Electronic Supporting Information

Addition reactions and diazomethane capture by the intramolecular P-O-B FLP: *t*Bu_2POBcat

Diya Zhu,[a] Zheng-Wang Qu,*[b] and Douglas W. Stephan [a*]

This PDF file includes:

2.1 catBOPtBu$_2$ 1

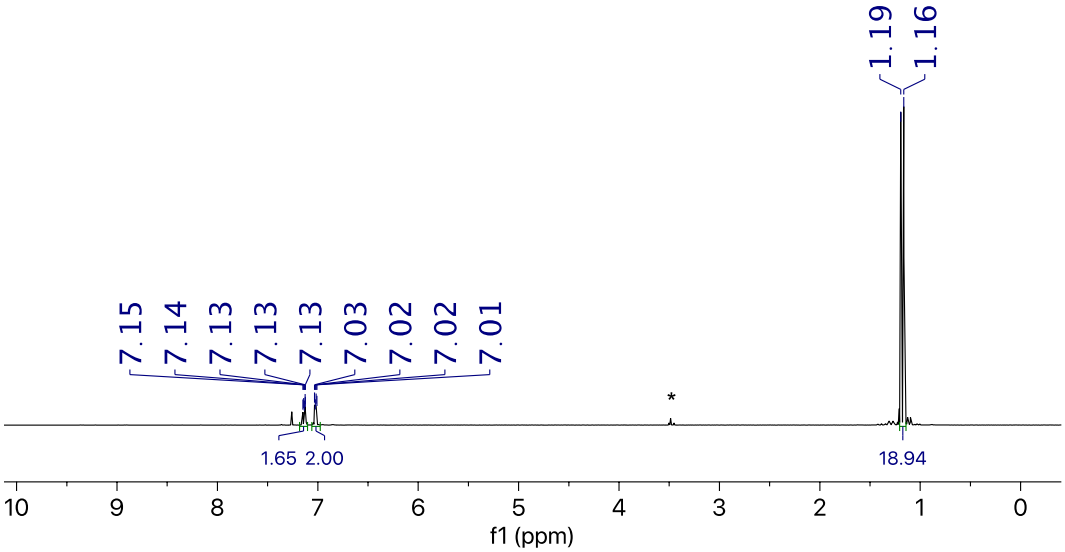

Figure S1. ^{1}H ($CDCl_3$) NMR spectrum of **1**. (Asterisks denote the solvent impurities)

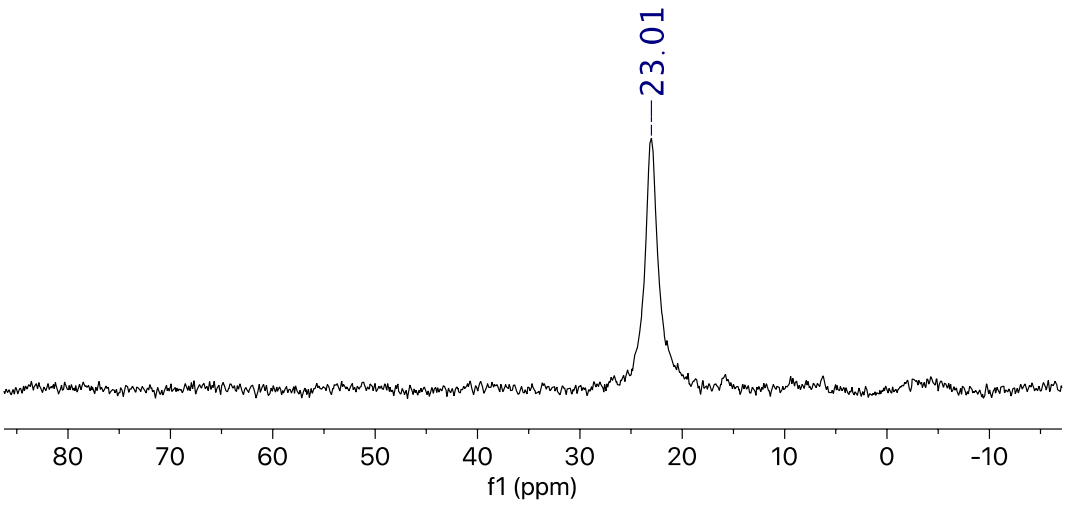

Figure S2. $^{11}B\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **1**.

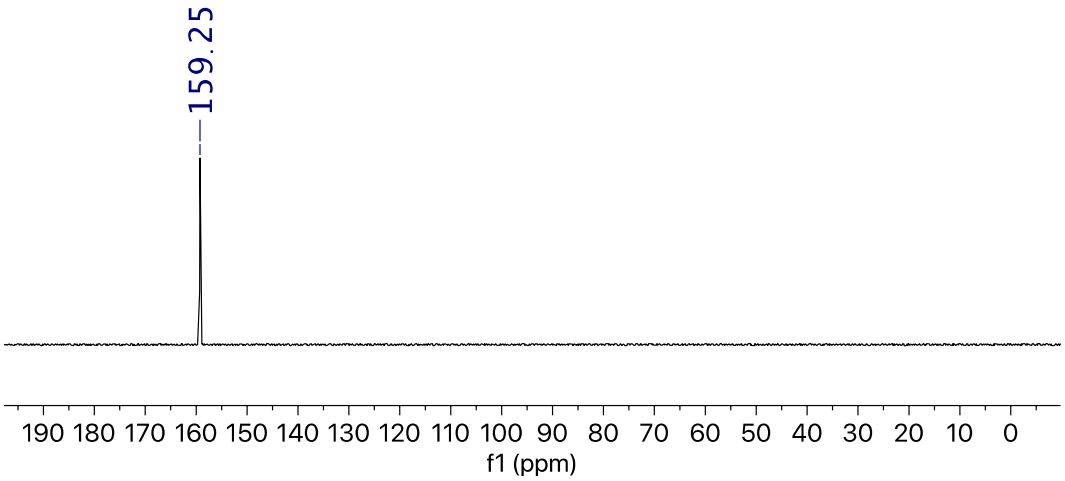

Figure S3. $^{31}P\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **1**.

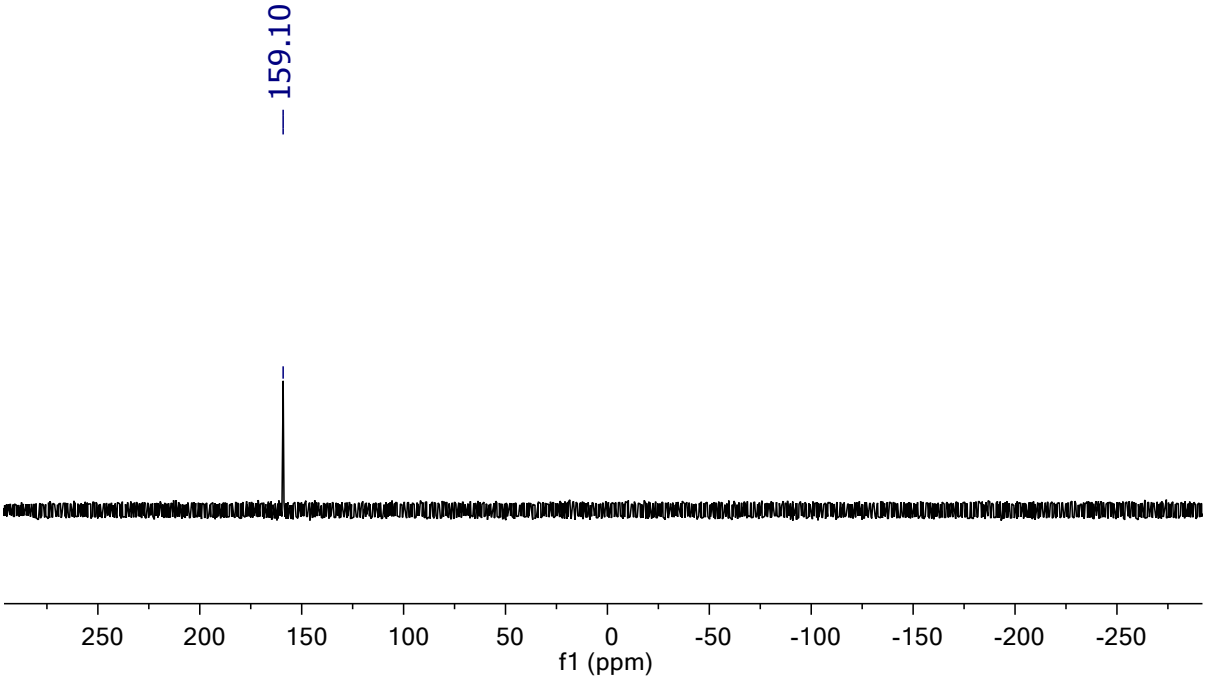

Figure S4. $^{31}P\{^{1}H\}$ ($CDCl_3$, 193 K) NMR spectrum of **1**.

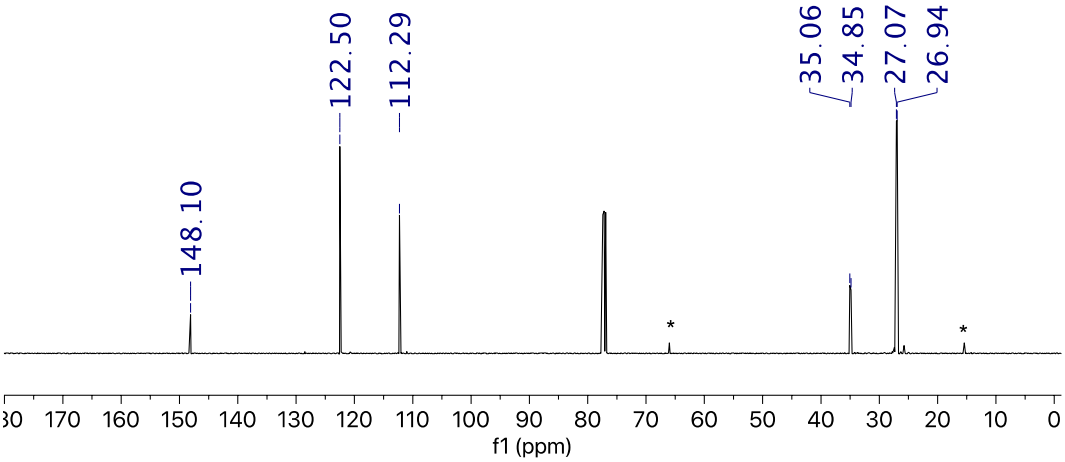

Figure S5. $^{13}C\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **1**. (Asterisks denote the solvent impurities)

2.2 catBOPMes$_2$ 2

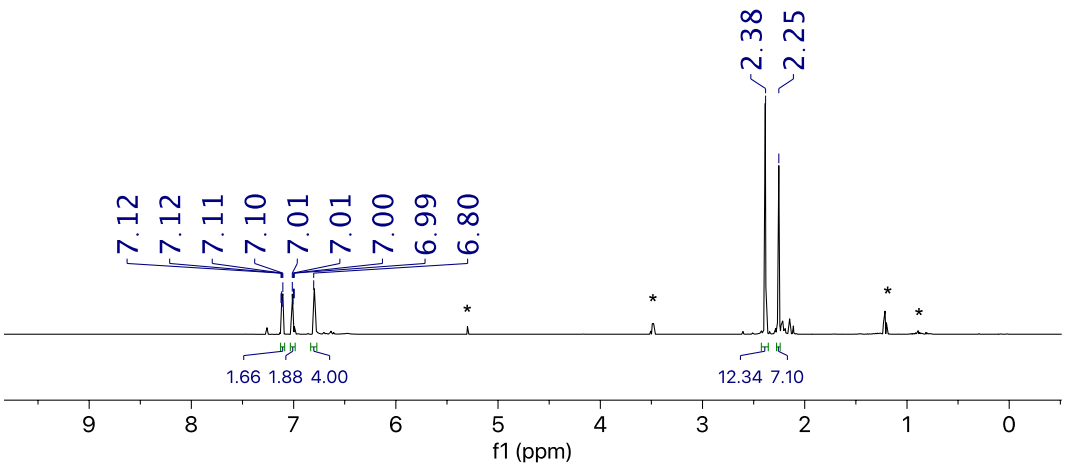

Figure S6. ^{1}H ($CDCl_3$) NMR spectrum of **2**. (Asterisks denote the solvent impurities)

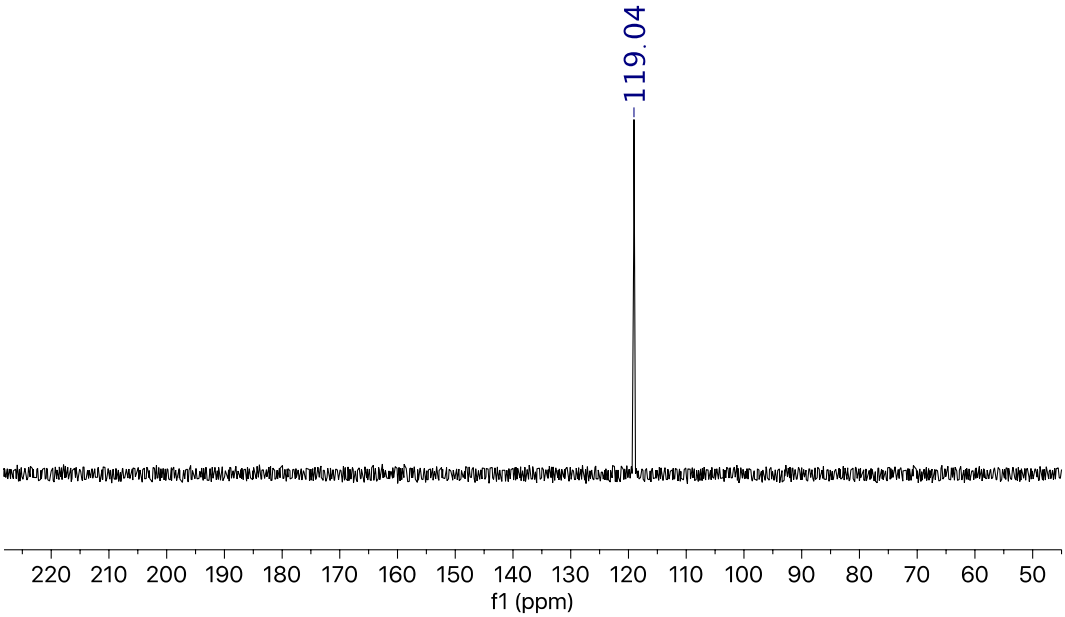

Figure S7. $^{31}P\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **2**.

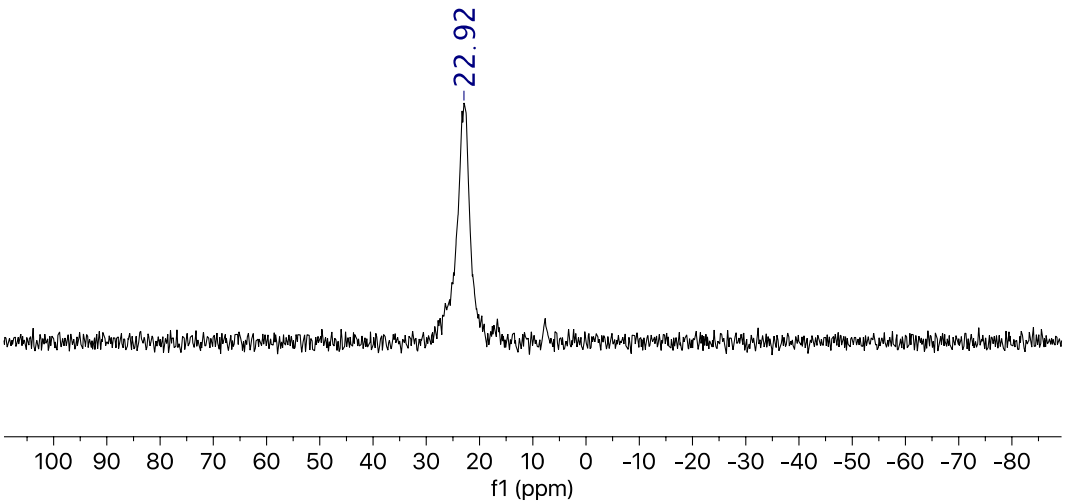

Figure S8. $^{11}B\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **2**.

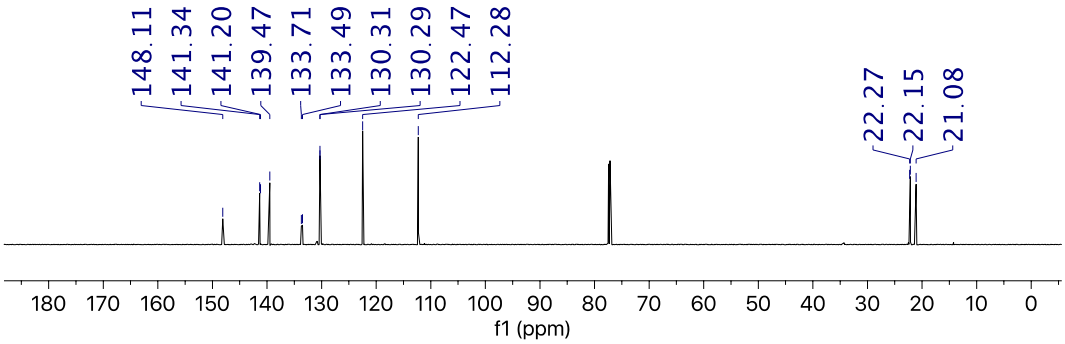

Figure S9. $^{13}C\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **2**.

2. 3 t*Bu$_2$P(H)OBcat(OPh) 3*

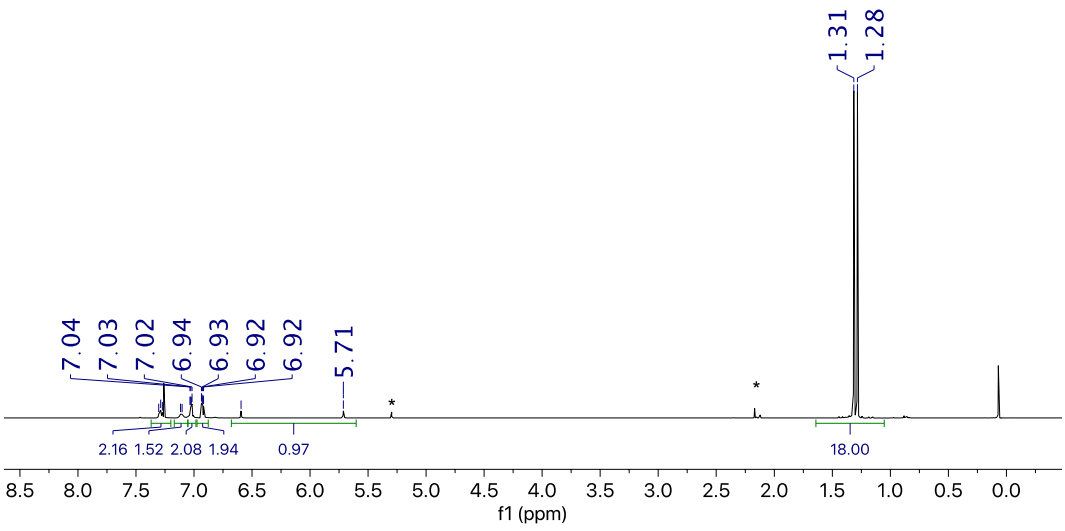

Figure S10. ^{1}H ($CDCl_3$) NMR spectrum of **3**. (Asterisks denote the solvent impurities)

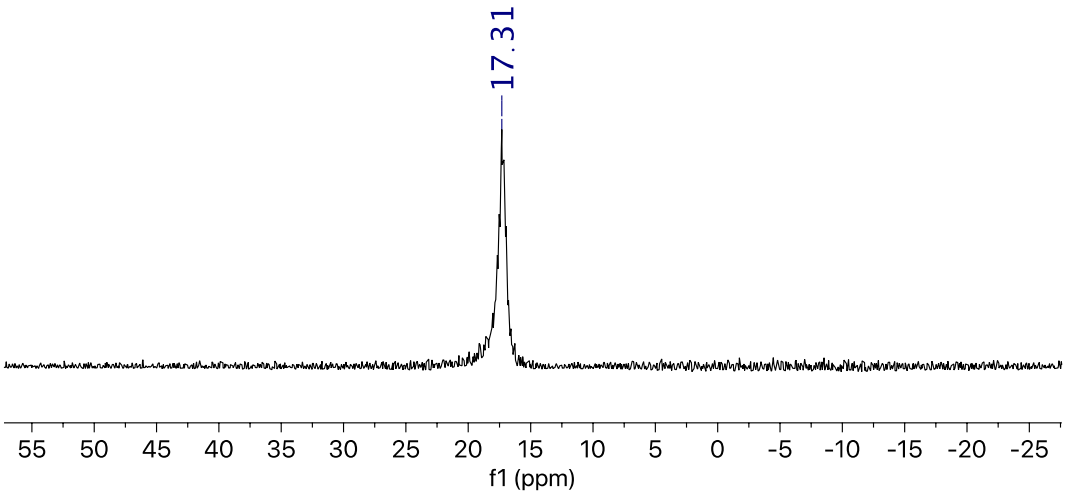

Figure S11. $^{11}B\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **3**.

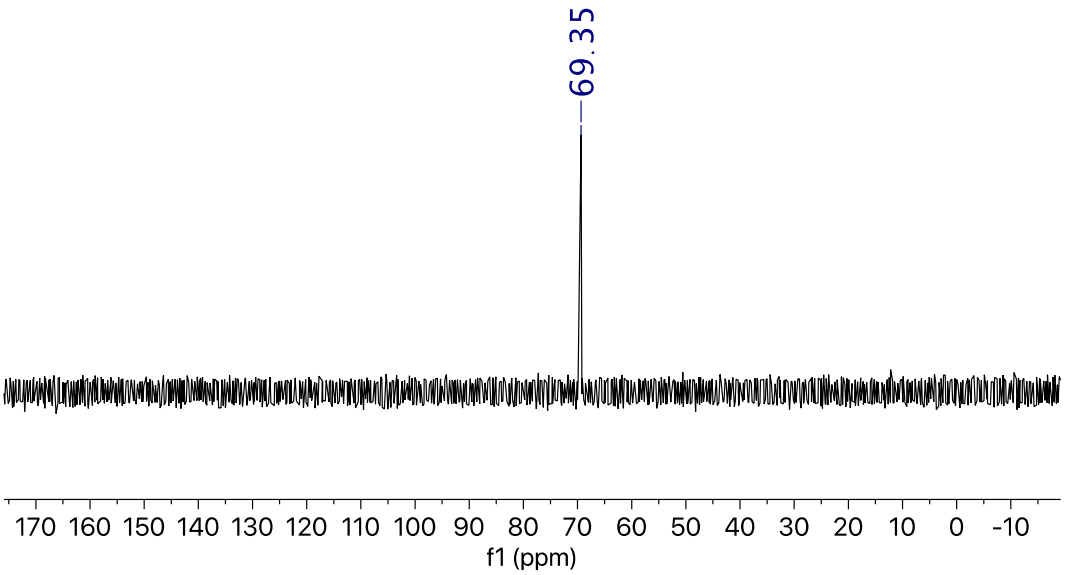

Figure S12. $^{31}P\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **3**.

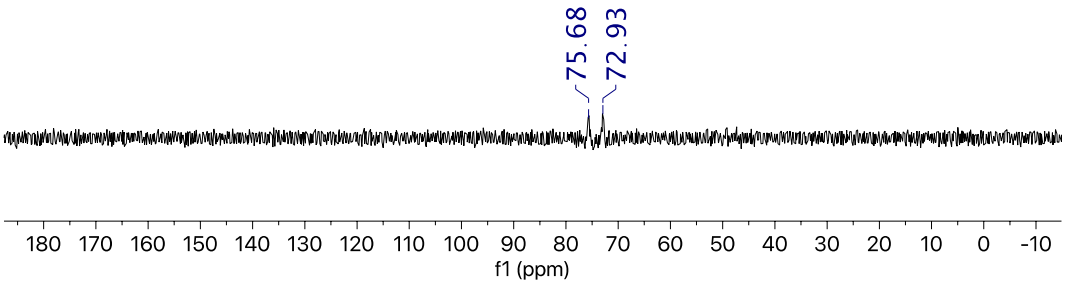

Figure S13. ^{31}P ($CDCl_3$) NMR spectrum of **3**.

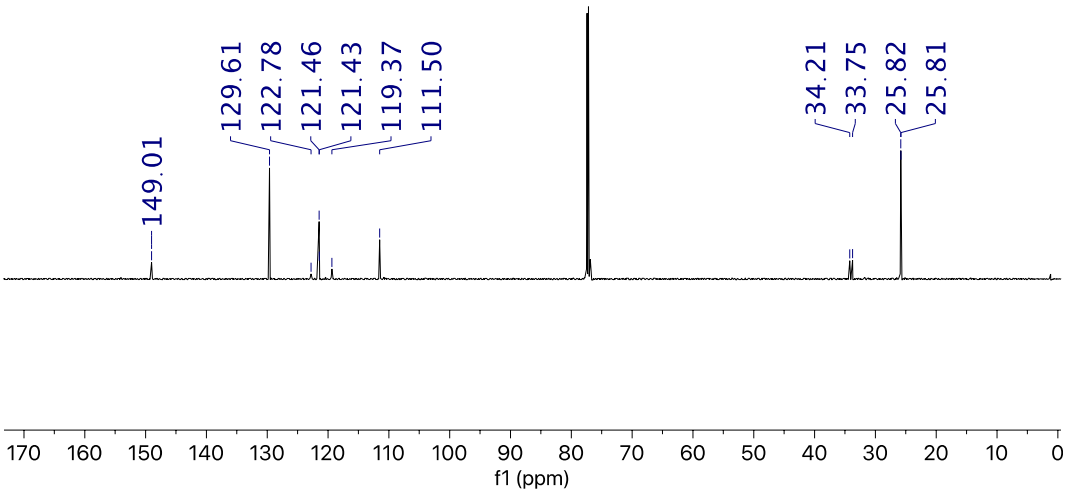

Figure S14. $^{13}C\{^1H\}$ ($CDCl_3$) NMR spectrum of **3**.

2.4 Generation of $tBu_2POBcat(CO_2)$ *4*

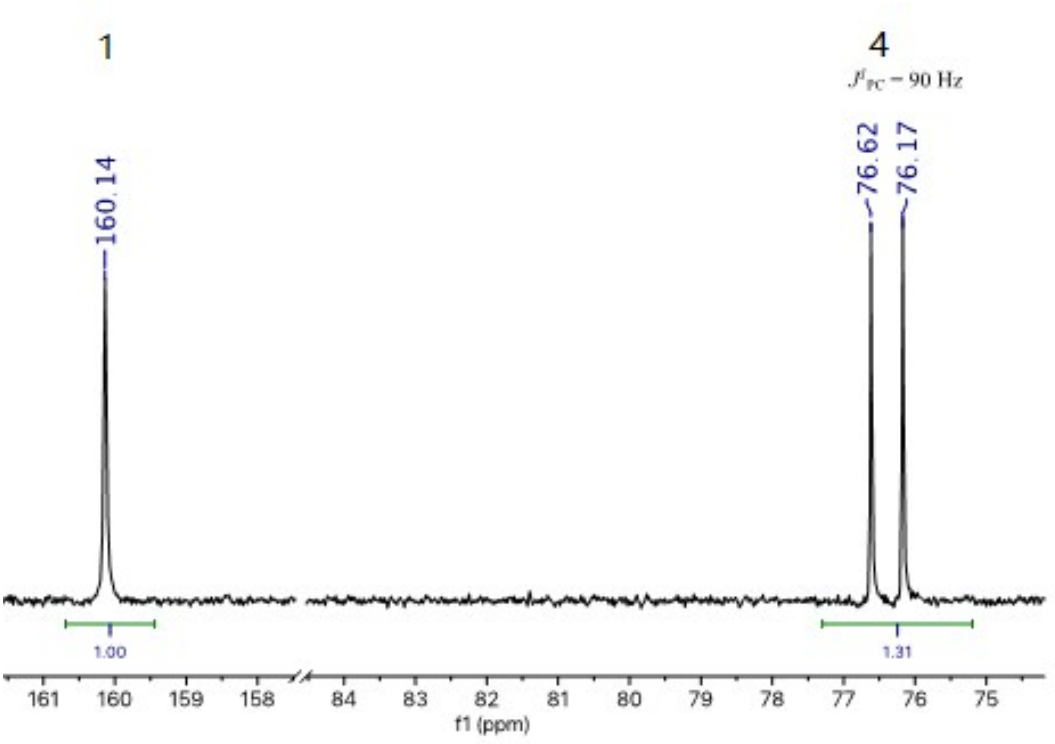

Figure S15. $^{31}P\{^1H\}$ ($CDCl_3$) NMR spectrum of rxn crude (expanded, 298 K).

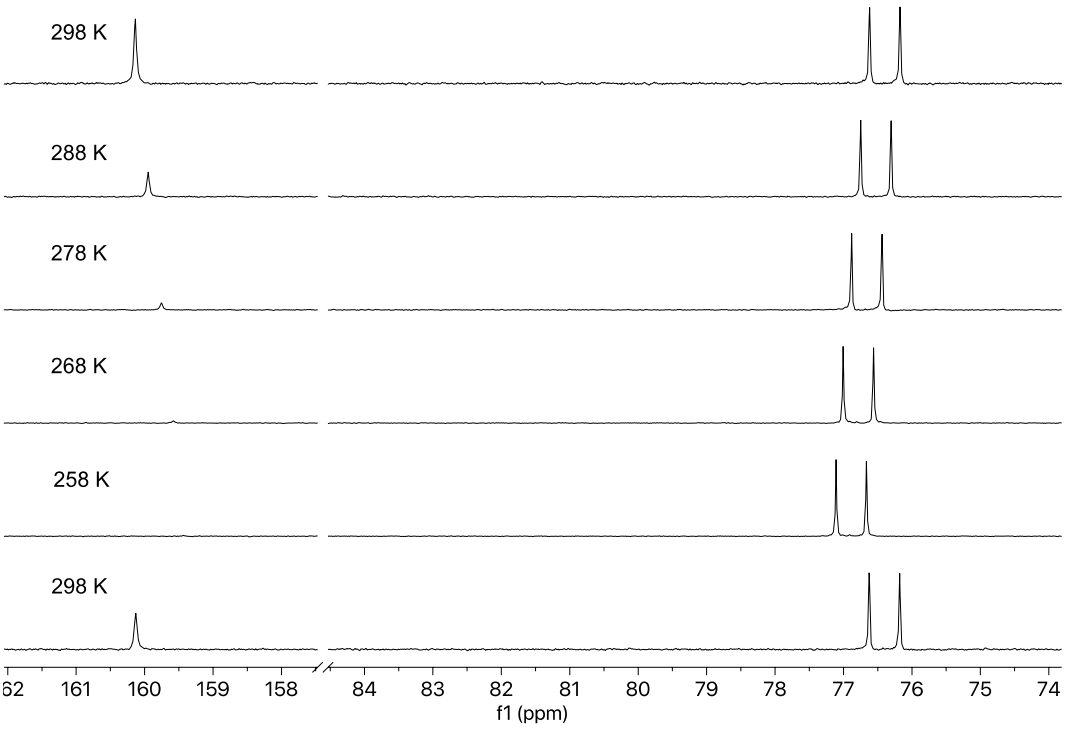

Figure S16. $^{31}P\{^1H\}$ ($CDCl_3$) NMR VT spectrum (expanded, from 298 to 258 K, and warm back to 298 K)

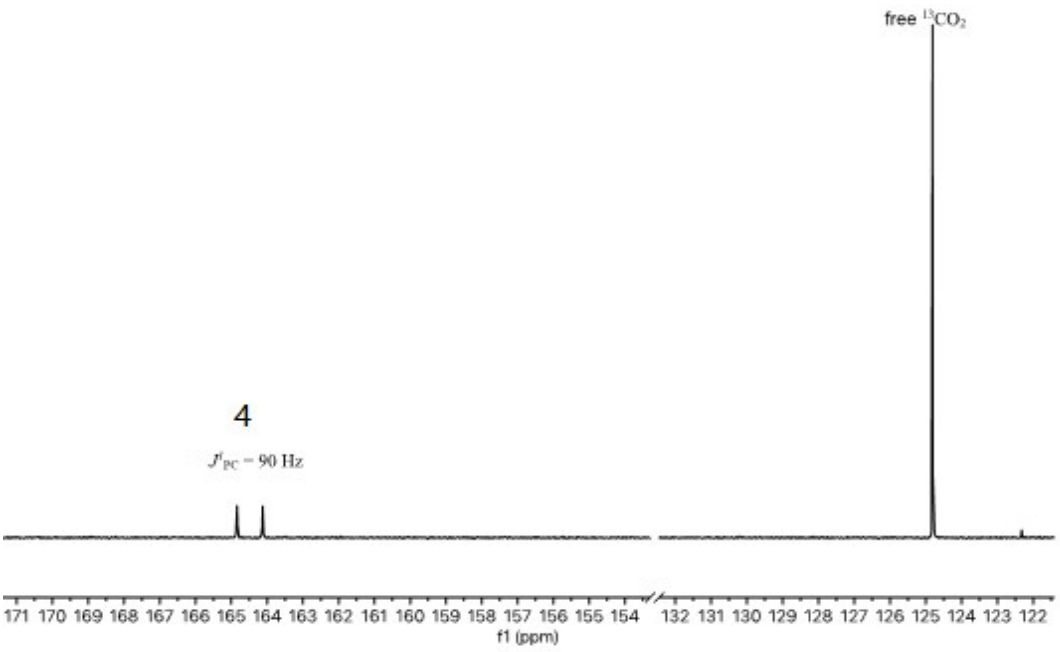

Figure S17. $^{13}C\{^1H\}$ ($CDCl_3$) NMR spectrum of rxn crude (expanded, 298 K).

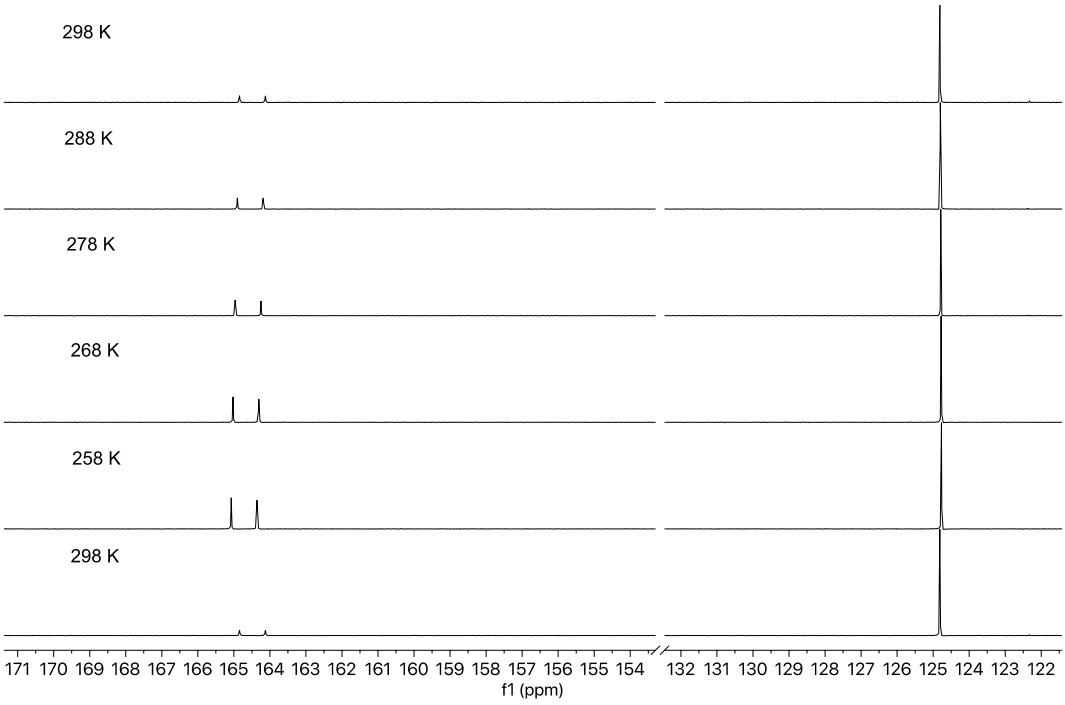

Figure S18. $^{13}C\{^1H\}$ ($CDCl_3$) NMR VT spectrum (expanded, from 298 to 258 K, and warm back to 298 K)

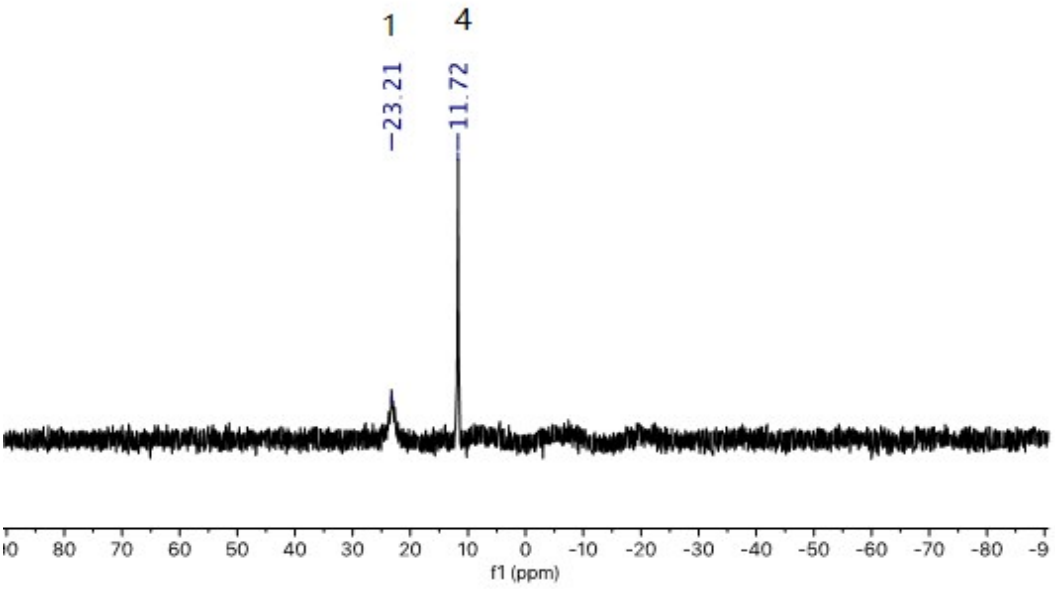

Figure S19. $^{11}B\{^{1}H\}$ ($CDCl_3$) NMR spectrum of rxn crude (298 K).

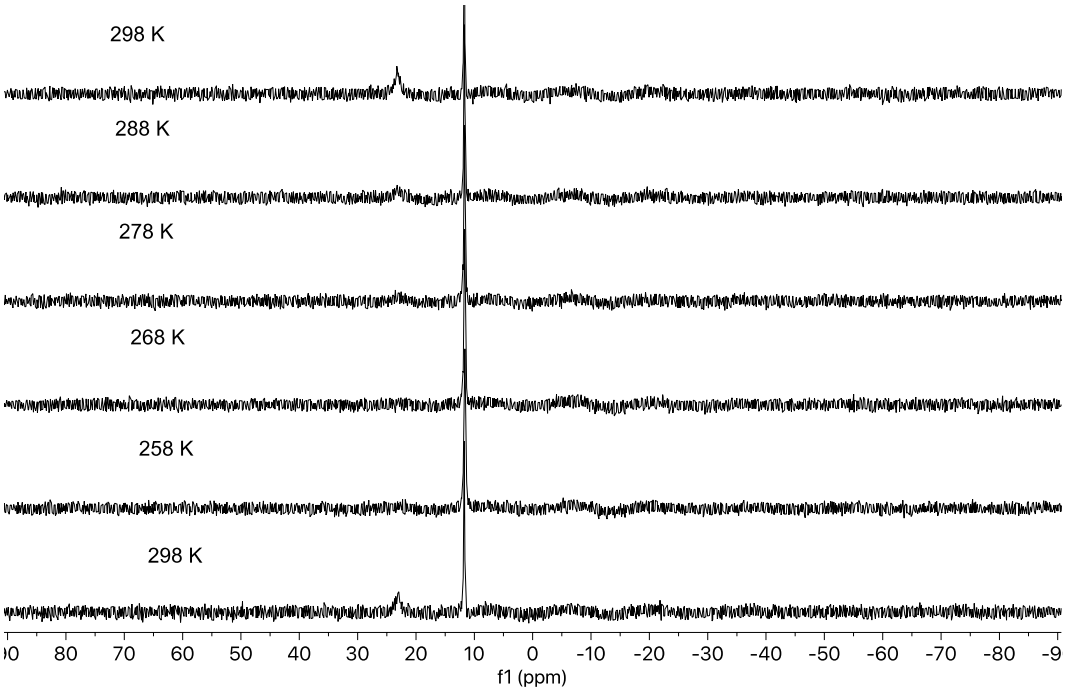

Figure S20. $^{11}B\{^{1}H\}$ ($CDCl_3$) NMR VT spectrum (from 298 to 258 K, and warm back to 298 K)

2.5 tBu_2POBcat(CS_2) 5

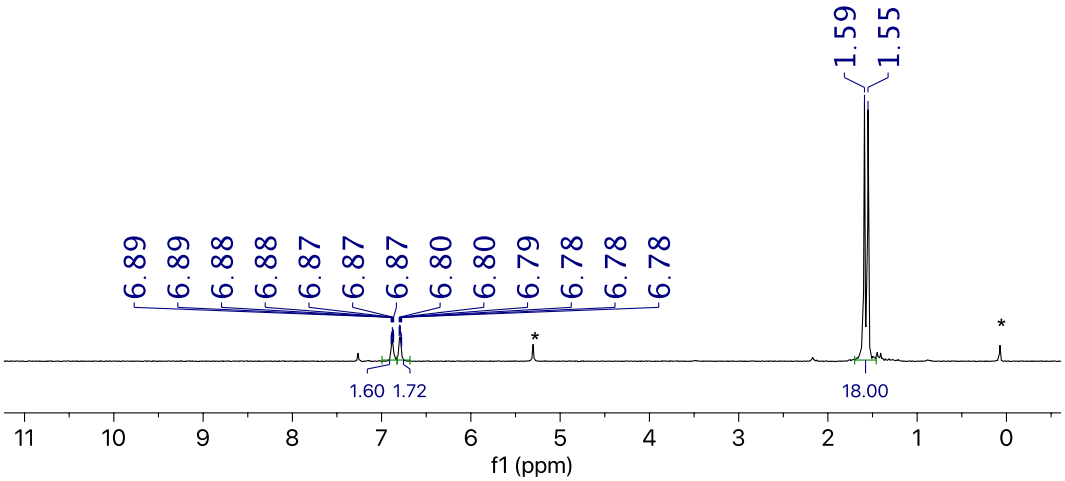

Figure S21. ^{1}H ($CDCl_3$) NMR spectrum of **5**. (Asterisks denote the solvent impurities)

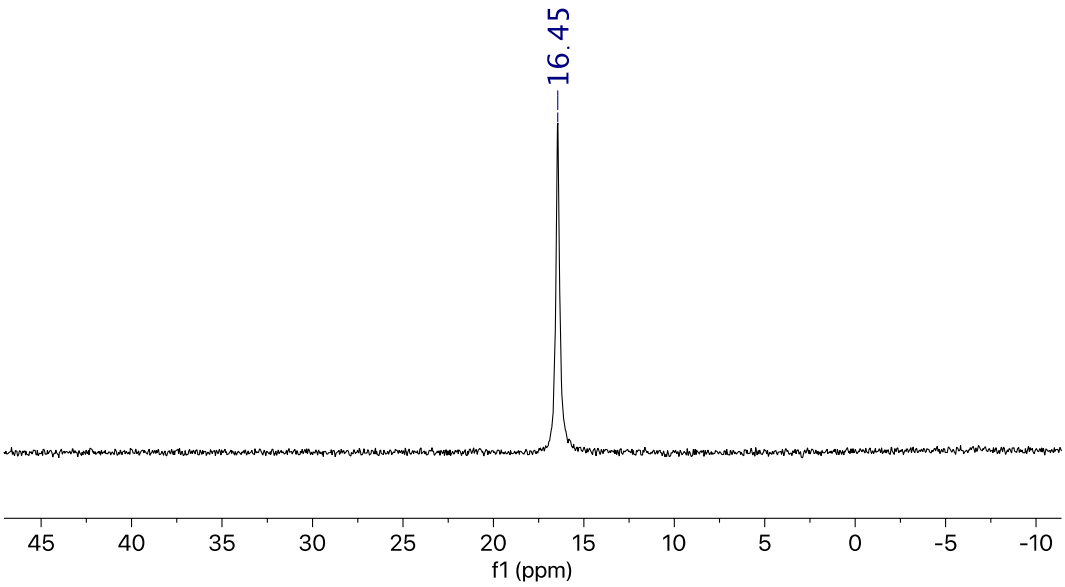

Figure S22. $^{11}B\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **5**.

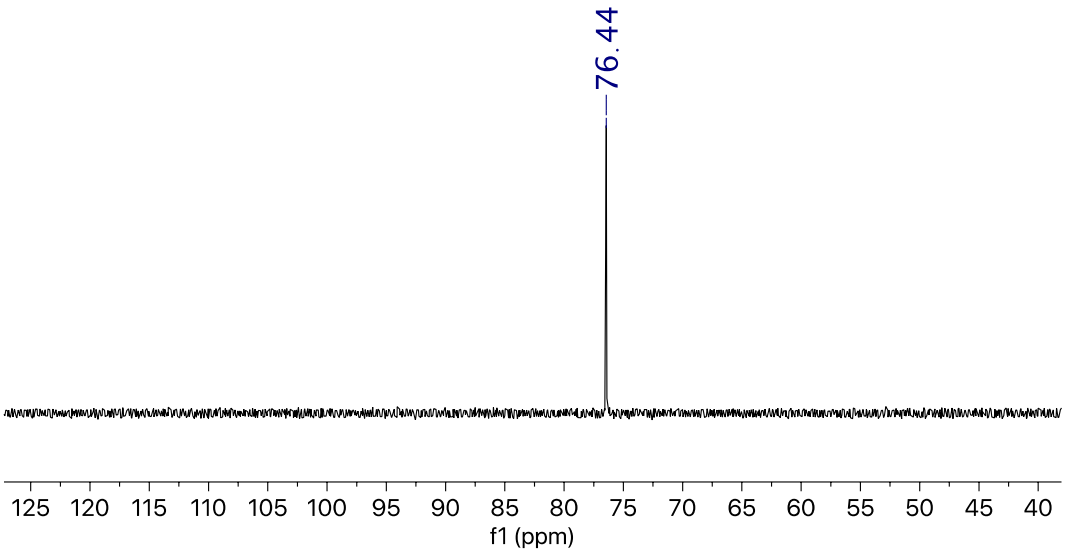

Figure S23. $^{31}P\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **5**.

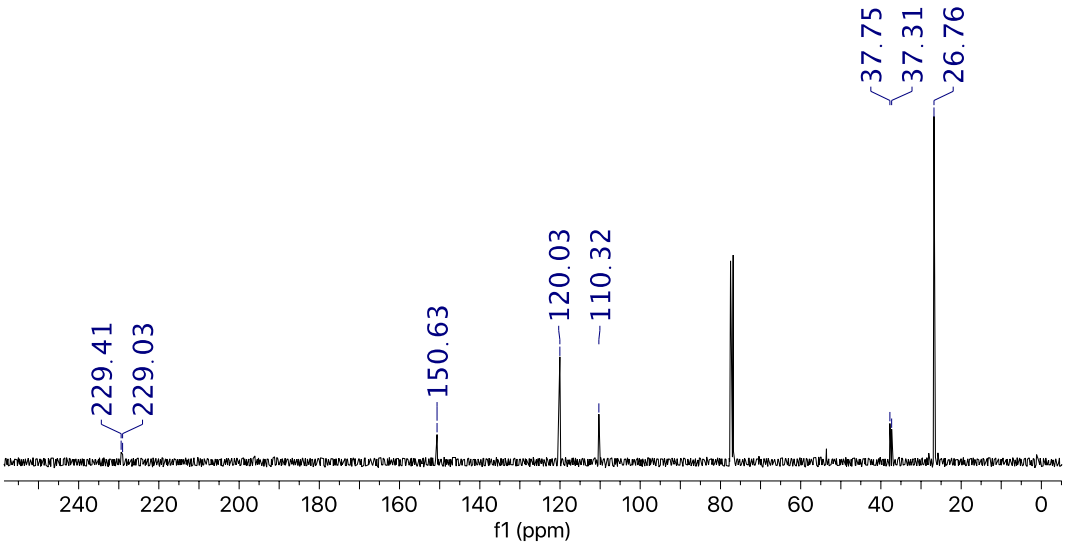

Figure S24. $^{13}C\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **5**.

2.6 tBu_2POBcat(PhNCO) 6

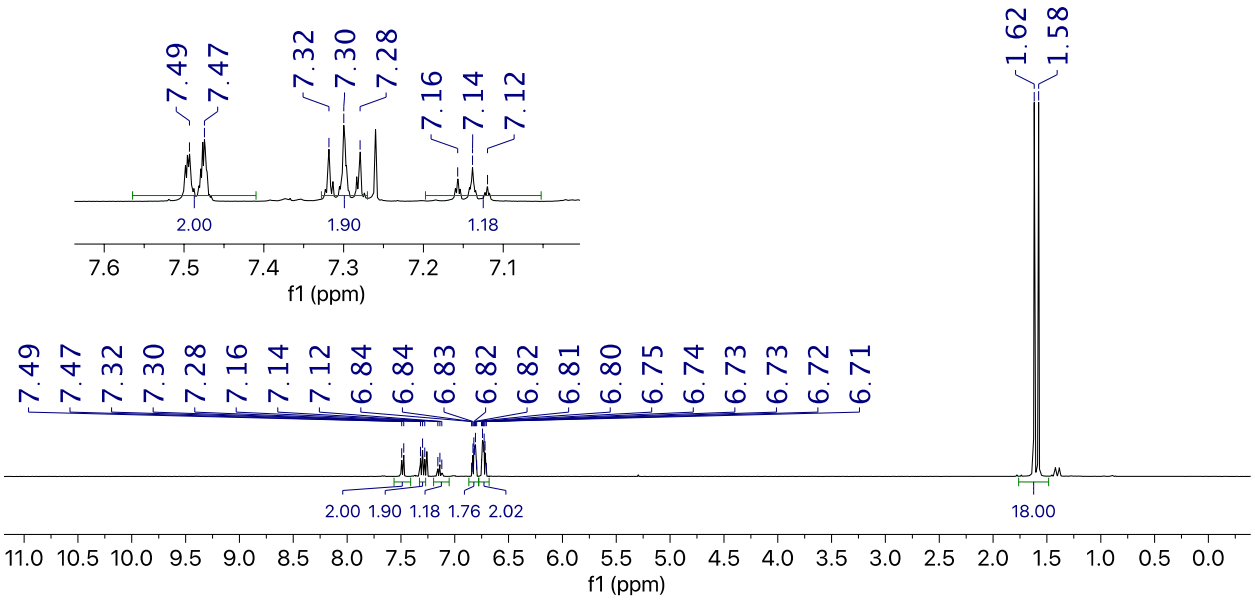

Figure S25. ^{1}H ($CDCl_3$) NMR spectrum of **6**.

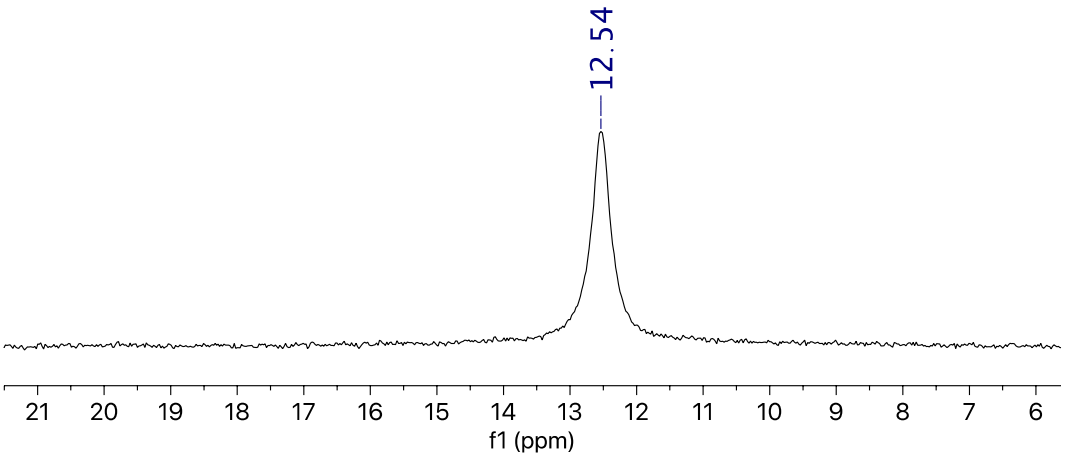

Figure S26. $^{11}B\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **6**.

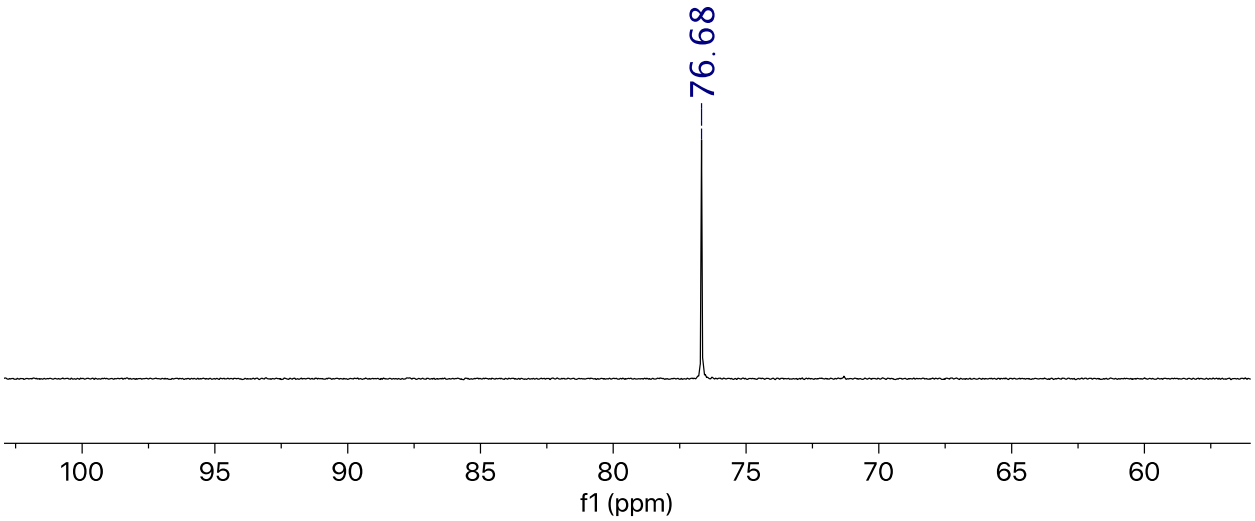

Figure S27. $^{31}P\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **6**.

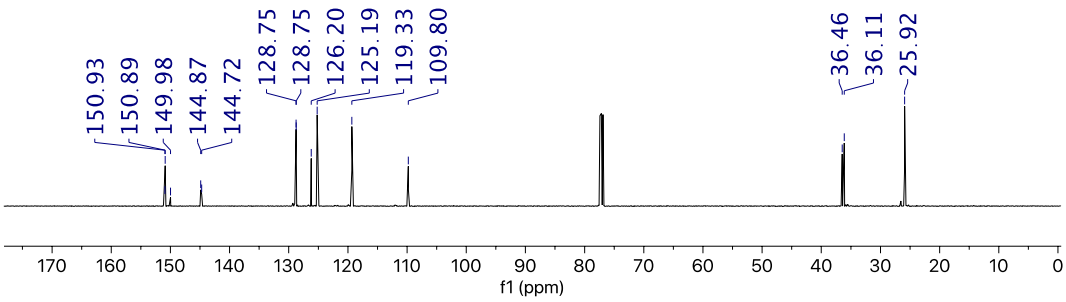

Figure S28. $^{13}C\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **6**.

2.7 tBu_2POBcat(MesCNO) 7

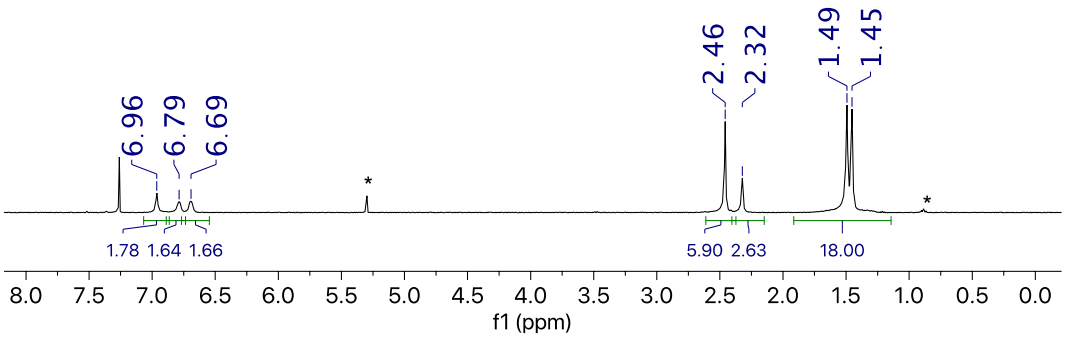

Figure S29. ^{1}H ($CDCl_3$) NMR spectrum of **7**. (Asterisks denote the solvent impurities)

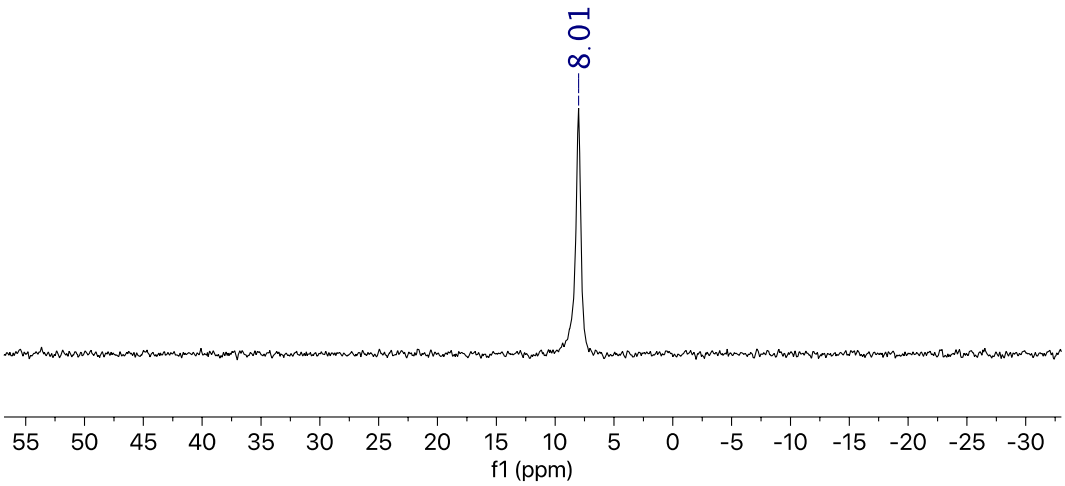

Figure S30. $^{11}B\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **7**.

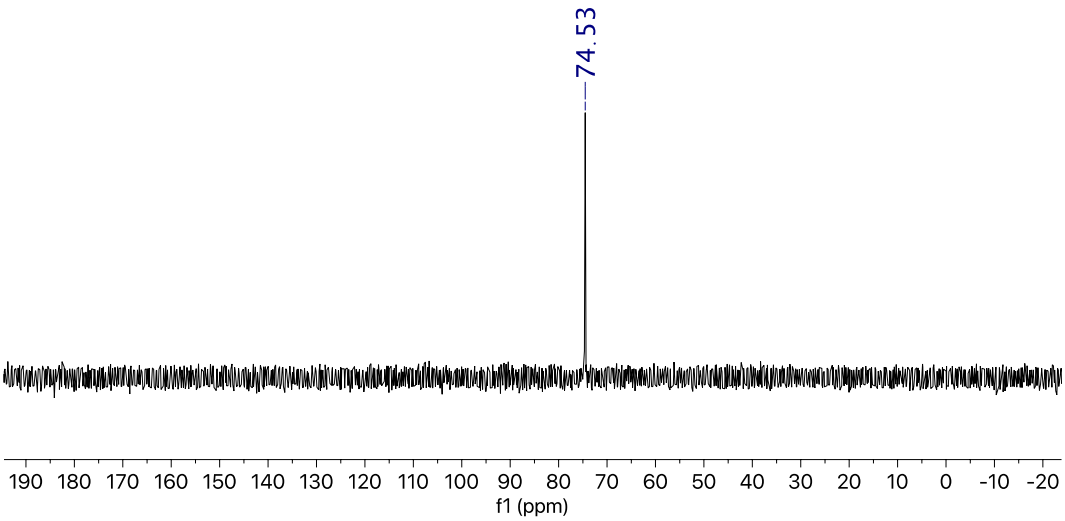

Figure S31. $^{31}P\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **7**.

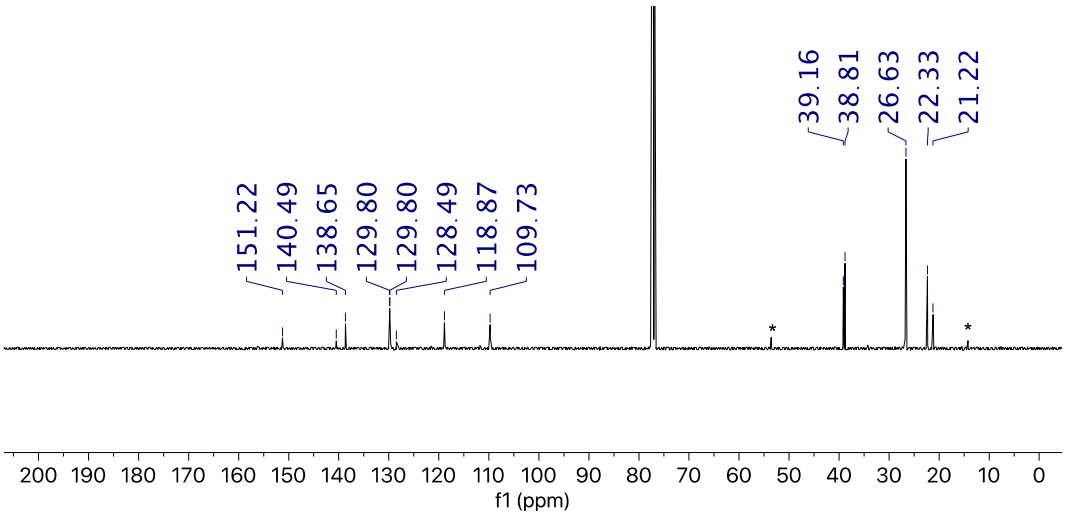

Figure S32. $^{13}C\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **7**. (Asterisks denote the solvent impurities)

2.8 ($tBu_2P(O)OBcat)_2$ 8

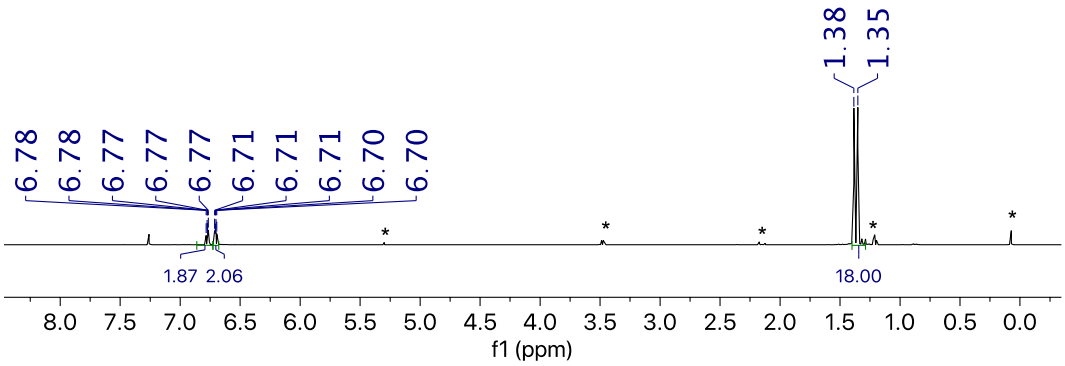

Figure S33. ^{1}H ($CDCl_3$) NMR spectrum of **8**. (Asterisks denote the solvent impurities)

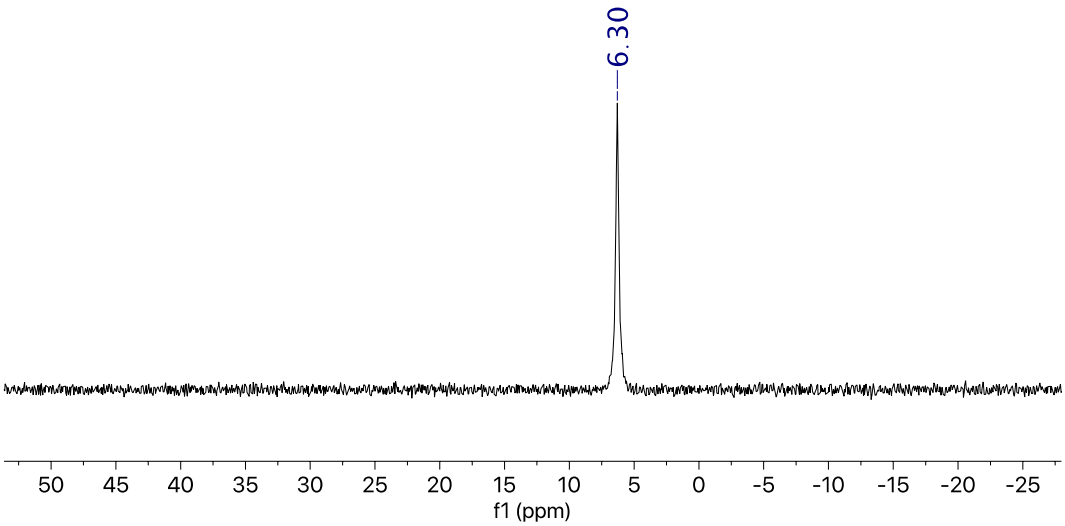

Figure S34. $^{11}B\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **8**.

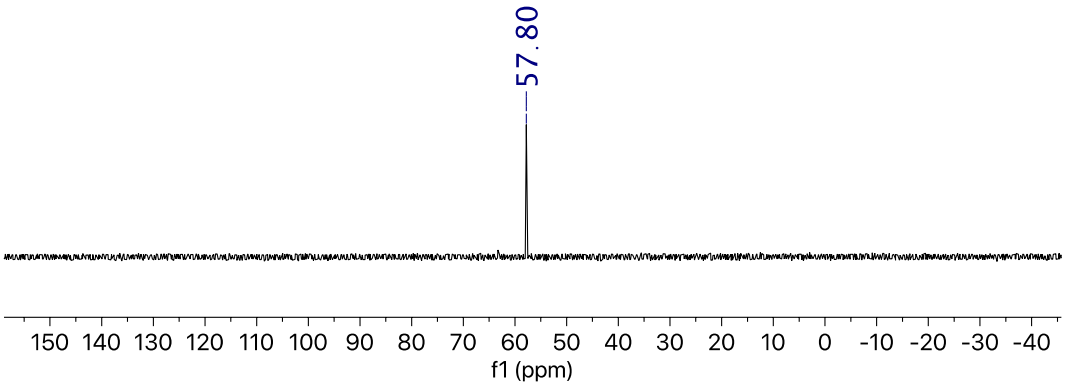

Figure S35. $^{31}P\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **8**.

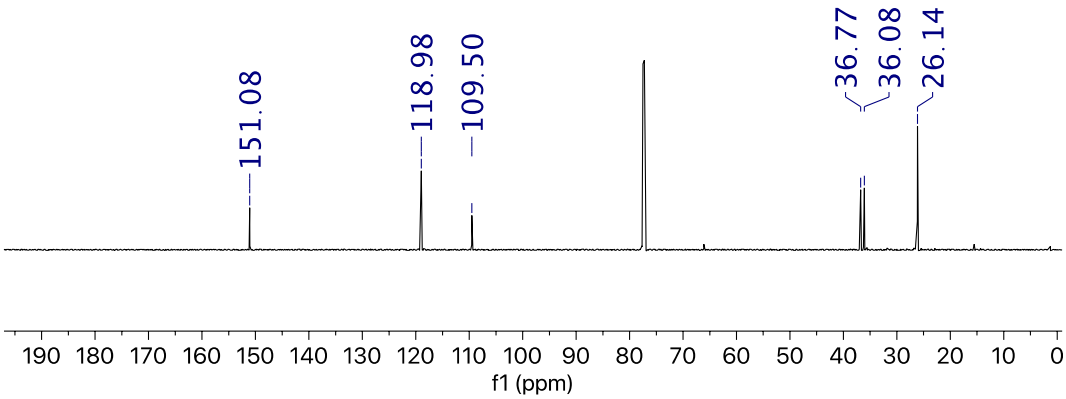

Figure S36. $^{13}C\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **8**.

2.9 $tBu_2POBcat(C_{14}H_8O_2)$ 9

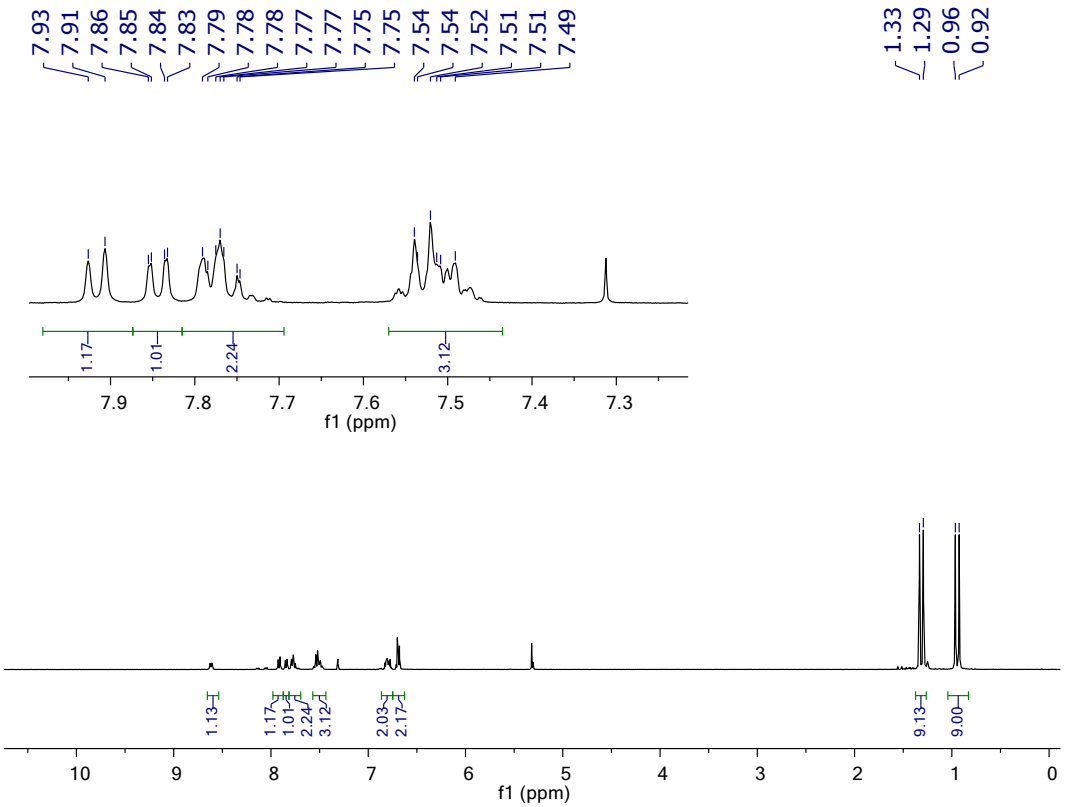

Figure S37. ^{1}H (CD_2Cl_2) NMR spectrum of **9**.

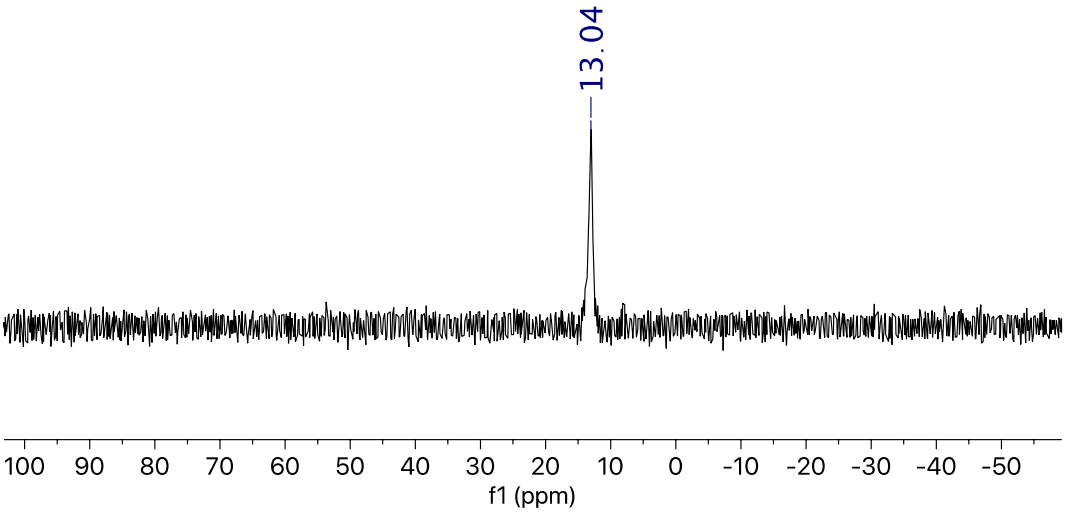

Figure S38. $^{11}B\{^{1}H\}$ (CD_2Cl_2) NMR spectrum of **9**.

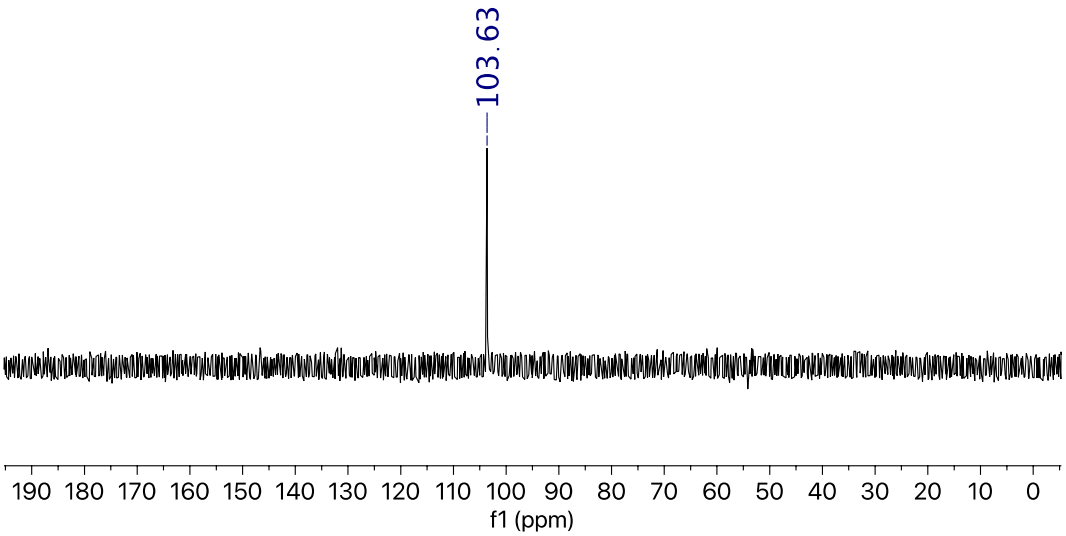

Figure S39. $^{31}P\{^{1}H\}$ (CD_2Cl_2) NMR spectrum of **9**.

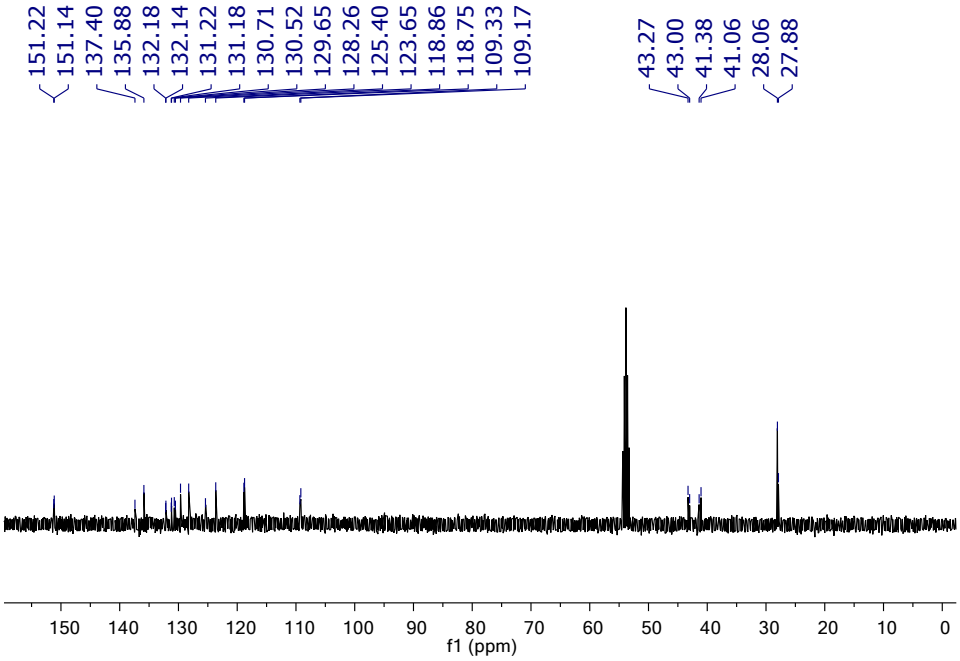

Figure S40. $^{13}C\{^{1}H\}$ (CD_2Cl_2) NMR spectrum of **9**.

2.10 $tBu_2POBcat(Ph_2CN_2)$ 10

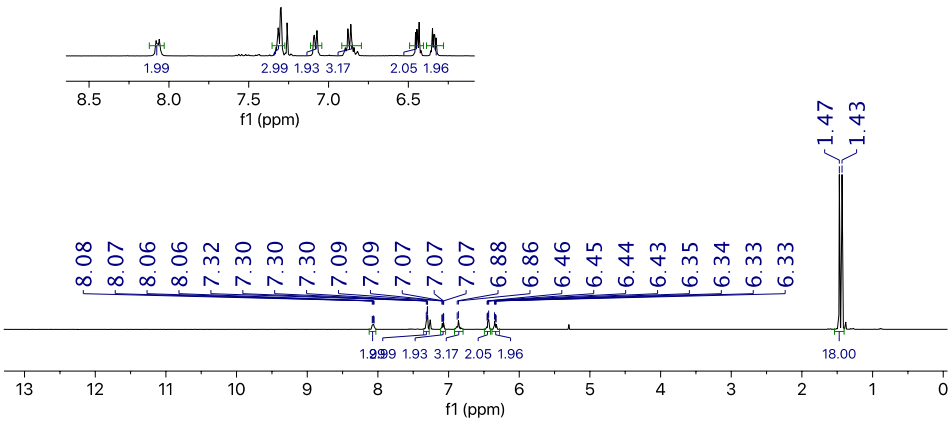

Figure S41. ^{1}H ($CDCl_3$) NMR spectrum of **10**.

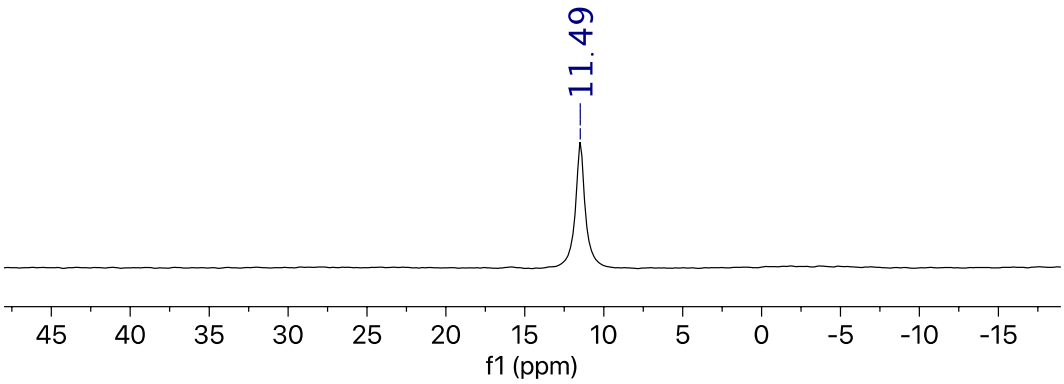

Figure S42. $^{11}B\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **10**.

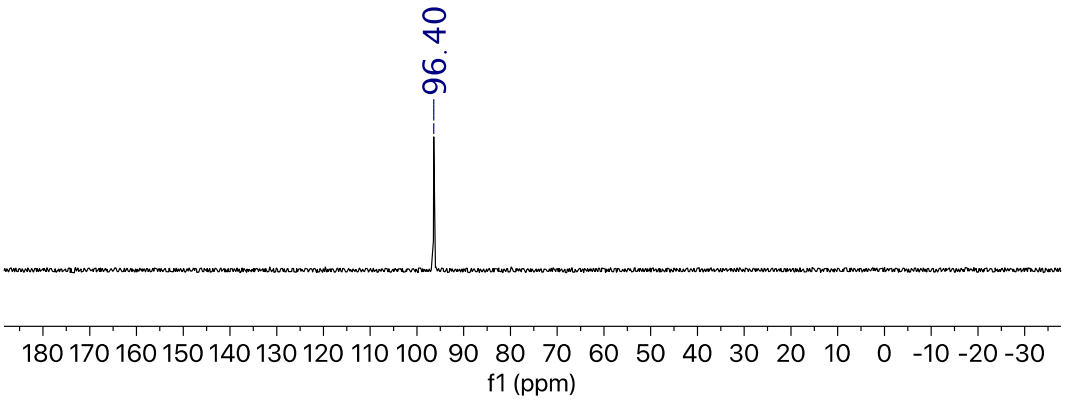

Figure S43. $^{31}P\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **10**.

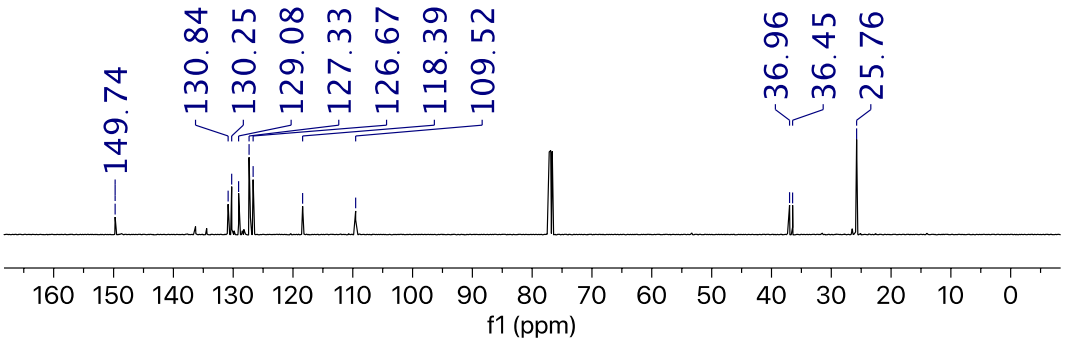

Figure S44. ^{13}C ($CDCl_3$) NMR spectrum of **10**.

2.11 $Mes_2POBcat(Ph_2CN_2)$ 11

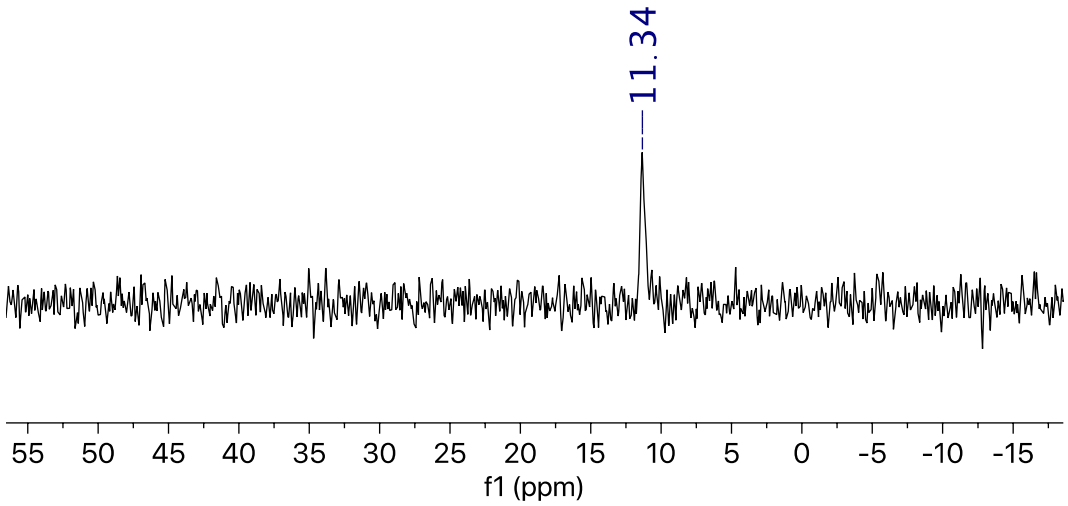

Figure S45. $^{11}B\{^1H\}$ ($CDCl_3$) NMR spectrum of **11**.

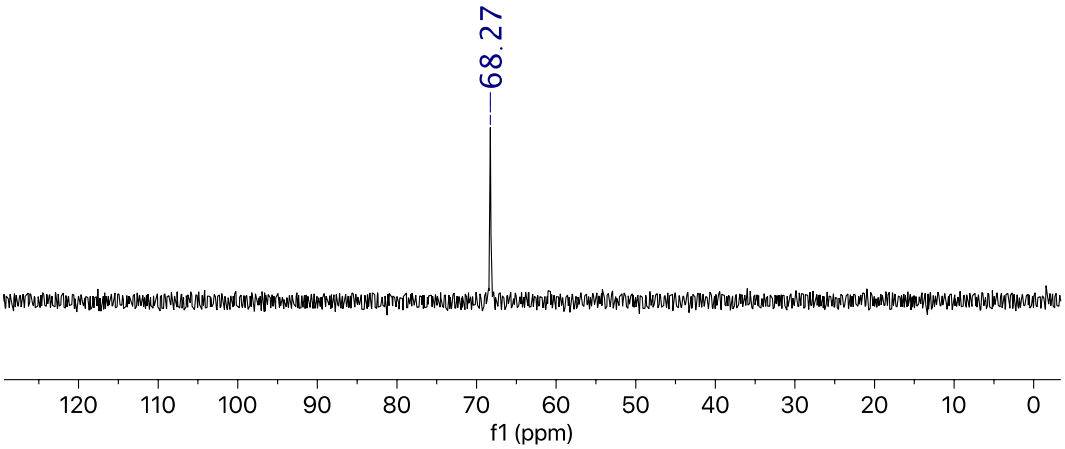

Figure S46. $^{31}P\{^1H\}$ ($CDCl_3$) NMR spectrum of **11**.

2.12 ($tBu_2POBcat)_2(EtO_2CCHN_2$) 12

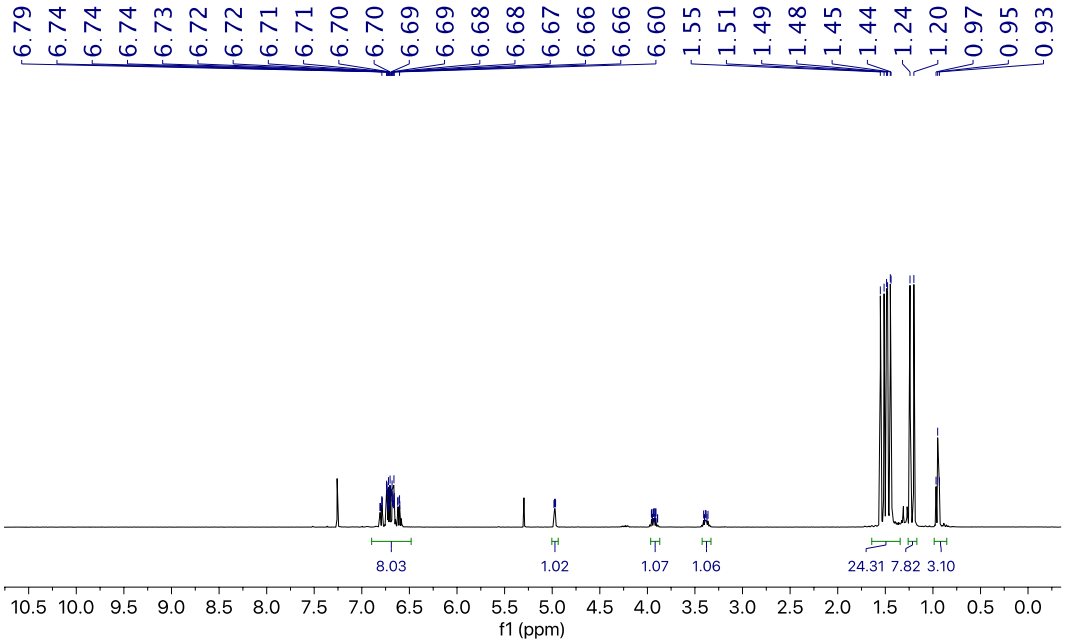

Figure S47. ^1H ($CDCl_3$) NMR spectrum of **12**.

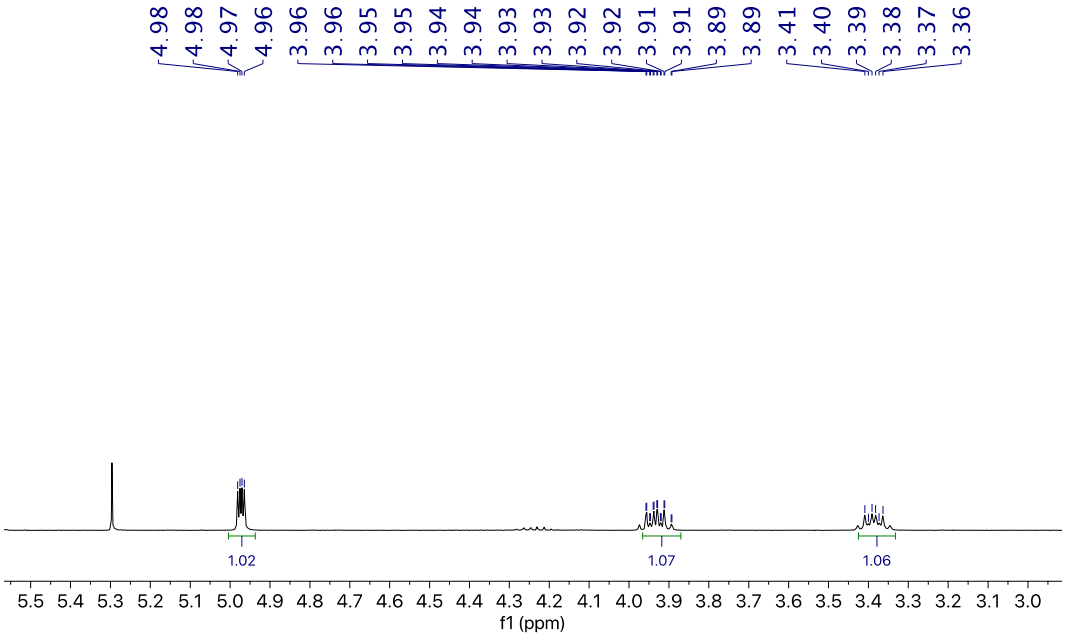

Figure S48. Expanded ^1H ($CDCl_3$) NMR spectrum of **12.**

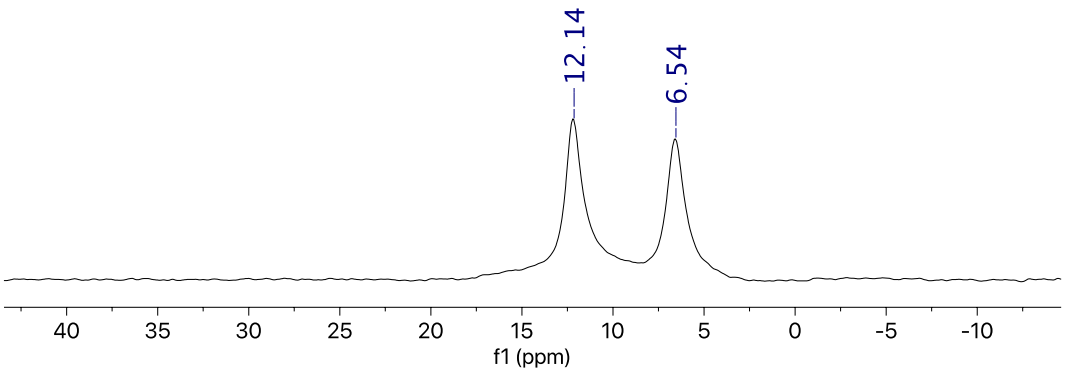

Figure S49. $^{11}B\{^{1}H\}$ ($CDCl_3$) NMR spectrum of **12**.

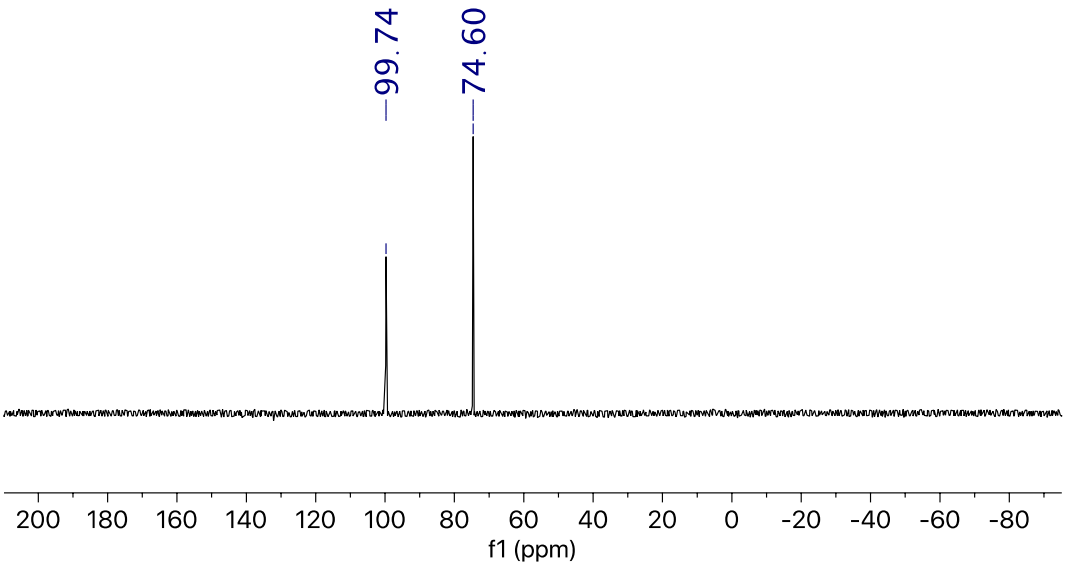

Figure S50. $^{31}P\{^{1}H\}$ ($CDCl_3$) NMR spectrum of**12**.

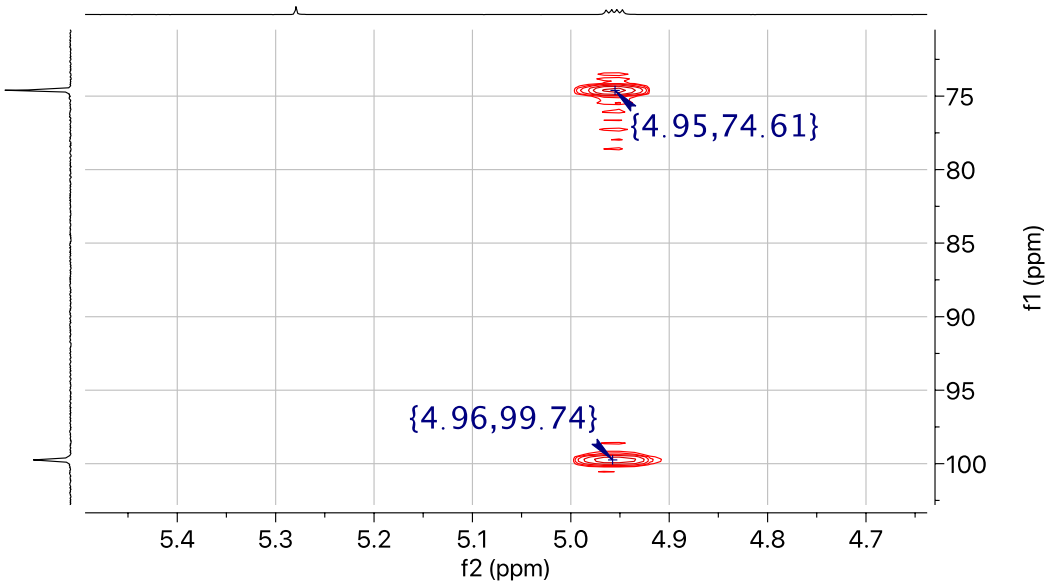

Figure S51. Expansion of HMQC spectrum (400 MHz) of**12** ($CDCl_3$) indicating the assignments of P^1 and P^2 signals.

3.1 Computation Details

All computations were performed using the Gaussian 09 program.[1] The geometry optimization of **1** was performed at the M06-2X functional with the def2-TZVP basis set. The stationary nature of the converged-upon geometry was confirmed by carrying out a frequency calculation and ensuring the absence of imaginary frequencies.

Table S1. Cartesian coordinates (Å) of the optimized structure of compound **1.**

P	-1.61984	0.00574	-0.6043
O	-0.36388	-0.03389	0.52776
C	2.95147	0.00801	-0.64037
C	3.12015	-0.02372	0.74061
C	4.02183	0.033	-1.50705
C	4.36906	-0.03201	1.32237
C	5.29663	0.02483	-0.92903
H	3.88123	0.05765	-2.57916
C	5.46612	-0.00683	0.45348
H	4.49255	-0.05658	2.39661
H	6.16675	0.04375	-1.57219
H	6.46596	-0.0122	0.86752
B	0.95929	-0.02211	0.30332
O	1.88466	-0.0429	1.35063
O	1.60376	0.00957	-0.93469
C	-2.49431	1.57502	-0.00547
C	-2.51853	-1.56429	-0.03832
C	-3.64027	1.8704	-0.9905

H	-4.45608	1.15305	-0.90874
H	-4.051	2.86125	-0.77752
H	-3.29164	1.87189	-2.02576
C	-3.01709	1.5781	1.43506
H	-3.33709	2.58988	1.70371
H	-3.87918	0.92321	1.55872
H	-2.24724	1.27526	2.14603
C	-1.43706	2.68875	-0.15633
H	-0.63273	2.58629	0.57281
H	-0.9965	2.69985	-1.15615
H	-1.91347	3.65887	0.00889
C	-3.91479	-1.60306	-0.67906
H	-4.60478	-0.90745	-0.20123
H	-3.88241	-1.37565	-1.74772
H	-4.33465	-2.60707	-0.57108
C	-2.61899	-1.77862	1.47743
H	-3.29691	-1.07365	1.9538
H	-3.00137	-2.78547	1.67237
H	-1.64489	-1.69502	1.95977
C	-1.67285	-2.70747	-0.64015
H	-1.59354	-2.62407	-1.72566
H	-0.66308	-2.72739	-0.22528
H	-2.14338	-3.66681	-0.40747

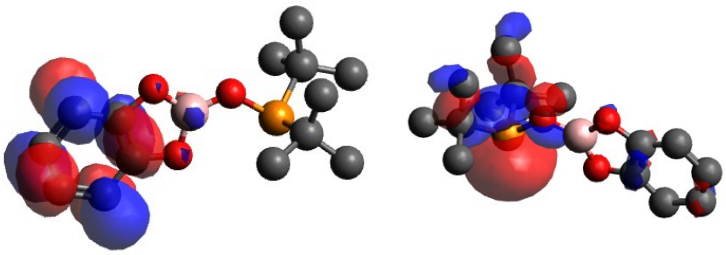

Figure S52. Computed LUMO (left) and HOMO (right) of compound **1**.

3.2 Global Electrophilicity Index (GEI) Calculations

The GEI values of **1**, $Mes_2POB(C_6F_5)_2$, and $Ph_2P(o\text{-}C_6H_4)Bpin$ were calculated using the Gaussian 09 program.[1] The geometry optimizations were carried out at the BP86 functional with the def2-TZVP basis set.[2] The stationary nature of the converged-upon geometry was confirmed by carrying out a frequency calculation and ensuring the absence of imaginary frequencies. The GEI (ω) is defined as $\omega = \mu^2/2\eta$ where μ is the chemical potential and η is the chemical hardness. These terms are defined as μ = 1/2 (E_{HOMO} + E_{LUMO}) and η = (E_{LUMO} − E_{HOMO}).

Table S2. Calculated GEI values (in eV) of **1**, $Mes_2POB(C_6F_5)_2$, and $Ph_2P(o\text{-}C_6H_4)Bpin$.

Compound	HOMO eV	LUMO eV	GEI (ω) eV
1	-6.261	-0.551	1.016
$Mes_2POB(C_6F_5)_2$	-6.055	-1.745	1.766
$Ph_2P(o\text{-}C_6H_4)Bpin$	-6.074	-1.579	1.629

(1) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, M. C. X. Li, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian 09, Revision E.01.* , Wallingford CT, 2016.

(2) (a) A. R. Jupp, T. C. Johnstone and D. W. Stephan, *Dalton Trans.*, 2018, **47**, 7029-7035 ; (b) A. R. Jupp, T. C. Johnstone and D. W. Stephan, *Inorg. Chem.*, 2018, **57**, 14764-14771

3.3 Computational Mechanistic Details

Figure S53. The detailed reaction free energy paths (in kcal/mol, at 298 K and 1 M in CH_2Cl_2 solution) for the reactions of Ph_2CN_2 and EtO_2CHN_2 with the FLP *t*Bu_2POBcat, computed at the PW6B95-D3/def2-QZVP + COSMO-RS // TPSS-D3/def2-TZVP + COSMO level of theory.

Table S3. TPSS-D3/def2-TZVP + COSMO computed lowest imaginary frequency (ImF), zero-point energies (ZPE), gas-phase enthalpic (Hc) and Gibbs free-energy (Gc) corrections; the COSMO-RS computed solvation enthalpic (Hsol) and Gibbs free-energy (Gsol) corrections in CH_2Cl_2 solution; TPSS-D3/def2-QZVP and PW6B95-D3/def2-QZVP single-point energies (TPSS-D3 and PW6B95-D3); the relative electronic energies (ΔET and ΔEP) and Gibbs free-energies (ΔGT and ΔGP) at the TPSS-D3 and PW6B95-D3 levels. Each structure is labeled either by its molecular formula or a specific name in bold. Transition structures (with only one imaginary frequency) are indicated by the "**TS**" prefix. See **Figure S53** for structural labellings.

Table S4. The TPSS-D3/def2-TZVP + COSMO optimized atomic Cartesian coordinates (in Å) in CH_2Cl_2 solution. Each structure is labeled by the specific name (See also **Figure S53** and **Table S3**), followed by the number of atoms, the total energy, and the detailed atomic coordinates (in double-column text list).

Computational Details: The quantum chemical DFT calculations have been performed with the TURBOMOLE 7.3 suite of programs[1] The structures are fully optimized at the TPSS-D3/def2-TZVP + COSMO(CH_2Cl_2) level of theory, which combines the TPSS meta-GGA density

functional[2] with the BJ-damped DFT-D3 dispersion correction[3, 4] and the def2-TZVP basis set,[5, 6] using the Conductor-like Screening Model (COSMO) continuum solvation model[7] for CH_2Cl_2 solvent (dielectric constant ε = 8.93 and solvent diameter R_{solv} = 2.94 Å). The density-fitting RI-J approach[5, 8, 9] is used to accelerate the geometry optimization and numerical harmonic frequency calculations[10] in solution. The optimized structures are characterized by frequency analysis to identify the nature of located stationary points (no imaginary frequency for true minima and only one imaginary frequency for transition state) and to provide thermal corrections (at 298.15 K and 1 atm) according to the modified ideal gas–rigid rotor–harmonic oscillator model.[11] This choice of dispersion-corrected meta-GGA functional makes the efficient exploration of all potential reaction paths possible.

The final solvation free energies in CH_2Cl_2 are computed with the COSMO-RS solvation model[12] (parameter file: BP_TZVP_C30_1601.ctd) using the COSMOtherm program package[13] on the above TPSS-D3 optimized structures, and corrected by +1.89 kcal·mol^{-1} to account for higher reference solute concentration of 1 mol·L^{-1} usually used in solution. To check the effects of the chosen DFT functional on the reaction energies and barriers, single-point calculations at the meta-GGA TPSS-D3[2] and hybrid-meta-GGA PW6B95-D3[14] levels are performed using a larger def2-QZVP basis set.[6, 15] The final reaction Gibbs free energies (ΔG) are determined from the electronic single-point energies plus TPSS-D3 thermal corrections and COSMO-RS solvation free energies. For the low-lying reaction channels, the computed reaction free energies from both DFT functionals are in good mutual agreement of 0.3 $\pm$ 1.0 kcal/mol but the barriers at PW6B95-D3 level are usually 3.3 $\pm$ 2.3 kcal/mol higher (average and standard deviations, see Table S1 below). Somewhat larger deviations of reaction energies and barriers are observed for less important high-lying channels. In our discussion, higher-level PW6B95-D3 Gibbs free energies (in kcal/mol, at 298.15 K and 1 mol/L standard state concentration) will be used in our discussion unless specified otherwise. Meta-GGA functionals like TPSS tend to underestimate reaction barriers that can be evidently improved by using hybrid meta-GGA functionals like PW6B95.

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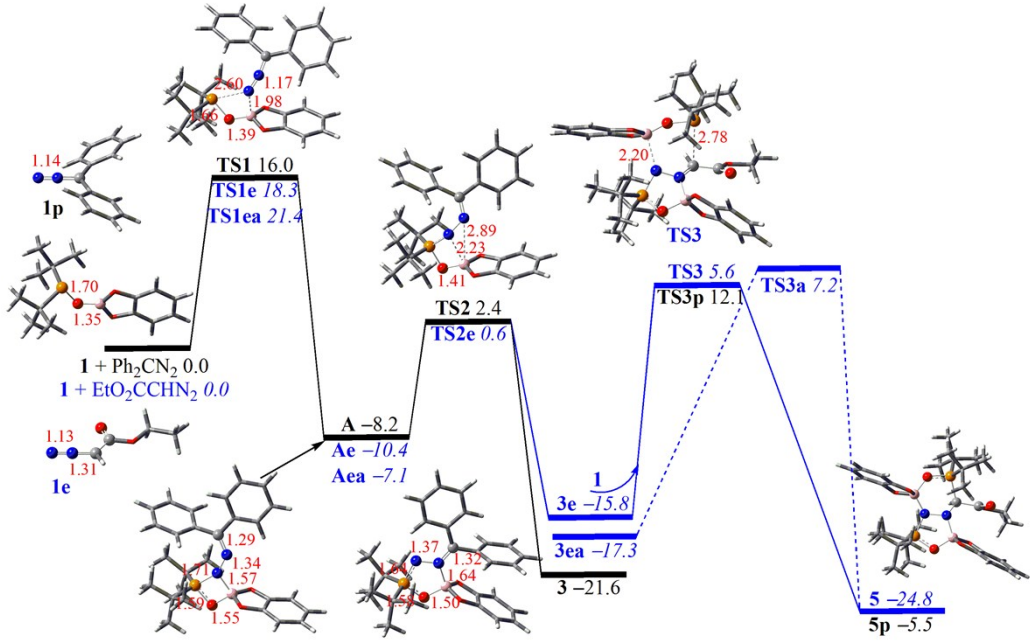
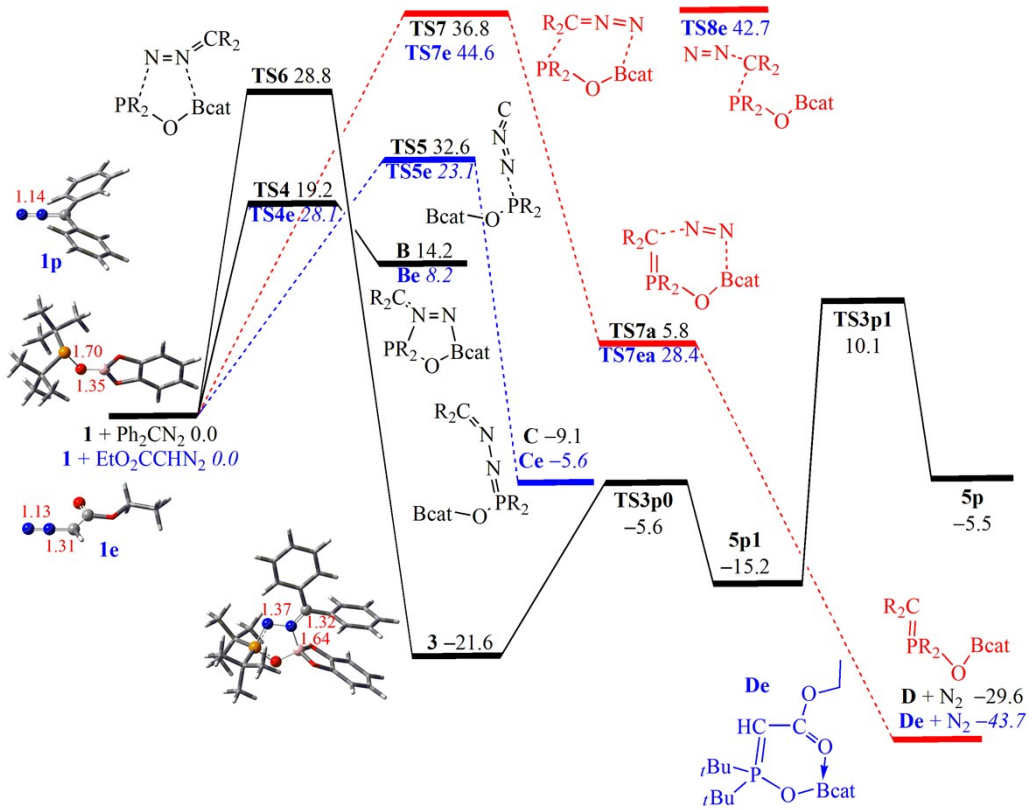


(a)



(b)

Figure S53. The detailed reaction free energy paths in CH_2Cl_2 solution (in kcal/mol, at 298 K and 1 mol/L reference concentration) for the reactions of Ph_2CN_2 (**1p**) and EtO_2CHN_2 (**1e**) with the FLP *t*Bu_2POBcat (**1**), computed at the PW6B95-D3/def2-QZVP + COSMO-RS // TPSS-D3/def2-TZVP + COSMO level of theory: (a) Low-lying competitive reaction channels; (b) unfavorable reaction channels. More detailed energies and brief description of potential reactions are given in SI **Table S3**.

It is clearly seen that the unusual adduct **3** (**3e**) with terminal N of **1p** (**1e**) bound to the Lewis-basic P rather than Lewis-acidic B center of **1** is actaully formed from a two-step mechanism, while further 1,3-addition of 3e and 1 is apparently favored by small steric hindrance of outward H (rather tan bulky ester or phenyl groups). Concerted additions of **1p** (**1e**) and **1** are kinetially less favorable.

Table S3. TPSS-D3/def2-TZVP + COSMO computed lowest imaginary frequency (ImF), zero-point energies (ZPE), gas-phase enthalpic (Hc) and Gibbs free-energy (Gc) corrections; the COSMO-RS computed solvation enthalpic (Hsol) and Gibbs free-energy (Gsol) corrections in CH_2Cl_2 solution; TPSS-D3/def2-QZVP and PW6B95-D3/def2-QZVP single-point energies (TPSS-D3 and PW6B95-D3); the relative electronic energies (ΔET and ΔEP) and Gibbs free-energies (ΔGT and ΔGP) at the TPSS-D3 and PW6B95-D3 levels. Each structure is labeled either by its molecular formula or a specific name in bold. Transition structures (with only one imaginary frequency) are indicated by the "**_ts**" appendix. See also Figure S1 for labellings.

Reactions	ImF cm^{-1}	ZPE kcal/mol	Hc kca/mol	Gc kcal/mol	Hsol kcal/mol	Gsol kcal/mol	TPSS-D3 E_h	PW6B95-D3 E_h	ΔET kcal/mol	ΔEP kcal/mol	ΔGP kcal/mol	ΔGT kcal/mol
*Reaction of Ph_2CN_2 (**1p**) with FLP **1** ($tBu_2POBcat$)*: two-step mechanism to unusual adduct **3**												
1p + **1**	0	333.21	354.83	281.60	-34.71	-24.41	-1750.63332	-1752.40675	0.0	0.0	0.0	0.0
1p.1	0	333.91	356.30	296.46	-28.60	-21.38	-1750.64954	-1752.42356	-10.2	-10.6	5.5	5.8
TS1	-164	333.18	354.92	296.68	-29.52	-22.10	-1750.64137	-1752.40593	-5.1	0.5	16.0	10.5
A	0	335.53	356.74	299.69	-37.14	-28.00	-1750.66775	-1752.43998	-21.6	-20.9	-8.3	-9.0
TS2	-280	334.71	355.88	298.91	-31.68	-23.69	-1750.65460	-1752.42867	-13.4	-13.8	2.4	2.8
3	0	336.03	356.97	300.57	-32.34	-24.31	-1750.69668	-1752.46853	-39.8	-38.8	-21.6	-22.6
*Unfavorable 1,3-addition of **3** and another FLP **1***: stepwise (**TS3p0** and **TS3p1**) or concerted (**TS3p**)												
3 + **1**	0	548.33	582.79	484.46	-51.93	-37.89	-2890.06322	-2892.94853	0.0	0.0	-21.6	0.0
TS3p0	-95	547.85	582.78	500.10	-43.27	-32.57	-2890.07052	-2892.95346	-4.6	-3.1	-5.6	14.5
5p1	0	549.79	584.17	503.25	-42.74	-32.20	-2890.08828	-2892.97441	-15.7	-16.3	-15.2	6.9
TS3p1	-39	548.94	583.03	502.23	-39.60	-30.32	-2890.05901	-2892.93543	2.6	8.2	10.1	26.1
TS3p	-122	547.93	582.84	499.96	-38.91	-29.90	-2890.05109	-2892.92922	7.6	12.1	12.1	29.2
5p	2	550.65	584.58	503.81	-42.11	-32.41	-2890.07574	-2892.95943	-7.9	-6.9	-5.5	15.1
Less competitive channels: usual N=N/BOP addition (**TS4**), N...P attack (**TS5**), concerted unusual addition (**TS6**), 1,3-addition of **1p** (**TS7**)												
1p + **1**	0	333.21	354.83	281.60	-34.71	-24.41	-1750.63332	-1752.40675	0.0	0.0	0.0	0.0
TS4	-50	333.40	354.94	297.20	-30.80	-22.90	-1750.63418	-1752.40044	-0.5	4.0	19.2	14.7
B	0	335.82	356.80	300.38	-39.67	-29.53	-1750.64008	-1752.40289	-4.2	2.4	14.2	7.5
TS5	-194	332.71	354.71	295.23	-32.33	-24.13	-1750.61045	-1752.37403	14.4	20.5	32.6	26.4
C	0	335.36	356.88	298.88	-30.90	-22.92	-1750.67308	-1752.44811	-25.0	-26.0	-9.1	-8.1
TS6	-163	333.29	354.88	296.96	-30.92	-23.15	-1750.61961	-1752.38428	8.6	14.1	28.8	23.3
3	0	336.03	356.97	300.57	-32.34	-24.31	-1750.69668	-1752.46853	-39.8	-38.8	-21.6	-22.6

TS7	-202	333.20	353.91	298.29	-32.21	-24.12	-1750.61073	-1752.37223	14.2	21.7	36.8	29.3
TS7a	-141	333.54	355.00	297.73	-28.90	-21.75	-1750.65690	-1752.42448	-14.8	-11.1	5.8	2.1
D + N_2	0	332.93	355.14	286.65	-30.46	-21.23	-1750.68699	-1752.46711	-33.7	-37.9	-29.7	-25.5
*Reaction of EtO_2CCHN_2 (**1e**) with FLP **1** ($tBu_2POBcat$)*: two-step mechanism to unusual adduct **3e** (selective via **TS1e** vs. **TS1ea**)												
1e + **1**	0	276.72	296.21	227.56	-31.40	-20.89	-1555.58560	-1557.11749	0.0	0.0	0.0	0.0
1e.1	0	276.94	297.42	240.71	-26.99	-19.08	-1555.59418	-1557.12593	-5.4	-5.3	7.8	7.7
TS1ea	-116	276.85	296.50	241.79	-22.96	-16.56	-1555.58715	-1557.10994	-1.0	4.7	21.4	15.7
Aea	0	280.15	298.62	247.09	-31.54	-23.33	-1555.62488	-1557.15302	-24.7	-22.3	-7.1	-9.5
3ea	0	279.55	298.44	245.68	-31.75	-22.62	-1555.63895	-1557.16820	-33.5	-31.8	-17.3	-19.0
TS1e	-113	276.60	296.39	241.13	-31.09	-21.90	-1555.58169	-1557.10536	2.5	7.6	18.3	13.1
Ae	0	279.22	298.11	245.47	-37.16	-27.00	-1555.61881	-1557.14993	-20.8	-20.4	-10.5	-10.9
TS2e	-17	278.47	297.36	244.56	-28.77	-20.21	-1555.60978	-1557.14166	-15.2	-15.2	0.6	0.6
3e	0	279.55	298.33	245.94	-32.72	-23.95	-1555.63424	-1557.16401	-30.5	-29.2	-15.8	-17.1
*favorable concerted 1,3-addition of **3e** and another FLP **1*** (**TS3**)												
3e + **1**	0	491.86	524.15	429.83	-52.31	-37.54	-2695.00078	-2697.64401	0.0	0.0	-15.8	0.0
TS3	-118	492.03	524.42	446.55	-39.90	-29.48	-2695.00822	-2697.64640	-4.7	-1.5	5.6	18.2
5	0	494.33	526.03	449.83	-42.38	-31.61	-2695.05159	-2697.69677	-31.9	-33.1	-24.8	-7.8
TS3a	-113	492.06	524.52	446.26	-39.72	-29.39	-2695.00464	-2697.64354	-2.4	0.3	7.2	20.3
Less competitive channels: usual N=N/BOP addition (**TS4e**), N...P attack (**TS5e**), concerted unusual addition (**TS6**), 1,3-addition of **1p** (**TS7e**)												
1e + **1**	0	276.72	296.21	227.56	-31.40	-20.89	-1555.58560	-1557.11749	0.0	0.0	0.0	0.0
TS4e	-209	277.34	296.64	242.88	-31.29	-22.24	-1555.57392	-1557.09197	7.3	16.0	28.1	19.4
Be	0	279.32	298.21	245.62	-41.04	-29.66	-1555.59319	-1557.11616	-4.8	0.8	8.2	2.6
TS5e	-178	277.35	296.70	243.09	-22.19	-16.01	-1555.58903	-1557.11027	-2.2	4.5	23.1	16.4
Ce	0	278.99	298.31	244.32	-31.19	-21.82	-1555.61578	-1557.14859	-18.9	-19.5	-5.6	-5.0
TS7e	-245	276.47	295.79	241.96	-27.13	-19.42	-1555.55270	-1557.06868	20.7	30.6	44.6	34.6
TS7ea	-386	278.07	296.42	245.24	-28.76	-20.80	-1555.57359	-1557.09752	7.5	12.5	28.4	23.4
TS8e	-518	276.23	296.02	241.26	-24.29	-17.14	-1555.55545	-1557.07425	18.9	27.1	42.7	34.5
De + N_2	0	276.69	296.67	232.38	-29.72	-19.21	-1555.65584	-1557.19745	-44.1	-50.2	-43.7	-37.6

Table S4. The TPSS-D3/def2-TZVP + COSMO optimized atomic Cartesian coordinates (in Å) in CH2Cl2 solution. Each structure is labeled by the specific name (See also **Figure S53** and **Table S3**), followed by the number of atoms, the total energy, and the detailed atomic coordinates (in double-column text list).

1e.1 loose complex of **1e** and **1**

55

Energy = -1555.520890002

N	-1.2215721	-0.4823225	-2.1145612
N	-0.4929577	0.2986348	-1.7348187
C	0.3675339	1.1943949	-1.3235363
C	1.3131124	1.7041125	-2.2974741
H	0.3607367	1.4369326	-0.2701019
O	1.3500836	1.4046909	-3.4850782
O	2.1719320	2.5683772	-1.6984938
C	3.2200742	3.1012081	-2.5686591
C	4.1740268	3.8798850	-1.6874202
H	2.7466507	3.7321705	-3.3263304
H	3.7067837	2.2593213	-3.0676620
H	4.9751435	4.2984360	-2.3053217
H	3.6596657	4.7034483	-1.1832618
H	4.6250571	3.2310776	-0.9302040
B	1.4092585	-2.8942992	-0.8292300
O	0.3323820	-3.5868909	-0.4152346
P	-1.0087031	-3.0227913	0.4665811
O	1.8382265	-1.6442255	-0.3556224
O	2.2799349	-3.3966932	-1.8119081
C	3.0070378	-1.3789389	-1.0561180
C	3.2704423	-2.4315752	-1.9349734
C	3.8401900	-0.2807980	-0.9521841
C	4.3762757	-2.4355553	-2.7655441
C	-0.4498388	-3.4899174	2.2126549
C	-2.2333956	-4.2970849	-0.1829744
C	4.9668362	-0.2719744	-1.7896773
H	3.6289904	0.5304121	-0.2646339
C	5.2271177	-1.3219974	-2.6760237
H	4.5740713	-3.2548750	-3.4486306
C	0.3634298	-2.2646112	2.6895258
C	-1.6845873	-3.6327611	3.1189683
C	0.4368155	-4.7394547	2.3121644
C	-2.2433878	-4.0793475	-1.7128199
C	-1.9121277	-5.7674542	0.1113597
C	-3.6282536	-3.9236568	0.3568962
H	5.6533235	0.5680570	-1.7439569
H	6.1080102	-1.2795149	-3.3092721
H	-0.2474007	-1.3556699	2.6742208
H	0.7045443	-2.4366963	3.7184291
H	1.2425816	-2.0922130	2.0612430
H	-2.3781056	-2.7922475	2.9975276
H	-2.2258701	-4.5626626	2.9245040
H	-1.3589207	-3.6456570	4.1666746

H 1.3111606 -4.6621256 1.6596007
H 0.7955266 -4.8365328 3.3452235
H -0.1026391 -5.6526610 2.0552959
H -3.0413519 -4.6923490 -2.1500851
H -2.4365985 -3.0317498 -1.9668149
H -1.2928807 -4.3751948 -2.1651185
H -0.8946303 -6.0206780 -0.2020712
H -2.0231889 -6.0032630 1.1734100
H -2.6074841 -6.4091738 -0.4458601
H -3.8494999 -2.8640768 0.1843301
H -4.3848967 -4.5173936 -0.1709245
H -3.7292374 -4.1271596 1.4255995

1e $C_2H_5O_2CCHN_2$
14
Energy = -416.2039241017
N -3.5723813 0.0458926 -0.3042481
N -2.5348425 -0.2549958 0.0384189
C -1.3277597 -0.5871998 0.4207249
C -0.2067342 0.1164903 -0.1752047
H -1.2478959 -1.3703091 1.1621780
O -0.2780020 1.0046974 -1.0170143
O 0.9542758 -0.3567451 0.3430639
C 2.1713258 0.2714328 -0.1747586
C 3.3392116 -0.3741513 0.5411696
H 2.1085122 1.3458624 0.0177946
H 2.2045982 0.1097794 -1.2557969
H 4.2730738 0.0693538 0.1806526
H 3.2727478 -0.2103871 1.6210431
H 3.3701707 -1.4506881 0.3474733

1p.1 loose complex of **1p** and **1**
66
Energy = -1750.564627829
B 0.8446142 -0.4170715 -2.6441891
O 1.7938935 -0.4708347 -1.6884475
P 1.4478074 -0.4240714 -0.0153613
O -0.5454512 -0.4394287 -2.4470314
O 1.1656607 -0.3342633 -4.0099806
C -1.0897336 -0.3557949 -3.7192412
C -0.0606981 -0.2944596 -4.6612222
C -2.4237685 -0.3290318 -4.0812208
C -0.3133990 -0.2037686 -6.0179396
C 1.7866797 -2.2233222 0.4268835
C 2.9114933 0.6584227 0.4712536
C -2.6947252 -0.2361787 -5.4559154

H	-3.2179210	-0.3742213	-3.3431260
C	-1.6648068	-0.1756273	-6.4003573
H	0.4889822	-0.1546622	-6.7465759
C	3.2253560	-2.7333687	0.2875028
C	1.2791934	-2.4034299	1.8731535
C	0.8679879	-3.0426463	-0.5048035
C	4.2214331	0.3989600	-0.2872325
C	2.4257321	2.0889835	0.1433983
C	3.1276997	0.5509766	1.9899262
H	-3.7275778	-0.2098042	-5.7893335
H	-1.9117877	-0.1036711	-7.4551381
H	3.8954228	-2.2660596	1.0146954
H	3.2436199	-3.8169361	0.4671567
H	3.6164359	-2.5524204	-0.7182894
H	1.8821194	-1.8465830	2.5956021
H	0.2382524	-2.0746718	1.9636406
H	1.3270772	-3.4664174	2.1410507
H	-0.1628915	-2.6743946	-0.4754050
H	1.2218218	-3.0175928	-1.5403981
H	0.8663005	-4.0884407	-0.1735289
H	4.6735677	-0.5574588	-0.0193870
H	4.0615211	0.4167285	-1.3686243
H	4.9372757	1.1924256	-0.0346747
H	2.1983081	2.2007692	-0.9224507
H	1.5309489	2.3438988	0.7190524
H	3.2157621	2.8063923	0.3993531
H	2.1904174	0.6805578	2.5418586
H	3.5704371	-0.4097262	2.2695534
H	3.8147994	1.3432634	2.3122991
N	-1.4491606	2.2216351	-0.5890872
N	-1.4942343	1.6670807	0.4097894
C	-1.5369835	1.0382732	1.5606202
C	-2.2598941	-0.2425710	1.5824805
C	-0.8037653	1.6605973	2.6708954
C	-2.3591695	-1.0333802	0.4236217
C	-2.8835576	-0.6917971	2.7605242
C	-0.3248957	0.8769906	3.7374428
C	-0.5203888	3.0397433	2.6759032
C	-3.0573434	-2.2378612	0.4464166
H	-1.8638473	-0.7132087	-0.4875069
C	-3.5675518	-1.9057117	2.7789784
H	-2.8424121	-0.0833860	3.6581365
C	0.3983711	1.4591577	4.7756252
H	-0.5020223	-0.1926612	3.7395787
C	0.2138701	3.6123321	3.7104500
H	-0.8816598	3.6692423	1.8670819

C -3.6595331 -2.6867717 1.6242791
H -3.1168281 -2.8376415 -0.4580014
H -4.0399009 -2.2361776 3.7001581
C 0.6741449 2.8281584 4.7711223
H 0.7613273 0.8327889 5.5859970
H 0.4192309 4.6790622 3.6913301
H -4.1940777 -3.6319841 1.6427609
H 1.2418862 3.2774220 5.5805721

1p Ph_2CN_2 (Ph = C_6H_5)
25
Energy = -611.2395455107
N 0.1294649 -0.1212320 -1.5569932
N 1.2695260 -0.0895588 -1.4574385
C 2.5757966 -0.0532147 -1.3433332
C 3.2118626 1.2688186 -1.4663555
C 3.2528779 -1.3386460 -1.1051381
C 2.6122805 2.2988016 -2.2142686
C 4.4261397 1.5353444 -0.8076940
C 2.5917801 -2.4018838 -0.4631988
C 4.5744986 -1.5360435 -1.5451323
C 3.2103271 3.5533099 -2.3015999
H 1.6787579 2.1137159 -2.7389035
C 5.0249484 2.7889773 -0.9097524
H 4.8924107 0.7629404 -0.2048959
C 3.2339856 -3.6215847 -0.2660179
H 1.5736808 -2.2697596 -0.1067740
C 5.2149476 -2.7548566 -1.3332782
H 5.0937714 -0.7376374 -2.0650143
C 4.4230773 3.8054316 -1.6553415
H 2.7313796 4.3333578 -2.8866709
H 5.9627464 2.9739216 -0.3933413
C 4.5512938 -3.8046914 -0.6939747
H 2.7057026 -4.4282165 0.2344046
H 6.2358973 -2.8865022 -1.6806853
H 4.8921115 4.7818959 -1.7305474
H 5.0534866 -4.7538819 -0.5328037

1 $tBu_2POBcat$ (tBu = Me_3C Bcat = $BO_2C_6H_4$)
41
Energy = -1139.312507766
B 0.4188312 -0.6700103 1.7511937
O 0.1892187 0.6462568 1.9369143
P -0.6627620 1.6474641 0.8545806
O 0.0246274 -1.4454925 0.6500358
O 1.1120855 -1.4370394 2.7017027

C	0.4885004	-2.7237284	0.9334330
C	1.1430184	-2.7182735	2.1666125
C	0.3650241	-3.8700955	0.1700454
C	1.7103789	-3.8603870	2.7018438
C	-2.2752918	1.8074480	1.8119192
C	0.4144517	3.1744532	1.0788310
C	0.9363257	-5.0375300	0.7019742
H	-0.1444978	-3.8650458	-0.7878390
C	1.5928493	-5.0324790	1.9370961
H	2.2187164	-3.8493021	3.6602231
C	-2.7945640	0.3569891	1.9295770
C	-2.1977258	2.4307566	3.2101565
C	-3.2551188	2.5949450	0.9188967
C	-0.3301526	4.3922306	0.5056639
C	0.8989690	3.4587297	2.5081228
C	1.6430389	2.8782020	0.1877927
H	0.8654173	-5.9628305	0.1384721
H	2.0232603	-5.9543104	2.3162984
H	-2.7890223	-0.1539260	0.9598207
H	-2.1970874	-0.2281833	2.6359368
H	-3.8268956	0.3778069	2.2996169
H	-1.9862879	3.5024818	3.1621053
H	-3.1635434	2.3046252	3.7173158
H	-1.4294426	1.9470975	3.8213108
H	-4.2593467	2.5426711	1.3575716
H	-2.9795649	3.6492467	0.8360279
H	-3.3036026	2.1706081	-0.0905632
H	-0.7569091	4.1796609	-0.4820348
H	-1.1349882	4.7213462	1.1693229
H	0.3738527	5.2258048	0.3924861
H	1.3532304	2.5709521	2.9563469
H	1.6592528	4.2499823	2.4724621
H	0.0905765	3.8010679	3.1563686
H	2.3263057	3.7361503	0.2173663
H	2.1901131	1.9978450	0.5424765
H	1.3477532	2.7052963	-0.8525910

3ea (*Z*)-1,2-adduct of **1e** and **1**

55

Energy = -1555.568941924

N	-0.9956276	-1.4791674	-0.0084749
N	0.1122899	-1.0331478	-0.6093202
C	0.2457655	0.1654704	-1.1307770
C	-0.7713908	1.2102757	-1.1103827
H	1.1964815	0.3628571	-1.6089133
O	-1.8619604	1.1728376	-0.5601724

O	-0.3156145	2.2806573	-1.8207297
C	-1.2280838	3.4181164	-1.8945323
C	-0.7447435	4.3151235	-3.0145616
H	-1.2131390	3.9235319	-0.9230686
H	-2.2372365	3.0388304	-2.0722183
H	-1.4043545	5.1861351	-3.0870061
H	0.2743619	4.6668297	-2.8275690
H	-0.7653052	3.7836854	-3.9709445
B	1.3828566	-2.0739912	-0.6897647
O	0.8031676	-3.2826969	-0.0483812
P	-0.6687866	-3.0335443	0.4786932
O	2.5293903	-1.5358551	0.0375542
O	1.7993517	-2.2912214	-2.0693979
C	3.5617801	-1.4936595	-0.8659767
C	3.1276257	-1.9425656	-2.1213700
C	4.8671928	-1.0855296	-0.6519974
C	3.9836821	-1.9980079	-3.2082517
C	-0.6141525	-3.1212088	2.3165699
C	-1.8402155	-4.1490454	-0.3949089
C	5.7444041	-1.1373140	-1.7509533
H	5.1967742	-0.7421206	0.3237771
C	5.3120919	-1.5831639	-3.0013432
H	3.6407547	-2.3468558	-4.1772652
C	0.2132772	-1.8917205	2.7549539
C	-2.0255004	-3.0441991	2.9237278
C	0.1099491	-4.4079424	2.7599607
C	-1.4514975	-4.0511818	-1.8875595
C	-1.7241532	-5.6043265	0.0888161
C	-3.2796341	-3.6206423	-0.2147987
H	6.7760212	-0.8233850	-1.6201030
H	6.0108686	-1.6113448	-3.8324017
H	-0.2966528	-0.9591694	2.5002211
H	0.3380041	-1.9393320	3.8422033
H	1.2065222	-1.8893134	2.2962577
H	-2.5763385	-2.1720805	2.5579095
H	-2.6062144	-3.9469313	2.7159324
H	-1.9269889	-2.9516945	4.0109910
H	1.1029505	-4.4784095	2.3083219
H	0.2285995	-4.3715971	3.8484471
H	-0.4565035	-5.3079763	2.5125127
H	-2.1532380	-4.6677303	-2.4595631
H	-1.5270197	-3.0218891	-2.2505081
H	-0.4370123	-4.4147011	-2.0674318
H	-0.6962098	-5.9739974	0.0237954
H	-2.0802646	-5.7185663	1.1161959
H	-2.3508556	-6.2325253	-0.5539172

H -3.3508685 -2.5675384 -0.4999809
H -3.9377484 -4.2051528 -0.8674795
H -3.6360525 -3.7348400 0.8109772

3e (*E*)-1,2-adduct of **1e** and **1**
55
Energy = -1555.564490161
N -0.5481390 -1.0110186 0.3688805
N 0.7111233 -0.6215765 0.0806652
C 0.9530173 0.6699207 0.0919046
C 2.2528863 1.2920870 -0.1375100
H 0.1128378 1.3162842 0.3184043
O 3.3306072 0.7654970 -0.3486860
O 2.0798288 2.6476802 -0.0684753
C 3.2955782 3.4280963 -0.2781017
C 2.9153381 4.8905029 -0.1748199
H 3.7002282 3.1710270 -1.2615178
H 4.0255895 3.1326074 0.4813111
H 2.1774566 5.1577165 -0.9374847
H 2.5017270 5.1184508 0.8123746
H 3.8077205 5.5065368 -0.3263489
B 1.7736369 -1.8508198 -0.2713090
O 0.8607385 -3.0395728 -0.1672301
P -0.6213431 -2.6570509 0.1959692
O 2.8681053 -1.9558071 0.6758125
O 2.3299533 -1.7301709 -1.6075527
C 4.0018205 -2.0438806 -0.0930271
C 3.6822605 -1.9117550 -1.4514097
C 5.3049648 -2.2324726 0.3296593
C 4.6537881 -1.9623127 -2.4339653
C -1.0801449 -3.3777561 1.8248425
C -1.6721069 -3.1083892 -1.2488958
C 6.3023391 -2.2861927 -0.6622288
H 5.5468556 -2.3290869 1.3838751
C 5.9837864 -2.1540488 -2.0146935
H 4.3994895 -1.8537802 -3.4841281
C 0.1250856 -3.0862832 2.7469591
C -2.3249955 -2.6532283 2.3793648
C -1.3222070 -4.8946449 1.7392288
C -3.1686444 -2.9201659 -0.9469449
C -1.2377107 -2.1462092 -2.3773868
C -1.3741868 -4.5593004 -1.6797566
H 7.3369587 -2.4341915 -0.3653613
H 6.7728639 -2.1993360 -2.7601873
H 1.0354672 -3.5738928 2.3908709
H 0.3116964 -2.0112186 2.8280660

H -0.1140284 -3.4694515 3.7449620
H -2.1740718 -1.5705082 2.3979866
H -3.2256105 -2.8757333 1.8032517
H -2.4871751 -2.9988146 3.4064519
H -0.4714770 -5.4183840 1.2926048
H -1.4591636 -5.2784489 2.7563543
H -2.2250375 -5.1305409 1.1694034
H -3.5328601 -3.6538774 -0.2226504
H -3.3842052 -1.9138890 -0.5744326
H -3.7283351 -3.0630746 -1.8780358
H -1.4866197 -1.1100608 -2.1343166
H -0.1631881 -2.2157785 -2.5732958
H -1.7722293 -2.4312714 -3.2902229
H -1.9174928 -4.7535545 -2.6113673
H -0.3070321 -4.7042919 -1.8681352
H -1.7052600 -5.2898007 -0.9388742

3 1,2-adduct of **1p** and **1**
66
Energy = -1750.613591009
B 0.1954733 -1.0370700 -0.1271317
O -1.0868087 -1.7729206 -0.3542677
P -2.3366864 -0.8076551 -0.3323259
O 1.1418608 -1.2902273 -1.2095948
O 0.8335072 -1.4629246 1.1208764
C 2.2202056 -1.9032011 -0.6289601
C 2.0344285 -2.0104442 0.7577448
C 3.3706820 -2.3684481 -1.2421543
C 2.9898069 -2.5897251 1.5745645
C -3.2180207 -0.8957261 -1.9461680
C -3.3190290 -1.2537260 1.1668072
C 4.3486800 -2.9553963 -0.4193905
H 3.5142617 -2.2689413 -2.3136126
C 4.1622099 -3.0640867 0.9597121
H 2.8421175 -2.6598773 2.6479536
C -3.9920642 -2.2123025 -2.1261721
C -4.1602129 0.3185876 -2.0834268
C -2.1048841 -0.7865095 -3.0122346
C -3.5316893 -2.7794460 1.2322774
C -2.4397647 -0.8151558 2.3591920
C -4.6637657 -0.5087585 1.2131772
H 5.2662363 -3.3251385 -0.8683506
H 4.9357126 -3.5180477 1.5729924
H -4.8466175 -2.2776472 -1.4470363
H -4.3769949 -2.2509358 -3.1515860
H -3.3496385 -3.0850257 -1.9737851

H	-5.0077432	0.2657454	-1.3965780
H	-3.6192059	1.2529553	-1.9093317
H	-4.5544231	0.3308385	-3.1059881
H	-1.5420968	0.1445737	-2.8967030
H	-1.4075722	-1.6256915	-2.9565133
H	-2.5790728	-0.7851202	-4.0000130
H	-4.1860462	-3.1431383	0.4372427
H	-2.5782245	-3.3115837	1.1757990
H	-4.0032034	-3.0185159	2.1924736
H	-1.4534821	-1.2878997	2.3259265
H	-2.3080217	0.2698979	2.3738931
H	-2.9400803	-1.1239233	3.2840114
H	-4.5311700	0.5718617	1.0981419
H	-5.3544416	-0.8656561	0.4440561
H	-5.1278938	-0.6896913	2.1894233
N	-1.6715356	0.6817815	-0.1962813
N	-0.3165153	0.5190148	-0.0539206
C	0.4923887	1.5486742	0.1256305
C	0.0834163	2.9541520	0.2360181
C	1.9553104	1.2535160	0.2113120
C	-1.2548529	3.4178233	0.2284471
C	1.1051448	3.9262993	0.3734315
C	2.5668487	1.0466201	1.4523435
C	2.7435584	1.2659219	-0.9457468
C	-1.5384571	4.7765039	0.3547457
H	-2.0538237	2.6998585	0.1229886
C	0.8112693	5.2791326	0.4932735
H	2.1415258	3.6092724	0.3850770
C	3.9425863	0.8339347	1.5332781
H	1.9577196	1.0343468	2.3509035
C	4.1184887	1.0552014	-0.8640119
H	2.2702525	1.4236196	-1.9099409
C	-0.5159110	5.7166362	0.4851839
H	-2.5755583	5.1018162	0.3481793
H	1.6224457	5.9947808	0.5940622
C	4.7209106	0.8374349	0.3759845
H	4.4030559	0.6535863	2.5002146
H	4.7170802	1.0490502	-1.7703809
H	-0.7473502	6.7739761	0.5787551
H	5.7907108	0.6605146	0.4381771

5p1 B...N adduct of **3** and **1**
107
Energy = -2889.947967508

B	1.7084790	-1.6060994	-0.1423642
O	0.7976416	-2.7732983	-0.1998934

P	-0.7446365	-2.4372851	-0.1318937
O	2.1168797	-1.1699530	-1.4799237
O	2.9172405	-1.8866831	0.6153500
C	3.4866899	-1.1970614	-1.4790847
C	3.9645254	-1.6216962	-0.2307133
C	4.3476857	-0.8331494	-2.5004748
C	5.3186412	-1.6976826	0.0414432
C	-1.3507462	-2.5619317	-1.8952855
C	-1.4310832	-3.6898862	1.0412131
C	5.7259406	-0.9054952	-2.2328767
H	3.9705165	-0.4930600	-3.4599734
C	6.2005986	-1.3265970	-0.9884830
H	5.6805855	-2.0101818	1.0158806
C	-2.8194136	-2.9903263	-2.0338587
C	-1.1151362	-1.2018784	-2.5735732
C	-0.4534517	-3.6090666	-2.6040681
C	-1.1129999	-5.0857947	0.4604092
C	-0.6720149	-3.4932134	2.3676231
C	-2.9358037	-3.5606768	1.3167729
H	6.4315252	-0.6227572	-3.0088419
H	7.2709562	-1.3654556	-0.8080474
H	-3.4908140	-2.3011911	-1.5244820
H	-3.0626648	-2.9853972	-3.1024596
H	-2.9861904	-4.0056097	-1.6637681
H	-1.7432522	-0.4172043	-2.1495333
H	-0.0654573	-0.9083593	-2.5059633
H	-1.3647934	-1.3148875	-3.6353259
H	0.5905998	-3.2927874	-2.6189783
H	-0.5173744	-4.6004297	-2.1504938
H	-0.8140485	-3.6855347	-3.6360823
H	-1.7021817	-5.3004386	-0.4345501
H	-0.0506414	-5.1994916	0.2289130
H	-1.3803214	-5.8270060	1.2216101
H	-0.9683579	-2.5516065	2.8334703
H	-0.9491164	-4.3130293	3.0391203
H	0.4127845	-3.5114527	2.2319723
H	-3.1745089	-2.6166434	1.8084059
H	-3.5427644	-3.6456063	0.4154740
H	-3.2162277	-4.3752649	1.9944721
N	-0.6056549	-0.8965603	0.5488162
N	0.7575749	-0.5549482	0.6456027
C	1.1805327	0.3642859	1.4890719
C	2.5290533	0.9250268	1.3315579
C	0.4001860	0.8149376	2.6591206
C	3.0299154	1.2961579	0.0734744
C	3.3100491	1.1665542	2.4781863

C	0.1166817	2.1685772	2.8729087
C	0.0675983	-0.1249024	3.6428227
C	4.2903691	1.8759938	-0.0387563
H	2.4123286	1.1574551	-0.8041037
C	4.5779274	1.7211337	2.3571479
H	2.9224681	0.8945911	3.4548564
C	-0.5500809	2.5666854	4.0270893
H	0.3970884	2.8983750	2.1227290
C	-0.5689832	0.2801772	4.8118323
H	0.3369820	-1.1642754	3.4978474
C	5.0710315	2.0795788	1.0974402
H	4.6635711	2.1594549	-1.0175381
H	5.1830656	1.8803453	3.2447655
C	-0.8969207	1.6235509	4.9972705
H	-0.7940934	3.6147360	4.1739453
H	-0.8130507	-0.4536464	5.5743842
H	6.0588693	2.5219010	1.0070239
H	-1.4097769	1.9382982	5.9016986
B	-1.8093518	0.1292218	0.6511748
O	-1.3691823	1.4206994	0.1809249
P	-2.0495995	2.3131628	-1.0374540
O	-2.3725177	0.1960903	2.0346524
O	-2.8884578	-0.5421092	-0.1428301
C	-3.6743029	-0.1659941	1.9557293
C	-4.0020126	-0.5819588	0.6559699
C	-4.6271619	-0.1571484	2.9635901
C	-5.2816186	-0.9790563	0.3138942
C	-3.0085301	3.6599791	-0.1011920
C	-0.4766725	3.1085171	-1.7316186
C	-5.9296796	-0.5707860	2.6300942
H	-4.3719275	0.1647625	3.9687892
C	-6.2538238	-0.9693713	1.3322240
H	-5.5276340	-1.2866391	-0.6979432
C	-3.9334895	2.8945768	0.8614211
C	-2.2079441	4.6803317	0.7169153
C	-3.8911470	4.3835455	-1.1374477
C	-0.8597076	4.2454731	-2.6923933
C	0.5369317	3.6010253	-0.6912840
C	0.1923742	1.9850415	-2.5477742
H	-6.6978958	-0.5723007	3.3987158
H	-7.2696247	-1.2761453	1.0995949
H	-3.3603374	2.4312049	1.6672114
H	-4.6537748	3.5967530	1.3019772
H	-4.4981491	2.1094110	0.3462933
H	-2.9007063	5.2841236	1.3202238
H	-1.5165225	4.1815732	1.4016139

H -1.6428425 5.3666212 0.0800191
H -4.6132311 5.0240185 -0.6139168
H -3.3094200 5.0166565 -1.8124793
H -4.4516263 3.6631723 -1.7437991
H -1.6469759 3.9354368 -3.3903206
H -1.2035031 5.1336699 -2.1543759
H 0.0189139 4.5328070 -3.2847514
H 0.7233970 2.8258821 0.0544715
H 1.4917607 3.8222986 -1.1869082
H 0.2070838 4.5062886 -0.1802582
H 1.1074909 2.3688756 -3.0183959
H 0.4667417 1.1427187 -1.9070655
H -0.4709381 1.6123641 -3.3352799

5p 1,3-adduct of **3** and **1**
107
Energy = -2889.936033247
B 1.5798366 -1.4263914 -0.3486844
O 0.7765301 -2.6431993 0.0204457
P -0.7580071 -2.3969832 0.1813853
O 2.1663488 -1.6800127 -1.7034729
O 2.7337186 -1.3211544 0.5626962
C 3.5040249 -1.8533335 -1.5116400
C 3.8418885 -1.6312658 -0.1649546
C 4.4745883 -2.1444248 -2.4582299
C 5.1546411 -1.6980982 0.2726893
C -1.5568325 -3.3176425 -1.2232947
C -1.1789685 -3.0544213 1.8757833
C 5.8097688 -2.2199340 -2.0194054
H 4.2109204 -2.2999420 -3.5002536
C 6.1431515 -2.0013177 -0.6810210
H 5.4070955 -1.5116232 1.3123179
C -3.0846033 -3.4077975 -1.0919137
C -1.1394927 -2.5794393 -2.5143676
C -0.9524152 -4.7402613 -1.3126923
C -1.2661117 -4.5934752 1.8734952
C 0.0051205 -2.6514534 2.7775147
C -2.4896043 -2.4797699 2.4351197
H 6.5921598 -2.4498351 -2.7377148
H 7.1819828 -2.0620545 -0.3682418
H -3.5571555 -2.4274446 -1.0157539
H -3.4819390 -3.9011762 -1.9865865
H -3.3781767 -4.0049685 -0.2236018
H -1.5924838 -1.5919407 -2.5785258
H -0.0509107 -2.4861811 -2.5771030
H -1.4813732 -3.1829039 -3.3637129

H	0.1400682	-4.7099572	-1.3019054
H	-1.3018938	-5.4047558	-0.5236670
H	-1.2737559	-5.1628288	-2.2715914
H	-2.1440610	-4.9614917	1.3373363
H	-0.3665053	-5.0565018	1.4596860
H	-1.3571711	-4.9121577	2.9187872
H	0.2068357	-1.5824188	2.7357425
H	-0.2557193	-2.9111045	3.8096901
H	0.9137918	-3.1856945	2.4932838
H	-2.4380046	-1.3979907	2.5431603
H	-3.3478382	-2.7179171	1.8009154
H	-2.6551986	-2.9310370	3.4209068
N	-0.7993278	-0.7373402	-0.0363595
N	0.5733836	-0.2329179	-0.2966560
C	0.8957577	0.9954286	0.4793001
C	2.2817175	1.5602673	0.1307025
C	0.6940289	0.8044599	1.9883691
C	3.0126614	1.1557522	-0.9892012
C	2.8126376	2.5961873	0.9158511
C	-0.5781791	0.7824300	2.5773090
C	1.8012870	0.5251245	2.8042230
C	4.2481324	1.7264257	-1.2912811
H	2.6194064	0.3877529	-1.6375600
C	4.0327842	3.1908373	0.6011739
H	2.2845282	2.9298010	1.8005574
C	-0.7330142	0.5471630	3.9446091
H	-1.4637194	0.9637079	1.9839163
C	1.6468392	0.2868529	4.1679398
H	2.7884245	0.4768463	2.3625817
C	4.7654220	2.7514908	-0.5025690
H	4.8000391	1.3618576	-2.1524008
H	4.4146967	3.9886872	1.2317329
C	0.3774142	0.3092866	4.7500857
H	-1.7310915	0.5462314	4.3736049
H	2.5226715	0.0776421	4.7761003
H	5.7259112	3.2002276	-0.7387399
H	0.2573426	0.1271152	5.8143100
B	-2.0371981	0.1124516	-0.3338804
O	-1.6929801	1.5710274	-0.2171953
P	-0.3037441	2.2855718	-0.2830333
O	-3.1051214	-0.1827124	0.6459866
O	-2.7082384	-0.0379530	-1.6651609
C	-4.2849395	-0.1886897	-0.0380782
C	-4.0458043	-0.0994583	-1.4194415
C	-5.5665191	-0.3120962	0.4722051
C	-5.0877986	-0.1275773	-2.3332651

C	0.0137996	2.6062925	-2.1180293
C	-0.5905913	3.9064864	0.6540964
C	-6.6294392	-0.3348178	-0.4497800
H	-5.7399652	-0.3905625	1.5415464
C	-6.3939015	-0.2438346	-1.8231497
H	-4.8996370	-0.0679294	-3.4010360
C	0.0829791	1.2548655	-2.8669800
C	-1.2434812	3.3344266	-2.6540658
C	1.2515289	3.4574586	-2.4766566
C	0.3043295	5.0407587	0.1191861
C	-2.0782399	4.2889382	0.4597845
C	-0.3764597	3.8048768	2.1783379
H	-7.6482278	-0.4256479	-0.0832522
H	-7.2324376	-0.2643391	-2.5138238
H	-0.8019841	0.6467555	-2.6783123
H	0.1069020	1.4980553	-3.9368340
H	0.9642449	0.6708381	-2.6171985
H	-1.1493953	3.3664264	-3.7455454
H	-2.1630907	2.7996688	-2.4047589
H	-1.3078842	4.3655770	-2.3001033
H	1.4428556	3.3102931	-3.5458018
H	1.0738760	4.5208621	-2.3194321
H	2.1503518	3.1682866	-1.9356938
H	1.3641557	4.7748116	0.1206755
H	0.0158598	5.3450788	-0.8876854
H	0.1693059	5.9063867	0.7767517
H	-2.7388740	3.5293334	0.8810987
H	-2.2368096	5.2309257	0.9975933
H	-2.3494643	4.4446435	-0.5839876
H	-0.5342917	4.8119980	2.5812062
H	-1.0959844	3.1355485	2.6472863
H	0.6250403	3.4818293	2.4611260

5 1,3-adduct of **3e** and **1**

96

Energy = -2694.922988750

N	-0.8258162	-0.5352348	0.1165175
N	0.5774768	-0.1298354	0.2449157
C	0.8634410	1.0310262	-0.6033022
C	2.3521985	1.3352512	-0.7154252
H	0.4594597	0.9269219	-1.6179169
O	3.1089332	1.5169593	0.2197367
O	2.6906113	1.4759290	-2.0115259
C	4.1038771	1.7631131	-2.2737313
C	4.3752004	1.3823582	-3.7133783
H	4.7003490	1.1856498	-1.5656427

H	4.2667515	2.8292346	-2.0861186
H	5.4237863	1.5895484	-3.9500583
H	4.1858431	0.3163365	-3.8709629
H	3.7460595	1.9573649	-4.3995161
B	1.5048036	-1.3644656	0.1342141
O	0.6043815	-2.4818591	-0.3614856
P	-0.9175086	-2.1077535	-0.4070448
O	2.1366110	-1.7518679	1.4174126
O	2.6126928	-1.1942911	-0.8256517
C	3.4669116	-1.8714102	1.1700183
C	3.7559902	-1.5472250	-0.1671280
C	4.4725778	-2.2476943	2.0484549
C	5.0465016	-1.5977409	-0.6664317
C	-1.7514415	-3.2174163	0.8143295
C	-1.4329242	-2.3096885	-2.1818805
C	5.7878498	-2.2969305	1.5502209
H	4.2490028	-2.4951742	3.0820962
C	6.0707379	-1.9810461	0.2198557
H	5.2577027	-1.3570048	-1.7042390
C	-1.0242023	-2.9538777	2.1518003
C	-3.2580783	-2.9914198	1.0071358
C	-1.5006749	-4.6736683	0.3655755
C	-0.9021788	-1.0589068	-2.9120444
C	-0.7486547	-3.5543276	-2.7864056
C	-2.9585211	-2.3978528	-2.3512501
H	6.5954429	-2.5895441	2.2158085
H	7.0945700	-2.0311885	-0.1402745
H	0.0525635	-3.1207344	2.0697692
H	-1.2001214	-1.9307865	2.4939636
H	-1.4326284	-3.6491665	2.8944527
H	-3.8266143	-3.1161776	0.0846943
H	-3.6127981	-3.7390042	1.7266485
H	-3.4723176	-2.0062659	1.4196098
H	-0.4449904	-4.8576445	0.1474307
H	-1.8014503	-5.3331050	1.1874547
H	-2.1009233	-4.9374753	-0.5095384
H	-1.4010899	-0.1536900	-2.5571370
H	0.1803567	-0.9518528	-2.7831365
H	-1.1050634	-1.1739834	-3.9825898
H	-1.1029538	-4.4835899	-2.3361715
H	-0.9886685	-3.5851776	-3.8557591
H	0.3366692	-3.4998799	-2.6739878
H	-3.4659530	-1.5727243	-1.8446749
H	-3.1899423	-2.3449654	-3.4214867
H	-3.3497167	-3.3465618	-1.9735798
B	-1.9230122	0.3763404	0.6094576

O	-1.5279682	1.8143536	0.3182322
P	-0.1083249	2.4321136	0.1524946
O	-2.2549484	0.3061866	2.0618929
O	-3.1912222	0.1098000	-0.0989524
C	-3.6153392	0.3418278	2.1278645
C	-4.1774229	0.2267788	0.8441795
C	-4.4154697	0.4303663	3.2566814
C	-5.5478048	0.1943706	0.6515653
C	0.4770393	2.9661715	1.8317845
C	-0.3301939	3.7759895	-1.1033749
C	-5.8091881	0.4044741	3.0690337
H	-3.9769454	0.5110501	4.2467627
C	-6.3649252	0.2895148	1.7932310
H	-5.9724280	0.0945663	-0.3429793
C	1.6012384	4.0152038	1.7589264
C	-0.7458382	3.5553779	2.5750588
C	0.9571811	1.7328980	2.6308643
C	-1.2105224	4.8963451	-0.5141524
C	1.0092070	4.3560850	-1.5954880
C	-1.0761343	3.1391473	-2.2994336
H	-6.4617394	0.4744295	3.9350216
H	-7.4448758	0.2704815	1.6761389
H	1.2556958	4.9550427	1.3196134
H	2.4679409	3.6494616	1.2045097
H	1.9215232	4.2282634	2.7850041
H	-0.4072567	3.8210201	3.5831201
H	-1.1376816	4.4578294	2.1026845
H	-1.5457606	2.8170367	2.6585277
H	1.8311405	1.2670301	2.1780404
H	1.2175031	2.0946084	3.6340017
H	0.1657382	0.9870824	2.7243976
H	-1.4589282	5.5908238	-1.3244813
H	-2.1444680	4.5029829	-0.1030475
H	-0.6865321	5.4608047	0.2611711
H	1.6175947	3.5968480	-2.0914403
H	0.7852780	5.1378493	-2.3299897
H	1.5916218	4.8094748	-0.7917332
H	-1.3073784	3.9387618	-3.0115972
H	-2.0105825	2.6679223	-1.9858022
H	-0.4595847	2.3999561	-2.8188700

Aea (*Z*)-1,1-adduct of **1e** and **1**
55
Energy = -1555.557010471

B	1.7485274	-0.2093715	-0.0833034
O	0.9772076	-1.5028338	0.0290960

P	-0.5077162	-0.8605297	0.0499431
O	2.6193351	-0.1150447	-1.2576538
O	2.5812391	0.0980685	1.0857601
C	3.8528429	0.2539378	-0.7930401
C	3.8270159	0.3845114	0.6048823
C	5.0074153	0.4880583	-1.5217877
C	4.9544726	0.7596758	1.3170444
C	-1.2865315	-1.6608363	-1.4447496
C	-1.1381942	-1.2846299	1.7613345
C	6.1576118	0.8719741	-0.8052196
H	5.0215004	0.3848708	-2.6031071
C	6.1315263	1.0051499	0.5844284
H	4.9255615	0.8639063	2.3976806
C	-1.0097506	-3.1772417	-1.3022279
C	-2.7902390	-1.4554476	-1.6749755
C	-0.5024456	-1.0990529	-2.6502747
C	-0.3561433	-2.5228629	2.2555033
C	-0.7858518	-0.0866506	2.6670408
C	-2.6414162	-1.5984601	1.8321865
H	7.0792952	1.0678942	-1.3465733
H	7.0323060	1.3053907	1.1125924
H	-1.5971962	-3.6196183	-0.4912054
H	-1.3169382	-3.6590270	-2.2371547
H	0.0485441	-3.3836404	-1.1334435
H	-3.0295053	-0.4205423	-1.9174973
H	-3.0740353	-2.0831751	-2.5281242
H	-3.3905910	-1.7595254	-0.8162963
H	-0.6987863	-0.0312858	-2.7872798
H	0.5748422	-1.2466976	-2.5431820
H	-0.8404285	-1.6299001	-3.5474879
H	-0.5322698	-3.3978536	1.6240255
H	0.7166497	-2.3325760	2.2965492
H	-0.7165808	-2.7533188	3.2645795
H	0.2808419	0.1511802	2.6154794
H	-1.3606218	0.8033092	2.4018475
H	-1.0288839	-0.3592286	3.7005685
H	-3.2557349	-0.7698312	1.4815446
H	-2.8901654	-2.4972567	1.2591873
H	-2.8888278	-1.7978973	2.8806390
N	0.3990376	0.5975266	-0.1569748
N	0.2616978	1.8977064	-0.2865199
C	-0.8781710	2.5322973	-0.2860467
C	-2.1543636	1.8865416	-0.1092306
H	-0.8351869	3.6085724	-0.4058852
O	-2.2965219	0.6580299	0.0370699
O	-3.1934037	2.7286122	-0.0990560

C -4.5215189 2.1345333 0.1149103
C -5.5204970 3.2710540 0.1187758
H -4.4964755 1.5972687 1.0664193
H -4.7012194 1.4197612 -0.6918613
H -6.5227138 2.8615037 0.2799693
H -5.3030185 3.9805098 0.9225980
H -5.5124382 3.8027947 -0.8372090

Ae (*E*)-1,1-adduct of **1e** and **1**
55
Energy = -1555.554952017
B 1.9624083 -0.1190378 -0.0903484
O 1.2297434 -1.4956451 0.1661740
P -0.2233048 -0.8939540 0.0259115
O 2.8271326 -0.1478618 -1.2550442
O 2.7627828 0.3015977 1.0454211
C 4.0769426 0.1968662 -0.8063651
C 4.0384873 0.4663387 0.5691632
C 5.2517729 0.2938846 -1.5330968
C 5.1727334 0.8434719 1.2683952
C -1.0692936 -1.5643870 -1.4635079
C -1.1057326 -1.0245905 1.6400267
C 6.4099538 0.6751801 -0.8314657
H 5.2748538 0.0844818 -2.5980940
C 6.3712955 0.9440458 0.5387646
H 5.1356909 1.0532212 2.3330171
C -1.5852150 -2.9903312 -1.1855005
C -2.2243740 -0.6404888 -1.9009977
C -0.0003698 -1.6025770 -2.5770510
C -0.8912076 -2.4590187 2.1768183
C -0.4073828 -0.0180658 2.5809146
C -2.6091896 -0.7138480 1.5500467
H 7.3500209 0.7604456 -1.3688988
H 7.2815050 1.2365033 1.0543822
H -2.4005546 -2.9986604 -0.4575372
H -1.9712159 -3.3987153 -2.1260280
H -0.7851700 -3.6489843 -0.8346540
H -1.8590172 0.3541560 -2.1708694
H -2.6857923 -1.0793595 -2.7923091
H -2.9998204 -0.5437760 -1.1377523
H 0.4073560 -0.6080682 -2.7771862
H 0.8241856 -2.2699815 -2.3187264
H -0.4828609 -1.9707873 -3.4888268
H -1.3988301 -3.2092564 1.5664753
H 0.1715685 -2.7057568 2.2341553
H -1.3133250 -2.5008298 3.1869927

H	0.6722790	-0.1851167	2.6214670
H	-0.5899493	1.0156558	2.2734747
H	-0.8186589	-0.1557297	3.5865963
H	-2.8063052	0.2900196	1.1622202
H	-3.1447007	-1.4411975	0.9348913
H	-3.0240474	-0.7619267	2.5625485
N	0.5680248	0.5865713	-0.2587504
N	0.2869432	1.8793617	-0.3707939
C	-0.9365632	2.2869441	-0.3130797
C	-1.2259960	3.7254356	-0.4346594
H	-1.7846715	1.6114999	-0.1727520
O	-0.4198472	4.6231507	-0.6162510
O	-2.5632898	3.9167172	-0.3092061
C	-3.0120237	5.3055469	-0.3962189
C	-4.5145189	5.3042684	-0.2078698
H	-2.7150015	5.6969258	-1.3735185
H	-2.4955595	5.8781154	0.3794122
H	-4.8857048	6.3324028	-0.2698683
H	-5.0059053	4.7117633	-0.9854930
H	-4.7851458	4.8972211	0.7710557

Aea 1,1-adduct of **1p** and **1**
66
Energy = -1750.590132960

B	1.9020642	-0.2308406	0.0671765
O	1.0146572	-1.4960666	0.0868998
P	-0.3520264	-0.6896600	0.1494624
O	2.7124538	-0.1220331	-1.1411767
O	2.8166857	-0.1473356	1.2041113
C	4.0074593	0.0146354	-0.7255284
C	4.0716242	-0.0023274	0.6767268
C	5.1470725	0.1506026	-1.5011240
C	5.2766112	0.1162052	1.3495101
C	-1.3038056	-1.0711693	-1.3910431
C	-1.1159792	-1.1427415	1.7862029
C	6.3757193	0.2692185	-0.8261564
H	5.0907426	0.1651031	-2.5855202
C	6.4393111	0.2532341	0.5687343
H	5.3196580	0.1031134	2.4346528
C	-1.2470954	-2.5981804	-1.6170257
C	-2.7672520	-0.6039753	-1.3585216
C	-0.5338039	-0.3510499	-2.5196423
C	-0.8225205	-2.6437405	2.0232152
C	-0.3565745	-0.3147763	2.8444624
C	-2.6301213	-0.9131616	1.9001534
H	7.2893196	0.3774364	-1.4041627

H	7.4017709	0.3469875	1.0639306
H	-1.8039816	-3.1429349	-0.8494766
H	-1.7168814	-2.8096304	-2.5846456
H	-0.2184500	-2.9646811	-1.6403373
H	-2.8714104	0.4205095	-0.9995972
H	-3.1574423	-0.6415662	-2.3816168
H	-3.3837337	-1.2588221	-0.7406035
H	-0.6219895	0.7344642	-2.4302367
H	0.5274943	-0.6137910	-2.5195157
H	-0.9713308	-0.6573517	-3.4762833
H	-1.3178446	-3.2808343	1.2855232
H	0.2484317	-2.8507143	2.0077642
H	-1.2203826	-2.9020049	3.0115050
H	0.7252056	-0.4513696	2.7616842
H	-0.5765167	0.7521903	2.7595618
H	-0.6766381	-0.6574086	3.8349708
H	-2.9290519	0.0913876	1.6017393
H	-3.1898064	-1.6365726	1.3026823
H	-2.9132424	-1.0579462	2.9488580
N	0.6395354	0.6978481	0.1283043
N	0.7631938	2.0194675	-0.0501039
C	-0.1577700	2.9032809	-0.2620264
C	-1.6315412	2.6967264	-0.3071078
C	-2.3209247	2.9107027	-1.5124182
C	-2.3656227	2.4420965	0.8569677
C	-3.7114609	2.8563596	-1.5532182
H	-1.7582526	3.1344676	-2.4141508
C	-3.7617520	2.3951378	0.8171948
H	-1.8448379	2.3247285	1.8024320
C	-4.4364243	2.6002639	-0.3857486
H	-4.2310901	3.0182712	-2.4930371
H	-4.3206463	2.2096944	1.7299416
H	-5.5214757	2.5668371	-0.4137494
C	0.3341953	4.2841313	-0.4987331
C	-0.5374686	5.3835204	-0.4247680
C	1.6887935	4.5213120	-0.8006198
C	-0.0698676	6.6809078	-0.6390981
H	-1.5858636	5.2255873	-0.1922140
C	2.1513365	5.8152038	-1.0140321
H	2.3613386	3.6721671	-0.8669837
C	1.2748885	6.9040634	-0.9346955
H	-0.7604336	7.5172328	-0.5729818
H	3.1987888	5.9794238	-1.2523440
H	1.6384582	7.9133076	-1.1061969

Be usual (*Z*)-1,2-adduct of **1e** and **1**

55
Energy = -1555.533659449

B	-2.1630058	0.3980761	0.1513212
O	-1.6737309	-1.1206808	0.2391199
P	-0.1474599	-1.2850536	0.1458863
O	-3.0327267	0.6646980	1.2933529
O	-2.9836567	0.5251726	-1.0548215
C	-4.3043886	0.7334732	0.7855762
C	-4.2746636	0.6454908	-0.6154206
C	-5.4960162	0.8774520	1.4769743
C	-5.4352634	0.6895850	-1.3704060
C	0.5084842	-1.9666699	1.7253500
C	0.2846607	-2.0426625	-1.4772686
C	-6.6802277	0.9264256	0.7176024
H	-5.5133456	0.9472700	2.5605715
C	-6.6507324	0.8320244	-0.6752977
H	-5.4055501	0.6151053	-2.4533976
C	0.0120960	-3.4271064	1.8292941
C	2.0420523	-1.9148098	1.8461463
C	-0.1334178	-1.1075376	2.8372058
C	-0.5935505	-3.3071273	-1.6297759
C	-0.1306334	-1.0066584	-2.5469726
C	1.7720497	-2.4018752	-1.6156523
H	-7.6324578	1.0376826	1.2284563
H	-7.5804429	0.8686632	-1.2361179
H	0.5221884	-4.0774528	1.1141813
H	0.2461582	-3.7854251	2.8376861
H	-1.0689360	-3.5030263	1.6813090
H	2.4101654	-0.8871013	1.8865446
H	2.3119046	-2.4017766	2.7893813
H	2.5489697	-2.4475445	1.0392907
H	0.2031825	-0.0677439	2.7863596
H	-1.2243086	-1.1304110	2.7893250
H	0.1862568	-1.5224362	3.7988542
H	-0.3220528	-4.0876868	-0.9154149
H	-1.6537624	-3.0698127	-1.5153934
H	-0.4302752	-3.6986094	-2.6395664
H	-1.1703024	-0.6899678	-2.4218661
H	0.5156848	-0.1247469	-2.5284902
H	-0.0318432	-1.4863731	-3.5262286
H	2.4223903	-1.5331998	-1.4814092
H	2.0709816	-3.1864001	-0.9163044
H	1.9310765	-2.7811644	-2.6306198
N	-0.8748871	1.2147512	0.1168440
N	0.2004114	0.5197767	0.0804180
C	1.4857078	0.9084818	0.0041365

C	1.9278207	2.2818191	-0.0362070
H	2.2145214	0.1123826	-0.0237507
O	1.2385139	3.2937357	-0.0153039
O	3.2988804	2.2931750	-0.0916359
C	3.9242096	3.6099878	-0.1695463
C	4.0184320	4.0782613	-1.6124902
H	4.9117175	3.4595966	0.2710244
H	3.3471932	4.3041006	0.4460984
H	4.5559239	5.0321483	-1.6513484
H	4.5635301	3.3490572	-2.2200620
H	3.0222647	4.2244969	-2.0392253

B usual 1,2-adduct of **1p** and **1**

66

Energy = -1750.565836640

B	-1.9664506	-0.0872718	-0.1621183
O	-1.2246000	-1.3923256	0.2223977
P	0.3002463	-1.4183729	-0.0748573
O	-2.7500744	0.3565479	1.0142496
O	-2.9536251	-0.3595231	-1.2264849
C	-4.0619195	0.2987987	0.6501756
C	-4.1850336	-0.1299952	-0.6835875
C	-5.1769842	0.6126860	1.4119898
C	-5.4235692	-0.2545837	-1.2920196
C	1.0700623	-2.0674543	1.4867096
C	0.4723340	-2.3833577	-1.6679060
C	-6.4390905	0.4895081	0.7998800
H	-5.0774329	0.9443134	2.4415552
C	-6.5603714	0.0664389	-0.5250006
H	-5.5081715	-0.5797298	-2.3246246
C	0.3221392	-3.3854139	1.8045723
C	2.5777022	-2.3447505	1.4360015
C	0.7470300	-1.0085402	2.5615218
C	-0.6820328	-3.4174117	-1.6782684
C	0.2355028	-1.4031039	-2.8362657
C	1.8045493	-3.1340153	-1.8106946
H	-7.3308786	0.7319933	1.3716817
H	-7.5451855	-0.0170342	-0.9762003
H	0.5571993	-4.1669110	1.0760851
H	0.6690687	-3.7274493	2.7863933
H	-0.7589159	-3.2410387	1.8446116
H	3.1593346	-1.4434928	1.2514528
H	2.8668360	-2.7402314	2.4165233
H	2.8343168	-3.0937725	0.6856331
H	1.2984383	-0.0814739	2.3828317
H	-0.3231302	-0.7872607	2.5996804

H	1.0542641	-1.4095994	3.5334281
H	-0.6153676	-4.1224133	-0.8461572
H	-1.6558180	-2.9270397	-1.6523446
H	-0.5914603	-3.9833715	-2.6126795
H	-0.7268302	-0.8937761	-2.7355968
H	1.0197109	-0.6474049	-2.9226276
H	0.2226451	-1.9876602	-3.7625601
H	2.6758402	-2.4904495	-1.6916794
H	1.8740384	-3.9540140	-1.0905648
H	1.8363844	-3.5700342	-2.8150704
N	-0.8707813	0.8622306	-0.5800172
N	0.3368635	0.4637317	-0.3295403
C	1.4147724	1.2586197	-0.1896029
C	1.2669780	2.7161369	-0.1054761
C	2.7627277	0.6832000	-0.1050847
C	0.1045632	3.3584788	0.3737140
C	2.3647892	3.5261114	-0.4701733
C	3.5976366	1.0389303	0.9755850
C	3.2871194	-0.1470064	-1.1061245
C	0.0661743	4.7424858	0.5117260
H	-0.7636861	2.7651090	0.6307278
C	2.3091058	4.9118220	-0.3543269
H	3.2657312	3.0597822	-0.8554268
C	4.8934307	0.5459516	1.0632801
H	3.2115027	1.6995412	1.7460189
C	4.5879959	-0.6494246	-1.0135695
H	2.6943090	-0.3470193	-1.9905443
C	1.1605025	5.5304074	0.1427371
H	-0.8336598	5.2128184	0.8993912
H	3.1639631	5.5096772	-0.6579722
C	5.3923619	-0.3079693	0.0706914
H	5.5166178	0.8164951	1.9105137
H	4.9764028	-1.2885946	-1.8013021
H	1.1130505	6.6120293	0.2316576
H	6.4055504	-0.6918357	0.1415705

Ce terminal N-to-P adduct of **1e** and **1**
55
Energy = -1555.543843096

N	-0.9658627	0.5170549	-0.9381013
N	-1.8822248	-0.1878312	-0.2106573
C	-2.5984140	-1.0369258	-0.8752093
C	-3.6278900	-1.7818927	-0.1421546
H	-2.4711032	-1.2058421	-1.9466820
O	-3.9056108	-1.6823568	1.0455969
O	-4.2790146	-2.6365926	-0.9852326

C	-5.3453075	-3.4216462	-0.3704041
C	-5.8525747	-4.3955402	-1.4139635
H	-6.1264650	-2.7319649	-0.0351901
H	-4.9373739	-3.9307346	0.5072702
H	-6.2428066	-3.8672209	-2.2896162
H	-5.0552366	-5.0723225	-1.7361618
H	-6.6617978	-4.9947500	-0.9832920
B	2.0592760	-0.1140810	0.5425997
O	1.1470501	0.8630339	0.7816714
P	-0.0939517	1.5488211	-0.0440029
O	2.4614151	-0.5974698	-0.7024223
O	2.7453835	-0.7270485	1.5936854
C	3.4414933	-1.5420618	-0.4116259
C	3.6114561	-1.6205392	0.9711330
C	4.1784485	-2.3135519	-1.2910461
C	4.5252099	-2.4808751	1.5521484
C	0.7062419	2.6793121	-1.2640032
C	-0.9834645	2.3397685	1.3799146
C	5.1100374	-3.1917659	-0.7149610
H	4.0422039	-2.2427192	-2.3649940
C	5.2778502	-3.2740503	0.6719112
H	4.6518724	-2.5380090	2.6280699
C	1.0802581	1.8549181	-2.5174774
C	-0.2995039	3.7715428	-1.6816738
C	1.9850232	3.3169716	-0.6870737
C	-0.1813968	3.5180990	1.9629461
C	-2.3741781	2.8096516	0.9066833
C	-1.1675591	1.2729663	2.4867805
H	5.7130457	-3.8208972	-1.3624473
H	6.0074768	-3.9665965	1.0802844
H	1.7775402	1.0480218	-2.2821552
H	0.1927150	1.4207563	-2.9796179
H	1.5636203	2.5389864	-3.2253499
H	-0.5332911	4.4549663	-0.8608998
H	0.1494640	4.3592159	-2.4902480
H	-1.2288321	3.3312608	-2.0548698
H	2.4097608	3.9763287	-1.4518166
H	1.7931147	3.9150088	0.2055944
H	2.7350266	2.5593964	-0.4442140
H	0.8207119	3.2076944	2.2724354
H	-0.0956506	4.3527215	1.2622649
H	-0.7114821	3.8808119	2.8512447
H	-2.9641193	1.9666490	0.5391133
H	-2.8933920	3.2494925	1.7660069
H	-2.3159540	3.5705045	0.1247950
H	-1.7332036	1.7432634	3.3001153

H -1.7242424 0.4103232 2.1147597
H -0.2054784 0.9421855 2.8854091

C terminal N-to-P adduct of **1p** and **1**
66
Energy = -1750.588369829
B -2.5175247 0.0117952 -0.3755375
O -2.0337605 1.2620582 -0.5758993
P -0.6508866 2.0020444 -0.0276221
O -3.6389120 -0.4539853 -1.0731159
O -2.0202203 -0.9481623 0.5097861
C -3.8342548 -1.7475773 -0.5992000
C -2.8577323 -2.0447540 0.3518930
C -4.8105393 -2.6587511 -0.9577253
C -2.8006019 -3.2661896 0.9966350
C -0.3120139 3.0885868 -1.4938676
C -1.2212965 2.8196773 1.5259993
C -4.7658555 -3.9045889 -0.3113336
H -5.5680793 -2.4231823 -1.6975104
C -3.7856899 -4.2015207 0.6419184
H -2.0361849 -3.4881579 1.7336844
C -1.3635890 4.1964760 -1.6742156
C 1.0942447 3.6999738 -1.3279522
C -0.3150594 2.1783024 -2.7453795
C -2.6297386 3.4280643 1.3905007
C -1.2555296 1.7319076 2.6242386
C -0.2019590 3.9046519 1.9250232
H -5.5111179 -4.6535677 -0.5602479
H -3.7847134 -5.1759555 1.1201634
H -1.3215094 4.9362592 -0.8697432
H -1.1565211 4.7168904 -2.6171749
H -2.3764505 3.7871003 -1.7299589
H 1.1557617 4.3705827 -0.4673197
H 1.8457850 2.9147675 -1.2165069
H 1.3238279 4.2835959 -2.2274035
H 0.3966531 1.3570325 -2.6310844
H -1.3106048 1.7717013 -2.9406181
H -0.0181562 2.7913273 -3.6052205
H -2.6704046 4.2384787 0.6605289
H -3.3686176 2.6719293 1.1114615
H -2.9153694 3.8381909 2.3659027
H -1.9650374 0.9353664 2.3815004
H -0.2716718 1.2814579 2.7625736
H -1.5810623 2.2092816 3.5563464
H 0.8097621 3.4918031 1.9766705
H -0.2080497 4.7468089 1.2265157

H	-0.4699061	4.2887612	2.9158776
N	0.5220820	1.0273000	0.4321024
N	1.3713531	0.5329704	-0.5428097
C	2.2096822	-0.3929319	-0.1658473
C	2.2535235	-0.9965120	1.1918063
C	3.1791255	-0.8352948	-1.1929149
C	1.0792206	-1.4114007	1.8408604
C	3.4801952	-1.1612097	1.8537838
C	3.7581362	-2.1157038	-1.1475939
C	3.5319416	0.0151351	-2.2586157
C	1.1356175	-1.9811605	3.1107729
H	0.1263228	-1.2823901	1.3449725
C	3.5350890	-1.7216689	3.1302391
H	4.3969321	-0.8444967	1.3640622
C	4.6491069	-2.5346614	-2.1360225
H	3.4976053	-2.7904093	-0.3378004
C	4.4208777	-0.4036003	-3.2441784
H	3.0983630	1.0092841	-2.2925575
C	2.3616566	-2.1365912	3.7634976
H	0.2175144	-2.3025631	3.5964225
H	4.4939736	-1.8368871	3.6283963
C	4.9858339	-1.6825272	-3.1894219
H	5.0787786	-3.5315624	-2.0837628
H	4.6852825	0.2723985	-4.0532779
H	2.4025112	-2.5783565	4.7555596
H	5.6837007	-2.0067662	-3.9562808

De C-to-P adduct of **1e** and **1** (N_2-loss)
53
Energy = -1446.029194786

C	-1.3964433	1.2276596	-0.1377550
C	-0.2088810	1.8205040	-0.4884290
H	-2.2448583	1.8484864	0.1167933
O	0.9039506	1.1876075	-0.7965638
O	-0.1543815	3.1602996	-0.5620003
C	1.1733544	3.7878654	-0.6199243
C	1.8537957	3.7581680	0.7375258
H	0.9470388	4.8056621	-0.9407095
H	1.7658039	3.2851358	-1.3854804
H	1.2320716	4.2478690	1.4933956
H	2.0570883	2.7298192	1.0490602
H	2.8061218	4.2959627	0.6720471
B	1.2156932	-0.1965615	-0.3090010
O	-0.0139689	-1.0377702	-0.3239566
P	-1.4893122	-0.5065839	-0.1886953
O	1.8110978	-0.1341901	1.0420096

O	2.2304344	-0.7818527	-1.1899620
C	3.0750443	-0.6314938	0.9200801
C	3.3266582	-1.0192714	-0.4074123
C	4.0365647	-0.7748289	1.9076241
C	4.5436998	-1.5624421	-0.7851319
C	-2.1969757	-1.1167748	1.4059539
C	-2.3355368	-1.1181457	-1.7213518
C	5.2768650	-1.3243737	1.5317196
H	3.8363508	-0.4740734	2.9316975
C	5.5255239	-1.7100009	0.2134092
H	4.7310418	-1.8608538	-1.8125915
C	-1.1290939	-0.7982905	2.4751380
C	-3.4903225	-0.3494403	1.7471702
C	-2.4615642	-2.6318308	1.3812129
C	-2.0307928	-2.6097807	-1.9619355
C	-3.8517607	-0.8684044	-1.6607379
C	-1.7234350	-0.2987153	-2.8793183
H	6.0512009	-1.4485864	2.2837550
H	6.4910367	-2.1321653	-0.0511422
H	-0.2051157	-1.3525184	2.2989431
H	-0.8892666	0.2689679	2.4895190
H	-1.5345746	-1.0799870	3.4535397
H	-4.2892873	-0.5292678	1.0244140
H	-3.8394833	-0.6937741	2.7271162
H	-3.3104756	0.7271644	1.8159031
H	-2.7183721	-2.9528518	2.3970449
H	-3.2998561	-2.8892802	0.7283789
H	-1.5769287	-3.1918473	1.0637489
H	-0.9533641	-2.7947468	-1.9611565
H	-2.5008755	-3.2570880	-1.2196770
H	-2.4263940	-2.8839588	-2.9466690
H	-4.0827996	0.1768068	-1.4284304
H	-4.2827347	-1.0953245	-2.6424609
H	-4.3417614	-1.5116243	-0.9245365
H	-2.1407089	-0.6738587	-3.8204976
H	-1.9630903	0.7638317	-2.7889180
H	-0.6357625	-0.4127685	-2.9185406

De C-to-P adduct of **1p** and **1** (N_2-loss)
64
Energy = -1641.013426095

B	0.2332189	-0.8191048	-1.8670587
O	0.8746085	-1.4791666	-0.8693624
P	1.1797838	-1.0042280	0.7013578
O	-0.1497561	-1.4871637	-3.0365711
O	-0.0972505	0.5375457	-1.9084501

C	-0.7346584	-0.5035570	-3.8260827
C	-0.7041598	0.7152437	-3.1465543
C	-1.2746631	-0.6270748	-5.0929615
C	-1.2135585	1.8774728	-3.6954040
C	1.6794260	-2.7028853	1.3146305
C	2.6543945	0.1559015	0.5073940
C	-1.7937477	0.5459255	-5.6639972
H	-1.2931730	-1.5777168	-5.6154438
C	-1.7644446	1.7674264	-4.9821154
H	-1.1858173	2.8221125	-3.1627110
C	2.8999780	-3.2940519	0.5896777
C	1.9360030	-2.6101413	2.8308797
C	0.4814931	-3.6545701	1.1064138
C	3.3886129	-0.2348228	-0.8008029
C	2.2015626	1.6234373	0.3413109
C	3.6634909	0.0765317	1.6691926
H	-2.2250380	0.5009689	-6.6592543
H	-2.1755254	2.6533149	-5.4562896
H	3.8146590	-2.7267919	0.7789355
H	3.0609775	-4.3138048	0.9604358
H	2.7329192	-3.3497055	-0.4898164
H	2.7881403	-1.9735387	3.0786473
H	1.0500697	-2.2278958	3.3474767
H	2.1467371	-3.6169112	3.2102042
H	-0.4099332	-3.2981920	1.6271125
H	0.2454862	-3.7854080	0.0477927
H	0.7559173	-4.6317661	1.5225525
H	3.6550895	-1.2907063	-0.8526501
H	2.7966936	0.0193860	-1.6837999
H	4.3114811	0.3541978	-0.8381626
H	1.3552771	1.7145873	-0.3426604
H	1.9341290	2.0789177	1.2943636
H	3.0503126	2.1763779	-0.0799677
H	3.2077526	0.3451511	2.6235708
H	4.1238183	-0.9103894	1.7559308
H	4.4631334	0.7975863	1.4621571
C	-0.1896171	-0.3187301	1.4437377
C	-1.5448803	-0.8829689	1.3716137
C	-0.0240976	0.9046967	2.2713999
C	-2.0310059	-1.7193955	0.3367970
C	-2.4779754	-0.5602021	2.3903270
C	0.8102481	0.9495237	3.3988274
C	-0.7343682	2.0751663	1.9380879
C	-3.3397717	-2.1927719	0.3234292
H	-1.3772876	-2.0252765	-0.4708027
C	-3.7893368	-1.0253026	2.3694619

H -2.1540181 0.0664307 3.2154101
C 0.9953368 2.1325367 4.1209806
H 1.3157581 0.0412926 3.7129547
C -0.5741453 3.2483251 2.6672510
H -1.3941546 2.0520371 1.0749690
C -4.2406424 -1.8497461 1.3346991
H -3.6598543 -2.8309171 -0.4970559
H -4.4621675 -0.7487927 3.1784025
C 0.3072202 3.2887248 3.7561601
H 1.6678837 2.1436201 4.9751513
H -1.1190578 4.1438400 2.3783563
H -5.2635172 -2.2150103 1.3174838
H 0.4446208 4.2098347 4.3159580

N_2
2
Energy = -109.5899318143
N 0.1001731 -0.0001040 0.0000039
N 1.1998290 0.0001039 -0.0000039

TS1ea (*Z*)-1,1-addition TS of **1e** and **1**
55
Energy = -1555.510894823
B 2.1178113 -0.5950844 -0.1421493
O 1.1194006 -1.5135855 -0.2563814
P -0.5146299 -1.2396969 -0.2259242
O 3.0158470 -0.3075167 -1.1816397
O 2.5119837 0.0163597 1.0597011
C 3.9473073 0.5519515 -0.6178437
C 3.6414327 0.7496817 0.7310298
C 5.0327342 1.1603132 -1.2219608
C 4.4048060 1.5665571 1.5453501
C -1.0457542 -2.4262806 -1.5770185
C -0.9628670 -1.8275954 1.5059576
C 5.8160331 1.9929098 -0.4062421
H 5.2639299 1.0026398 -2.2702525
C 5.5097073 2.1910476 0.9442879
H 4.1615219 1.7155619 2.5921422
C -0.6951430 -3.8945488 -1.2943592
C -2.5566005 -2.2567558 -1.8237504
C -0.2865024 -1.9422745 -2.8322884
C -0.0657719 -2.9757695 1.9974549
C -0.7383093 -0.5864264 2.3989495
C -2.4441055 -2.2330833 1.5748998
H 6.6778909 2.4933944 -0.8370391
H 6.1380061 2.8425503 1.5440187

H	-1.2881362	-4.2998327	-0.4696617
H	-0.9153633	-4.4909144	-2.1895632
H	0.3667841	-4.0135735	-1.0597590
H	-2.8234837	-1.2034875	-1.9485738
H	-2.8217681	-2.7985091	-2.7398164
H	-3.1549455	-2.6626504	-1.0055500
H	-0.4909331	-0.8861505	-3.0387030
H	0.7933153	-2.0729617	-2.7250583
H	-0.6250312	-2.5321577	-3.6925151
H	-0.2022885	-3.8863537	1.4099835
H	0.9909575	-2.6985111	1.9692767
H	-0.3329286	-3.1993375	3.0383934
H	0.2949691	-0.2299789	2.3411761
H	-1.4070385	0.2284987	2.1070625
H	-0.9500333	-0.8561653	3.4411439
H	-3.0917590	-1.4536527	1.1637178
H	-2.6308341	-3.1734613	1.0480105
H	-2.7120965	-2.3831051	2.6283639
N	0.1248148	0.9562886	-0.6178188
N	-0.5595031	1.9081829	-0.5200724
C	-1.6873751	2.5592346	-0.3308259
C	-2.9140606	1.8289699	-0.1199937
H	-1.6501859	3.6401084	-0.3609531
O	-3.0356717	0.6044974	-0.0940947
O	-3.9675389	2.6848512	0.0517937
C	-5.2559039	2.0389520	0.2760753
C	-6.2848933	3.1378060	0.4471452
H	-5.1744891	1.4067057	1.1653597
H	-5.4745607	1.3974584	-0.5827857
H	-7.2688656	2.6887948	0.6184133
H	-6.0404175	3.7721324	1.3048291
H	-6.3416989	3.7632678	-0.4491197

TS1e (*E*)-1,1-addition TS of **1e** and **1**
55
Energy = -1555.510857382

B	2.2567575	0.3414526	-0.0165219
O	1.9355185	-0.9829082	-0.0458702
P	0.4381538	-1.6794165	-0.0286809
O	2.9865884	0.9638688	-1.0344789
O	2.0422176	1.1976725	1.0693332
C	3.1914027	2.2603008	-0.5777267
C	2.6172949	2.4023968	0.6871902
C	3.8455239	3.3017642	-1.2101401
C	2.6630554	3.5945021	1.3863254
C	0.6626556	-2.9896215	-1.3414405

C	0.3501062	-2.3584326	1.7203727
C	3.9004275	4.5180485	-0.5109000
H	4.2890283	3.1842010	-2.1932138
C	3.3232099	4.6609495	0.7555868
H	2.2128157	3.6981794	2.3678544
C	1.7146751	-4.0554410	-1.0029311
C	-0.7116511	-3.6337102	-1.6112814
C	1.0960607	-2.2126770	-2.6046791
C	1.7009487	-2.8758518	2.2408944
C	-0.0992879	-1.1526512	2.5762930
C	-0.7228335	-3.4560030	1.7953834
H	4.4018123	5.3660439	-0.9673010
H	3.3845247	5.6179044	1.2647151
H	1.3938939	-4.6938181	-0.1752129
H	1.8646745	-4.6962855	-1.8810768
H	2.6760096	-3.5996469	-0.7479839
H	-1.4741220	-2.8741455	-1.8175901
H	-0.6292571	-4.2757629	-2.4959300
H	-1.0528883	-4.2521483	-0.7784245
H	0.3867012	-1.4148679	-2.8482823
H	2.0879994	-1.7706232	-2.4828212
H	1.1281993	-2.9139848	-3.4467096
H	2.0426951	-3.7583834	1.6963527
H	2.4731178	-2.1049776	2.1763556
H	1.5816190	-3.1519533	3.2961303
H	0.6086461	-0.3213634	2.5075158
H	-1.0860397	-0.7911646	2.2684221
H	-0.1595278	-1.4665481	3.6252244
H	-1.6725248	-3.1299819	1.3550825
H	-0.4027491	-4.3750003	1.2970639
H	-0.9107423	-3.6919949	2.8493548
N	-0.3431838	0.4318117	-0.8214146
N	-1.4860408	0.6796666	-0.7136072
C	-2.6732899	0.2584526	-0.3440655
C	-3.8284226	1.1120067	-0.4520418
H	-2.7154877	-0.7628704	0.0403734
O	-3.8589658	2.2619019	-0.8856870
O	-4.9343521	0.4562665	0.0082523
C	-6.1770484	1.2148886	-0.0490055
C	-7.2735244	0.3158634	0.4858413
H	-6.3560025	1.5101159	-1.0873498
H	-6.0580471	2.1216812	0.5518506
H	-8.2280549	0.8517962	0.4581090
H	-7.3668415	-0.5893507	-0.1220488
H	-7.0695857	0.0250809	1.5210041

TS1 1,1-addition TS of **1p** and **1**
66
Energy = -1750.556982390

B	1.8401517	-0.2190693	0.2485857
O	1.8500355	-1.6065431	0.2943722
P	0.4234939	-2.4380608	0.4995192
O	1.5990761	0.4767592	-0.9841623
O	2.7347619	0.5530649	1.0579821
C	2.1563172	1.7223130	-0.8081059
C	2.8344021	1.7702855	0.4174823
C	2.0956745	2.8180704	-1.6527146
C	3.4712908	2.9200752	0.8532018
C	0.2720268	-3.2823759	-1.1791493
C	0.9279908	-3.6441760	1.8478358
C	2.7411437	3.9883529	-1.2211711
H	1.5607113	2.7756799	-2.5958832
C	3.4111185	4.0390765	0.0045098
H	3.9874595	2.9545396	1.8074055
C	1.6140512	-3.7281194	-1.7799263
C	-0.7059139	-4.4638857	-1.0824592
C	-0.3476513	-2.1984669	-2.0904341
C	2.0258919	-4.6471223	1.4685181
C	1.4309301	-2.7452172	2.9985747
C	-0.3407121	-4.3765929	2.3271573
H	2.7075491	4.8731970	-1.8500247
H	3.8934333	4.9618887	0.3128923
H	2.0806715	-4.5301334	-1.2047555
H	1.4374369	-4.0992220	-2.7983183
H	2.3137068	-2.8899512	-1.8365603
H	-1.6434100	-4.1712755	-0.5956729
H	-0.9501583	-4.8085889	-2.0951054
H	-0.2750767	-5.3081744	-0.5365227
H	-1.3405317	-1.9039841	-1.7380334
H	0.2818065	-1.3044423	-2.1361076
H	-0.4453018	-2.6010788	-3.1069043
H	1.6740182	-5.3741294	0.7310617
H	2.9074179	-4.1368516	1.0683416
H	2.3318547	-5.2031193	2.3649060
H	2.3478037	-2.2184704	2.7215402
H	0.6776424	-2.0014154	3.2808822
H	1.6392652	-3.3751861	3.8721817
H	-1.1321626	-3.6648360	2.5883423
H	-0.7319809	-5.0663794	1.5753321
H	-0.0990109	-4.9591156	3.2246586
N	0.1451133	0.0455140	1.2455610
N	-0.6835228	0.7629678	0.8321091

C	-1.7277024	1.3112901	0.2905693
C	-2.7034819	0.3570448	-0.2835432
C	-3.3068611	0.6107816	-1.5261263
C	-2.9752098	-0.8529129	0.3761586
C	-4.1762385	-0.3226320	-2.0853874
H	-3.0823872	1.5311351	-2.0560989
C	-3.8432511	-1.7840303	-0.1911564
H	-2.5047783	-1.0601896	1.3317286
C	-4.4476679	-1.5226487	-1.4218801
H	-4.6359229	-0.1163161	-3.0477476
H	-4.0479805	-2.7147823	0.3300928
H	-5.1234058	-2.2489005	-1.8639376
C	-1.8301061	2.7759255	0.2630023
C	-3.0746691	3.3953905	0.0525916
C	-0.6975335	3.5855184	0.4678237
C	-3.1776935	4.7851547	0.0373800
H	-3.9625226	2.7867814	-0.0866318
C	-0.8081013	4.9718256	0.4545015
H	0.2747508	3.1275560	0.6205013
C	-2.0472966	5.5809911	0.2362091
H	-4.1477395	5.2466143	-0.1250753
H	0.0805254	5.5781695	0.6044061
H	-2.1302751	6.6638204	0.2211738

TS2e 1,2-boryl shift TS of adduct **Ae**

55

Energy = -1555.537311487

B	1.1463626	-0.7524389	0.4888958
O	0.2926979	-1.8136723	0.6834723
P	-1.3385980	-1.6517099	0.6084046
O	1.3260666	-0.0846378	-0.7235999
O	1.9918702	-0.2658190	1.4885606
C	2.2281687	0.9284175	-0.4321111
C	2.6376346	0.8149575	0.8985614
C	2.6726548	1.9461615	-1.2555194
C	3.5248319	1.7057321	1.4742212
C	-1.9030378	-2.6591949	-0.8235014
C	-1.8187094	-2.2579705	2.2955465
C	3.5653278	2.8633232	-0.6811058
H	2.3377987	2.0357831	-2.2833833
C	3.9850144	2.7433324	0.6481422
H	3.8358866	1.6155519	2.5097890
C	-1.7403491	-4.1690849	-0.5820367
C	-3.3730351	-2.3110376	-1.1398025
C	-1.0260441	-2.2277681	-2.0215564
C	-1.0738826	-3.5472755	2.6917076

C	-1.4330532	-1.1398848	3.2902953
C	-3.3426829	-2.4739103	2.3452744
H	3.9342329	3.6898774	-1.2800275
H	4.6765220	3.4742847	1.0553554
H	-2.4176893	-4.5353761	0.1941674
H	-1.9868660	-4.6921373	-1.5128037
H	-0.7130357	-4.4304489	-0.3102869
H	-3.4841640	-1.2357979	-1.2982168
H	-3.6565149	-2.8395881	-2.0573243
H	-4.0532163	-2.6264894	-0.3445815
H	-1.0969189	-1.1499856	-2.1858935
H	0.0227656	-2.4968207	-1.8701110
H	-1.3923526	-2.7538867	-2.9107230
H	-1.3507508	-4.3994148	2.0682495
H	0.0090713	-3.4105262	2.6420625
H	-1.3425505	-3.7862696	3.7277183
H	-0.3613252	-0.9250201	3.2609547
H	-1.9725546	-0.2132460	3.0872077
H	-1.6901752	-1.4895668	4.2974586
H	-3.8858098	-1.5832145	2.0135915
H	-3.6553584	-3.3265572	1.7358576
H	-3.6298125	-2.6797391	3.3828189
N	-1.7260240	-0.1374136	0.1721981
N	-1.0747768	0.7988268	0.9215395
C	-0.9652859	2.0130734	0.4648075
C	-1.3586716	2.5227368	-0.8572435
H	-0.4163870	2.7016062	1.1009770
O	-2.0290733	1.9754855	-1.7188391
O	-0.7852530	3.7572491	-1.0336167
C	-0.9644403	4.3449753	-2.3527470
C	-0.0764602	5.5710009	-2.4229125
H	-2.0231251	4.5934099	-2.4816485
H	-0.6953613	3.5957585	-3.1033325
H	-0.1817979	6.0424465	-3.4056129
H	-0.3560711	6.3010130	-1.6571997
H	0.9736857	5.2968179	-2.2802796

TS2 1,2-boryl shift TS of adduct **A**

66

Energy = -1750.572152076

B	0.2511744	-2.5387693	0.1885185
O	-1.1125681	-2.6928450	-0.1518808
P	-1.7062364	-1.1903952	0.1243289
O	1.2306291	-2.3307276	-0.8050449
O	0.8275158	-3.0738120	1.3585771
C	2.4327853	-2.5870076	-0.1759593

C	2.1913930	-3.0363891	1.1259442
C	3.7141411	-2.4531881	-0.6792978
C	3.2202944	-3.3737637	1.9866963
C	-2.4351106	-0.7302056	-1.5213197
C	-2.9178821	-1.4982917	1.4929927
C	4.7682039	-2.7896011	0.1860150
H	3.8941313	-2.1042139	-1.6909110
C	4.5270665	-3.2394104	1.4878142
H	3.0266534	-3.7208076	2.9964219
C	-3.1062076	-1.9433086	-2.1980114
C	-3.4457738	0.4196764	-1.3780376
C	-1.2384684	-0.2932616	-2.3952876
C	-4.0727805	-2.3947408	1.0088450
C	-2.1471835	-2.2290047	2.6139212
C	-3.4702853	-0.1800109	2.0582759
H	5.7911873	-2.6961996	-0.1660480
H	5.3656315	-3.4897038	2.1307116
H	-3.9883236	-2.2899487	-1.6570194
H	-3.4268814	-1.6285681	-3.1985230
H	-2.4073987	-2.7758084	-2.3046187
H	-3.0326123	1.2648957	-0.8229084
H	-3.7144809	0.7735241	-2.3799271
H	-4.3629620	0.0847015	-0.8847424
H	-0.7812566	0.6248056	-2.0260024
H	-0.4691052	-1.0694244	-2.4417770
H	-1.6081048	-0.1109401	-3.4108806
H	-4.7301077	-1.8722172	0.3084284
H	-3.7053166	-3.3116165	0.5391405
H	-4.6737563	-2.6768940	1.8812988
H	-1.8169704	-3.2198360	2.2947847
H	-1.2736387	-1.6549213	2.9323404
H	-2.8251617	-2.3446085	3.4674827
H	-2.6714042	0.4097878	2.5100817
H	-3.9686183	0.4300224	1.3020876
H	-4.2013162	-0.4216853	2.8387722
N	-0.3975751	-0.4720411	0.7012382
N	0.6257677	0.3240101	0.2856121
C	0.5095710	1.5827820	-0.0216014
C	-0.7308748	2.3966254	0.0257445
C	-1.1266706	3.1665382	-1.0799868
C	-1.4996305	2.4496859	1.1952350
C	-2.2765250	3.9511163	-1.0243437
H	-0.5281750	3.1451448	-1.9863496
C	-2.6464224	3.2405119	1.2548918
H	-1.1796560	1.8807582	2.0612633
C	-3.0420893	3.9878763	0.1437581

H	-2.5756872	4.5336212	-1.8910361
H	-3.2309993	3.2744911	2.1698288
H	-3.9388183	4.5992123	0.1893754
C	1.7709351	2.2335682	-0.4515851
C	1.9375036	3.6264004	-0.3749274
C	2.8398951	1.4549270	-0.9332156
C	3.1391269	4.2224772	-0.7591783
H	1.1272166	4.2447414	-0.0007961
C	4.0375241	2.0515028	-1.3138806
H	2.7067251	0.3804459	-0.9968269
C	4.1942116	3.4395999	-1.2306815
H	3.2510608	5.3008635	-0.6858866
H	4.8512236	1.4351556	-1.6873345
H	5.1274903	3.9047469	-1.5354123

TS3a 1,3-addition TS of **3ea** and **1**
96
Energy = -2694.872739772

N	-0.4355424	-0.9382919	-0.5906899
N	0.8663905	-0.4847637	-0.6679416
C	1.2538542	0.5655936	-1.3407893
C	0.5865988	1.1074207	-2.5380153
H	2.2898172	0.8413365	-1.1924151
O	-0.4260861	0.6773809	-3.0598243
O	1.3851763	2.0569808	-3.0823897
C	0.9900038	2.5182354	-4.4131009
C	1.8730268	3.6990375	-4.7562379
H	-0.0708548	2.7794481	-4.3868053
H	1.1236655	1.6829205	-5.1073832
H	1.6170987	4.0613733	-5.7570805
H	1.7249922	4.5166278	-4.0440082
H	2.9290168	3.4135983	-4.7495177
B	1.9596397	-1.4459282	0.0491821
O	1.2802523	-2.7525401	-0.1257962
P	-0.2608896	-2.6120422	-0.4622694
O	2.1787972	-1.1097038	1.4511386
O	3.2441462	-1.3500539	-0.6313861
C	3.5056112	-0.7929942	1.5617716
C	4.1470689	-0.9442763	0.3239698
C	4.1949327	-0.3781658	2.6890974
C	5.4992825	-0.6942220	0.1686448
C	-1.1386231	-3.4346400	0.9371935
C	-0.5456819	-3.3417341	-2.1318226
C	5.5695963	-0.1192212	2.5417424
H	3.6919091	-0.2590640	3.6436062
C	6.2080705	-0.2742024	1.3096025

H	5.9889989	-0.8144876	-0.7928736
C	-1.0344230	-2.4954289	2.1561792
C	-2.5976943	-3.7946464	0.6136842
C	-0.3589662	-4.7320145	1.2697190
C	0.5322350	-2.7253120	-3.0510565
C	-0.3957035	-4.8735069	-2.1229292
C	-1.9347835	-2.9198786	-2.6493575
H	6.1415536	0.2089453	3.4049494
H	7.2708251	-0.0661966	1.2251014
H	0.0078214	-2.2295114	2.3578301
H	-1.6106787	-1.5819242	2.0143006
H	-1.4250539	-3.0360607	3.0260318
H	-2.6553240	-4.5800063	-0.1447235
H	-3.0607102	-4.1800940	1.5287004
H	-3.1839011	-2.9374357	0.2817122
H	0.6762111	-4.5171894	1.5408835
H	-0.8587681	-5.1888933	2.1311351
H	-0.3710334	-5.4552949	0.4526160
H	0.4051381	-1.6434379	-3.1307065
H	1.5440719	-2.9541524	-2.7068338
H	0.4005340	-3.1566888	-4.0495893
H	-1.1934844	-5.3631806	-1.5590190
H	-0.4579722	-5.2228860	-3.1597472
H	0.5723075	-5.1854513	-1.7195531
H	-2.0276787	-1.8311276	-2.6628041
H	-2.0394641	-3.2931634	-3.6745274
H	-2.7484751	-3.3403765	-2.0543480
B	-1.9928741	0.4187565	-0.3643539
O	-1.3516389	1.6266727	-0.3569431
P	-0.2451863	2.7143234	0.1983913
O	-2.6340494	-0.0483840	0.8462570
O	-2.8616162	0.1129757	-1.4739824
C	-3.8363759	-0.5852679	0.4573670
C	-3.9580660	-0.5086797	-0.9361552
C	-4.8256449	-1.1391274	1.2516604
C	-5.0637913	-1.0213965	-1.5939903
C	-0.4017629	2.6086483	2.0786446
C	-1.0863143	4.2837054	-0.4378821
C	-5.9560908	-1.6525921	0.5927626
H	-4.7222394	-1.1902773	2.3309035
C	-6.0686352	-1.6006913	-0.7992966
H	-5.1480510	-0.9740574	-2.6748497
C	0.4121040	3.7629526	2.6900847
C	-1.8182787	2.5798487	2.6696707
C	0.3072187	1.2820236	2.4141794
C	-2.4792470	4.5821422	0.1301957

C	-0.1338891	5.4718434	-0.2076584
C	-1.2059039	4.0653003	-1.9598560
H	-6.7521776	-2.1019557	1.1790303
H	-6.9508976	-2.0125586	-1.2805846
H	-0.1235809	4.7142123	2.6297440
H	1.3862820	3.8779308	2.1992528
H	0.5952239	3.5484459	3.7506333
H	-1.7441679	2.3282501	3.7366885
H	-2.3181455	3.5462873	2.5916930
H	-2.4359491	1.8186846	2.1884408
H	1.3418468	1.2819514	2.0625449
H	0.3137580	1.1390039	3.5024896
H	-0.2040072	0.4254916	1.9679549
H	-2.9509761	5.3736042	-0.4675175
H	-3.1236998	3.6981453	0.0887078
H	-2.4294024	4.9334757	1.1634491
H	0.8769571	5.2422052	-0.5644794
H	-0.5020251	6.3401863	-0.7686401
H	-0.0706429	5.7571482	0.8449228
H	-1.6195241	4.9723835	-2.4182589
H	-1.8592617	3.2214565	-2.1949138
H	-0.2230006	3.8778969	-2.4000720

TS3p0 N-to-B addition TS of **3** and **1**
107
Energy = -2889.928972670

B	1.8056214	-2.0166990	0.3912699
O	0.8059089	-3.0751967	0.1085406
P	-0.6623769	-2.5208128	-0.0745309
O	2.6541920	-1.7674354	-0.7792712
O	2.6865319	-2.3856029	1.4949486
C	3.9376487	-1.9948122	-0.3663424
C	3.9582236	-2.3540733	0.9908946
C	5.1053855	-1.8717110	-1.1004503
C	5.1456220	-2.5889140	1.6607767
C	-1.0734138	-2.8734821	-1.8530421
C	-1.7189411	-3.4009371	1.1610931
C	6.3169512	-2.1111906	-0.4275704
H	5.0832460	-1.5823456	-2.1468055
C	6.3367698	-2.4588485	0.9247140
H	5.1529300	-2.8394592	2.7167315
C	-2.5710072	-2.8343077	-2.1985050
C	-0.2897262	-1.8397830	-2.6857534
C	-0.5165294	-4.2793820	-2.1888451
C	-2.0097375	-4.8624258	0.7756929
C	-0.9089055	-3.3971170	2.4759447

C	-3.0336938	-2.6227757	1.3486203
H	7.2527335	-2.0156765	-0.9712803
H	7.2879032	-2.6271517	1.4218519
H	-2.9977320	-1.8486863	-2.0235817
H	-2.6723691	-3.0703849	-3.2643660
H	-3.1404160	-3.5826115	-1.6405363
H	-0.6464670	-0.8254182	-2.5165879
H	0.7790672	-1.8714599	-2.4541219
H	-0.4220365	-2.0903264	-3.7448426
H	0.5519079	-4.3477432	-1.9765930
H	-1.0375108	-5.0779224	-1.6577115
H	-0.6702393	-4.4349154	-3.2628352
H	-2.6404913	-4.9404429	-0.1130359
H	-1.0880767	-5.4279091	0.6113175
H	-2.5478954	-5.3306098	1.6081986
H	-0.5974594	-2.3913425	2.7673944
H	-1.5457176	-3.8008073	3.2708791
H	-0.0135869	-4.0165550	2.3902583
H	-2.8477323	-1.5846770	1.6347577
H	-3.6420920	-2.6204827	0.4413195
H	-3.6136366	-3.1046936	2.1437681
N	-0.4996820	-0.9211262	0.3647066
N	0.8273009	-0.7804705	0.7945299
C	1.1893336	0.1888326	1.6121174
C	2.6325845	0.4613826	1.7925163
C	0.2660533	1.0028572	2.4213839
C	3.4662592	0.7190600	0.6962054
C	3.1677992	0.5416645	3.0905218
C	0.6138211	2.3274352	2.7343007
C	-0.8792199	0.4511722	3.0191965
C	4.8084930	1.0433109	0.8916799
H	3.0531689	0.6748990	-0.3040473
C	4.5118658	0.8386340	3.2798222
H	2.5249487	0.3497692	3.9442293
C	-0.1690699	3.0834775	3.6027725
H	1.5006519	2.7642327	2.2885016
C	-1.6304550	1.1886695	3.9243189
H	-1.1787841	-0.5561740	2.7649624
C	5.3365457	1.0956861	2.1788373
H	5.4417380	1.2398613	0.0323869
H	4.9199971	0.8717051	4.2860751
C	-1.2872375	2.5134506	4.2115962
H	0.1030937	4.1134212	3.8146704
H	-2.4993261	0.7367110	4.3934900
H	6.3860524	1.3321800	2.3286043
H	-1.8890212	3.0953043	4.9041194

B -1.5407536 0.8536957 -0.5578322
O -0.4755237 1.2373645 -1.3213692
P -0.0547315 2.3038718 -2.5339149
O -1.9867990 1.6139611 0.5586299
O -2.6431184 0.0984131 -1.0722518
C -3.2984324 1.2595632 0.7608971
C -3.6998622 0.3545846 -0.2267833
C -4.1732700 1.7049747 1.7370891
C -4.9898827 -0.1422892 -0.2882979
C -1.6822313 2.6516799 -3.4330616
C 0.4781759 3.8151609 -1.5272905
C -5.4826015 1.1983217 1.6936530
H -3.8580617 2.4122764 2.4956184
C -5.8823817 0.2951408 0.7040587
H -5.2969020 -0.8369701 -1.0633688
C -2.0601290 1.3015283 -4.0837747
C -2.8705722 3.1757867 -2.6149166
C -1.3586499 3.6396333 -4.5725484
C 0.9823901 4.8946454 -2.5035411
C -0.5280800 4.4154770 -0.5369616
C 1.6927479 3.2828329 -0.7400662
H -6.1988302 1.5200619 2.4440596
H -6.9034691 -0.0746136 0.6969977
H -2.3571666 0.5625485 -3.3374526
H -2.9063773 1.4615962 -4.7645181
H -1.2248047 0.8963127 -4.6661389
H -3.7785952 3.1337099 -3.2316624
H -3.0580182 2.5804552 -1.7181857
H -2.7233929 4.2141614 -2.3109693
H -2.1884260 3.6372141 -5.2905299
H -1.2357638 4.6616459 -4.2070830
H -0.4479587 3.3503561 -5.1108062
H 1.6023870 4.4634104 -3.2990876
H 0.1600788 5.4461113 -2.9656566
H 1.5989292 5.6154228 -1.9512423
H -0.9576366 3.6529484 0.1164744
H -0.0101772 5.1501366 0.0955018
H -1.3395221 4.9369418 -1.0500322
H 2.1360882 4.1000469 -0.1569405
H 1.3956614 2.4903700 -0.0509663
H 2.4605013 2.8843811 -1.4124065

TS3p1 C-to-P addition TS of **5p1**
107
Energy = -2889.916385143
B 1.5286756 -1.7389414 -0.1011237

O	0.5147194	-2.7667099	0.2714294
P	-0.9855428	-2.3085195	0.2502999
O	2.0452239	-1.9870891	-1.4577416
O	2.6705868	-1.8136982	0.8088736
C	3.3752839	-2.2751196	-1.3051608
C	3.7469663	-2.1663911	0.0439904
C	4.2991108	-2.5855082	-2.2891861
C	5.0534465	-2.3709475	0.4538433
C	-1.7102702	-3.1723930	-1.2343659
C	-1.6985404	-2.8268045	1.8813378
C	5.6282543	-2.7981026	-1.8806300
H	4.0070336	-2.6542380	-3.3326509
C	5.9971067	-2.6927074	-0.5375476
H	5.3363834	-2.2708902	1.4972112
C	-3.2461662	-3.2140670	-1.2383521
C	-1.1545295	-2.4866163	-2.4993524
C	-1.1642248	-4.6245320	-1.2409905
C	-1.6905832	-4.3660130	1.9846282
C	-0.7524639	-2.2449175	2.9491805
C	-3.1209085	-2.2979528	2.1335139
H	6.3785553	-3.0455759	-2.6263102
H	7.0318718	-2.8573256	-0.2506214
H	-3.6968153	-2.2242969	-1.1613645
H	-3.5697447	-3.6585043	-2.1866179
H	-3.6290009	-3.8449369	-0.4308668
H	-1.5638756	-1.4869633	-2.6230441
H	-0.0621808	-2.4380729	-2.4758069
H	-1.4488826	-3.1026889	-3.3573438
H	-0.0730948	-4.6419192	-1.2149151
H	-1.5528498	-5.2342038	-0.4256347
H	-1.4958422	-5.0755516	-2.1831229
H	-2.4550363	-4.8227440	1.3520182
H	-0.7136149	-4.7929785	1.7409782
H	-1.9229132	-4.6222926	3.0245029
H	-0.7944750	-1.1556562	2.9550040
H	-1.0899054	-2.6076540	3.9263387
H	0.2816969	-2.5635452	2.7975453
H	-3.1418622	-1.2085406	2.1225647
H	-3.8421087	-2.6725946	1.4035808
H	-3.4298359	-2.6514241	3.1242949
N	-0.7504451	-0.6380879	0.1209612
N	0.6834867	-0.3952709	0.1031419
C	1.1630168	0.6559163	0.8170892
C	2.5579361	1.1005152	0.5636501
C	0.5954862	0.9027289	2.1854531
C	3.2512436	0.7381227	-0.6016879

C	3.1952222	1.9819419	1.4578053
C	-0.6601253	1.4125568	2.5072881
C	1.4048854	0.4005147	3.2268875
C	4.5493016	1.1766539	-0.8349392
H	2.7631244	0.1208707	-1.3429777
C	4.4875108	2.4361232	1.2152679
H	2.6716432	2.3286192	2.3407102
C	-1.0949127	1.4483196	3.8340274
H	-1.3168420	1.7711965	1.7317017
C	0.9700915	0.4385307	4.5475341
H	2.3611970	-0.0507747	2.9848346
C	5.1808965	2.0254076	0.0742990
H	5.0633575	0.8560788	-1.7361012
H	4.9535576	3.1171539	1.9218085
C	-0.2837807	0.9696724	4.8593711
H	-2.0808133	1.8463967	4.0560792
H	1.6089872	0.0410447	5.3310150
H	6.1931303	2.3740087	-0.1090035
H	-0.6261065	0.9971871	5.8899256
B	-1.8461684	0.4161825	-0.2861576
O	-1.3586248	1.7698908	-0.5060062
P	0.0368337	2.5552058	-0.6652147
O	-2.9122465	0.4756333	0.7671471
O	-2.5988735	-0.0113200	-1.5097817
C	-4.1074957	0.4544757	0.1197145
C	-3.9212889	0.1736983	-1.2438230
C	-5.3741103	0.6324925	0.6533135
C	-4.9935499	0.0714110	-2.1156265
C	0.3658653	2.4642235	-2.5304727
C	-0.4659878	4.3262358	-0.2038547
C	-6.4685584	0.5343864	-0.2262561
H	-5.5133100	0.8416559	1.7100285
C	-6.2824112	0.2607228	-1.5825774
H	-4.8418306	-0.1517024	-3.1675776
C	0.3292770	0.9642579	-2.8884157
C	-0.7135050	3.1642242	-3.3706769
C	1.7633761	3.0199961	-2.8602610
C	0.5259274	5.3291905	-0.8163817
C	-1.9105617	4.6589840	-0.6122718
C	-0.3543431	4.4458616	1.3303107
H	-7.4741345	0.6755453	0.1605679
H	-7.1441408	0.1916026	-2.2407935
H	-0.6646977	0.5470285	-2.7199215
H	0.5672427	0.8601752	-3.9547023
H	1.0524315	0.3756193	-2.3219359
H	-0.5521591	2.9099149	-4.4272810

H	-1.7136354	2.8201327	-3.0898204
H	-0.6716838	4.2526909	-3.2814961
H	2.0030104	2.7705829	-3.9018246
H	1.8162746	4.1055306	-2.7583374
H	2.5321356	2.5769959	-2.2214504
H	1.5634751	5.0717254	-0.5746447
H	0.4266745	5.4006474	-1.9015913
H	0.3230357	6.3219434	-0.3960510
H	-2.6028460	3.8913681	-0.2561396
H	-2.1901624	5.6182380	-0.1568618
H	-2.0249051	4.7512582	-1.6936415
H	-0.5173790	5.4940238	1.6113832
H	-1.1074684	3.8426469	1.8396664
H	0.6332503	4.1406850	1.6913218

TS3p 1,3-addition TS of **3** and **1**
107
Energy = -2889.907895090

B	1.7223159	-1.6656170	-0.2533675
O	0.8496014	-2.8494258	-0.0013065
P	-0.6667204	-2.4668924	0.2331020
O	2.0187936	-1.5176447	-1.6858947
O	2.9975017	-1.8078162	0.4401202
C	3.3767207	-1.6500303	-1.7993952
C	3.9587912	-1.8168310	-0.5327011
C	4.1465871	-1.5909519	-2.9491913
C	5.3289590	-1.9386940	-0.3755968
C	-1.5600019	-3.1820005	-1.2306031
C	-1.2080925	-3.1991714	1.8446119
C	5.5396110	-1.7153621	-2.7983763
H	3.6904065	-1.4486146	-3.9241806
C	6.1178494	-1.8856143	-1.5383382
H	5.7727051	-2.0556326	0.6082569
C	-3.0756083	-3.3319414	-1.0202451
C	-1.2467762	-2.2991014	-2.4531751
C	-0.9484820	-4.5786732	-1.5100690
C	-1.3518105	-4.7309071	1.7967160
C	-0.1128390	-2.8445217	2.8671184
C	-2.5296067	-2.5328684	2.2765593
H	6.1735988	-1.6757189	-3.6796685
H	7.1970381	-1.9744050	-1.4506623
H	-3.5596121	-2.3989784	-0.7302795
H	-3.5193461	-3.6533011	-1.9692757
H	-3.3042541	-4.0945705	-0.2717311
H	-1.6973408	-1.3126370	-2.3697633
H	-0.1674316	-2.1852003	-2.5899027

H	-1.6556067	-2.8021195	-3.3376898
H	0.1249437	-4.5114458	-1.6958673
H	-1.1265769	-5.2931493	-0.7056023
H	-1.4360936	-4.9618991	-2.4138550
H	-2.1768474	-5.0572708	1.1599404
H	-0.4285586	-5.2137637	1.4631427
H	-1.5620361	-5.0766252	2.8156535
H	0.0053188	-1.7658098	2.9605660
H	-0.4216545	-3.2364378	3.8427130
H	0.8494384	-3.2890632	2.5992395
H	-2.4178708	-1.4468522	2.3244558
H	-3.3572217	-2.7724113	1.6049958
H	-2.7864510	-2.9032280	3.2756924
N	-0.5852462	-0.7983338	0.3691359
N	0.8002705	-0.5038672	0.3976107
C	1.2805158	0.3725410	1.2862574
C	2.5439279	1.0608115	1.0071020
C	0.6401543	0.5494783	2.6136992
C	3.0778251	1.0709683	-0.2971319
C	3.1744193	1.8743194	1.9720385
C	-0.6786062	0.9340148	2.8587823
C	1.4392237	0.1518415	3.7086048
C	4.2399544	1.7642919	-0.5991019
H	2.5463338	0.5612195	-1.0879023
C	4.3294224	2.5867034	1.6640494
H	2.7552202	1.9678047	2.9657285
C	-1.1938300	0.9181433	4.1559907
H	-1.3066450	1.2533243	2.0461568
C	0.9209098	0.1323401	4.9989768
H	2.4507059	-0.1979776	3.5305218
C	4.8816263	2.5215759	0.3831787
H	4.6312503	1.7316150	-1.6113795
H	4.7944487	3.2023302	2.4286901
C	-0.4021762	0.5176749	5.2297964
H	-2.2254467	1.2174599	4.3182243
H	1.5483697	-0.1997303	5.8210293
H	5.7841626	3.0779649	0.1465270
H	-0.8092308	0.4995907	6.2367747
B	-2.0065355	0.7885327	-0.2186770
O	-1.2144678	1.8926704	-0.1511895
P	0.0948406	2.7373159	-0.7505585
O	-2.9725782	0.5669275	0.8284840
O	-2.6006150	0.3899820	-1.4643857
C	-4.0950270	0.0777233	0.2118956
C	-3.8814446	-0.0102164	-1.1685870
C	-5.2927753	-0.3129509	0.7865571

C -4.8617169 -0.4565370 -2.0370099
C -0.1539532 2.7236832 -2.6235087
C -0.4140158 4.4059145 -0.0214889
C -6.2930513 -0.7796711 -0.0839361
H -5.4501945 -0.2587898 1.8590354
C -6.0853565 -0.8437254 -1.4646786
H -4.6856614 -0.5199177 -3.1059337
C 0.0832213 1.2492159 -3.0209926
C -1.5029521 3.1895691 -3.1829003
C 1.0019850 3.5540054 -3.2188711
C 0.5848017 5.4794437 -0.4867693
C -1.8589830 4.8495922 -0.2824119
C -0.2294321 4.2070132 1.5001369
H -7.2471662 -1.0942359 0.3287503
H -6.8807489 -1.2047823 -2.1098541
H -0.7785723 0.6284171 -2.7792806
H 0.2549140 1.1926751 -4.1036946
H 0.9580404 0.8284853 -2.5157328
H -1.5590228 2.9399138 -4.2517198
H -2.3348865 2.6903676 -2.6785175
H -1.6287871 4.2712742 -3.0901936
H 1.0922768 3.3250968 -4.2882037
H 0.8351431 4.6289208 -3.1184610
H 1.9576504 3.3058913 -2.7400822
H 1.6194654 5.1212354 -0.4177561
H 0.3957268 5.7947466 -1.5161603
H 0.4913504 6.3638123 0.1560825
H -2.5625475 4.0460018 -0.0426316
H -2.0968461 5.7107826 0.3570181
H -2.0154844 5.1520315 -1.3197976
H -0.3241958 5.1778656 2.0035335
H -0.9883951 3.5341488 1.9061230
H 0.7571650 3.7917757 1.7345704

TS3 1,3-addition of **3e** and **1** (into **5**)
96
Energy = -2694.876807754
N -0.4327934 -0.8585124 -0.4094519
N 0.8846275 -0.3901317 -0.4897925
C 1.1193487 0.6934771 -1.1758349
C 2.4143959 1.4058535 -1.1514809
H 0.3584001 1.0337033 -1.8656396
O 3.1895273 1.4872993 -0.2201219
O 2.5816915 2.0290070 -2.3462507
C 3.7828778 2.8561860 -2.4408050
C 3.7704059 3.5158922 -3.8028551

H	4.6523545	2.2085435	-2.2973312
H	3.7560957	3.5832544	-1.6238582
H	4.6637869	4.1395960	-3.9091723
H	3.7740699	2.7671073	-4.6005799
H	2.8884729	4.1530447	-3.9216807
B	1.9867415	-1.3459675	0.2047827
O	1.2585138	-2.6490209	0.1610356
P	-0.2451964	-2.5173952	-0.2975001
O	2.3250972	-0.9632298	1.5709935
O	3.2227066	-1.3941705	-0.5668792
C	3.6891617	-0.8722975	1.5991557
C	4.2255726	-1.1378858	0.3295674
C	4.5011862	-0.5656274	2.6770558
C	5.5892587	-1.1114929	0.0972571
C	-1.2398664	-3.3327230	1.0258114
C	-0.3652318	-3.2872512	-1.9740130
C	5.8897676	-0.5383728	2.4514964
H	4.0801463	-0.3527886	3.6550355
C	6.4230015	-0.8053465	1.1886330
H	5.9948309	-1.3100348	-0.8902151
C	-1.2988199	-2.3456582	2.2095043
C	-2.6454039	-3.7563201	0.5684071
C	-0.4604927	-4.5892070	1.4869687
C	0.7329944	-2.6025816	-2.8195425
C	-0.0944823	-4.8012873	-1.9134656
C	-1.7311082	-2.9932812	-2.6197488
H	6.5561220	-0.3038227	3.2771440
H	7.4991894	-0.7748636	1.0420682
H	-0.2924057	-2.0324971	2.5058565
H	-1.8813829	-1.4576197	1.9676550
H	-1.7631951	-2.8621703	3.0571854
H	-2.5962345	-4.5750047	-0.1546905
H	-3.1932174	-4.1187620	1.4452757
H	-3.2181817	-2.9355549	0.1355343
H	0.5452618	-4.3337720	1.8252413
H	-1.0157553	-5.0202512	2.3275488
H	-0.3896955	-5.3486105	0.7057436
H	0.5293868	-1.5357346	-2.9433895
H	1.7270617	-2.7253894	-2.3824871
H	0.7276065	-3.0658824	-3.8124308
H	-0.9013716	-5.3417514	-1.4114800
H	-0.0294796	-5.1788527	-2.9405176
H	0.8513937	-5.0224595	-1.4099352
H	-1.9193629	-1.9174152	-2.6524680
H	-1.7107680	-3.3723810	-3.6480165
H	-2.5566848	-3.4801481	-2.0975636

B	-2.1092080	0.5699862	-0.4431420
O	-1.4906617	1.7880647	-0.4844088
P	-0.2683427	2.7454965	0.0876385
O	-2.8386250	0.1677706	0.7221176
O	-2.8041928	0.1173652	-1.6120423
C	-3.9286528	-0.5299074	0.2556378
C	-3.8954724	-0.5787872	-1.1433341
C	-4.9431761	-1.1218392	0.9874500
C	-4.8642919	-1.2513145	-1.8686952
C	-0.6242716	2.8591155	1.9294544
C	-0.7252233	4.3181577	-0.8373158
C	-5.9340173	-1.8017380	0.2599898
H	-4.9602156	-1.0760560	2.0714614
C	-5.8912067	-1.8702790	-1.1354808
H	-4.8316218	-1.2965717	-2.9524345
C	0.2285226	3.9958330	2.5185866
C	-2.0976394	3.0251283	2.3261063
C	-0.0941223	1.5100855	2.4673176
C	-2.0929968	4.9223132	-0.4966393
C	0.4007976	5.3454516	-0.6148457
C	-0.7026870	3.9038178	-2.3263834
H	-6.7437333	-2.2881239	0.7955011
H	-6.6684521	-2.4096198	-1.6685801
H	-0.1844164	4.9796188	2.2780250
H	1.2645503	3.9514502	2.1623021
H	0.2460736	3.8970149	3.6110638
H	-2.1750338	2.9542658	3.4196050
H	-2.4986166	3.9949779	2.0251249
H	-2.7163231	2.2359912	1.8930395
H	0.9699165	1.3793967	2.2486792
H	-0.2353901	1.4792777	3.5554598
H	-0.6358450	0.6642995	2.0343084
H	-2.3243711	5.7237203	-1.2109119
H	-2.8859798	4.1706879	-0.5614025
H	-2.1023287	5.3580894	0.5061656
H	1.3832194	4.9053683	-0.8215881
H	0.2559579	6.1882830	-1.3017548
H	0.4093964	5.7405508	0.4034018
H	-0.8859142	4.7929801	-2.9423052
H	-1.4753169	3.1633102	-2.5486131
H	0.2721404	3.4900236	-2.6085100

TS4e usual 1,2-addition of **1e** and **1**
55
Energy = -1555.504098185

B	-1.6607494	0.1018219	0.3731493

O	-1.1448939	-1.1856298	0.4646842
P	0.2491277	-1.8845190	0.0204517
O	-2.4295998	0.6186538	1.4479669
O	-2.1013111	0.6522655	-0.8632132
C	-3.1936727	1.6187819	0.8808061
C	-2.9937437	1.6413934	-0.5051758
C	-4.0566131	2.4997939	1.5090808
C	-3.6451745	2.5472474	-1.3236363
C	0.4251382	-3.1942214	1.3438918
C	-0.1114956	-2.5437303	-1.6990337
C	-4.7239996	3.4232518	0.6874467
H	-4.2070879	2.4773066	2.5836033
C	-4.5231526	3.4464953	-0.6963226
H	-3.4836601	2.5601502	-2.3966068
C	-0.6491956	-4.2907314	1.2906245
C	1.8385725	-3.7995419	1.2359913
C	0.3218136	-2.4202462	2.6759798
C	-1.5526103	-3.0597278	-1.8462017
C	0.0996506	-1.3346278	-2.6372928
C	0.9050727	-3.6417489	-2.0527958
H	-5.4086434	4.1342301	1.1402336
H	-5.0541093	4.1752493	-1.3014858
H	-0.5560152	-4.9073228	0.3922957
H	-0.5261705	-4.9477544	2.1610417
H	-1.6557711	-3.8640480	1.3255795
H	2.6074844	-3.0192696	1.2341088
H	2.0107648	-4.4403748	2.1084710
H	1.9618291	-4.4118446	0.3401250
H	1.0629202	-1.6148532	2.7302912
H	-0.6725528	-1.9902680	2.8160900
H	0.5196044	-3.1196806	3.4965139
H	-1.7537015	-3.9152816	-1.1981455
H	-2.2772209	-2.2727077	-1.6224540
H	-1.7010289	-3.3772132	-2.8860506
H	-0.5810478	-0.5131906	-2.3951484
H	1.1288339	-0.9650761	-2.5851888
H	-0.1015121	-1.6509677	-3.6678789
H	1.9368692	-3.3113360	-1.8900795
H	0.7336394	-4.5573585	-1.4803572
H	0.7970544	-3.8854025	-3.1162140
N	0.1020256	1.0292999	0.6169021
N	1.0808637	0.4646800	0.3108751
C	2.3787437	0.5261736	0.0413775
C	3.0135825	1.8276773	0.0727151
H	2.8962793	-0.3879355	-0.1902021
O	2.4724765	2.8980770	0.3313606

O	4.3372370	1.7015733	-0.2342586
C	5.0950910	2.9501323	-0.2272663
C	6.5318817	2.6012464	-0.5568666
H	4.9971505	3.4065974	0.7619882
H	4.6531025	3.6247827	-0.9664551
H	7.1336740	3.5160865	-0.5581990
H	6.9479664	1.9148163	0.1869620
H	6.6053715	2.1378862	-1.5455537

TS4 usual 1,2-addition of **1p** and **1**

66

Energy = -1750.551702874

B	-1.5971107	-0.6025907	0.8181354
O	-0.7645942	-1.7153512	0.6856561
P	0.8370831	-1.8416109	0.2552995
O	-2.6977468	-0.7460435	1.7480307
O	-2.1071081	0.0725998	-0.3726333
C	-3.7473744	-0.0536230	1.1981059
C	-3.3964510	0.4368245	-0.0677580
C	-5.0039480	0.1681155	1.7370225
C	-4.2824428	1.1691178	-0.8391269
C	1.2781558	-3.3326754	1.3136179
C	0.6839055	-2.3260599	-1.5630341
C	-5.9122468	0.9102794	0.9608797
H	-5.2729327	-0.2142562	2.7168309
C	-5.5601097	1.4003091	-0.2989526
H	-4.0029292	1.5434133	-1.8191556
C	0.5071734	-4.6250156	1.0186380
C	2.7982296	-3.5631285	1.2099874
C	0.9601806	-2.8671579	2.7523524
C	-0.5236594	-3.2112812	-1.9008857
C	0.5324708	-0.9708890	-2.2917022
C	1.9941162	-2.9833338	-2.0261243
H	-6.9060258	1.1053142	1.3533237
H	-6.2828716	1.9713795	-0.8742709
H	0.8122263	-5.0669102	0.0652765
H	0.7095963	-5.3622964	1.8073766
H	-0.5715263	-4.4428542	0.9930012
H	3.3494509	-2.6255838	1.3428107
H	3.1115546	-4.2583941	1.9990630
H	3.0857389	-3.9958476	0.2489050
H	1.4437116	-1.9087196	2.9785104
H	-0.1162008	-2.7513114	2.9031025
H	1.3359592	-3.6147889	3.4619834
H	-0.4168318	-4.2221723	-1.5015939
H	-1.4476359	-2.7787244	-1.5069566

H -0.6195980 -3.2865579 -2.9924039
H -0.3750804 -0.4468518 -1.9773412
H 1.3941229 -0.3229492 -2.0984512
H 0.4675355 -1.1465552 -3.3734568
H 2.8706816 -2.4131143 -1.6946341
H 2.0859370 -4.0090553 -1.6574386
H 2.0137321 -3.0169732 -3.1228409
N -0.5589357 0.6675676 1.5554531
N 0.3518794 1.1031394 0.9648070
C 1.2837198 1.7578302 0.3491381
C 2.6675859 1.2704356 0.4413986
C 3.5430563 1.4577018 -0.6394483
C 3.1144306 0.5747978 1.5757690
C 4.8434013 0.9615264 -0.5801348
H 3.1982605 1.9739935 -1.5294645
C 4.4176196 0.0906826 1.6330678
H 2.4433608 0.4214252 2.4151207
C 5.2862390 0.2799285 0.5555593
H 5.5095027 1.1036054 -1.4260989
H 4.7554132 -0.4376543 2.5196911
H 6.3017141 -0.1024664 0.6002491
C 0.8520817 2.9345098 -0.4356206
C 1.7058186 4.0443611 -0.5472410
C -0.4079854 2.9657688 -1.0543905
C 1.3025548 5.1622004 -1.2741339
H 2.6736515 4.0331271 -0.0566199
C -0.8058514 4.0915566 -1.7705671
H -1.0608190 2.1005796 -0.9876108
C 0.0471770 5.1917474 -1.8863754
H 1.9689628 6.0160999 -1.3538772
H -1.7804192 4.1050158 -2.2501264
H -0.2630329 6.0656801 -2.4513700

TS5e terminal N-to-P add. of **1e** and **1**
55
Energy = -1555.512503347
N -1.4739600 2.0499777 -1.5462602
N -2.2202636 1.1459096 -1.7572808
C -2.6633810 -0.0753041 -1.5136791
C -2.1616923 -0.8784653 -0.4353538
H -3.4582390 -0.4367209 -2.1532594
O -1.3323261 -0.5426803 0.4190490
O -2.7501195 -2.1113364 -0.4308972
C -2.3095879 -3.0118843 0.6289331
C -3.0592925 -4.3158795 0.4498428
H -2.5203065 -2.5396801 1.5929799

H	-1.2291058	-3.1474920	0.5390363
H	-4.1402297	-4.1638106	0.5287818
H	-2.8357330	-4.7624533	-0.5239843
H	-2.7510301	-5.0193419	1.2303715
B	1.0927762	-0.4193246	0.4985880
O	1.0771593	0.9183978	0.7651931
P	0.1384270	2.0551672	0.0021883
O	1.1674998	-1.0004023	-0.7781738
O	1.2905213	-1.3669601	1.5130675
C	1.2740465	-2.3590776	-0.5328566
C	1.3595099	-2.5792034	0.8454022
C	1.2796125	-3.3998806	-1.4434757
C	1.4655939	-3.8503449	1.3805811
C	1.4281105	2.9774052	-0.9979370
C	-0.4742575	3.0310022	1.4803587
C	1.3813784	-4.6959579	-0.9125217
H	1.2020368	-3.2223677	-2.5109474
C	1.4739885	-4.9157137	0.4656276
H	1.5259239	-4.0140339	2.4514425
C	1.6302954	2.1180595	-2.2676686
C	0.9097241	4.3683990	-1.4068432
C	2.7810220	3.1062719	-0.2762286
C	0.6415629	3.7552491	2.2500220
C	-1.5452850	4.0348990	1.0098478
C	-1.1458126	2.0009825	2.4139105
H	1.3851127	-5.5445097	-1.5897910
H	1.5487086	-5.9319908	0.8402676
H	1.9857795	1.1134389	-2.0198973
H	0.7016174	2.0269954	-2.8374515
H	2.3837877	2.6022245	-2.9008727
H	0.8443645	5.0445664	-0.5496762
H	1.6180805	4.8048916	-2.1218190
H	-0.0694477	4.3114512	-1.8894706
H	3.5047827	3.5342716	-0.9811982
H	2.7281775	3.7640756	0.5929535
H	3.1568902	2.1318545	0.0462328
H	1.4457595	3.0690406	2.5310536
H	1.0643058	4.5824300	1.6736304
H	0.2151907	4.1731415	3.1710471
H	-2.3639530	3.5283077	0.4916211
H	-1.9555327	4.5375924	1.8940516
H	-1.1378445	4.8003086	0.3455299
H	-1.6139687	2.5465221	3.2421430
H	-1.9125955	1.4232436	1.8917380
H	-0.4152907	1.3004124	2.8260611

TS5 terminal N-to-P add. of **1p** and **1**
66
Energy = -1750.527630136

B	-2.4956060	-0.3075955	-0.6013804
O	-2.4677845	1.0345031	-0.3911744
P	-1.3337300	1.9658564	0.3984465
O	-3.4891954	-0.8916307	-1.3963958
O	-1.6070012	-1.2540680	-0.0913190
C	-3.1960650	-2.2523265	-1.3740633
C	-2.0617563	-2.4674250	-0.5897264
C	-3.8648669	-3.2884470	-1.9994140
C	-1.5318524	-3.7282760	-0.3883780
C	-0.9999932	3.2692512	-0.8988403
C	-2.3265488	2.5201531	1.8712558
C	-3.3384803	-4.5756180	-1.8026659
H	-4.7459271	-3.1157740	-2.6082917
C	-2.2005217	-4.7905592	-1.0173008
H	-0.6479770	-3.8831920	0.2214332
C	-2.1832381	4.1671911	-1.2806390
C	0.1909522	4.1052739	-0.3856696
C	-0.5441435	2.4488425	-2.1293383
C	-3.7444978	3.0061790	1.5309120
C	-2.4255330	1.2655804	2.7724296
C	-1.5303047	3.6137821	2.6055239
H	-3.8286692	-5.4220774	-2.2736495
H	-1.8233701	-5.8005229	-0.8898451
H	-2.4556996	4.8448107	-0.4673260
H	-1.8959021	4.7797806	-2.1453260
H	-3.0603252	3.5764655	-1.5606083
H	-0.1005280	4.7750920	0.4269265
H	1.0028510	3.4641972	-0.0267665
H	0.5747423	4.7188883	-1.2087803
H	0.2521654	1.7411945	-1.8751283
H	-1.3779087	1.8960866	-2.5700734
H	-0.1548869	3.1420368	-2.8841573
H	-3.7368427	3.9400069	0.9658979
H	-4.2972299	2.2546819	0.9603065
H	-4.2821339	3.1831859	2.4709636
H	-2.9860158	0.4635250	2.2812637
H	-1.4380843	0.8853704	3.0426827
H	-2.9641566	1.5409582	3.6867951
H	-0.4930388	3.3075212	2.7791492
H	-1.5323274	4.5560267	2.0503863
H	-1.9977036	3.7968025	3.5800258
N	0.2901690	0.6513264	1.2484821
N	1.2463012	0.4990535	0.5215453

C	2.3668445	-0.2058654	0.4534739
C	2.6893313	-1.1505003	1.5339164
C	3.1966009	0.0011591	-0.7419059
C	1.6737082	-1.6642958	2.3661023
C	4.0168306	-1.5470071	1.8010411
C	4.0044924	-1.0205510	-1.2791882
C	3.1715227	1.2345926	-1.4235449
C	1.9685247	-2.5516905	3.3983280
H	0.6436048	-1.3661002	2.1906608
C	4.3084004	-2.4283657	2.8396064
H	4.8261276	-1.1454269	1.1996261
C	4.7518304	-0.8141237	-2.4376382
H	4.0262769	-1.9936979	-0.7986188
C	3.9089324	1.4368467	-2.5862290
H	2.5659137	2.0413036	-1.0209251
C	3.2874339	-2.9437876	3.6431400
H	1.1631167	-2.9394077	4.0171511
H	5.3421896	-2.7073803	3.0274778
C	4.7122526	0.4145897	-3.1015581
H	5.3600543	-1.6248730	-2.8309626
H	3.8682561	2.4013193	-3.0864471
H	3.5169248	-3.6317146	4.4519536
H	5.2968076	0.5736076	-4.0032506

TS6 unusual 1,3-addition of **1p** and **1**

66

Energy = -1750.536745002

B	-0.5090305	-1.5329421	0.1702945
O	-1.7005393	-1.2123697	-0.4027802
P	-2.7433056	0.0484333	-0.3084533
O	0.3397868	-2.4649457	-0.4347564
O	-0.0367705	-1.1314256	1.4249894
C	1.4117094	-2.5800176	0.4398017
C	1.1911614	-1.7682345	1.5539142
C	2.5599863	-3.3346554	0.2967297
C	2.1142530	-1.6533508	2.5760233
C	-3.6636485	-0.2368467	-1.9209165
C	-3.7599598	-0.3170576	1.2258342
C	3.5042064	-3.2332883	1.3297724
H	2.7303122	-3.9514559	-0.5786171
C	3.2890092	-2.4102815	2.4402443
H	1.9417869	-1.0076779	3.4304498
C	-4.4362379	-1.5620720	-1.9850950
C	-4.5947431	0.9655574	-2.1674375
C	-2.5574492	-0.2211261	-2.9998571
C	-3.9407311	-1.8255482	1.4656437

C	-2.9850404	0.3016834	2.4112526
C	-5.1299375	0.3752817	1.1140531
H	4.4273851	-3.8002433	1.2576750
H	4.0469296	-2.3509349	3.2155051
H	-5.2843537	-1.5723234	-1.2949397
H	-4.8307932	-1.6922348	-3.0014147
H	-3.7861338	-2.4131840	-1.7623507
H	-5.4485483	0.9787083	-1.4871461
H	-4.0543815	1.9132830	-2.0680350
H	-4.9812995	0.9022552	-3.1913683
H	-1.9744328	0.7054455	-2.9575374
H	-1.8784294	-1.0702852	-2.8942220
H	-3.0353436	-0.2767741	-3.9849183
H	-4.4990366	-2.3094971	0.6615676
H	-2.9783737	-2.3326064	1.5758177
H	-4.5004587	-1.9597756	2.3997980
H	-1.9800553	-0.1176954	2.5032869
H	-2.8935830	1.3855560	2.3029758
H	-3.5393107	0.0859032	3.3330309
H	-5.0328015	1.4381960	0.8689976
H	-5.7710135	-0.1025678	0.3684693
H	-5.6327013	0.3017362	2.0855533
N	-1.1777019	1.6213014	0.1373873
N	-0.1370796	1.2023206	-0.3211178
C	1.1652557	1.4473764	-0.3278929
C	1.6850763	2.5734519	0.4562733
C	2.0004477	0.5360823	-1.1270517
C	0.9069944	3.1741569	1.4672680
C	2.9615831	3.1217769	0.2027640
C	3.2931275	0.1592766	-0.7170063
C	1.4985712	-0.0253177	-2.3160321
C	1.3896934	4.2531961	2.2039428
H	-0.0846810	2.7823616	1.6773793
C	3.4370295	4.2045606	0.9372573
H	3.5751445	2.7050207	-0.5890959
C	4.0513296	-0.7332864	-1.4701631
H	3.6884414	0.5395275	0.2193945
C	2.2517246	-0.9279962	-3.0609394
H	0.5020724	0.2540120	-2.6463172
C	2.6594571	4.7768791	1.9482933
H	0.7685686	4.6888857	2.9825747
H	4.4202800	4.6098560	0.7117102
C	3.5384170	-1.2830378	-2.6471811
H	5.0383670	-1.0227714	-1.1198720
H	1.8368625	-1.3504188	-3.9726195
H	3.0334130	5.6212483	2.5204017

H 4.1291191 -1.9847404 -3.2294059

TS7a N_2-loss after 1,3-add. of **1p** and **1**
66
Energy = -1750.572406225
B 0.0583249 -0.0796114 -2.0274018
O 0.1069045 -0.9026928 -0.8953404
P 0.5094348 -0.9511928 0.6652755
O -1.2061906 0.0179510 -2.7051132
O 1.1177127 -0.1760660 -2.9971920
C -0.8866214 0.1120351 -4.0428036
C 0.4985154 -0.0076793 -4.2173660
C -1.7442027 0.2802687 -5.1154022
C 1.0813288 0.0363420 -5.4714587
C -0.3639681 -2.5407243 1.1267968
C 2.3848478 -1.1141380 0.6436805
C -1.1620050 0.3295531 -6.3945333
H -2.8162050 0.3713720 -4.9727569
C 0.2188997 0.2101498 -6.5685319
H 2.1548716 -0.0591169 -5.5987884
C 0.2524796 -3.7658891 0.4254945
C -0.3179477 -2.7098256 2.6557089
C -1.8459930 -2.4392080 0.6953445
C 2.8044418 -1.9051040 -0.6201218
C 3.0255122 0.2862332 0.5387073
C 2.9702166 -1.8462718 1.8668895
H -1.8021074 0.4645227 -7.2612909
H 0.6391530 0.2526462 -7.5689849
H 1.2519375 -4.0014070 0.7992815
H -0.3902374 -4.6310423 0.6258407
H 0.3008301 -3.6260994 -0.6580850
H 0.7019773 -2.7468905 3.0465036
H -0.8590575 -1.8991235 3.1532907
H -0.8067781 -3.6558570 2.9158677
H -2.4000426 -1.7375936 1.3198672
H -1.9478425 -2.1378779 -0.3495434
H -2.2925631 -3.4337793 0.8120974
H 2.5046560 -2.9526364 -0.5743844
H 2.4147674 -1.4650710 -1.5381556
H 3.8991325 -1.8713673 -0.6620190
H 2.6936681 0.8197742 -0.3548601
H 2.8253594 0.9040875 1.4146582
H 4.1091018 0.1434798 0.4532661
H 2.8165694 -1.2953253 2.7945036
H 2.5694456 -2.8564104 1.9775328
H 4.0509467 -1.9366419 1.7066998

N	0.2817670	1.5807889	-1.3510088
N	0.3248174	1.9940676	-0.3018944
C	-0.0696652	0.4666714	1.4895646
C	-1.5417515	0.6909721	1.5714225
C	0.7076185	1.1169564	2.5878063
C	-2.3892760	0.7790796	0.4489419
C	-2.1425734	0.8341290	2.8412712
C	1.2363336	0.3962863	3.6710028
C	0.8364740	2.5186788	2.6192002
C	-3.7625437	0.9703423	0.5907503
H	-1.9930661	0.6649651	-0.5514647
C	-3.5123279	1.0409220	2.9818493
H	-1.5175492	0.7818544	3.7277590
C	1.9263960	1.0300494	4.7059855
H	1.0747656	-0.6745048	3.7187604
C	1.5159013	3.1569001	3.6544692
H	0.4009049	3.1084646	1.8220614
C	-4.3372577	1.1059880	1.8556655
H	-4.3848319	1.0230272	-0.2991236
H	-3.9379830	1.1414370	3.9772635
C	2.0785411	2.4160927	4.6981702
H	2.3264489	0.4397309	5.5263004
H	1.6080066	4.2400030	3.6464276
H	-5.4068388	1.2627350	1.9625947
H	2.6115501	2.9157310	5.5023454

TS7ea N_2-loss after 1,3-add. of **1e** and **1**
55
Energy = -1555.503226620

N	3.2091780	-0.7637889	-1.1406156
N	3.0247911	0.3947705	-1.3660287
C	1.3559521	0.5435849	-0.9701036
C	0.7258892	1.6803892	-0.3226065
H	0.9803188	0.3882514	-1.9810139
O	-0.2199326	1.5717701	0.5310567
O	1.2392144	2.8604710	-0.5844882
C	0.6496873	4.0311011	0.1096992
C	1.4212362	5.2439201	-0.3549908
H	0.7443448	3.8542986	1.1829275
H	-0.4079947	4.0687181	-0.1593938
H	2.4802702	5.1573723	-0.0963553
H	1.3256632	5.3792398	-1.4358978
H	1.0137458	6.1292355	0.1432608
B	-1.0027127	0.1749481	0.5434012
O	-0.0328917	-0.8512275	0.7557201
P	1.3814296	-1.0906058	-0.0307491

O	-1.7344691	0.0914530	-0.7333823
O	-1.9914253	0.2734213	1.6059116
C	-3.0583624	0.2112436	-0.4084535
C	-3.2123750	0.3185928	0.9831809
C	-4.1508662	0.2156261	-1.2596099
C	-4.4625308	0.4359960	1.5669900
C	0.9787221	-2.6780100	-0.9501489
C	2.4547189	-1.1785298	1.5226119
C	-5.4251805	0.3371655	-0.6750511
H	-4.0256003	0.1278397	-2.3346991
C	-5.5777517	0.4456003	0.7083780
H	-4.5750184	0.5159651	2.6441919
C	0.6212945	-2.2587802	-2.3912239
C	2.1789982	-3.6390894	-0.9713220
C	-0.2347574	-3.3877119	-0.3217270
C	1.7397630	-2.1156465	2.5217168
C	3.8936719	-1.6871741	1.3385030
C	2.4990925	0.2502562	2.1011754
H	-6.3028635	0.3454751	-1.3152178
H	-6.5728689	0.5377861	1.1341912
H	-0.2443542	-1.5879621	-2.4063669
H	1.4655264	-1.7751810	-2.8939510
H	0.3628158	-3.1589243	-2.9605339
H	2.3995362	-4.0256036	0.0282283
H	1.9189868	-4.4936037	-1.6068788
H	3.0761165	-3.1678641	-1.3763819
H	-0.4177546	-4.3066192	-0.8919291
H	-0.0542343	-3.6619874	0.7207061
H	-1.1289610	-2.7639957	-0.3646865
H	0.7145997	-1.8021873	2.7179319
H	1.7363480	-3.1507196	2.1659818
H	2.3046686	-2.0883602	3.4608115
H	4.5039607	-1.0127606	0.7367051
H	4.3432691	-1.7523945	2.3367528
H	3.9285748	-2.6798913	0.8868131
H	3.0626125	0.2215782	3.0409155
H	3.0145599	0.9421599	1.4259236
H	1.4976630	0.6306826	2.3173380

TS7e 1,3-addition of **1e** and **1**
55
Energy = -1555.481833842

B	-1.6384934	-0.0456855	-0.6035179
O	-0.5962435	0.8198503	-0.1731334
P	0.8684692	0.6117881	0.5268520
O	-2.1678451	-1.0077124	0.3818702

O	-2.7746434	0.6760839	-1.1545778
C	-3.5318579	-0.9324367	0.2718983
C	-3.8902541	0.0761216	-0.6372322
C	-4.4822503	-1.6892708	0.9376093
C	-5.2185337	0.3657011	-0.9067476
C	1.7673254	2.0873721	-0.2162357
C	0.5121907	0.8484742	2.3651576
C	-5.8306817	-1.4000409	0.6696684
H	-4.1937539	-2.4666874	1.6380957
C	-6.1897077	-0.3951022	-0.2335348
H	-5.4933728	1.1462650	-1.6092871
C	1.2218048	3.4441054	0.2547449
C	3.2700407	1.9594876	0.0929424
C	1.5637428	1.9718035	-1.7421411
C	-0.6187833	1.8533772	2.6327612
C	0.0724973	-0.5490103	2.8558789
C	1.8005627	1.2442933	3.1034324
H	-6.6053862	-1.9697995	1.1742327
H	-7.2405985	-0.1968611	-0.4233014
H	1.4414026	3.6322923	1.3090318
H	1.6985863	4.2390690	-0.3334716
H	0.1408712	3.5103940	0.0991965
H	3.6648866	1.0015191	-0.2603922
H	3.8094724	2.7592399	-0.4283136
H	3.4868572	2.0479016	1.1598753
H	1.9032931	1.0062909	-2.1294824
H	0.5140599	2.1084855	-2.0121584
H	2.1541206	2.7575422	-2.2291702
H	-0.3354539	2.8747798	2.3721468
H	-1.5199947	1.5891547	2.0728944
H	-0.8612848	1.8286978	3.7029086
H	-0.8142600	-0.9008586	2.3200535
H	0.8762343	-1.2825169	2.7271901
H	-0.1699010	-0.4918596	3.9243145
H	2.6294887	0.5703595	2.8570366
H	2.1050176	2.2703529	2.8804584
H	1.6259429	1.1726068	4.1839194
N	-1.1093655	-1.1614517	-1.7537503
N	-0.0097237	-1.5972477	-1.5658978
C	1.0128349	-1.7104461	-0.7454852
C	2.3862151	-1.6611272	-1.2995237
H	0.8167626	-2.2918888	0.1534120
O	2.6712487	-1.3271303	-2.4369142
O	3.2653973	-2.0152684	-0.3481562
C	4.6809945	-1.9370301	-0.7290514
C	5.4909481	-2.1500779	0.5309861

H	4.8552914	-0.9572218	-1.1810694
H	4.8652193	-2.7075304	-1.4824683
H	6.5560991	-2.1030751	0.2834738
H	5.2726427	-1.3742405	1.2710532
H	5.2801067	-3.1289814	0.9709914

TS7e 1,3-addition of **1p** and **1**

66

Energy = -1750.529617400

B	0.0420452	0.2865130	-1.7766092
O	0.2574353	-0.8626734	-0.9401791
P	0.7744424	-1.0457901	0.5863296
O	-1.1572279	0.1078426	-2.6230093
O	1.1555626	0.6055303	-2.6846125
C	-0.7900821	0.5322493	-3.8709989
C	0.5865903	0.8163937	-3.9089562
C	-1.5883088	0.6568197	-4.9960960
C	1.2062623	1.2244510	-5.0789663
C	0.3500046	-2.8554197	0.8932458
C	2.6416106	-0.7759120	0.4646873
C	-0.9666871	1.0782939	-6.1861771
H	-2.6501561	0.4327709	-4.9589344
C	0.4010125	1.3559966	-6.2259432
H	2.2706986	1.4372431	-5.1055757
C	1.2191520	-3.8508445	0.1103369
C	0.4491510	-3.1153956	2.4086080
C	-1.1216098	-3.0336939	0.4683779
C	3.2548508	-1.3853771	-0.8080564
C	2.8278668	0.7558275	0.4022205
C	3.3446262	-1.3112225	1.7218468
H	-1.5649588	1.1901565	-7.0858552
H	0.8557761	1.6826332	-7.1568329
H	2.2543971	-3.8578607	0.4609823
H	0.8104385	-4.8596542	0.2540850
H	1.2087273	-3.6312428	-0.9612701
H	1.4557583	-2.9523468	2.8019174
H	-0.2495861	-2.4763650	2.9595840
H	0.1762652	-4.1585457	2.6088682
H	-1.7910788	-2.4264958	1.0829559
H	-1.2727102	-2.7648016	-0.5796229
H	-1.3938620	-4.0876331	0.6044463
H	3.2509097	-2.4759568	-0.7925437
H	2.7302969	-1.0381131	-1.7014993
H	4.2990527	-1.0521459	-0.8737757
H	2.3672969	1.1788214	-0.4954228
H	2.4161065	1.2518902	1.2850019

H 3.9017648 0.9754227 0.3557968
H 2.9334670 -0.8681162 2.6350130
H 3.2793674 -2.4000192 1.7984086
H 4.4074458 -1.0445904 1.6699560
N -0.3392398 1.6758254 -0.9949789
N -0.5972948 1.7128206 0.1872287
C -0.6688474 0.9521458 1.3094875
C -1.9822161 0.2863277 1.5112384
C 0.1032524 1.5199698 2.4544904
C -2.8109889 0.0036071 0.4103135
C -2.4018330 -0.0900568 2.7978008
C 0.6274853 0.6926814 3.4577481
C 0.3206757 2.9032652 2.5317264
C -4.0166131 -0.6643563 0.5955720
H -2.5125294 0.2885793 -0.5928336
C -3.6022693 -0.7737361 2.9726511
H -1.7910423 0.1519090 3.6599042
C 1.3575196 1.2354543 4.5107137
H 0.4850963 -0.3805601 3.3885602
C 1.0653434 3.4425750 3.5810832
H -0.1008588 3.5512609 1.7701380
C -4.4133047 -1.0651441 1.8738782
H -4.6456831 -0.8804423 -0.2627071
H -3.9084013 -1.0697574 3.9715675
C 1.5842094 2.6133179 4.5748696
H 1.7623659 0.5795330 5.2757869
H 1.2339372 4.5147479 3.6200783
H -5.3512953 -1.5941849 2.0133636
H 2.1634359 3.0335338 5.3916778

TS8e N_2-loss & C-to-P add. of **1e** and **1**
55
Energy = -1555.482048013
B 1.2866271 -1.0559545 -0.2191974
O 0.0608080 -1.4150329 -0.6436703
P -1.3633536 -0.4256293 -0.4785909
O 1.5845652 -0.0301500 0.6957710
O 2.4564738 -1.7052804 -0.6537949
C 2.9663933 -0.0483456 0.8183083
C 3.4909124 -1.0562031 0.0064970
C 3.7708907 0.7681807 1.5914620
C 4.8500247 -1.3004338 -0.0733215
C -2.2599092 -1.2570270 -1.9192262
C -1.9955984 -1.0479108 1.1932465
C 5.1529696 0.5314394 1.5195176
H 3.3555038 1.5491081 2.2196565

C	5.6791678	-0.4782320	0.7070408
H	5.2523606	-2.0843980	-0.7063049
C	-2.2827605	-2.7893229	-1.7713826
C	-3.7004392	-0.7554649	-2.1288475
C	-1.4287800	-0.8865317	-3.1685952
C	-1.3858377	-2.4110069	1.5656619
C	-1.5478889	-0.0088500	2.2428874
C	-3.5262505	-1.1539405	1.2254834
H	5.8251003	1.1476660	2.1087518
H	6.7534424	-0.6323632	0.6759263
H	-2.9523986	-3.1092492	-0.9683153
H	-2.6574897	-3.2210112	-2.7077963
H	-1.2843702	-3.1907973	-1.5838773
H	-3.7362317	0.2947847	-2.4282960
H	-4.1447378	-1.3389797	-2.9447761
H	-4.3273872	-0.8870663	-1.2458708
H	-1.3636117	0.1993858	-3.3023458
H	-0.4149363	-1.2898723	-3.1074677
H	-1.9179260	-1.3074848	-4.0554637
H	-1.6048348	-3.1850651	0.8276472
H	-0.3015295	-2.3503601	1.6900912
H	-1.8166350	-2.7203368	2.5257967
H	-0.4663462	0.1538398	2.2128985
H	-2.0475550	0.9518585	2.0988226
H	-1.8122014	-0.3841444	3.2393376
H	-4.0211337	-0.2320035	0.9011388
H	-3.8903886	-1.9818292	0.6114285
H	-3.8388191	-1.3419308	2.2602642
N	-4.7191631	1.8467866	0.1650825
N	-3.6978776	2.1081960	-0.2700113
C	-2.3003189	1.5346865	-0.5965864
C	-1.3395533	2.5109574	0.0322520
H	-2.2699462	1.6093871	-1.6853936
O	-1.5573375	3.1517807	1.0487729
O	-0.1797979	2.5532568	-0.6497789
C	0.8913727	3.3429487	-0.0358026
C	2.0882471	3.2617836	-0.9588692
H	1.0949066	2.9159425	0.9498620
H	0.5313351	4.3671523	0.0911168
H	2.9152716	3.8343343	-0.5267816
H	2.4153401	2.2262260	-1.0849986
H	1.8530117	3.6818542	-1.9412737

3.4 Boron chemical shift calculations of 12

All computations were performed using the Gaussian 09 program.[1] The geometry optimization of **12** was performed at the TPSS-D3/def2-TZVP + COSMO (Table S4). Boron chemical shifts were calculated at the B97D function with def2-TZVP basis with solvent effect (chloroform, ε=4.7113).

Table S3. Calculated boron chemical shifts of **12.**

compound	Calculated isotropic value	Calculated boron chemical shift	Experimental boron chemical shift
*t*Bu$_2$POBcat (reference)	-81.7	--	23.0
12 (boron in five-membered ring)	-89.9	14.8	12.1
12 (boron in six-membered ring)	-95.9	8.8	6.5

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, M. C. X. Li, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian 09, Revision E.01.* , Wallingford CT, 2016.