006	2.92618899293991	16.72700151611881
C	8.90202855997853	2.61486082646550	16.40149989675554
H	9.15009495542162	2.31122425814546	15.39102743711245
C	9.90351643131484	2.69849882332280	17.35641389863989
H	10.92425610115791	2.46006528007965	17.08500342848563
C	9.59786837625747	3.07549346212754	18.65519289402339
H	10.37763811314502	3.13118841301226	19.40323057119712
C	8.28861196182749	3.38138739745530	18.99259694424969
H	8.04147707735663	3.68087943225580	20.00377430007358
C	7.28934252119680	3.31359658731941	18.03488848080871
H	6.26582978574245	3.54895642995057	18.30057362599706
C	3.37659106806125	4.18376953697454	14.30955516429233
C	2.15864534217153	3.51725894973006	14.29819687101799
H	2.14900789077798	2.43810210037357	14.36724530595070
C	0.97296254111525	4.23266905892320	14.21198911752958
H	0.02945266700205	3.70112536899885	14.20415343573380
C	0.99341569888155	5.61713215046439	14.13819818042538
H	0.06766396277241	6.17409734476466	14.06754531161685
C	2.20832430096391	6.28761846349043	14.14709478118126

H	2.23398721608048	7.36798365093982	14.07876065737116
C	3.39391117416259	5.57391035724219	14.23118312482343
H	4.33862709240350	6.10779116268909	14.22934323683145

S.4.12 Parent 2-phosphafuran

Final Gibbs Free Enthalpy: 532.68572255 Eh

Total Enthalpy: 532.65367275 Eh

Number of Imaginary Frequencies: 0

C	-2.95550634801028	-0.25084590602478	0.02126767582032
C	-2.40314991565462	-1.49477564937720	0.01088470197165
C	-0.98558988861464	-1.41931719325705	-0.00280624977757
O	-2.06113884021435	0.75231668985337	0.01611495164810
P	-0.46839212905460	0.20192766267816	-0.00253305255851
H	-2.97745273531101	-2.40757822254489	0.01345357772670
H	-0.33506728239386	-2.28037702615678	-0.01261548913632
H	-3.99183286074663	0.04801964482917	0.03304388430563