General. All manipulations were carried out under an atmosphere of ultra-high purity nitrogen using standard Schlenk techniques under Ar or in a glovebox under N_2. Solvents were purchased from commercial sources, purified using Innovative Technology SPS-400 PureSolv solvent system or by distilling from conventional drying agents and stored over activated 4 Å molecular sieves. Glassware was oven-dried at 170 °C overnight or flame dried prior to use. NMR spectra were recorded in various deuterated solvents at 25 °C on a Varian Inova-400 or 500 spectrometers (1H: 400.11 MHz, 500.11 MHz, respectively). Proton chemical shifts are reported in ppm versus solvent protic impurity, but referenced finally to $SiMe_4$. Mass spectrometry analyses were performed in an Agilent 6130 MSD (Agilent Technologies, Santa Clara, CA) quadrupole mass spectrometer equipped with a Multimode (ESI and APCI) source. All starting materials have been obtained from commercial sources and used as received without further purification. Tetrazines were synthesized from corresponding nitriles[1] and NaOCP was synthesized using Grutzmacher method[2].

DFT[1] calculations were carried out using Gaussian 09[3]. Geometry optimizations were performed at the B3LYP/6-31G(d,p) level of theory[4]. Reoptimization of the dimethyl tetrazine species, with the 6-311G(d) basis set did not show significant differences in bond length data or thermodynamic data, and therefore analysis was focused on the 6-31G(d,p) calculations. All optimized structures were confirmed to be minima by analyzing the harmonic frequencies.[5-7] Cartesian coordinates, frequencies, and thermodynamic data are summarized in Tables S2-S4.

X-ray crystallography

The sample was investigated with synchrotron radiation at the ChemMatCARS beamline, Advanced Photon Source, Argonne National Laboratory, Chicago, utilizing the SCrAPS program (http://www.iumsc.indiana.edu/projects/SCrAPS/index.html). A yellow crystal (approximate dimensions 0.030 x 0.030 x 0.15 mm3) was placed onto the tip of a glass capillary and mounted on a Huber three-circle diffractometer and measured at 100 K.

Data collection

The data collection was carried out using synchrotron radiation (λ = 0.41328, silicon 111 and 311 monochromators, two mirrors to exclude higher harmonics) with a frame time of 0.5 seconds and a detector distance of 5.0 cm. A randomly oriented region of reciprocal space was surveyed to the extent of hemispheres. Two major sections of frames were collected with 0.50º steps in φ and a detector position of 0° in 2θ. Data to a resolution of 0.77 Å were initially considered in the reduction but was changed to

0.84 due to lack of reflections at higher angle. Final cell constants were calculated from the xyz centroids of 9550 strong reflections from the actual data collection after integration (SAINT).[8] The intensity data were corrected for absorption (SADABS).[9]

Structure solution and refinement

The space group *Pbca* was determined based on intensity statistics and systematic absences. The structure was solved using Superflip[10] and refined (full-matrix-least squares) using the Oxford University Crystals for Windows system.[11] The charge-flipping solution was calculated, which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed, which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were placed in ideal positions and refined as riding atoms. The final full matrix least squares refinement converged to R1 = 0.0649 and wR2 = 0.1889 (F2, all data).

ChemMatCARS Sector 15 is principally supported by the Divisions of Chemistry (CHE) and Materials Research (DMR), National Science Foundation, under grant number NSF/CHE-1346572. Use of the Advanced Photon Source, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science by Argonne National Laboratory, was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

General procedure for tetrazine + NaOCP reaction

In 20 ml scintillation vial 0.1 mmol of tetrazine was dissolved in 3 ml of THF, in separate vial 0.1 mmol of NaOCP was dissolved in 3 ml of THF. Both solution was precooled to -78^{o}C and then NaOCP solution was added to tetrazine solution using Pasteur pipette. Reaction immediately turned color from deep violet to yellow-orange and intense gas evolution was observed. Reaction mixture was removed from cold and stirred at r.t. for 1 h. Volatiles were removed under vacuum yielded yellow amorphous solid.

Sodium 3,6-dimethyl-1,2,4-diazaphosphinin-5-olate 2a.

Off-white solid. **^{1}H NMR** (400 MHz, [d_8]THF, 298K): δ(ppm) 2.43 (d, $J_{H,P}$ = 11.9 Hz, 3H), 2.18 (s, 3H). **^{31}P NMR** (162 MHz, [d_8]THF, 298K): δ(ppm) 117.54. **^{13}C NMR** (126 MHz, [d_8]THF) δ(ppm) 204.76 (d, $J_{C,P}$ = 47.7 Hz), 187.64 (d, $J_{C,P}$ = 70.7 Hz), 168.44 (d, $J_{C,P}$ = 50.7) Hz), 27.14 (d, $J_{C,P}$ = 40.8 Hz), 26.18. **MS (APCI-)** m/z = 141.0.

Sodium 3,6-diethyl-1,2,4-diazaphosphinin-5-olate 2b.

Off-white solid. **^{1}H NMR** (400 MHz, [d_8]THF, 298K): δ(ppm) 2.74 (m, 4H), 1.23 (t, $J_{H,H}$ = 7.7 Hz, 3H), 1.23 (t, $J_{H,H}$ = 7.6 Hz, 3H). **^{31}P NMR** (162 MHz, [d_8]THF, 298K): δ(ppm) 117.56. **^{13}C NMR** (126 MHz, [d_8]THF) δ(ppm) 204.56 (d, $J_{C,P}$ = 46.8 Hz), 194.38 (d, $J_{C,P}$ = 70.9 Hz), 153.74 (d, $J_{C,P}$ = 19.8) Hz), 35.20 (d, $J_{C,P}$ = 35.0 Hz), 26.37, 16.69 (d, $J_{C,P}$ = 7.6 Hz), 13.03. **MS (APCI-)** m/z = 169.1.

Sodium 3,6-diphenyl-1,2,4-diazaphosphinin-5-olate 2c. Off-white solid. **^{1}H NMR** (400 MHz, CD_3CN, 298K): δ(ppm) 8.00-7.94 (m; 4H), 7.45-7.27 (m, 6H). **^{31}P NMR** (162 MHz, CD_3CN, 298K): δ(ppm) 125.11. **^{13}C NMR** (120 MHz, CD_3CN, 298K): δ(ppm) 201.87 (d, $J_{C,P}$ = 45.7 Hz), 190.27 (d, $J_{C,P}$ = 72.0 Hz), 171.22, 148.92 (d, $J_{C,P}$ = 23.1 Hz), 144.60 (d, $J_{C,P}$ = 24.7 Hz), 139.32, 130.59, 129.45, 129.25, 128.21, 128.12, 127.51 (d, $J_{C,P}$ = 13.1 Hz). **MS (ESI-)**: m/z: 265.0 (M-Na); **(APCI+)**: m/z: 267.1 (M^-+2H)

Sodium 3,6-dipyridyl-1,2,4-diazaphosphinin-5-olate 2d. Yellow solid. **^{1}H NMR** (400 MHz, CD_3CN, 298K): δ(ppm) 8.54 (m, 2H), 8.24 (d, $J_{H,H}$ = 8.2 Hz, 1H), 8.17 (d, $J_{H,H}$ = 7.7 Hz, 1H), 7.81 (dt, $J_{H,H}$ = 14.7, 7.6 Hz, 2H), 7.35 (t, 1H), 7.28 (t, 1H). **^{31}P NMR** (162 MHz, CD_3CN, 298 K): δ(ppm) 143.02. **^{13}C NMR** (126 MHz, [d_6]DMSO, 298K): δ(ppm) 201.20 (d, $J_{C,P}$ = 46.3 Hz), 189.33 (d, $J_{C,P}$ = 71.9 Hz), 160.09 (d, $J_{C,P}$ = 21.1 Hz), 158.43, 149.18 149.05, 148.01 (d, $J_{C,P}$ = 24.3 Hz), 137.08, 135.88, 125.42, 124.19, 122.36, 119.34 (d, $J_{C,P}$ = 5.3 Hz). **MS (APCI+)**: m/z: 269.2 (M^-+2H).

Sodium 3-methyl-6-phenyl-1,2,4-diazaphosphinin-5-olate 2ea and Sodium 6-methyl-3-phenyl-1,2,4-diazaphosphinin-5-olate 2eb. Mixture of two regio isomers in 5:1 ratio. **^{1}H NMR** (400 MHz, CD_3CN, 298K): δ(ppm) *major isomer* 7.84-7.81 (m, 2H, *Ph*), 7.31-7.23 (m, 3H, *Ph*), 2.53 (d, $J_{H,P}$ = 11.6 Hz, 3H, *Me*), *minor isomer* 7.90-7.87 (m; 2H, *Ph*), 7.37-7.35 (m, 2H, *Ph*), 2.24 (s, 3H) **^{31}P NMR** (162 MHz, CD_3CN, 298K): δ(ppm) *major isomer* 129.7; *minor isomer* 112.5. **^{13}C NMR** (120 MHz, CD_3CN, 298K): δ(ppm) *major isomer* 203.05 (d, $J_{C,P}$ = 46.8 Hz), 190.00 (d, $J_{C,P}$ = 67.1 Hz), 139.91, 130.49, 128.19, 127.99, 27.20 (d, $J_{C,P}$ = 29.3 Hz) *minor isomer* 203.82 (d, $J_{C,P}$ = 44.3 Hz), 188.90 (d, $J_{C,P}$ = 74.1 Hz), 149.25 (d, $J_{C,P}$ = 19.7 Hz), 129.99, 129.19, 127.54 (d, $J_{C,P}$ = 13.2 Hz), 26.25. **MS (APCI-):** m/z: 203.1.

Sodium 3-methyl-6-pyridyl-1,2,4-diazaphosphinin-5-olate 2fa and Sodium 6-methyl-3-pyridyl-1,2,4-diazaphosphinin-5-olate 2fb. Mixture of two regio isomers in 3:1 ratio. **^{1}H NMR** (400 MHz, CD_3CN, 298K): δ(ppm) *major isomer* 8.55 (d, $J_{H,H}$ = 4.6 Hz, 1H, *Py*), 8.05 (d, $J_{H,H}$ = 7.9 Hz, 1H, *Py*), 7.82-7.76 (m, 1H, *Py*),

7.31-7.23 (m, 1H, *Py*) 2.59 (d, $J_{H,P}$ = 12.3 Hz, 3H, *Me*), *minor isomer* 8.57-8.55 (m, 1H, *Py*), 8.17 (d, $J_{H,H}$ = 7.9 Hz, 1H, *Py*), 7.82-7.76 (m, 1H, *Py*), 7.34-7.29 (m, 1H, *Py*), 2.27 (s, 3H, *Me*). **^{31}P NMR** (162 MHz, CD_3CN, 298 K): δ(ppm) 140.1, 119.51. **^{13}C NMR** *major isomer* (126 MHz, [d_8]THF): δ(ppm) 202.57 (d, $J_{C,P}$ = 45.6 Hz), 190.95 (d, $J_{C,P}$ = 70.9 Hz), 159.50, 148.64, 146.14 (d, $J_{C,P}$ = 20.1 Hz), 136.43, 126.27, 122.21, 29.86 (d, $J_{C,P}$ = 14.2 Hz) *minor isomer* not resolved during overnight ^{13}C NMR. **MS:** (ESI+): m/z: 206.1 (M^-+2H)

3,6-diphenyl-5-trimethylsiloxy-1,2,4-diazaphosphinin 3. To a stirring solution of sodium 3,6-diphenyl-1,2,4-diazaphosphinin-5-olate (37.1 mg, 0.073 mmol) at -78°C in a 20 mL scintillation vial was added dropwise 9.26 μL (0.073 mmol) TMSCl at -78°C. The solution changed colors from yellow to orange, and the reaction was stirred at r.t. for 30 minutes before volatiles were removed to afford an amorphous solid. **^{1}H NMR** (400 MHz, CD_3CN, 298K): δ(ppm) 8.20-8.11 (m, 2H), 7.86-7.80 (m, 2H), 7.60-7.55 (m, 3H), 7.54-7.49 (m, 3H), 0.33 (s, 9H, *TMS*). **^{31}P NMR** (162 MHz, CD_3CN, 298K): δ(ppm) 141.15. **MS (ESI-)**: m/z: 265.0 (M-TMS)

3,6-diethyl-5-methoxy-1,2,4-diazaphosphinin-5-olate 4a

To a freshly prepared solution of 2a in [d_8]THF 1 eq. of MeI was added and reaction was monitored with 1H and 31P NMR. After 5 min two products were detected and after 5h only a complete rearrangement to a major one was observed. ***4a*** *major* **^{1}H NMR** (400 MHz, [d_8]THF, 298K): δ(ppm) 3.97 (s, 3H), 2.91 (dq, $J_{H,H}$ = 7.4, $J_{H,P}$ = 13.5 Hz 2H), 2.55 (q, $J_{H,H}$ = 7.5 Hz, 2H), 1.27 (t, $J_{H,H}$ = 7.4 Hz, 3H), 1.07 (t, $J_{H,H}$ = 7.4 Hz, 3H). **^{31}P NMR** (162 MHz, [d_8]THF, 298K): δ(ppm) 119.68. **^{13}C NMR** (120 MHz, CD_3CN, 298K): δ(ppm) 201.56 (d, $J_{C,P}$ = 48.7 Hz), 193.61 (d, $J_{C,P}$ = 72.5 Hz), 155.53 (d, $J_{C,P}$ = 23.2 Hz), 47.00, 32.44 (d, $J_{C,P}$ = 26.6 Hz), 23.83, 13.61 (d, $J_{C,P}$ = 15.0 Hz), 11.29 . **MS (ESI+)**: m/z: 219.1 (M+H). **MS (ESI+)**: m/z: 185.1 (M+H). ***4a*** *minor* **^{1}H NMR** (400 MHz, [d_8]THF, 298K): δ(ppm) 4.29 (s, 3H), 3.01 (m 2H), 2.69 (m, 2H), 1.21 (m, 3H), 1.17 (m, 3H). **^{31}P NMR** (162 MHz, [d_8]THF, 298K): δ(ppm) 144.99.

3-phenyl-6-methyl-5-methoxy-1,2,4-diazaphosphinin-5-olate 4b

In 20 ml scintillation vial 17.2 mg (0.1 mmol) of 3-methyl-6-phenyltetrazine **1e** was dissolved in 3 ml of THF, in separate vial 30.2 mg (0.1 mmol) of NaOCP was dissolved in 3 ml of THF. Both solution was precooled to -78°C and then NaOCP solution was added to tetrazine solution using Pasteur pipette. Reaction immediately turned color from deep violet to yellow-orange and intense gas evolution was observed. Reaction mixture was removed from cold and stirred at r.t. for 1 h. One equivalent of MeI was

added and reaction mixture was stirred at r.t. for 6 h, then filtered. Volatiles were removed, yielding light-yellow amorphous solid in 70% yield. Only one isomer was detected with NMR. **^{1}H NMR** (400 MHz, CD_3CN, 298K): δ(ppm) 7.77 (m, 2H), 7.40 (m, 3H), 4.00 (s, 3H), 2.64 (d, $J_{H,P}$ = 14.4 Hz, 3H). **^{31}P NMR** (162 MHz, CD_3CN, 298K): δ(ppm) 136.33. **^{13}C NMR** (120 MHz, CD_3CN, 298K): δ(ppm) 202.62 (d, $J_{C,P}$ = 51.5 Hz), 188.47 (d, $J_{C,P}$ = 68.41 Hz), 150.33 (d, $J_{C,P}$ = 23.3 Hz), 134.79, 130.21, 130.04, 128.60, 67.51, 26.06 (d, $J_{C,P}$ = 33.14 Hz). **MS (ESI+)**: m/z: 219.1 (M+H)

Bis(triphenylphosphine)(hydrido)(carbonyl)ruthenium(3,6-diphenyl-1,2,4-diazaphosphinin-5-olate) 5

In 20 ml scintillation vial 23.5 mg (0.1 mmol) of **2c** was dissolved in 3 ml of THF, in separate vial 30.2 mg (0.1 mmol) of NaOCP was dissolved in 3 ml of THF. Both solution was precooled to -78°C and then NaOCP solution was added to tetrazine solution using Pasteur pipette. Reaction immediately turned color from deep violet to yellow-orange and intense gas evolution was observed. Reaction mixture was removed from cold and stirred at r.t. for 1 h and then cooled back to -78°C and transferred to a precooled vial containing 95.2 mg (0.1 mmol) of $(PPh_3)_3RuH(CO)Cl$ in 5 ml of THF. Reaction mixture was removed from cold and stirred for 12h. A deep red-brown solution was filtered through Celite pad and concentrated to ~2 ml. Pentane was added causing precipitation of tan solid. Precipitate was filtered and dried in vacuum. Yield 51% (mixture of isomers). *Major isomer* **^{1}H NMR** (400 MHz, CD_2Cl_2, 298K): δ(ppm) 7.70-7.11 (m, 40H) -14.43 (t, $J_{H,P}$ = 18.2 Hz, 1H), **^{31}P NMR** (162 MHz, CD_3CN, 298K): δ(ppm) 139.27 (t, $J_{P,P}$ = 5.8 Hz, 1P), 43.83 (d, $J_{P,P}$ = 5.7 Hz, 2P) fully decoupled ^{31}PNMR spectra require careful placement of the decoupling central frequency to avoid the hydride at -15 ppm from escaping decoupler power. **IR (KBr):** 2227 cm^{-1} (ν_{RuH}), 1924 cm^{-1} (ν_{CO}). *Minor isomer* **^{1}H NMR** (400 MHz, CD_2Cl_2, 298K): δ(ppm) -15.32 (t, $J_{H,P}$ = 18.4 Hz, 1H), aryl protons overlaps with major isomer signals. **^{31}P NMR** (162 MHz, CD_3CN, 298K): δ(ppm) 135.50 (t, $J_{P,P}$ = 5.8 Hz, 1P), 43.22 (d, $J_{P,P}$ = 5.7 Hz, 2P).

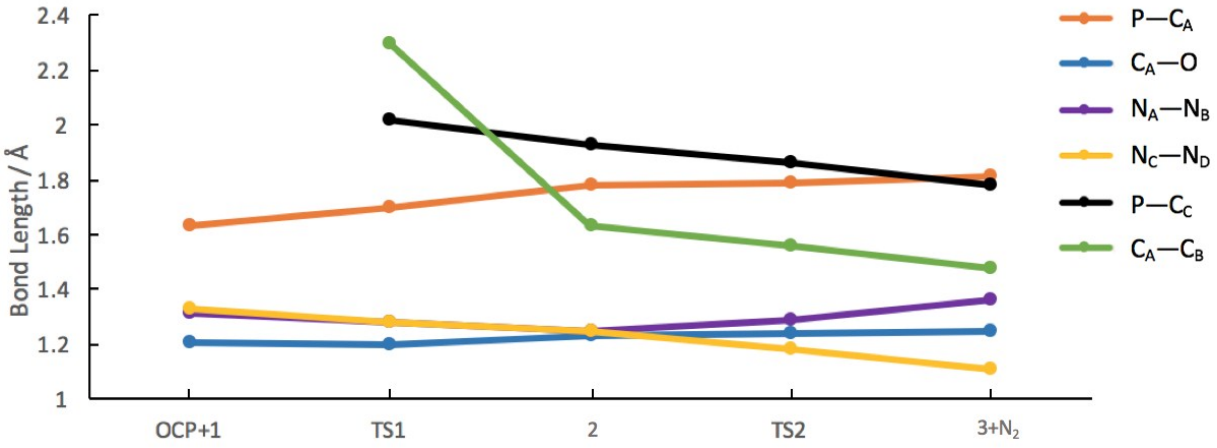
DFT calculations

Bond lengths for dimethyl tetrazine

Key bond lengths (Table S1 and Figure S1) in the various stationary states are revealing of reaction progress. At **TSI** the PC_C distance is shorter than the C_AC_B distance; since P is inherently larger than C_A of PCO^{-1}, this inequality shows that the main stabilization in reaching **TSI** is from PC_C bond formation, and the C_AC_B bond forms later. The reaction mechanism is thus asynchronous with regard to the ultimate formation of these two bonds. The PCO angle undergoes most of its bending in forming **TSI** and adduct **II**, but the DFT results (Figure S1) show that half of the bending has occurred by **TSI**; **TSI** thus prepares C_A for C_AC_B interaction.

Table S1. Bond lengths (in Å) and angle (in degrees)

	P—C_A	C_A—O	N_A—N_B	N_C—N_D	C_A—C_B	P—C_C	O-C-P
1 + OCP	1.631	1.206	1.317	1.326	-	-	180.0
TS1	1.697	1.196	1.278	1.278	2.299	2.017	153.7
2	1.778	1.234	1.248	1.248	1.631	1.928	131.8
TS2	1.788	1.243	1.289	1.179	1.556	1.865	128.6
3 + N_2	1.812	1.250	1.362	1.106	1.475	1.778	123.0



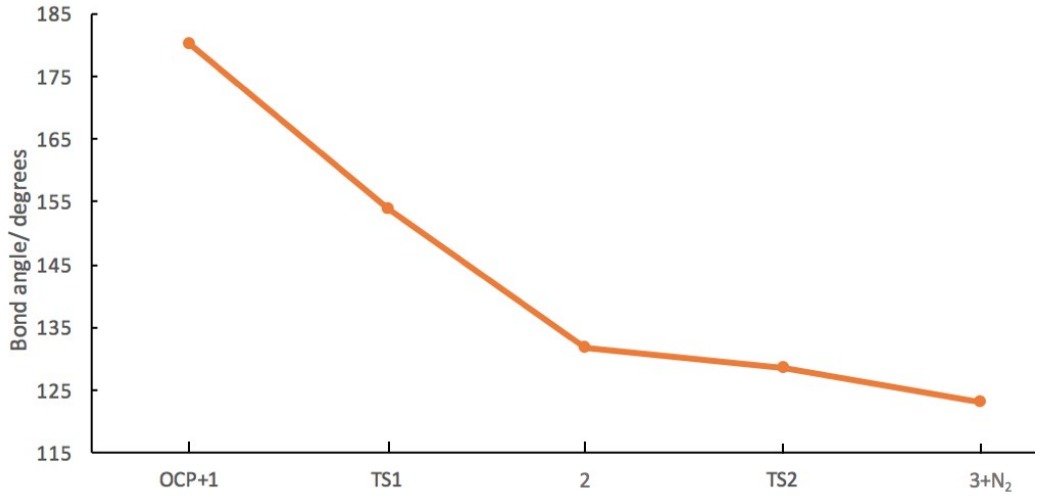


Figure S1. Graph of bond length changes across PES (top) and of OCP angle changes (bottom)

As shown by the green line in Figure S1 most of the C_AC_B bond forms following **TSI**, to give **II**. Following formation of **II**, the bond length changes become monotonic and with similar rate of change. Thus, the reaction starts with P-C_C attraction, but at cost of PCO bending, which rehybridizes at that carbon, allowing subsequent C_AC_B bond formation; during the formation of **TSI**, the animations show how the tetrazine folds from planar to boat shape, with an energy penalty, to prepare (pyramidalize) C_C and C_B to form the bonds present in **II**.

Substituent effect

As seen in Figure S2, The $–CF_3$ and $–C_6F_5$ groups have the lowest energy products, and they are ~15 kcal/mol lower in energy than the products containing electron donating groups. However, we believed that pentafluorobenzene would act as the *most* electron withdrawing substituent, yielding the lowest energy product, but in reality $–CF_3$ is the winner. One plausible explanation for this discrepancy from prediction lies in the optimized structures of each of these species compared to other tetrazines that contained a ring (i.e. phenyl and pyridyl). Each structure shows that the $–C_6F_5$ ring has been rotated nearly perpendicular to the tetrazine ring, whereas the other ring systems that were calculated have the substituent ring oriented nearly parallel to the tetrazine. A comparison of the optimized structure of the transition state and product for methyl/phenyl compared to methyl/pentafluorobenzene is shown in Figure S2.

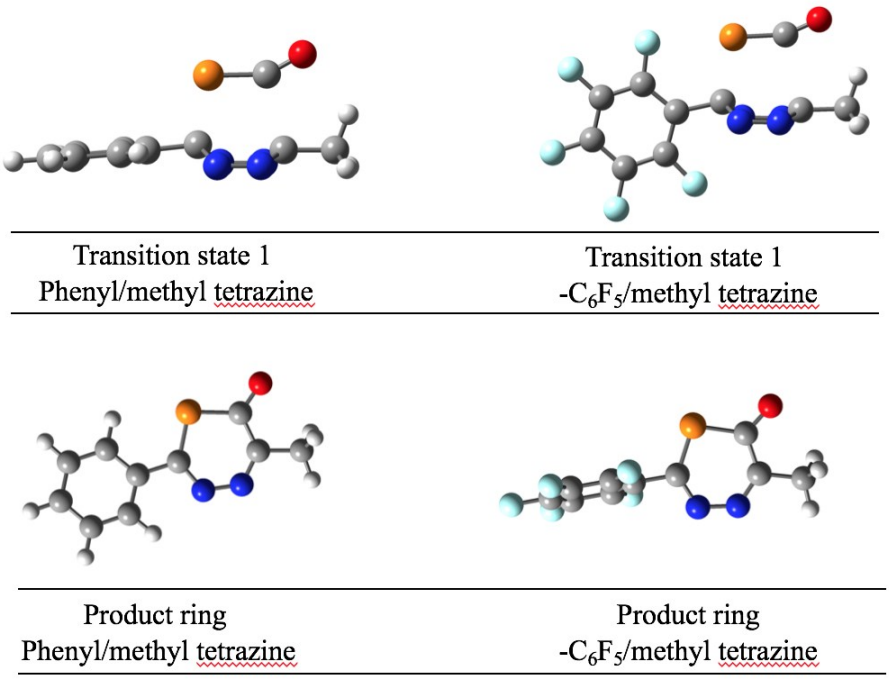


Figure S2. structural comparisons between Me/Ph and Me/C_6F_5

The ring rotation is likely due to the repulsion of the lone pairs on fluorine unfavorably interacting with the nitrogen lone pair in the tetrazine. This twist effectively shuts off the pi electron donating capabilities by breaking the conjugation, making it a sigma withdrawer only and therefore unexpectedly yielding products that are slightly less thermodynamically favorable than when $-CF_3$ is used.

Additionally, the pentafluorobenzene substituent was the only tetrazine where the computed isomers had significantly different energies of TSI. This is due to the orientation of the -C_6F_5 ring between the two isomers; in one, the ring is oriented nearly perpendicular to the tetrazine, and in the other isomer it is closer to parallel (Figure S3). When it is perpendicular it shuts of pi conjugation and weakens the amount of electron withdrawing ability of the ring. The reason there is a difference in the optimized geometries of these two isomers is because of repulsion between the PCO^- oxygen lone pairs and the fluorides when the oxygen is on the same side as the ring. Repulsion of the lone pairs cause the C_6F_5 ring to orient away from the oxygen of PCO, and therefore that isomer is lower in energy (~6 kcal/mol) than the isomer where the phosphorous is on the same side as C_6F_5 ring, where the ring prefers to be perpendicular to the tetrazine. Not as much repulsion. Efforts to "force" the C_6F_5 ring planar in both isomers fails (multiple attempts).

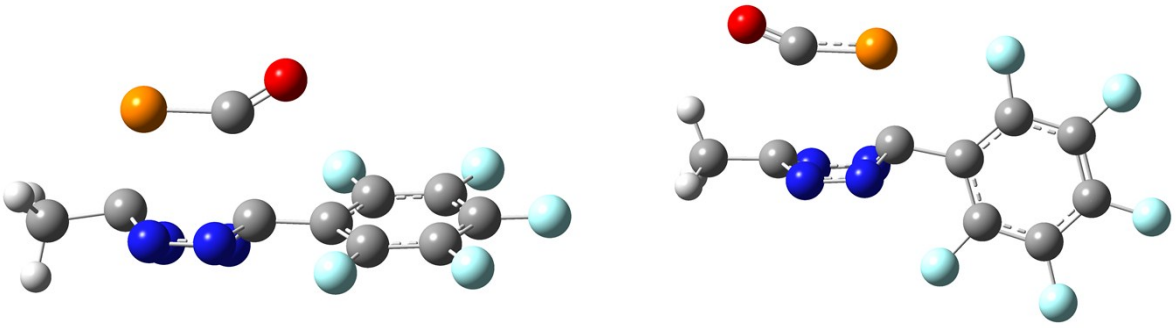
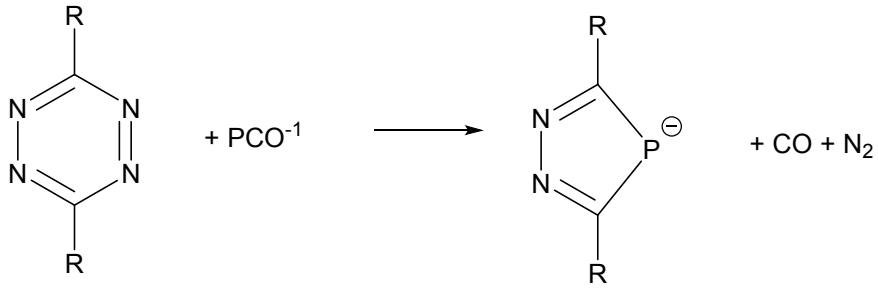


Figure S3. Comparison of TSI for both regioisomers of methyl/C_6F_5 tetrazine

Alternative products

In addition to reacting as a dienophile, PCO^{-1} can also lose CO, and thus be a formal equivalent for transfer of the anion P^{1-}, hence a 2 electron oxidant[12-16]. We therefore used DFT to compare the energy of this behavior with a tetrazine, to make a diazaphosphole anion (Scheme S1).



Scheme S1. Alternative tetrazine/OCP reaction pathway.

The ΔG^o calculated for this reaction is -52.3 kcal/mol showing it is highly competitive with the observed product, and so the observed selectivity may have a kinetic origin. Note that this preference rests on the $T\Delta S$ advantage for the diazaphospholide liberating two moles of gas; in fact, the reluctance of phosphorus to participate in π bonding tends to destabilize, enthalpically, the diazaphospholide, since it leaves negative charge more localized on the less appropriate P vs. N atom. There is increasing evidence that PCO(-)[17] can be a source of P(-1), by release of CO from primary products. Our report here thus contrasts to this, and apparently originates in the fact that the CO unit is incorporated into an aromatic ring, in which the CO bond moves towards single bond character.

In addition to reacting as a dienophile, PCO^{-1} can also lose CO, and thus be a formal equivalent for transfer of the anion P^{1-}, hence a 2 electron oxidant. We therefore used DFT to compare the energy of this behavior with a tetrazine, to make a diazaphosphole anion, as shown in Figure S4.

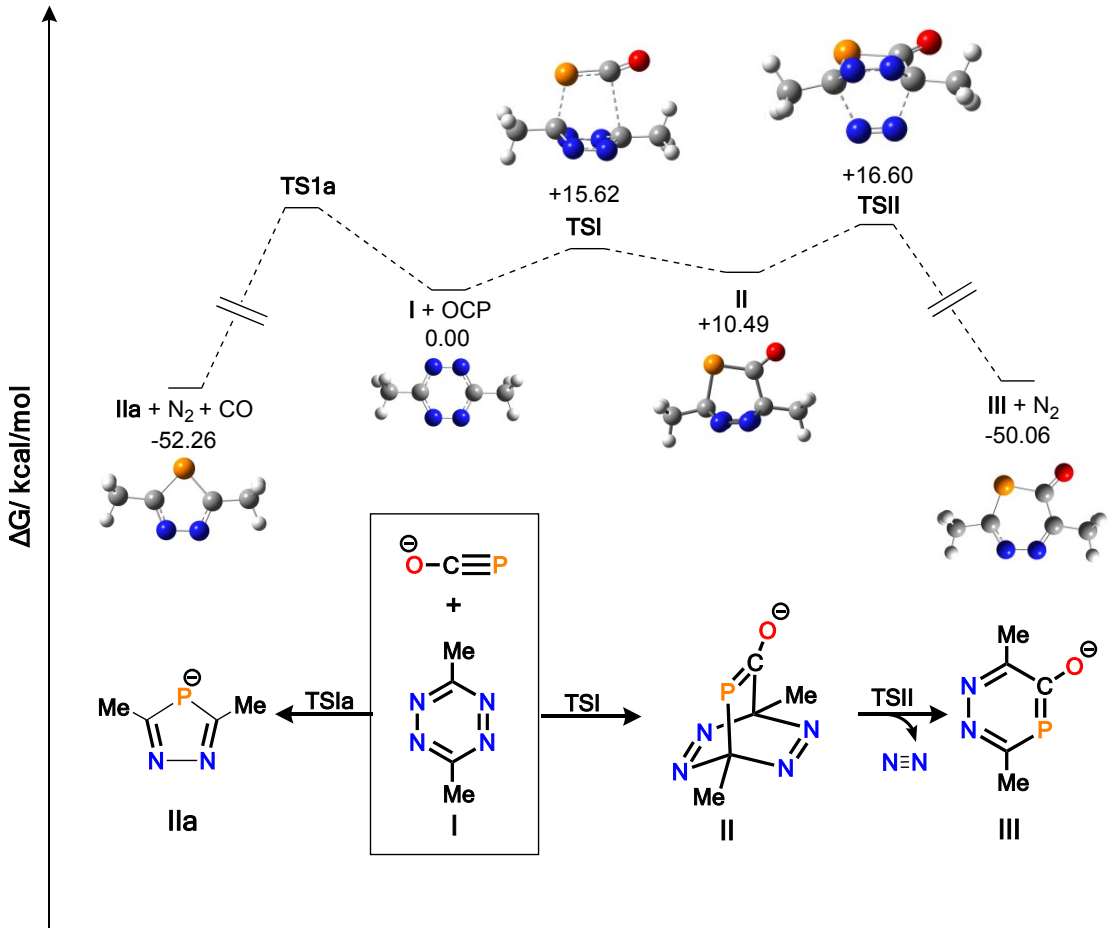


Figure S4. PES of two potential reactions of dimethyl tetrazine with PCO^{-}

NMR spectra

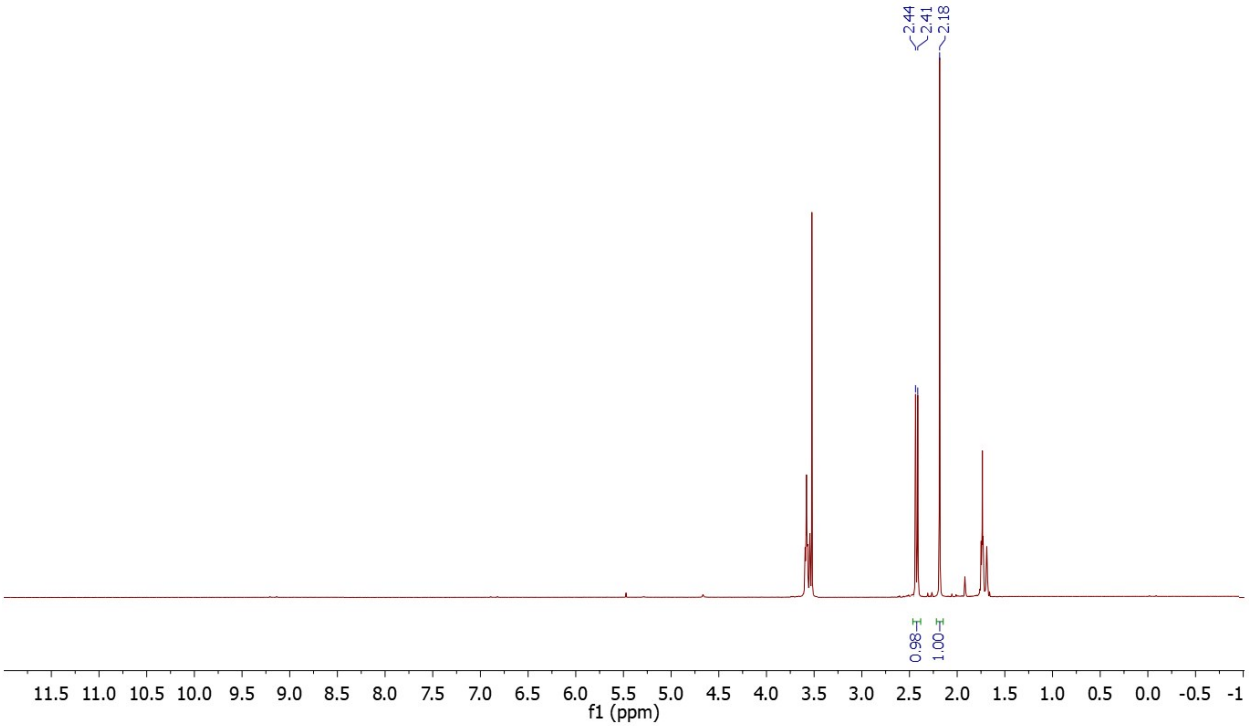


Figure S5. ^{1}H NMR spectrum of **2a** sodium 3,6-dimethyl-1,2,4-diazaphosphinin-5-olate in THF-d_8.

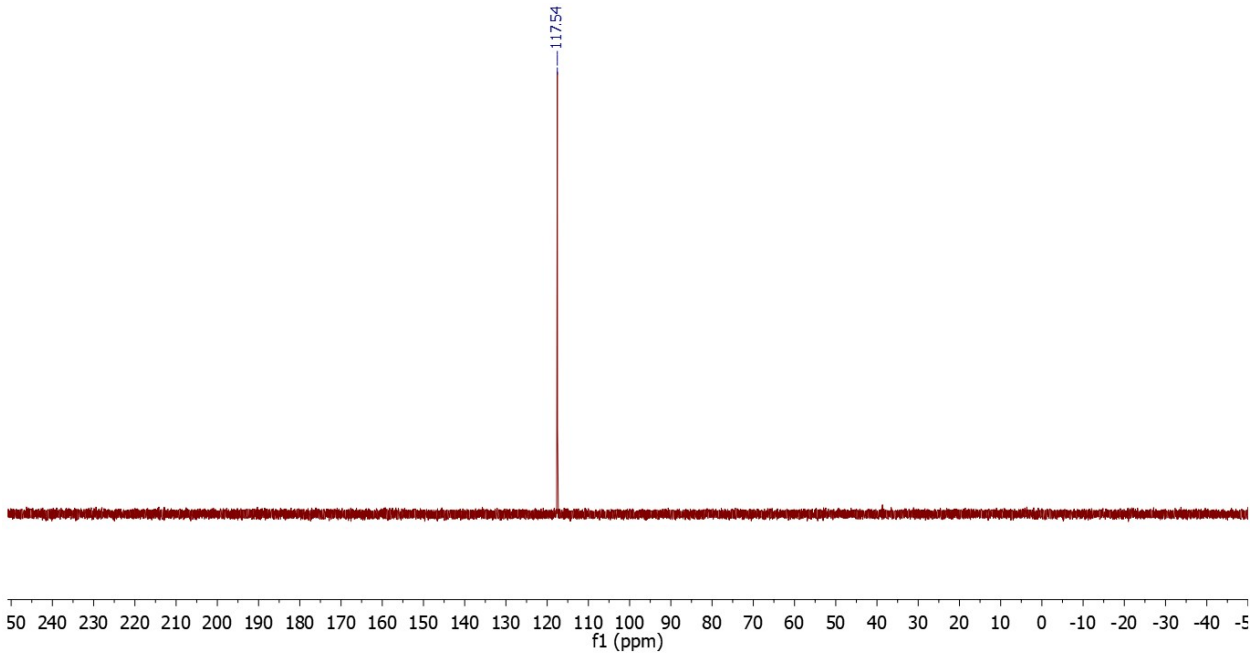


Figure S6. ^{31}P NMR spectrum of **2a** sodium 3,6-dimethyl-1,2,4-diazaphosphinin-5-olate in THF-d_8.

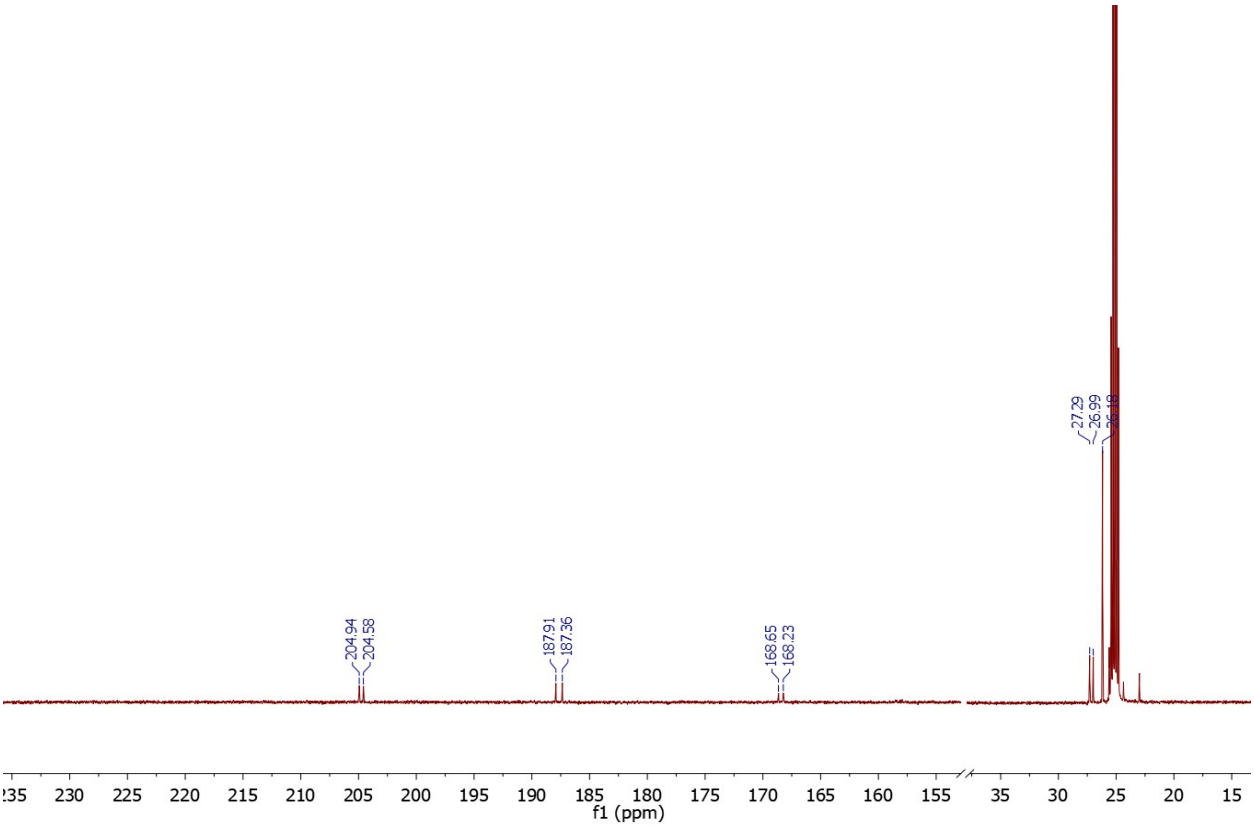


Figure S7. ^{13}C NMR spectrum of **2a** sodium 3,6-dimethyl-1,2,4-diazaphosphinin-5-olate in THF-d_8.

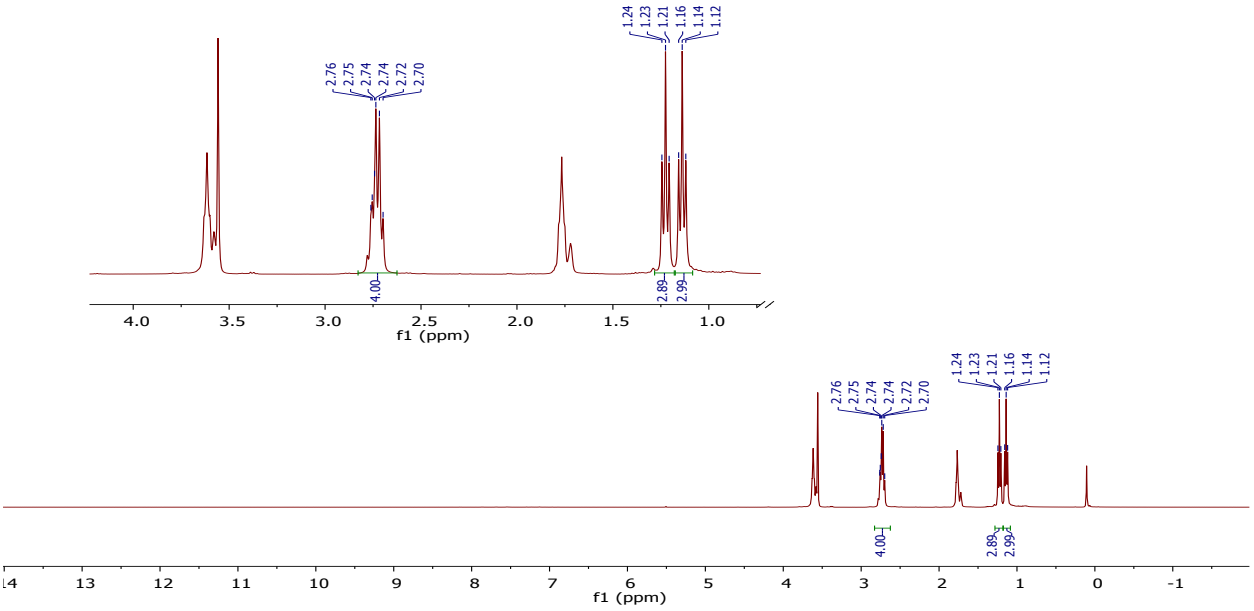


Figure S8. ^{1}H NMR spectrum of sodium **2b** 3,6-diethyl-1,2,4-diazaphosphinin-5-olate in THF-d_8.

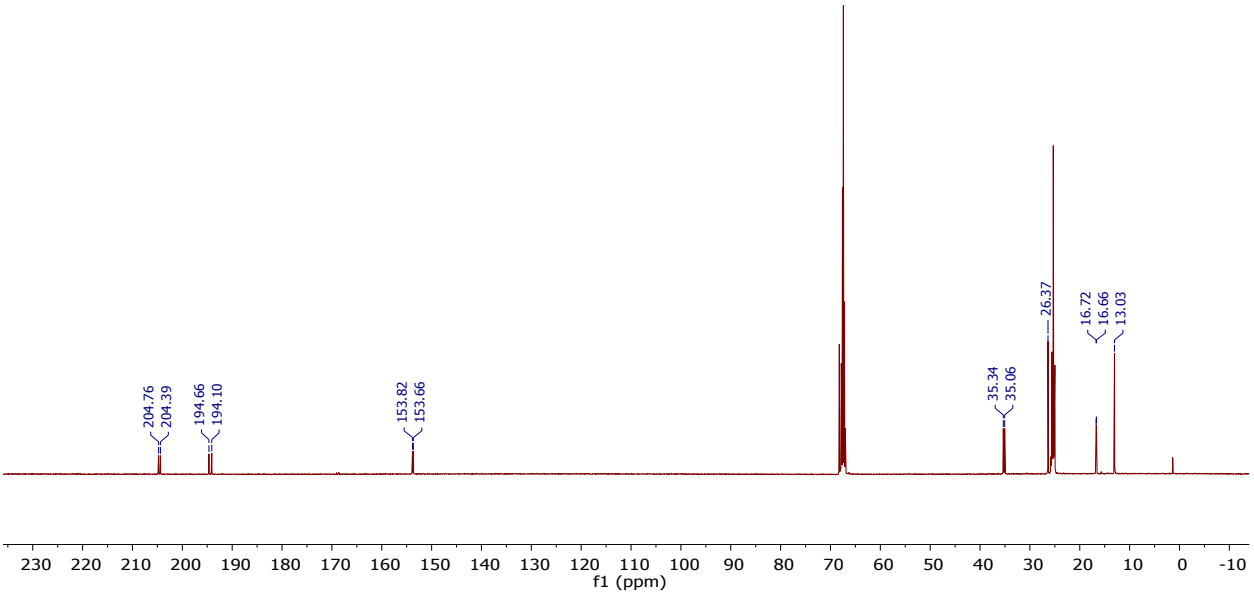


Figure S9. ^{13}C NMR spectrum of **2b** sodium 3,6-diethyl-1,2,4-diazaphosphinin-5-olate in THF-d_8.

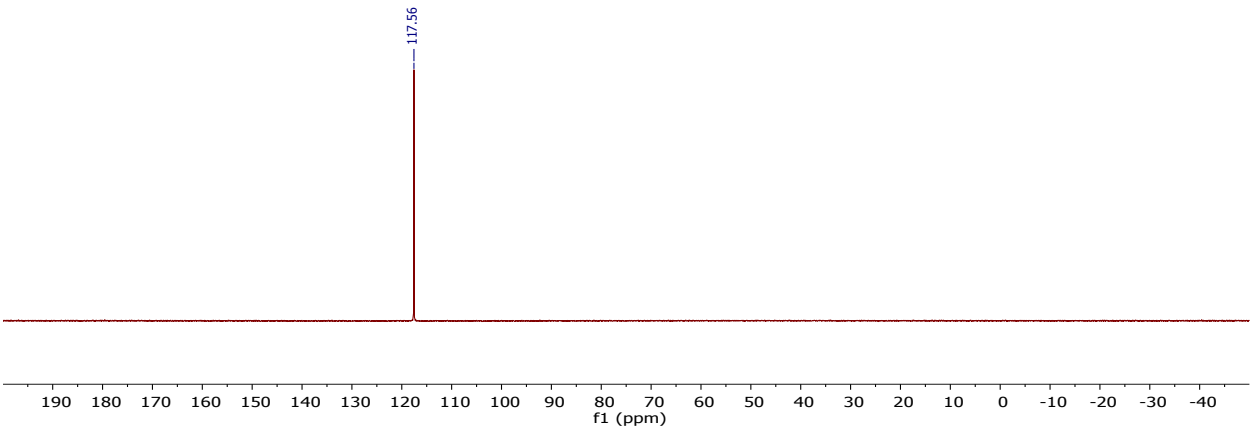


Figure S10. ^{31}P NMR spectrum of **2b** sodium 3,6-diethyl-1,2,4-diazaphosphinin-5-olate in THF-d_8.

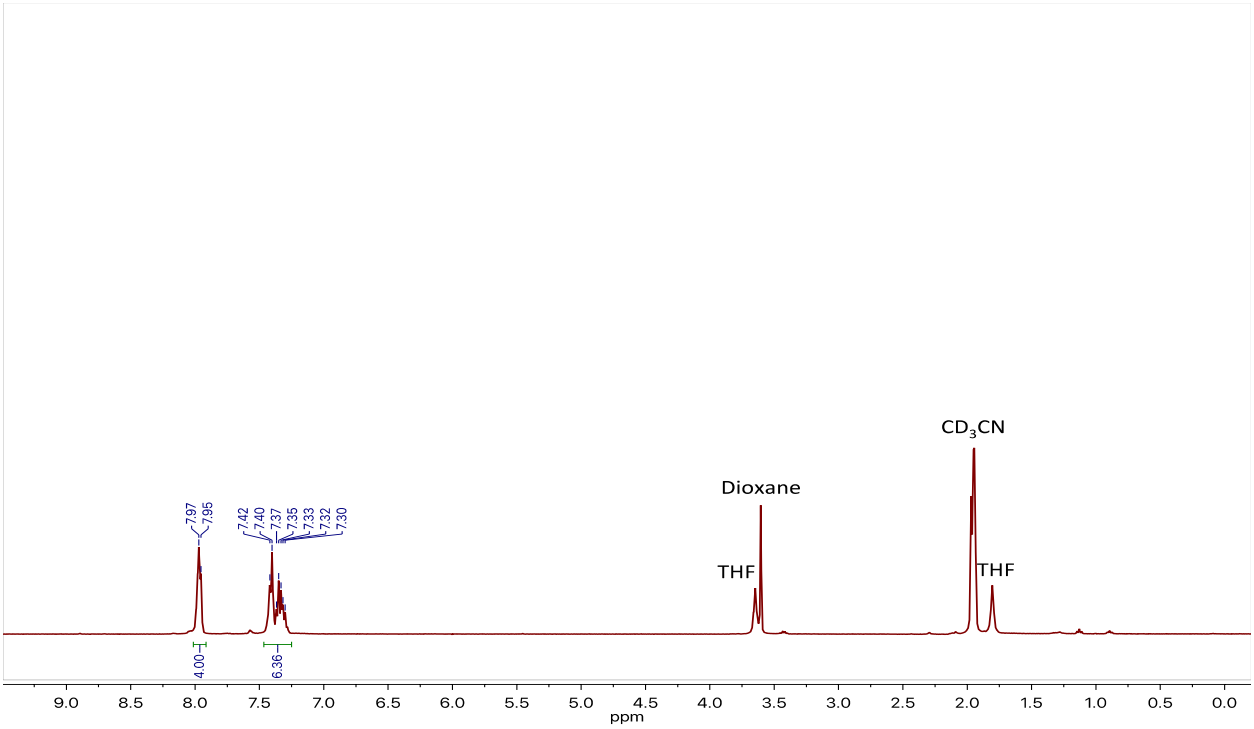


Figure S11. ^{1}H NMR spectrum of **2c** sodium 3,6-diphenyl-1,2,4-diazaphosphinin-5-olate

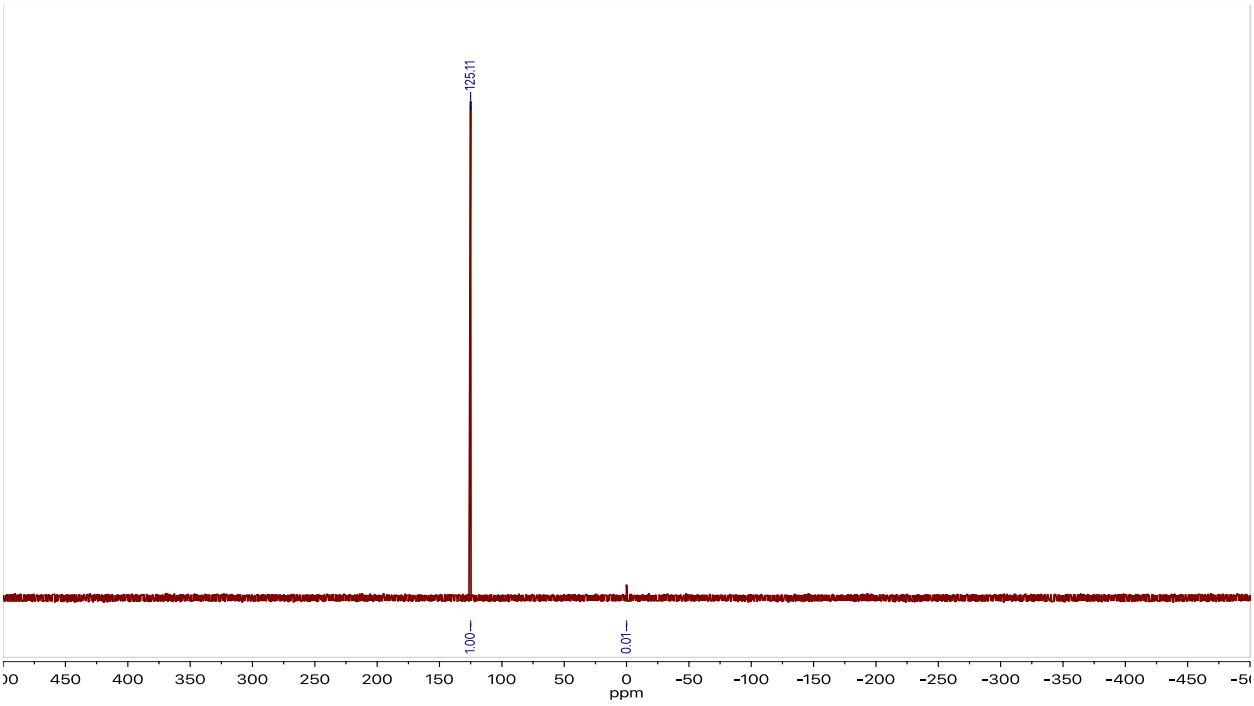


Figure S12. ^{31}P NMR spectrum of **2c** sodium 3,6-diphenyl-1,2,4-diazaphosphinin-5-olate

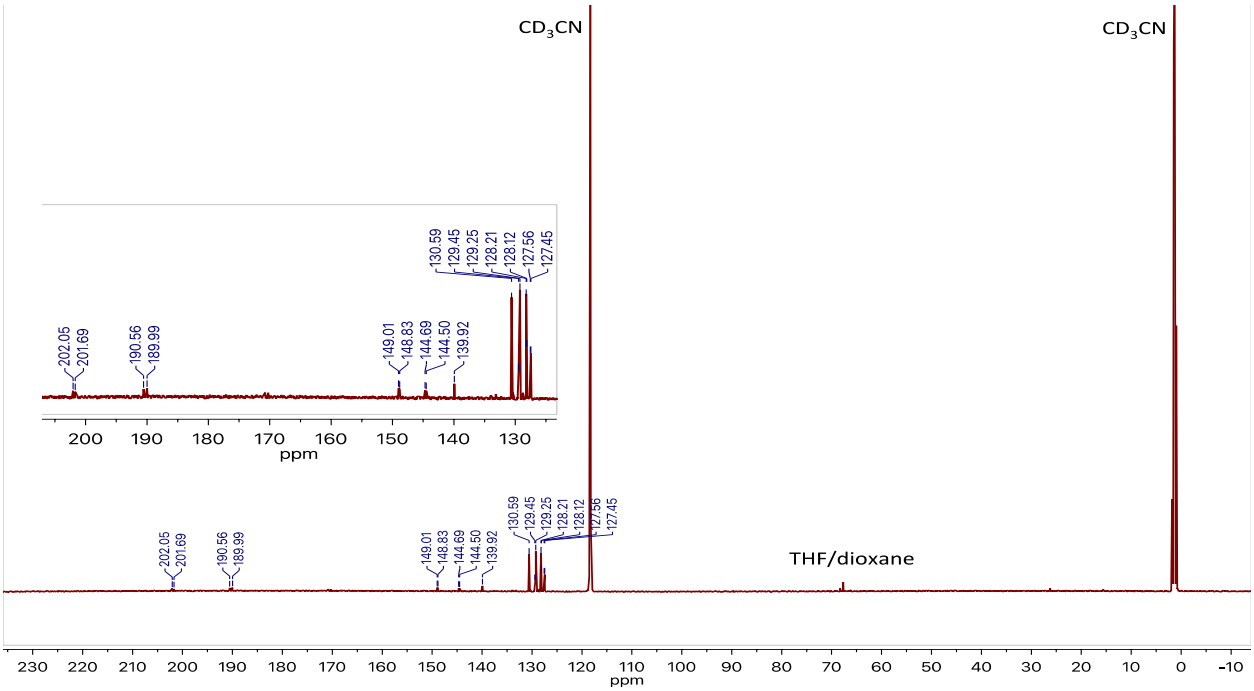


Figure S13. ^{13}C NMR spectrum of **2c** sodium 3,6-diphenyl-1,2,4-diazaphosphinin-5-olate

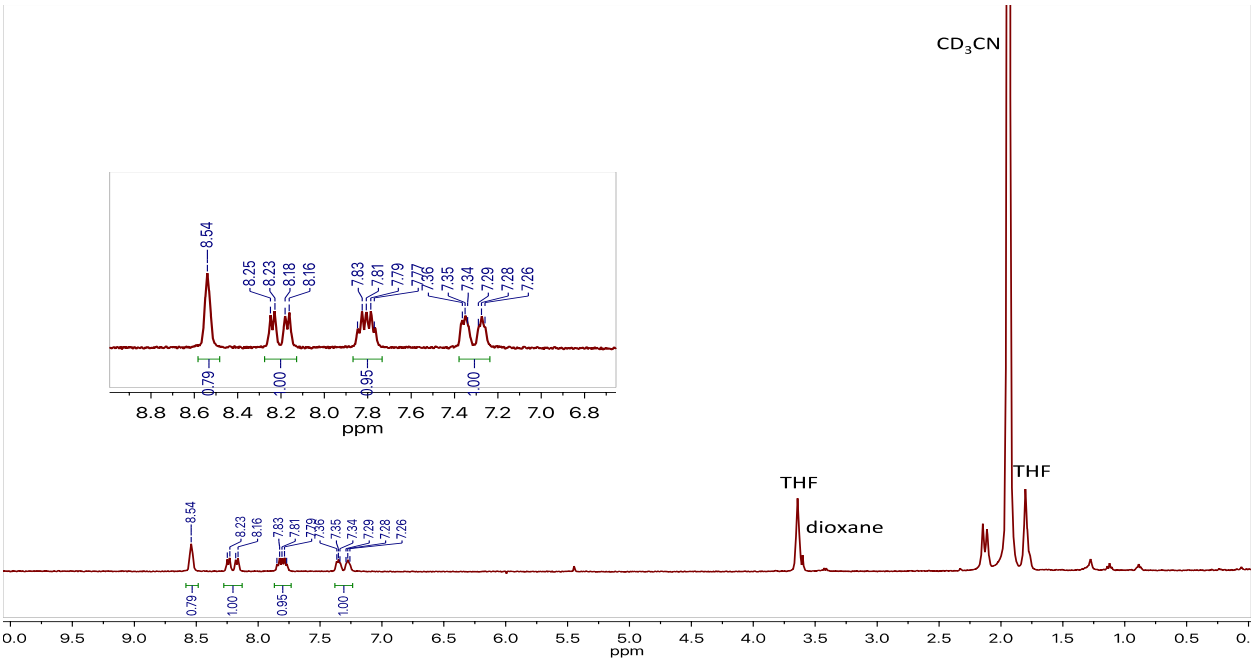


Figure S14. ^{1}H NMR spectrum of **2d** sodium 3,6-dipyridyl-1,2,4-diazaphosphinin-5-olate

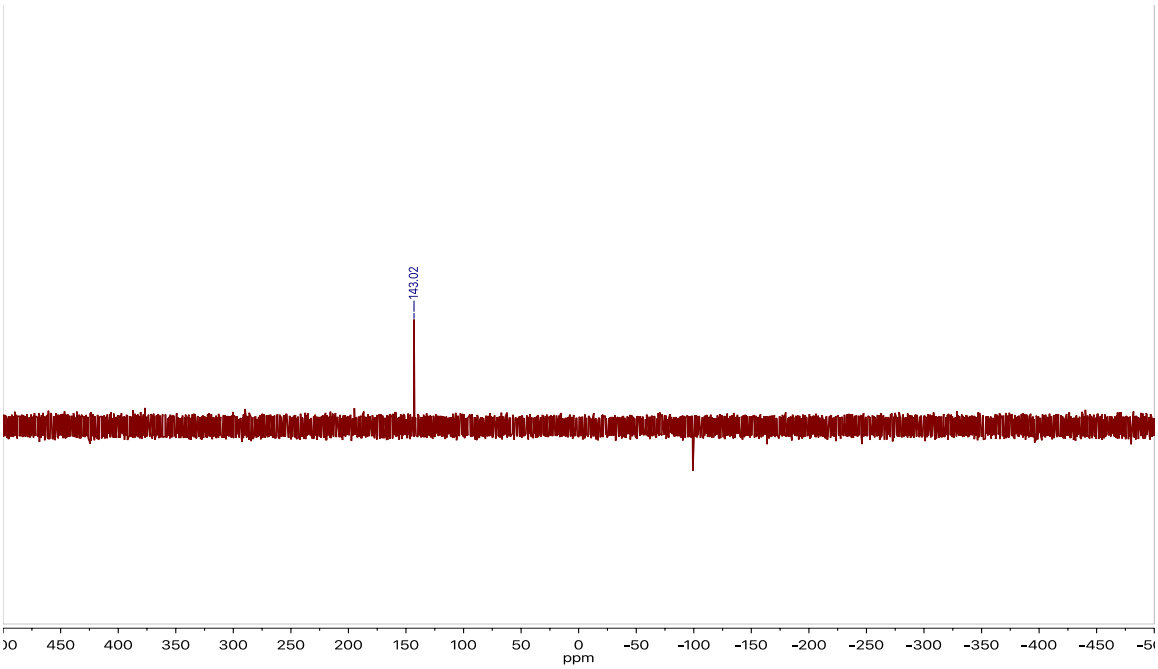


Figure S15. ^{31}P NMR spectrum of **2d** sodium 3,6-dipyridyl-1,2,4-diazaphosphinin-5-olate.

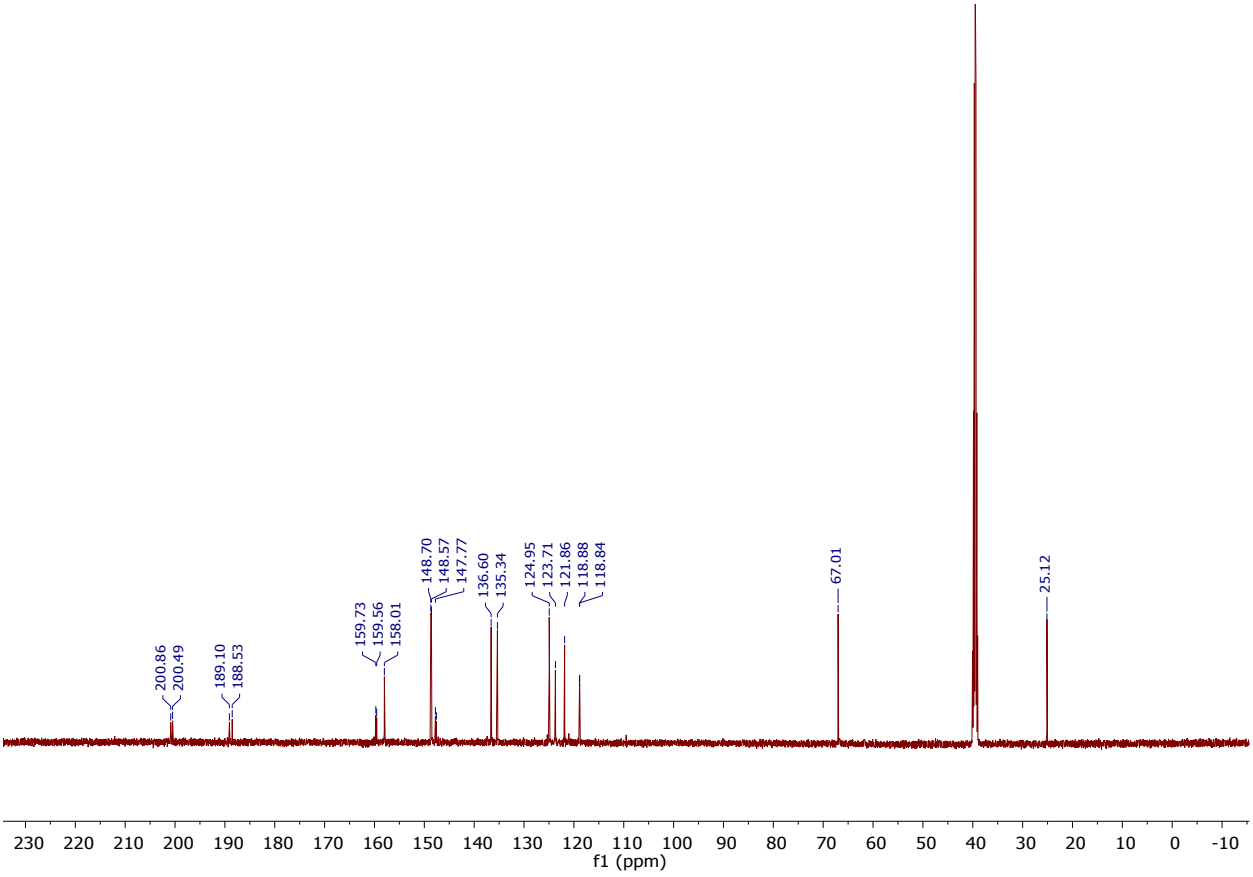


Figure S16. ^{13}C NMR spectrum of **2d** sodium 3,6-dipyridyl-1,2,4-diazaphosphinin-5-olate.

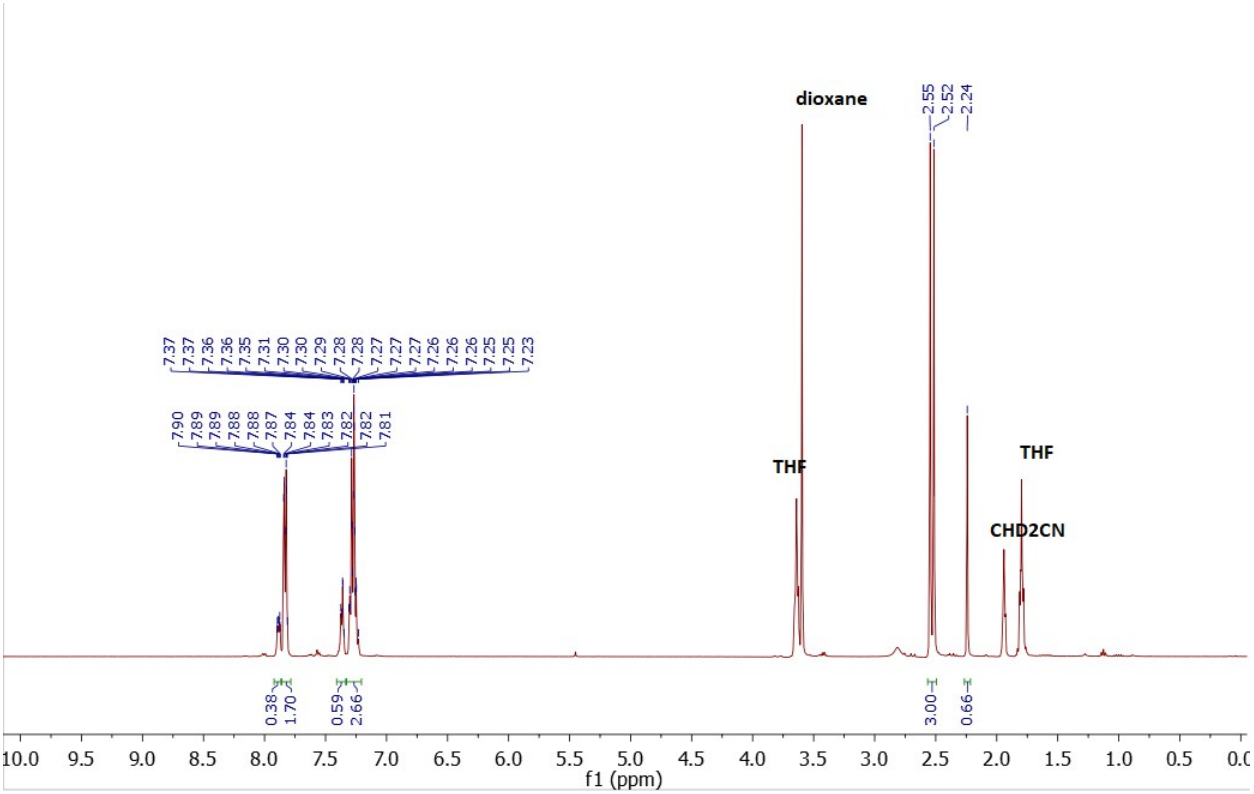


Figure S17. ^{1}H NMR spectrum of sodium **2e** 3-methyl-6-phenyl-1,2,4-diazaphosphinin-5-olate and sodium 6-methyl-3-phenyl-1,2,4-diazaphosphinin-5-olate mixture

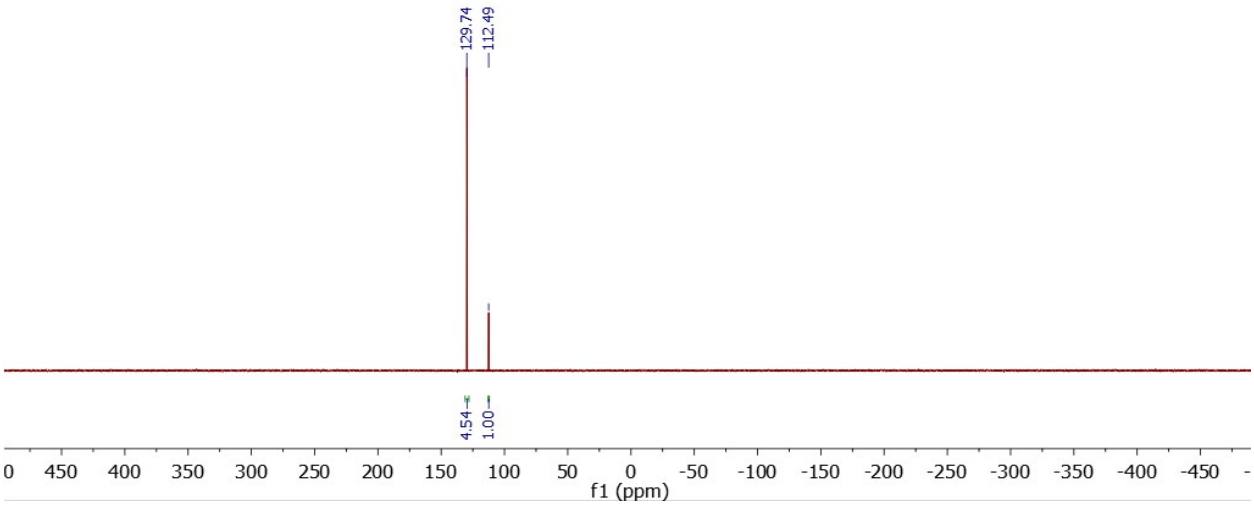


Figure S18. ^{31}P NMR spectrum of **2e** sodium 3-methyl-6-phenyl-1,2,4-diazaphosphinin-5-olate and sodium 6-methyl-3-phenyl-1,2,4-diazaphosphinin-5-olate mixture

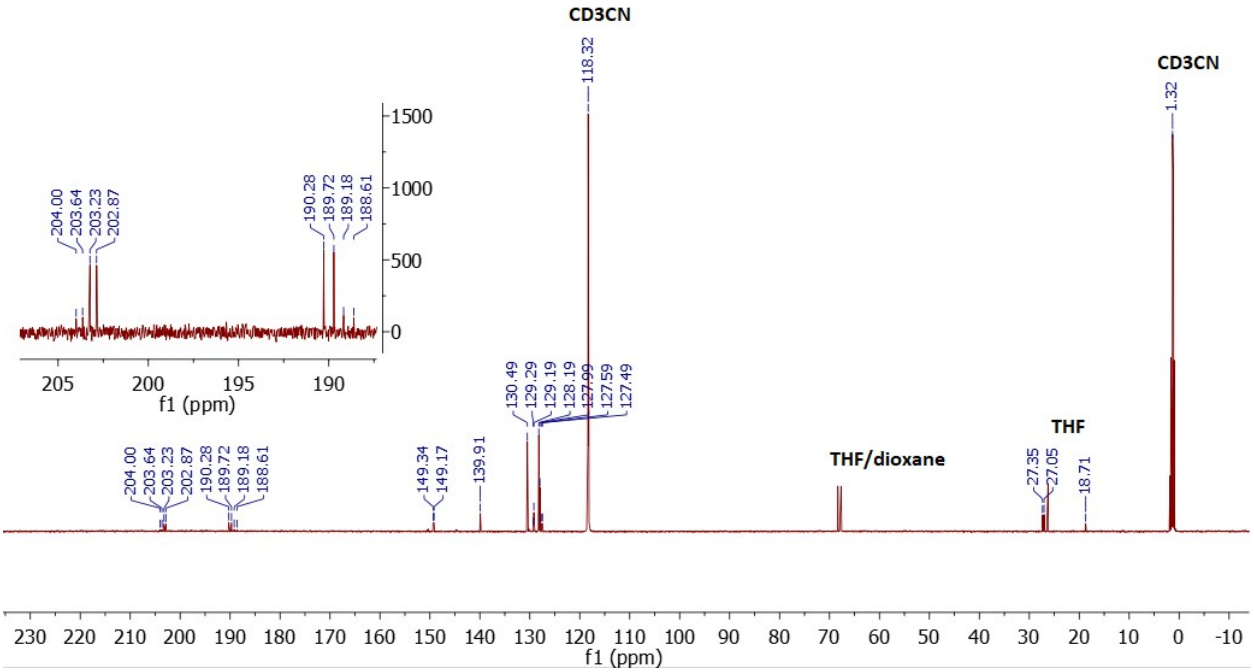


Figure S19. ^{13}C NMR spectrum of **2e** sodium 3-methyl-6-phenyl-1,2,4-diazaphosphinin-5-olate and sodium 6-methyl-3-phenyl-1,2,4-diazaphosphinin-5-olate mixture

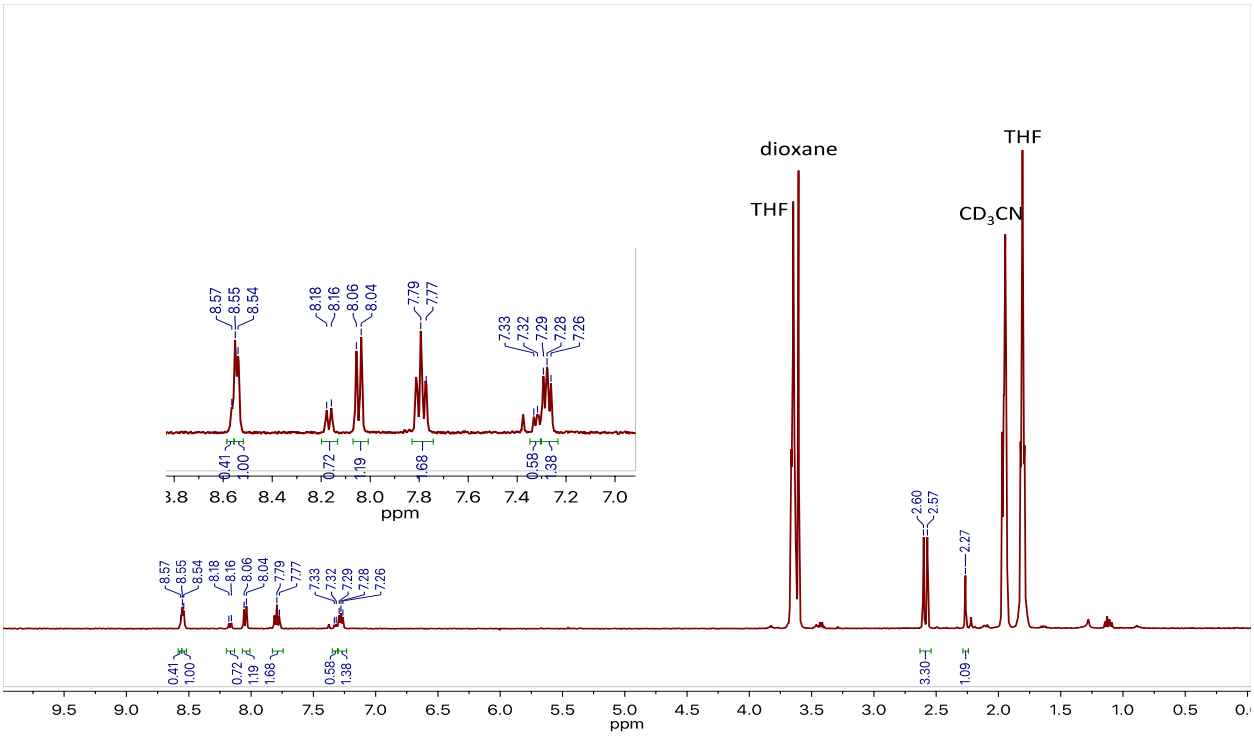


Figure S20. ^{1}H NMR spectrum of **2f** sodium 3-methyl-6-dipyridyl-1,2,4-diazaphosphinin-5-olate and 3-pyridyl-6-methyl-1,2,4-diazaphosphinin-5-olate

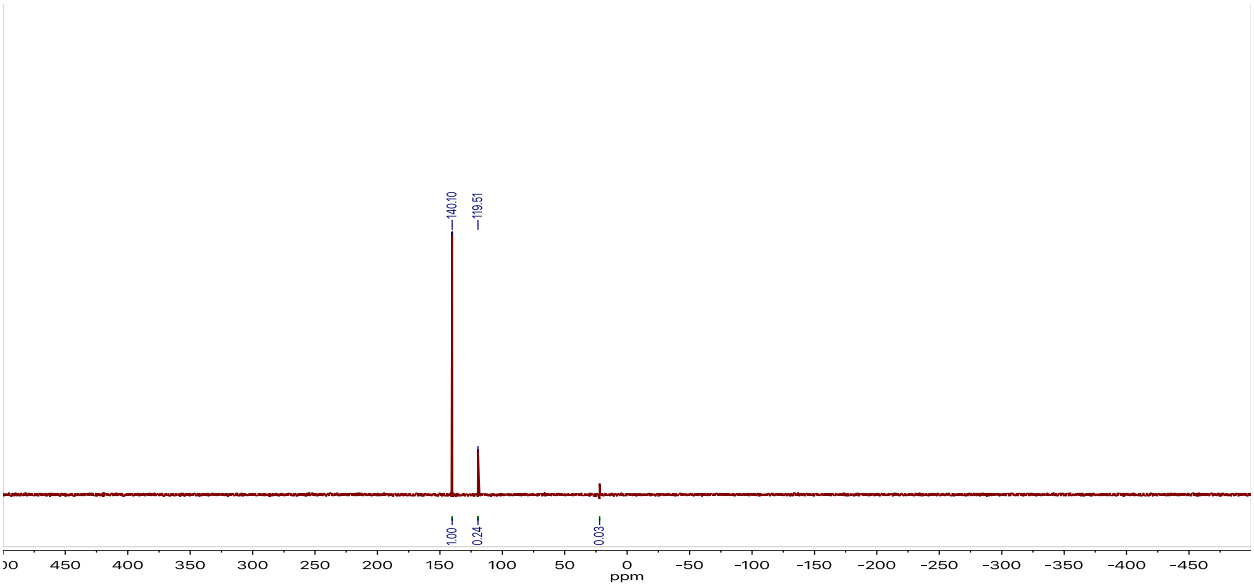


Figure S21. ^{31}P NMR spectrum of **2f** sodium 3-methyl-6-dipyridyl-1,2,4-diazaphosphinin-5-olate and 3-pyridyl-6-methyl-1,2,4-diazaphosphinin-5-olate

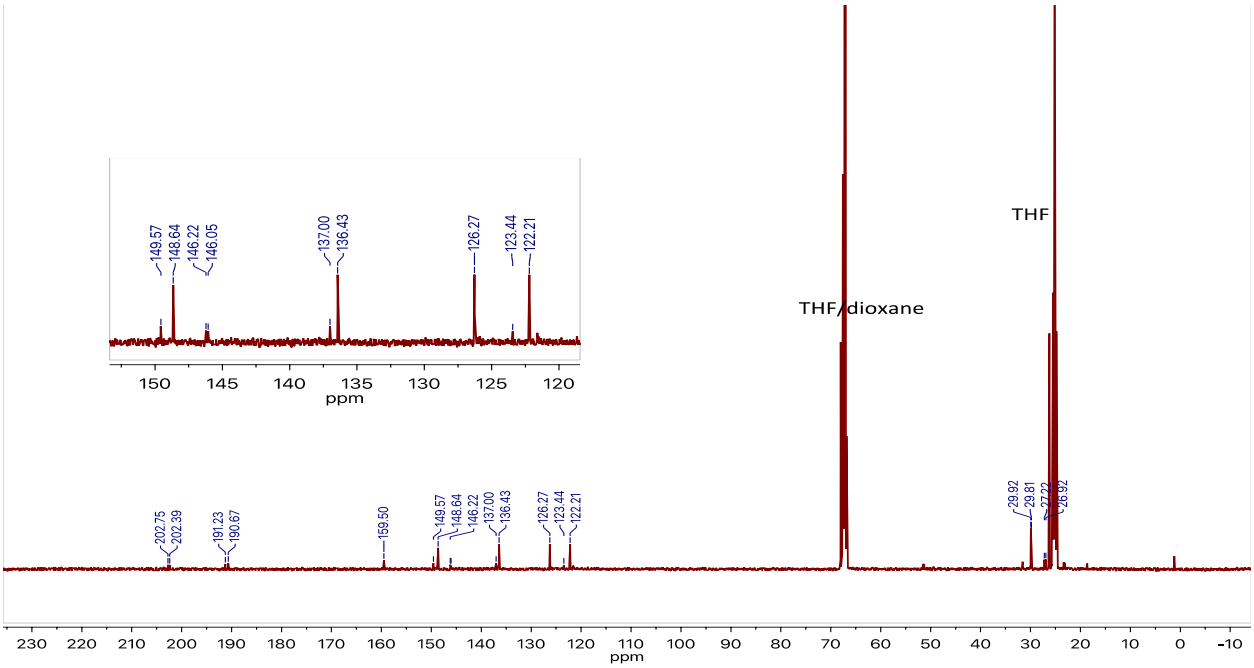


Figure S22. [1]13 NMR spectrum of **2f** sodium 3-methyl-6-dipyridyl-1,2,4-diazaphosphinin-5-olate and 3-pyridyl-6-methyl-1,2,4-diazaphosphinin-5-olate

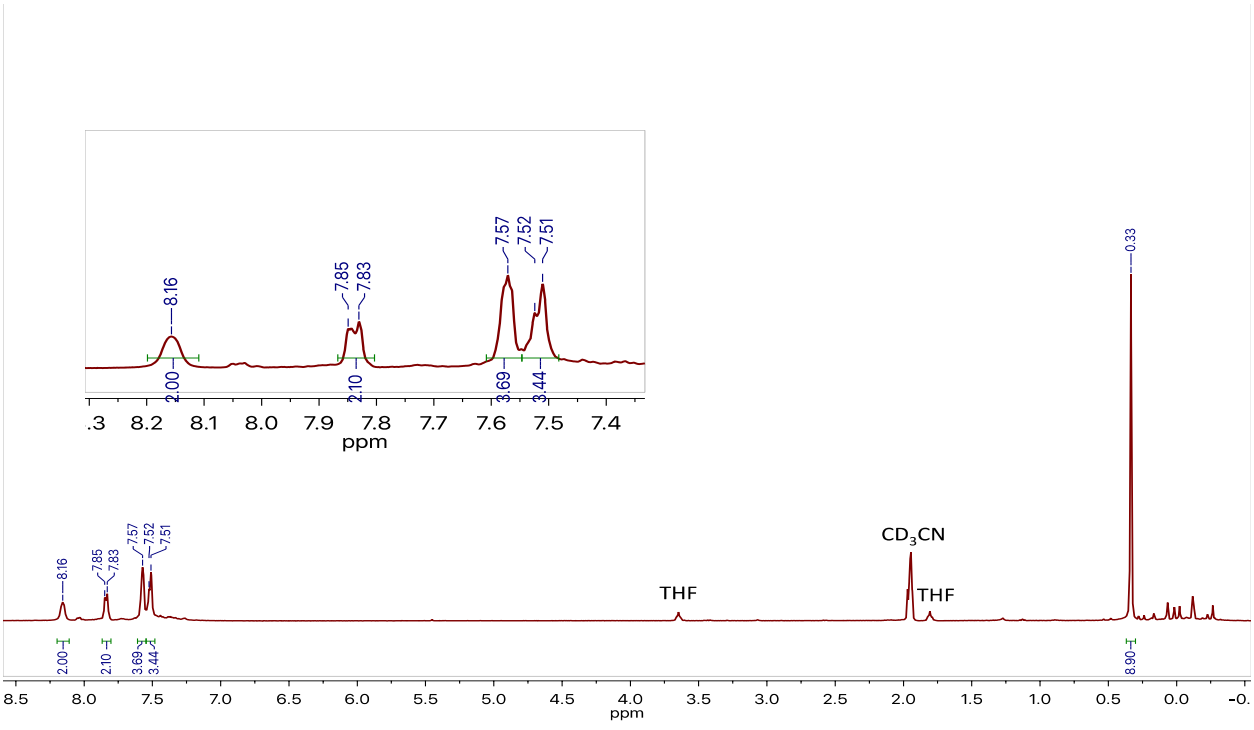


Figure S23. [1]H NMR spectrum of sodium 3,6-dipheynyl-1,2,4-diazaphosphinin-5-trimethoxysilane **3**

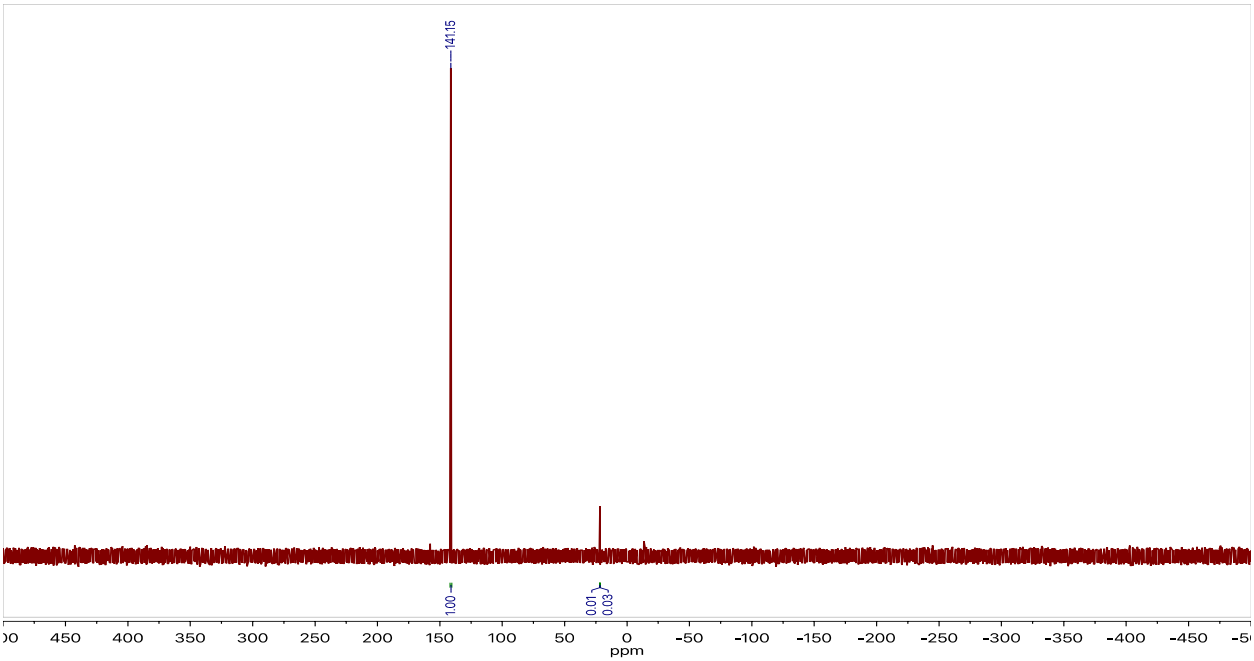


Figure S24. ^{31}P NMR spectrum of sodium 3,6-dipheynyl-1,2,4-diazaphosphinin-5-trimethoxysilane **3**

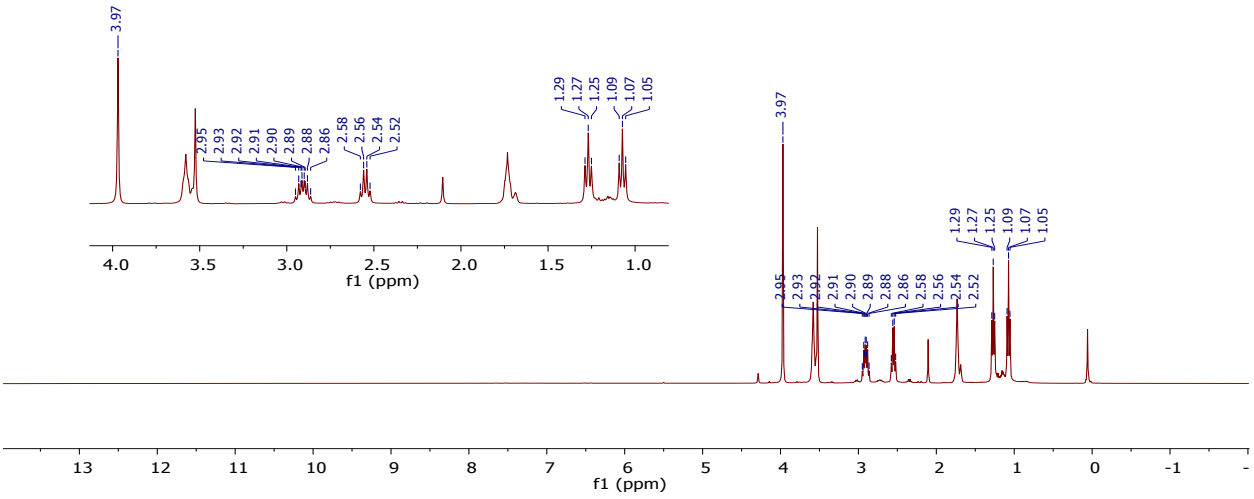


Figure S25. ^{1}H NMR spectrum of sodium **4a major** 3,6-diethyl-5-methoxy-1,2,4-diazaphosphinin in THF-d_8.

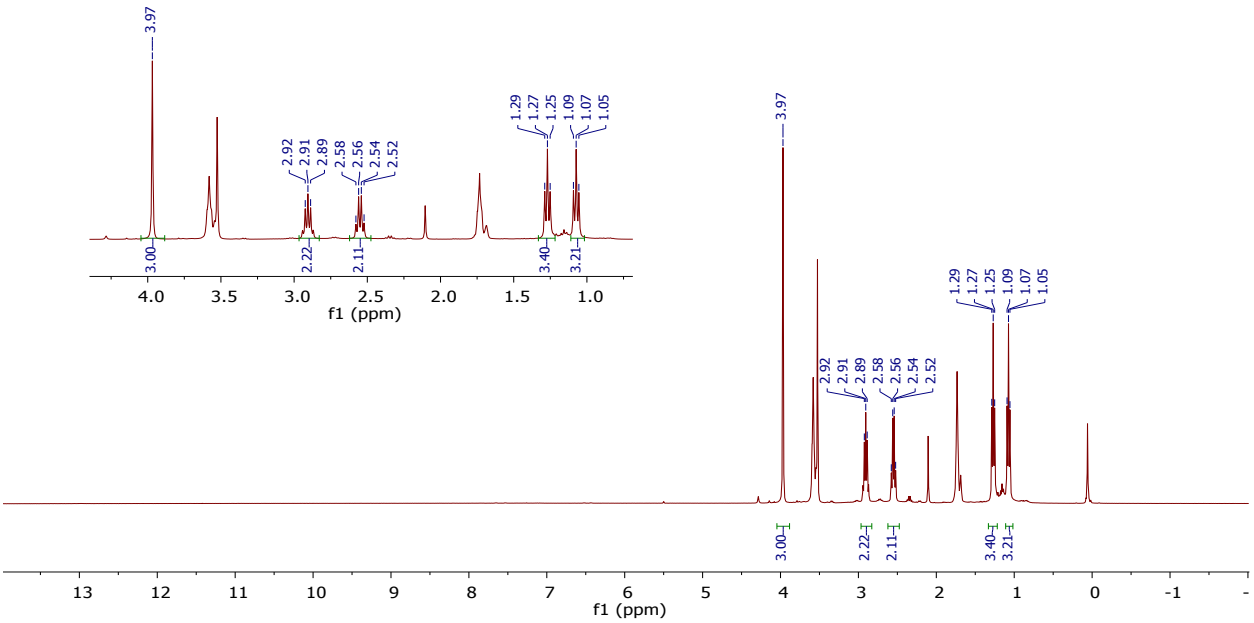


Figure S26. $^{1}H^{31}P$ NMR spectrum of **4a major** 3,6-diethyl-5-methoxy-1,2,4-diazaphosphinin in THF-d_8.

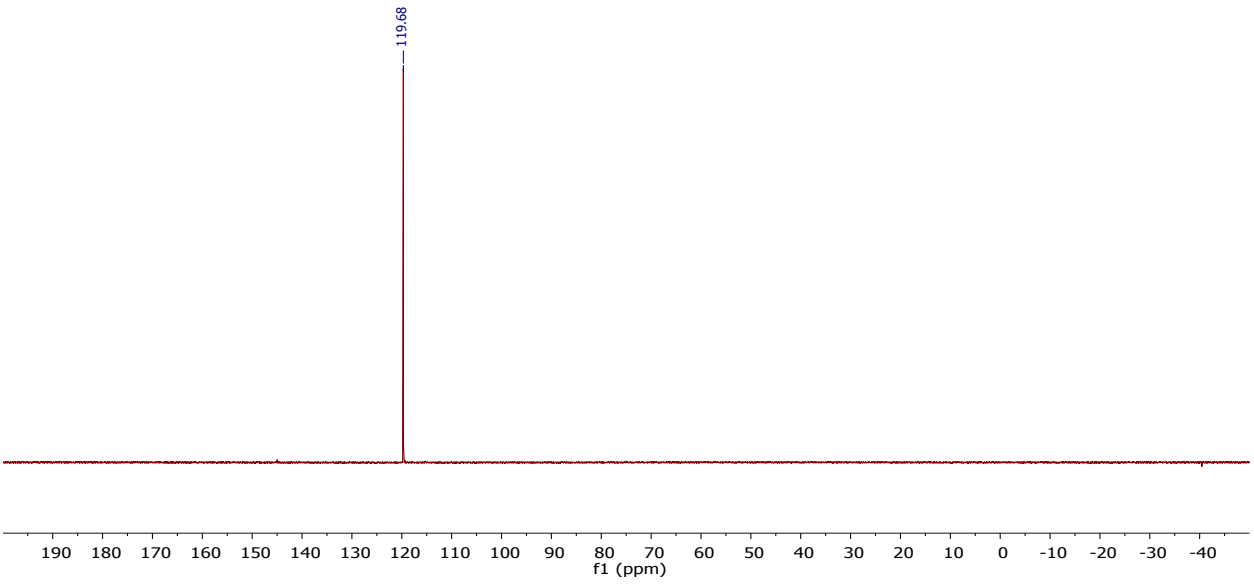


Figure S27. ^{31}P NMR spectrum of **4a major** 3,6-diethyl-5-methoxy-1,2,4-diazaphosphinin in THF-d_8.

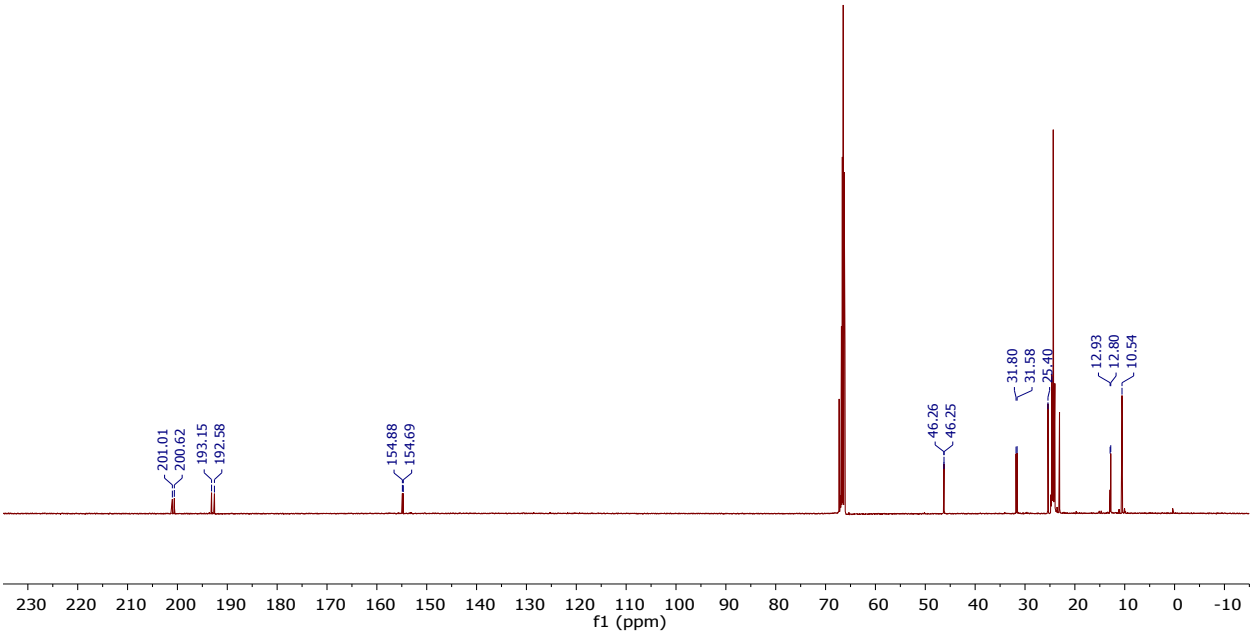


Figure S28I. ^{13}C NMR spectrum of **4a major** 3,6-diethyl-5-methoxy-1,2,4-diazaphosphinin in THF-d_8.

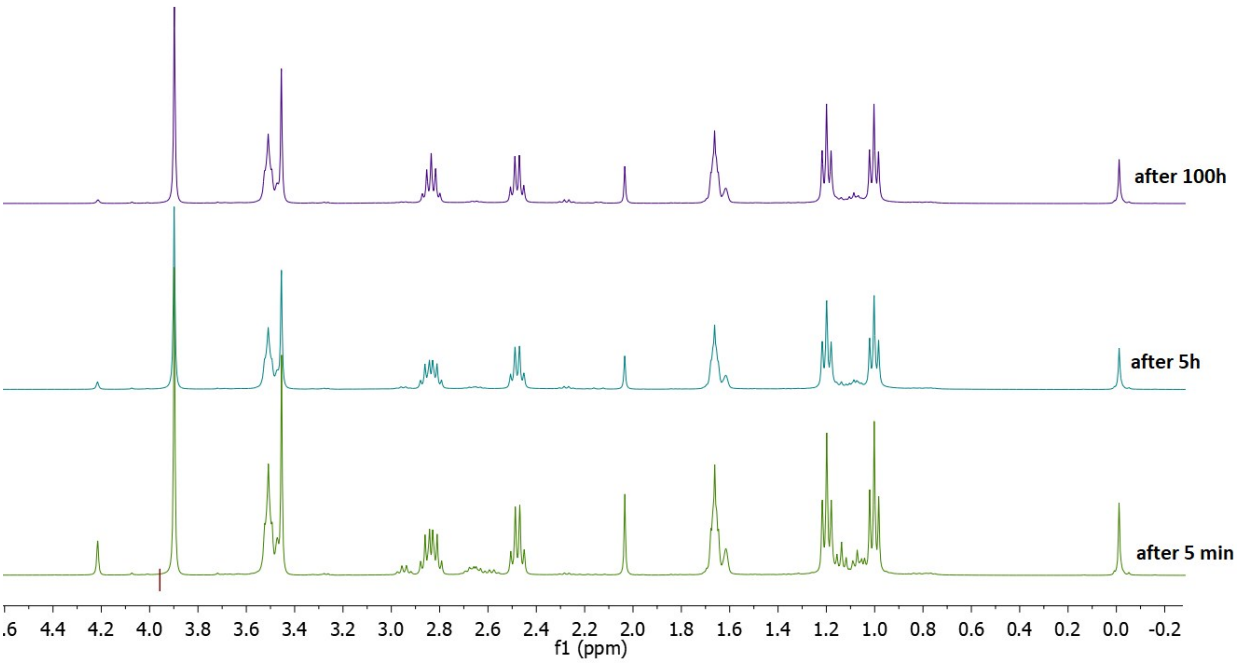


Figure S29. ^{1}H NMR monitoring of the reaction between **2a** and MeI

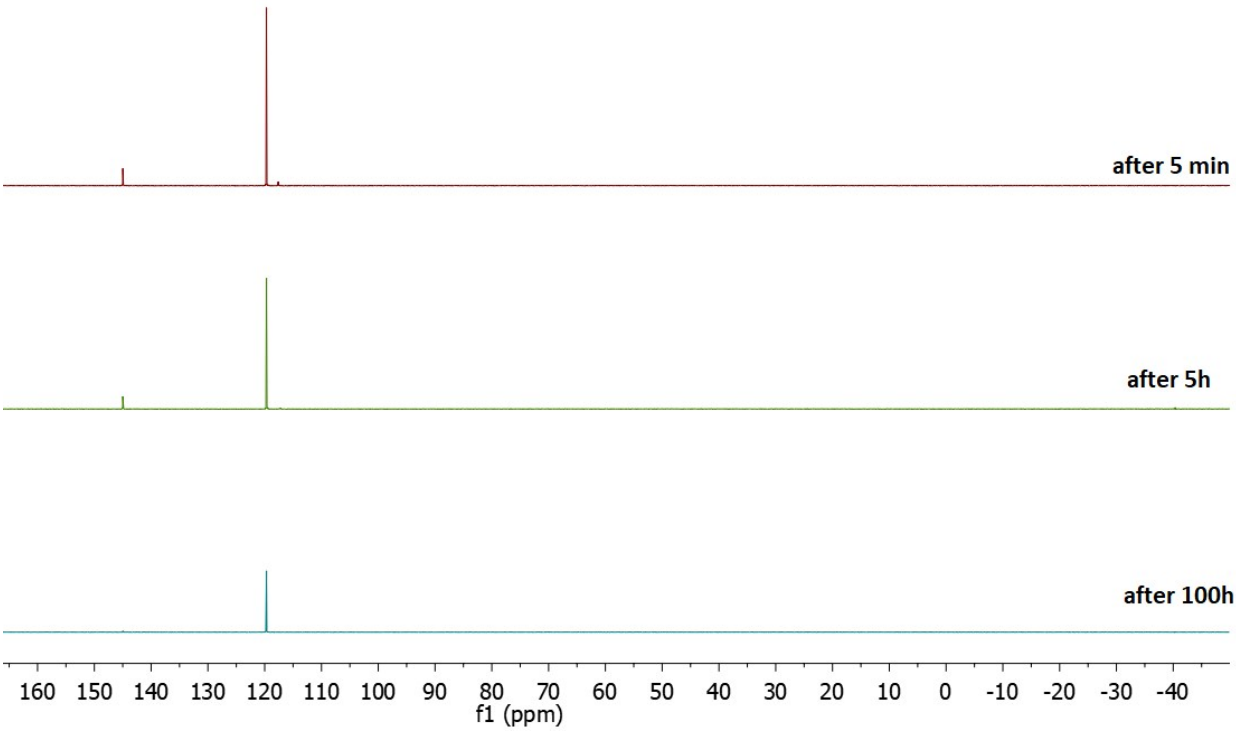


Figure S30. ^{31}P NMR monitoring of the reaction between **2a** and MeI

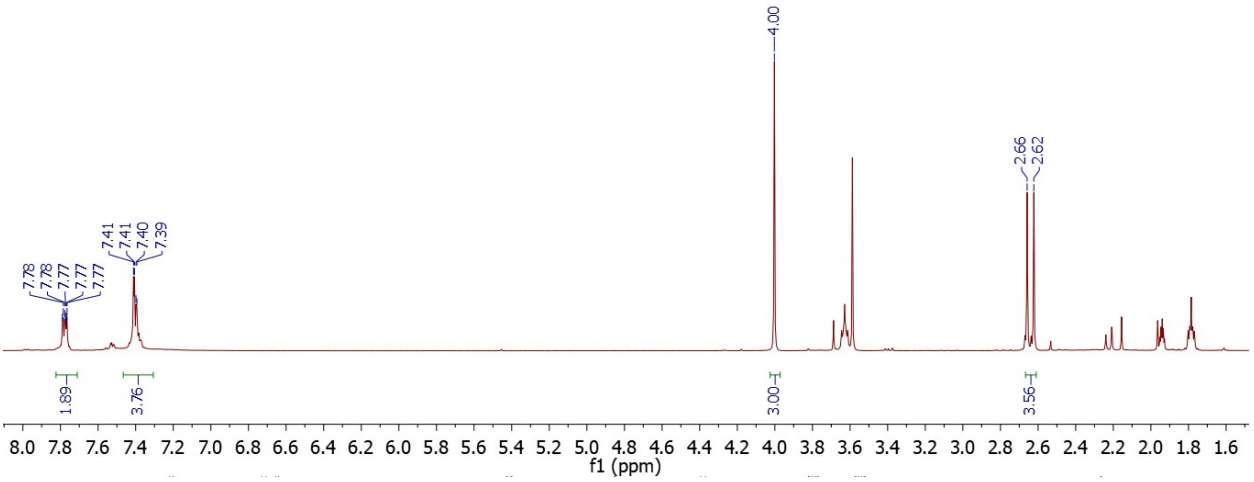


Figure S31. ^{1}H NMR spectrum of **4b** 6-methyl-3-phenyl-5-methoxy-1,2,4-diazaphosphinin in CD_3CN.

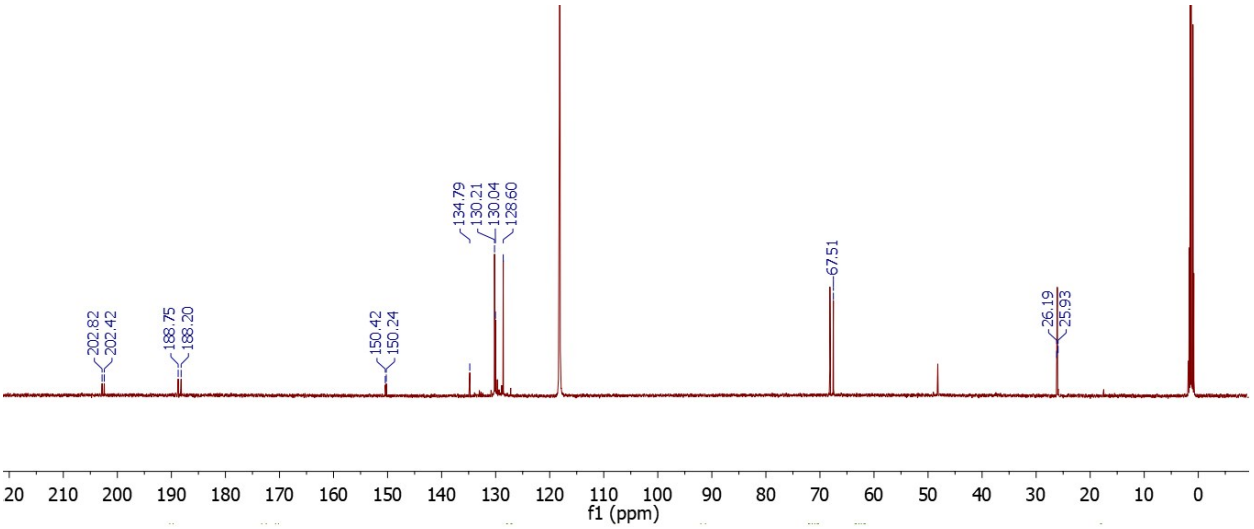


Figure S32. ^{13}C NMR spectrum of **4b** 6-methyl-3-phenyl-5-methoxy-1,2,4-diazaphosphinin in CD_3CN.

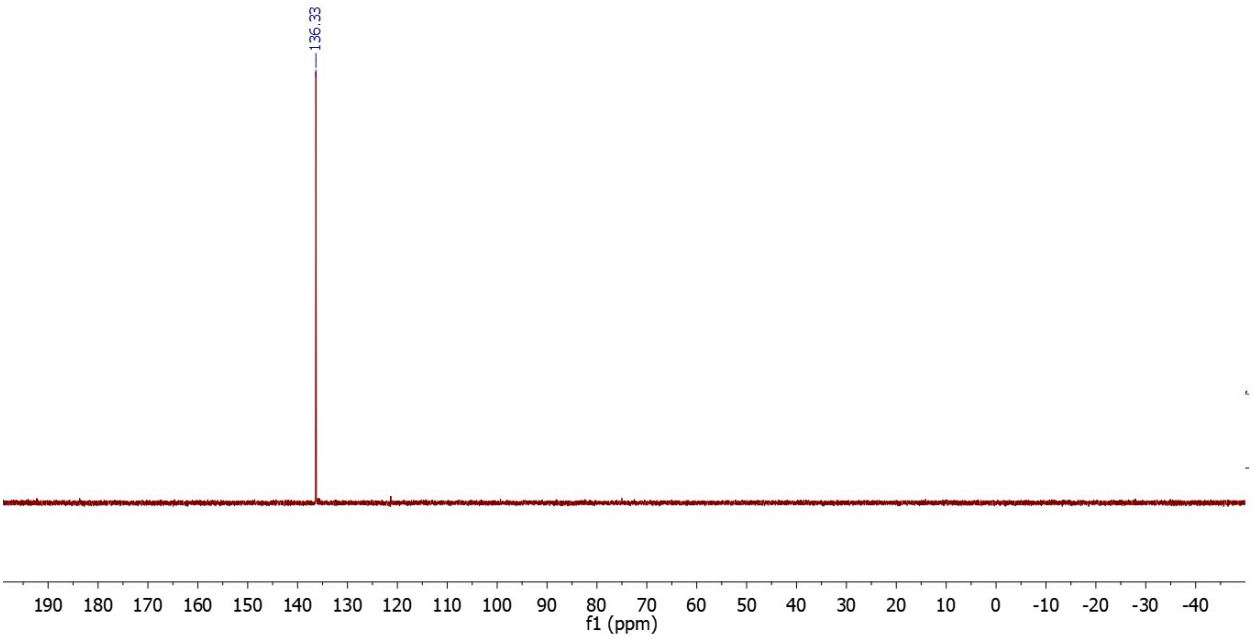


Figure S33. ^{31}P NMR spectrum of **4b** 6-methyl-3-phenyl-5-methoxy-1,2,4-diazaphosphinin in CD_3CN.

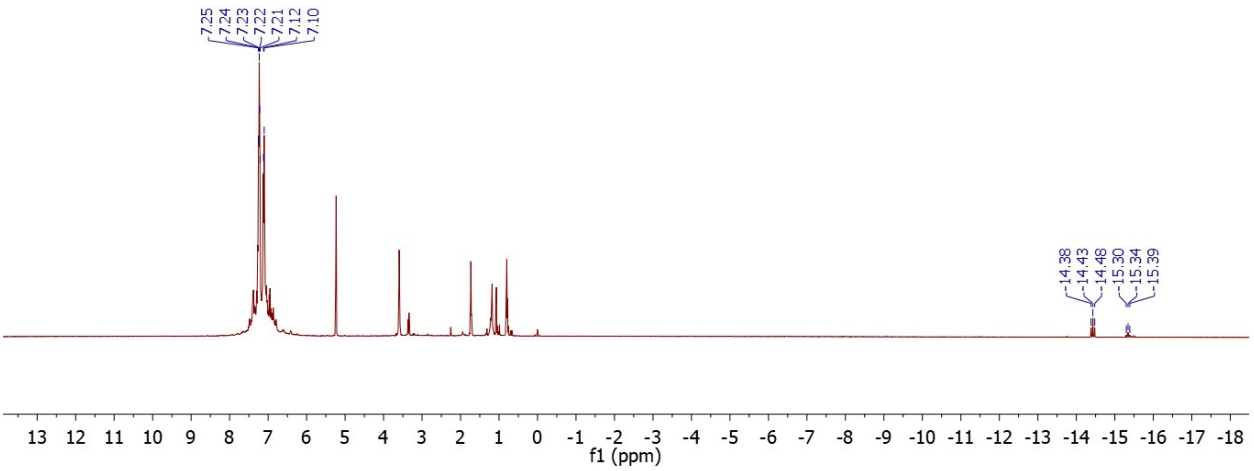


Figure S34. ^{1}H NMR spectrum of **5** bis(triphenylphosphine)(hydrido)(carbonyl)ruthenium(3,6-diphenyl-1,2,4-diazaphosphinin-5-olate)

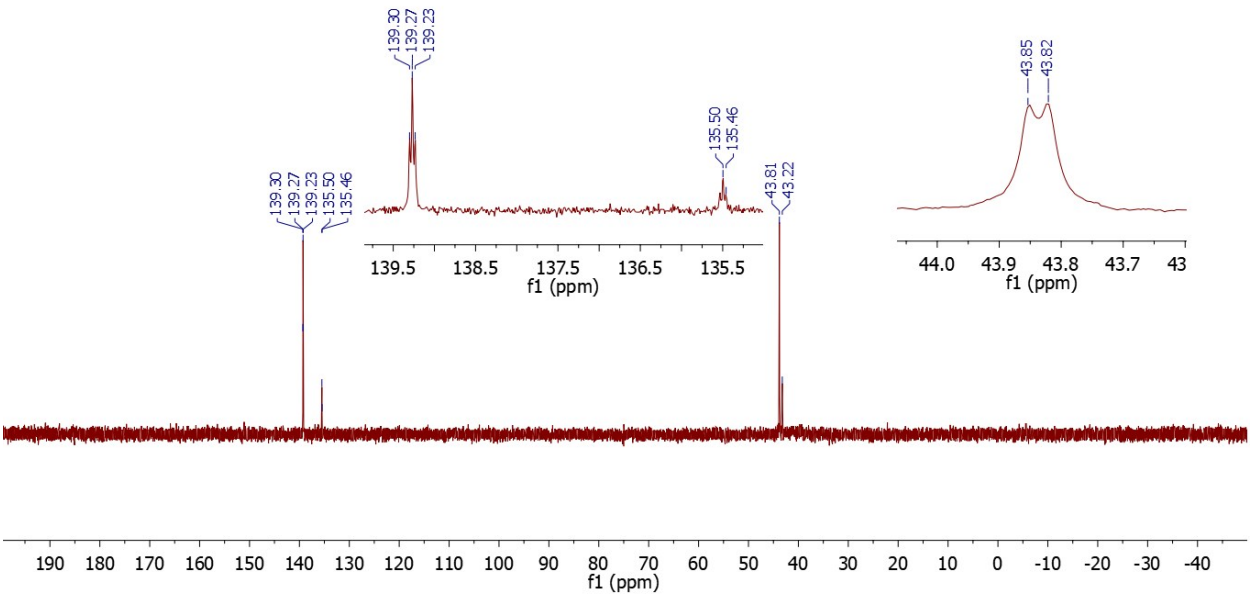
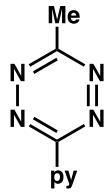
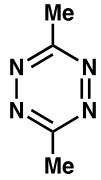
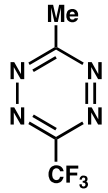
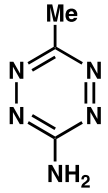
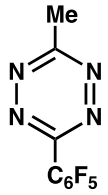


Figure S35. ^{31}P NMR spectrum of **5** bis(triphenylphosphine)(hydrido)(carbonyl)ruthenium(3,6-diphenyl-1,2,4-diazaphosphinin-5-olate)

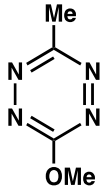
Table S2. Thermodynamics for Tetrazines plus OCP at double zeta

Tetrazine	Species	E(SCF) / E_h	G(gas) / E_h	ΔG(gas) / kcal/mol
	IA + PCO^-	–1037.460534	–1037.366265	0.00
	TSIaA	–1037.459250	–1037.343095	14.54
	TSIbA	–1037.463374	–1037.346650	12.31
	IIaA	–1037.466056	–1037.348277	11.29
	IIbA	–1037.468260	–1037.350411	9.95
	TSIIaA	–1037.453959	–1037.338356	17.51
	TSIIbA	–1037.456535	–1037.341012	15.85
	IIIaA + N_2	–1037.544817	–1037.449103	–51.98
	IIIbA + N_2	–1037.543997	–1037.449519	–52.24
	IB + PCO^-	–829.686817	-829.629332	0.00
	TSIB	–829.684990	-829.604442	15.62
	IIB	–829.694916	-829.612620	10.49
	TSIIB	–829.682287	-829.602876	16.60
	IIIB + N_2	–829.767847	-829.709105	–50.06
	IC + PCO^-	–1127.385205	–1127.354673	0.00
	TSIaC	–1127.404078	–1127.350257	2.77
	TSIbC	–1127.403134	–1127.349215	3.42
	IIaC	–1127.413530	–1127.357995	–2.08
	IIbC	–1127.410075	–1127.353976	0.44
	TSIIaC	–1127.401200	–1127.348176	4.08
	TSIIbC	–1127.397345	–1127.343884	6.77
	IIIaC + N_2	–1127.491087	–1127.458237	–64.99
	IIIbC + N_2	–1127.486535	–1127.454893	–62.89
	ID + PCO^-	–845.735315	–845.686847	0.00
	TSIaD	–845.720003	–845.650745	22.65
	TSIbD	–845.723885	–845.653067	21.20

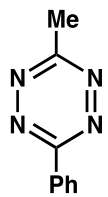
IIaD	–845.728233	–845.656959	18.75
IIbD	–845.734170	–845.661589	15.85
TSIIaD	–845.720698	–845.650975	22.51
TSIIbD	–845.722065	–845.652111	21.80
IIIaD + N_2	–845.810704	–845.760618	–46.29
IIIbD + N_2	–845.813434	–845.763370	–48.02



IE + PCO^-	–1517.542291	–1517.482671	0.00
TSIaE	–1517.544255	–1517.464322	11.51
TSIbE	–1517.555704	–1517.474082	5.39
IIaE	–1517.558439	–1517.476239	4.04
IIbE	–1517.558710	–1517.476030	4.17
TSIIaE	–1517.547996	–1517.467204	9.71
TSIIbE	–1517.548275	–1517.467408	9.58
IIIaE + N_2	–1517.642323	–1517.582441	–62.61
IIIbE + N_2	–1517.642358	–1517.582599	–62.71



IF + PCO^-	–904.896888	–904.833678	0.00
TSIaF	–904.888810	–904.805110	17.93
TSIbF	–904.887638	–904.803564	18.90
IIaF	–904.898054	–904.813536	12.64
IIbF	–904.894358	–904.809275	15.31
TSIIaF	–904.889523	–904.806555	17.02
TSIIbF	–904.884389	–904.801436	20.23
IIIaF + N_2	–904.982058	–904.918602	–53.29
IIIbF + N_2	–904.975926	–904.913008	–49.78



IG + PCO^-	–1021.431477	–1021.324554	0.00
TSIaG	–1021.427506	–1021.299594	15.66
TSIbG	–1021.430974	–1021.302580	13.79

IIaG	–1021.436566	–1021.306972	11.03
IIbG	–1021.433767	–1021.304533	12.56
TSIIaG	–1021.426048	–1021.298414	16.40
TSIIbG	–1021.422511	–1021.294766	18.69
IIIaG + N_2	–1021.516048	–1021.408428	–52.63
IIIbG + N_2	–1021.513978	–1021.408368	–52.59

Table S3. Thermodynamics for species optimized at B3LYP/6-311G(d,p) level of theory

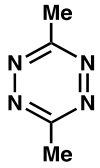
Tetrazine	**Species**	**E(SCF) / E_h**	**G(gas) / E_h**	**ΔG(gas) / kcal/mol**
	IB + PCO^-	–829.836312	-829.779594	0.00
	TSIB	–829.829926	-829.750172	18.46
	IIB	–829.838961	-829.757702	13.74
	TSIIB	–829.828456	-829.749818	18.68
	IIIB + N_2	–829.920362	-829.862446	–51.99

Table S?. Frequencies for all optimized species at B3LYP/6-31G(d,p) level of theory

SI Computational details

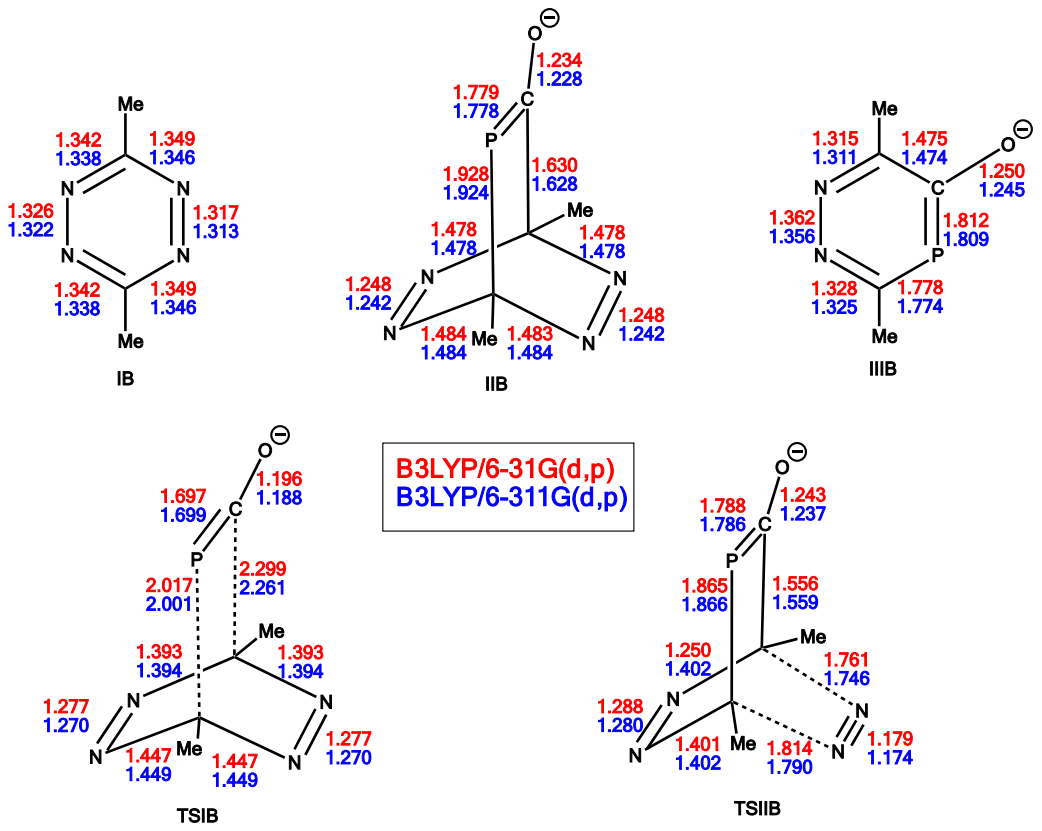


Figure S36. All frequencies/coordinates/thermo data is based on this labelling scheme.

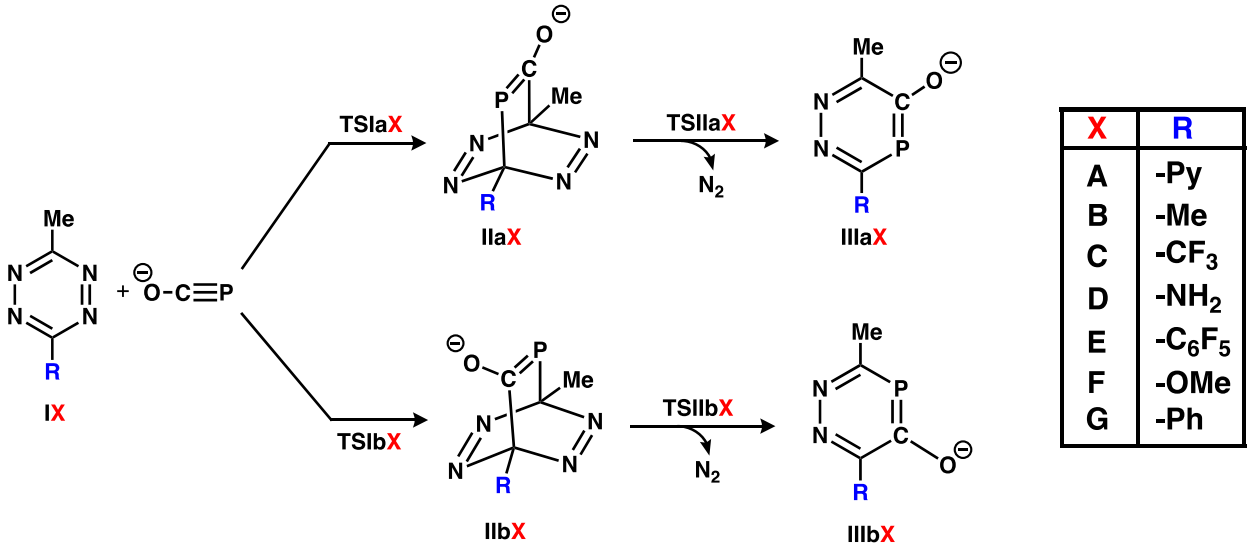


Table S4. Cartesian coordinates for all optimized species at B3LYP/6-31G(d,p) level of theory

IA

N	-0.970816	-1.206117	-0.091911
C	-0.330916	-0.019986	-0.026289
C	-2.908312	0.006993	0.003156
N	-2.287620	-1.187435	-0.076046
N	-2.270938	1.190246	0.021426
N	-0.951419	1.172484	0.007474
C	1.158006	-0.009894	-0.008634
C	1.851410	1.208837	-0.038685
N	1.772912	-1.201723	0.039988
C	3.243183	1.179741	-0.020137
H	1.300149	2.140267	-0.075043
C	3.106498	-1.210019	0.057661
C	3.890224	-0.053225	0.028371
H	3.810682	2.105167	-0.043762
H	3.576013	-2.191074	0.098405
H	4.973078	-0.123573	0.044224
C	-4.404110	0.011024	0.068318
H	-4.815739	-0.732671	-0.617777
H	-4.737398	-0.254313	1.078032
H	-4.787519	1.003182	-0.173164

TSIbA

TSIaA

C	0.112666	-0.225432	-0.069690
C	-2.318526	-0.817348	-0.251306
C	-2.225094	1.329049	0.428182
N	-0.367341	-0.550236	-1.409502
N	-1.618807	-0.767910	-1.460339
N	-1.629757	-1.437317	0.788763
N	-0.375071	-1.217510	0.860267
P	-0.547096	1.610452	0.456818
O	-3.359420	1.685402	0.562342
C	-3.793802	-1.072921	-0.333581
H	-4.069904	-1.332336	-1.360230
H	-4.069001	-1.893439	0.336736
H	-4.359614	-0.180148	-0.036866
C	1.621866	-0.133518	-0.035756
C	2.374479	-0.916639	0.853778
C	3.528808	0.827147	-0.883244
C	3.760266	-0.798590	0.849639
H	1.849281	-1.593147	1.516135
C	4.361652	0.091731	-0.040892
H	3.956448	1.537818	-1.591258
H	4.364021	-1.394062	1.530836
H	5.440256	0.217272	-0.081577

C	-2.478352	-0.469496	-0.057662	N	2.196179	0.729713	-0.888839
C	0.024379	-0.426356	-0.082485				
C	-0.582829	1.554501	0.207066	**IIaA**			
N	-1.812365	-1.183917	1.033016	C	-2.340841	0.557546	0.187443
N	-0.550155	-1.094107	1.021457	C	0.130866	0.145825	0.064884
N	-0.574364	-0.771743	-1.319410	N	-1.614912	1.415037	-0.762583
N	-1.832871	-0.860249	-1.319688	N	-0.385390	1.204462	-0.824939
C	-3.957664	-0.821744	-0.093252	N	-0.397855	0.432994	1.426963
H	-4.453554	-0.299947	-0.916326	N	-1.624150	0.635428	1.482663
H	-4.075466	-1.900432	-0.241899	C	-3.776281	1.015848	0.341867
H	-4.438231	-0.544416	0.849053	H	-4.294834	0.371519	1.053904
P	-2.308088	1.457928	0.207459	H	-3.806770	2.050080	0.697722
O	0.369469	2.269972	0.312280	H	-4.291413	0.946323	-0.617817
C	1.502557	-0.348547	-0.068075	C	1.637961	0.116464	0.049465
C	2.215793	-0.582902	1.123403	C	2.356680	0.694962	-1.010037
C	3.597912	-0.455437	1.121592	C	3.744493	0.608051	-1.010582
H	1.666061	-0.869822	2.011638	H	1.812486	1.201370	-1.797153
C	3.451164	0.136833	-1.185481	C	3.581813	-0.590373	1.047147
C	4.244293	-0.088688	-0.061447	C	4.382471	-0.049040	0.042400
H	4.166638	-0.637267	2.030898	H	4.321016	1.047017	-1.821586
H	3.914122	0.435392	-2.127248	H	4.038697	-1.113935	1.887631
H	5.323414	0.028079	-0.110709	H	5.464116	-0.142621	0.085186
N	2.121049	0.020120	-1.205017	N	2.247419	-0.519989	1.062523

P	-0.588833	-1.561294	-0.532793
C	-2.258271	-0.977178	-0.347830
O	-3.342491	-1.531062	-0.547116

IIbA

C	2.495715	-0.459656	0.092698
C	0.001720	-0.208774	0.052752
C	0.551525	1.350563	-0.278729
N	1.792515	-1.224851	-0.957564
N	0.548849	-1.093740	-0.978031
N	0.556431	-0.622255	1.355147
N	1.795143	-0.753376	1.370264
C	3.944861	-0.905544	0.182507
H	4.457078	-0.356890	0.977176
H	4.001739	-1.977336	0.403935
H	4.455386	-0.716662	-0.765506
C	-1.503186	-0.231393	0.055787
C	-2.215082	-0.644847	-1.080607
C	-3.604638	-0.611540	-1.054884
H	-1.665675	-0.990502	-1.947392
C	-3.452474	0.230411	1.173633
C	-4.248635	-0.164145	0.099305
H	-4.177868	-0.928329	-1.923185
H	-3.915335	0.591431	2.092811
H	-5.332186	-0.117376	0.166227
N	-2.117092	0.204962	1.165494

TSIIaA

C	1.438916	-0.080109	0.139274
C	-1.100348	-0.482675	-0.218537
N	-0.328656	-0.108329	-1.339721
N	0.929772	0.049888	-1.170623
P	0.637471	0.935301	1.486543
C	-1.022171	0.488576	0.995335
O	-2.096235	0.855449	1.497084
N	0.841281	-1.791352	0.495207
N	-0.324189	-1.886437	0.337298
C	-2.509559	-0.882940	-0.588601
H	-2.977428	-1.413142	0.243214
H	-3.101889	0.013161	-0.787748
H	-2.500942	-1.519898	-1.477305
C	2.932061	-0.205748	0.147398
C	3.729970	0.482483	1.076444
C	4.795717	-1.178297	-0.789579
C	5.110269	0.318561	1.042797
H	3.258010	1.133493	1.803807

P	2.324698	1.418888	-0.288040	C	5.666956	-0.531391	0.086030
O	-0.317921	2.188340	-0.478176	H	5.188163	-1.857089	-1.547855
				H	5.742597	0.847474	1.751874
	TSIIbA			H	6.739488	-0.692731	0.020800
C	-2.542408	-0.455201	0.015442	N	3.468137	-1.032242	-0.770448
C	0.026030	-0.124094	0.084261				
N	-0.508729	-1.196752	0.802924		**IIIaA**		
N	-1.780544	-1.378217	0.750798	N	-0.424639	-1.361852	-0.289680
C	-3.958981	-0.939363	-0.215723	C	0.069653	-0.154659	-0.027752
H	-3.963007	-2.005144	-0.465807	C	-2.669838	-0.645629	-0.130646
H	-4.556330	-0.796441	0.690319	N	-1.760759	-1.579851	-0.327686
H	-4.424072	-0.376937	-1.029486	C	1.568024	-0.109976	-0.018326
P	-2.356823	1.353294	0.419939	C	2.254790	0.992961	-0.564751
C	-0.566293	1.297182	0.421694	N	2.234252	-1.149564	0.525245
O	0.230948	2.203869	0.681312	C	3.644262	1.018090	-0.544481
N	-1.736315	-0.610182	-1.579376	H	1.684573	1.806101	-0.999951
N	-0.572637	-0.433424	-1.554088	C	3.568848	-1.109130	0.531922
C	1.524116	-0.168985	0.012326	C	4.330024	-0.059797	0.016435
C	2.263661	-0.892414	0.961476	H	4.184286	1.861795	-0.968092
C	3.651442	-0.892121	0.879158	H	4.065988	-1.969148	0.983734
H	1.730361	-1.440673	1.728304	H	5.415501	-0.090118	0.054701
C	3.444543	0.503231	-1.047904	C	-4.106282	-1.101487	-0.215034
C	4.266263	-0.175872	-0.148807	H	-4.141257	-2.173726	-0.421736

H	4.245751	-1.441153	1.606119	H	-4.637638	-0.881756	0.718655
H	3.885184	1.069765	-1.869053	H	-4.642558	-0.551904	-0.997971
H	5.347299	-0.143998	-0.254263	P	-0.773914	1.376397	0.311459
N	2.110988	0.517152	-0.981291	C	-2.480293	0.784850	0.156100
				O	-3.467163	1.537541	0.297851

IIIbA

N	-0.609156	-1.290137	-0.252904
C	-0.050188	-0.102426	-0.041540
C	-2.822555	-0.557032	-0.081652
N	-1.925501	-1.527783	-0.297722
C	1.444712	-0.149884	-0.011066
C	2.231477	0.941679	-0.438573
N	2.019163	-1.292572	0.426984
C	3.617188	0.828568	-0.434260
H	1.732546	1.852721	-0.737751
C	3.349987	-1.377146	0.425288
C	4.205107	-0.358445	0.003712
H	4.232035	1.661048	-0.770243
H	3.765335	-2.317912	0.792375
H	5.283717	-0.490674	0.028882
C	-4.255738	-1.058641	-0.127946
H	-4.450418	-1.566131	-1.080028
H	-4.428682	-1.794276	0.667054

IB

N	-0.662788	1.192266	0.000040
C	-1.288488	0.005295	0.000009
C	1.288488	0.005295	0.000009
N	0.662788	1.192266	0.000040
N	0.658656	-1.187768	0.000040
N	-0.658656	-1.187768	0.000040
C	2.786888	-0.003215	-0.000057
H	3.163991	1.019822	0.000350
H	3.163682	-0.532287	0.880495
H	3.163603	-0.531506	-0.881118
C	-2.786889	-0.003215	-0.000057
H	-3.163603	-0.531495	-0.881125
H	-3.163683	-0.532298	0.880488
H	-3.163991	1.019822	0.000361

TSIB

H	-4.974658	-0.242121	-0.009092
P	-2.556532	1.151470	0.225332
C	-0.738162	1.190645	0.140095
O	-0.136801	2.281853	0.248746

IIB

C	-1.386559	-0.177084	0.000000
C	1.089871	-0.576900	0.000000
C	0.982345	1.049746	0.000000
N	-0.853971	-0.886525	1.188949
N	0.377765	-1.086878	1.190344
N	0.377765	-1.086878	-1.190344
N	-0.853971	-0.886525	-1.188949
C	-2.904419	-0.229086	-0.000001
H	-3.296226	0.271290	-0.889517
H	-3.253529	-1.268166	-0.000017
H	-3.296227	0.271262	0.889530
P	-0.700623	1.624829	0.000001
O	2.057795	1.654138	-0.000001
C	2.533418	-1.036774	0.000000
H	2.582656	-2.130074	-0.000023
H	3.044631	-0.650794	-0.883804
H	3.044619	-0.650833	0.883828
C	-1.361969	-0.255682	0.000000
C	1.071438	-0.869435	0.000038
C	0.957264	1.426472	0.000016
N	-0.874741	-0.933972	1.181494
N	0.382640	-1.158967	1.175358
N	0.382703	-1.158866	-1.175351
N	-0.874671	-0.933880	-1.181547
C	-2.881727	-0.183592	-0.000068
H	-3.239680	0.338730	-0.891706
H	-3.294785	-1.198011	-0.000113
H	-3.239773	0.338688	0.891558
P	-0.723852	1.657864	0.000069
O	2.091506	1.804928	-0.000037
C	2.550575	-1.112860	-0.000005
H	2.836220	-1.676730	0.893865
H	2.836269	-1.676292	-0.894137
H	3.102485	-0.163382	0.000240

TSIIB

C	1.420492	-0.096863	-0.151852
C	-1.135643	-0.519540	-0.147249
N	-0.375610	-1.147366	-1.142595
N	0.897421	-0.955247	-1.128483

IIIB

N	-0.364204	1.614286	-0.000004
C	-1.223827	0.619324	-0.000005
C	1.536821	0.240413	0.000005
N	0.987916	1.449824	0.000007
C	3.058016	0.278019	0.000002
H	3.388053	1.321035	0.000148
H	3.472925	-0.226497	0.881209
H	3.472908	-0.226234	-0.881365
P	0.767377	-1.361037	-0.000005
C	-0.965518	-0.832926	0.000000
O	-1.922820	-1.637414	0.000009
C	-2.682583	1.012564	-0.000001
H	-3.197498	0.595763	-0.873926
H	-3.197500	0.595740	0.873911
H	-2.770417	2.101923	0.000011

TSIaC

C	0.616769	-0.175307	0.000002
C	-1.762385	-0.919799	-0.000012
C	-1.746297	1.393902	0.000023
N	0.184241	-0.879200	-1.184588
C	2.929321	-0.188878	-0.053289
H	3.257339	-1.226791	-0.171239
H	3.396691	0.411143	-0.841051
H	3.270001	0.188122	0.914810
C	-2.565397	-1.003813	-0.098948
H	-3.161575	-0.463310	-0.838542
H	-2.608601	-2.077035	-0.304405
H	-2.996405	-0.798551	0.883631
P	0.697996	1.614933	0.003428
C	-0.989533	1.024462	-0.016979
O	-2.041659	1.682249	0.052967
N	0.805085	-0.939991	1.331490
N	-0.362547	-1.101365	1.324095

IC

N	-0.295897	1.191462	0.007525
C	0.307824	-0.000121	-0.018764
C	-2.244176	-0.000039	0.008517
N	-1.616628	1.193045	0.022129
N	-1.616722	-1.193133	0.022132
N	-0.295938	-1.191629	0.007544
C	-3.739439	0.000070	-0.024203
H	-4.127555	0.896263	0.462370

N	-1.059948	-1.165497	-1.174295	H	-4.086968	0.003372	-1.063835
N	-1.059988	-1.165402	1.174317	H	-4.127487	-0.899032	0.456957
N	0.184201	-0.879122	1.184649	C	1.831332	-0.000022	-0.011446
P	-0.082004	1.722435	-0.000062	F	2.285486	0.001576	1.256919
O	-2.896252	1.713595	0.000018	F	2.311856	1.087257	-0.629501
C	-3.228775	-1.224205	-0.000019	F	2.312108	-1.088627	-0.626910
H	-3.490668	-1.799177	-0.893567				
H	-3.490873	-1.797908	0.894278		**TSIbC**		
H	-3.818735	-0.298003	-0.000730	C	1.932514	-0.538978	0.000062
C	2.138587	-0.072140	0.000010	C	-0.544476	-0.425139	-0.000122
F	2.600874	0.586675	-1.087282	C	0.195428	1.740654	0.000088
F	2.600878	0.586706	1.087279	N	1.267605	-1.059995	-1.188100
F	2.726408	-1.288976	0.000025	N	0.003524	-0.915452	-1.180459
				N	0.003413	-0.915573	1.180189
	IIaC			N	1.267486	-1.060156	1.188024
C	1.790374	-0.621506	0.000477	C	3.404374	-0.924381	0.000065
C	-0.63762	-0.076068	0.000022	H	3.902870	-0.532583	0.890859
N	1.049496	-1.085404	-1.188949	H	3.492237	-2.015732	0.002119
N	-0.168216	-0.818283	-1.191542	H	3.901764	-0.535961	-0.892817
N	-0.168034	-0.817198	1.192727	P	1.877977	1.446399	0.000094
N	1.050144	-1.084703	1.189455	O	-0.752343	2.456314	-0.000062
C	3.205266	-1.160735	-0.000331	C	-2.041305	-0.321407	0.000006
H	3.736345	-0.803392	0.883476	F	-2.493524	0.335148	1.090806

H	3.193248	-2.254693	-0.000886
H	3.735263	-0.802531	-0.884421
P	0.131596	1.697791	0.00001
C	1.771786	1.011223	-0.000212
O	2.878271	1.553311	-0.000478
C	-2.157476	-0.067975	-0.000171
F	-2.657606	0.55704	1.087213
F	-2.667802	-1.324093	0.00067
F	-2.657111	0.555582	-1.088444

TSIIaC

C	0.662015	-0.005469	-0.138112
C	-1.844562	-0.555400	-0.147921
N	-1.051368	-1.135577	-1.151462
N	0.208377	-0.884515	-1.125378
P	-0.118404	1.677964	0.021784
C	-1.770679	0.997737	-0.027064
O	-2.851780	1.604393	0.026602
N	0.088570	-0.904617	1.349731
N	-1.072320	-1.101133	1.303841
C	-3.250698	-1.103892	-0.116777
H	-3.719795	-0.873685	0.841816
H	-3.844522	-0.625302	-0.899143
F	-2.493509	0.333533	-1.091755
F	-2.670877	-1.534067	0.001032

IIbC

C	1.984430	-0.423635	-0.000156
C	-0.490785	-0.175193	0.000031
C	0.015990	1.390970	-0.000363
N	1.286594	-0.966717	-1.189682
N	0.044634	-0.847173	-1.194228
N	0.044870	-0.847703	1.193679
N	1.286497	-0.967168	1.189146
C	3.437014	-0.866221	-0.000293
H	3.943833	-0.483885	0.889318
H	3.504864	-1.959855	-0.000219
H	3.943446	-0.484001	-0.890166
P	1.791048	1.494031	0.000886
O	-0.862297	2.248273	-0.000946
C	-2.008830	-0.302015	0.000144
F	-2.562787	0.258118	-1.091115
F	-2.562527	0.259824	1.090701
F	-2.388527	-1.608056	0.001165

TSIIbC

H	-3.239532	-2.185587	-0.274925
C	2.173930	-0.052764	-0.035909
F	2.774982	0.525830	-1.104031
F	2.622608	0.592166	1.064145
F	2.642554	-1.320262	0.034358

IIIaC

N	-0.185393	1.351107	-0.000151
C	-0.639965	0.105462	-0.000355
C	2.065095	0.664844	-0.000094
N	1.143708	1.607487	-0.000264
C	3.495148	1.145770	-0.000126
H	3.518026	2.237942	-0.000936
H	4.032515	0.760080	0.874244
H	4.032906	0.758808	-0.873708
P	0.198421	-1.450915	-0.000826
C	1.893624	-0.797986	0.000257
O	2.891827	-1.547204	0.000985
C	-2.158191	0.093495	0.000070
F	-2.683795	0.716937	-1.084544
F	-2.682916	0.714697	1.086586
F	-2.670716	-1.164428	-0.001008
C	2.042366	-0.338847	-0.160554
C	-0.514543	-0.113735	-0.120935
N	0.029601	-0.906398	-1.130465
N	1.308844	-1.031645	-1.138762
C	3.481297	-0.805178	-0.088850
H	3.534924	-1.895344	-0.170311
H	4.055686	-0.370035	-0.912559
H	3.935304	-0.491147	0.854459
P	1.773174	1.498514	0.000899
C	-0.011205	1.356508	-0.012136
O	-0.861691	2.253515	0.047751
N	1.267769	-1.003978	1.317847
N	0.096768	-0.880645	1.351329
C	-2.022428	-0.289195	-0.042386
F	-2.660556	0.273203	-1.090064
F	-2.533541	0.237385	1.086580
F	-2.361879	-1.604806	-0.042911

IIIbC

N	-0.137906	-1.371644	0.000932
C	0.485920	-0.212492	0.000256
C	-2.276743	-0.437852	0.000250
N	-1.474843	-1.510144	0.001493

ID

N	0.685921	-1.200300	-0.040340
C	1.308514	0.000040	0.006438
C	-1.261439	0.000080	-0.006716
N	-0.630103	-1.188170	-0.042061
N	-0.630114	1.188234	-0.042040
N	0.686017	1.200313	-0.040360
C	-2.759851	-0.000002	0.054222
H	-3.157536	-0.890819	-0.435591
H	-3.101977	-0.008797	1.095646
H	-3.156540	0.899158	-0.420793
N	2.660760	-0.000079	0.103239
H	3.142592	-0.868805	-0.066012
H	3.142748	0.868567	-0.065976

TSIbD

C	1.366910	-0.218996	-0.000759
C	-1.034234	-0.903021	-0.027498
C	-1.023808	1.338344	0.001506
N	0.898750	-0.851798	-1.211622
N	-0.344759	-1.141557	-1.214320
N	-0.346568	-1.213979	1.136565
N	0.905771	-0.946673	1.150603
C	-3.749333	-0.812711	-0.000287
H	-3.986980	-1.417862	-0.883174
H	-3.986130	-1.423256	0.879057
H	-4.392571	0.072294	0.002505
P	-1.877277	1.277056	-0.001159
C	-0.056419	1.154254	0.000672
O	0.676860	2.157458	0.001997
C	1.998277	-0.324537	-0.000369
F	2.557830	0.265938	-1.088709
F	2.437715	-1.604872	-0.001701
F	2.558788	0.264030	1.088513

TSIaD

C	1.376733	-0.194196	0.003366
C	-1.045507	-0.843083	0.000147
C	-0.976463	1.367429	-0.000387
N	0.896413	-0.883840	-1.188682
N	-0.352639	-1.122076	-1.185701
N	-0.338852	-1.166018	1.163126
N	0.911855	-0.924593	1.166497
P	0.706808	1.666754	0.033797
O	-2.109494	1.754469	-0.008616
C	-2.515023	-1.148245	0.003503

C	2.880590	-0.077020	-0.000052
H	3.215543	0.428815	0.909746
H	3.344015	-1.068825	-0.038587
H	3.209330	0.495775	-0.871415
P	0.628071	1.690607	0.063517
O	-2.196098	1.608567	-0.035355
N	-2.423482	-1.170116	-0.026025
H	-2.905419	-0.308251	-0.299683
H	-2.680488	-1.342138	0.944435

IIbD

C	1.379467	-0.143742	-0.013308
C	-1.087347	-0.629578	0.035223
C	-1.015695	1.006695	0.007197
N	0.856858	-0.900626	-1.167083
N	-0.369626	-1.140478	-1.143125
N	-0.332632	-1.090816	1.234967
N	0.884445	-0.838515	1.210177
C	2.898461	-0.146527	-0.029640
H	3.283211	0.381416	0.846818
H	3.279992	-1.173767	-0.015423
H	3.265522	0.349875	-0.931926
P	0.636591	1.635814	-0.033355
H	-2.779827	-1.725976	-0.887920
H	-2.774874	-1.721544	0.898981
H	-3.102873	-0.221109	0.001766
N	2.825591	-0.093548	0.026396
H	3.158026	-0.889312	0.570210
H	3.138371	-0.240015	-0.932307

IIaD

C	1.081311	-0.572555	-0.004716
C	-1.397375	-0.178250	0.028290
N	0.366032	-1.082196	-1.191771
N	-0.865986	-0.886165	-1.175807
N	-0.856853	-0.908676	1.195800
N	0.377005	-1.097835	1.183951
C	2.528387	-1.020349	-0.012201
H	3.039523	-0.633985	0.871516
H	2.586700	-2.113157	-0.016651
H	3.032979	-0.626128	-0.896109
P	-0.724834	1.620823	0.033499
C	0.960663	1.053725	-0.006890
O	2.030178	1.667137	-0.024814
N	-2.840660	-0.202770	0.068467
H	-3.175781	0.414077	-0.668177

O	-2.119797	1.567031	0.004720
N	-2.446000	-1.080865	0.057149
H	-3.008719	-0.224114	0.042370
H	-2.611129	-1.568851	-0.820712

TSIIbD

C	1.403594	-0.077529	-0.112905
C	-1.134977	-0.569910	-0.185027
N	-0.327390	-1.196437	-1.147082
N	0.933470	-0.965889	-1.104474
C	2.916987	-0.090429	-0.017915
H	3.293345	-1.117427	-0.070724
H	3.351165	0.477508	-0.846625
H	3.243082	0.362842	0.922137
P	0.619069	1.626828	-0.043324
C	-1.037294	0.977766	-0.036599
O	-2.121469	1.581631	0.089921
N	0.836414	-0.873511	1.325163
N	-0.325463	-1.099852	1.321238
N	-2.472925	-1.015458	-0.183828
H	-3.028330	-0.272324	0.239488
H	-2.572143	-1.887423	0.323778
H	-3.147008	-1.142174	-0.185927

TSIIaD

C	1.437172	-0.105918	-0.147252
C	-1.107902	-0.532627	-0.108964
N	-0.355351	-1.162012	-1.125764
N	0.913332	-0.973577	-1.118456
P	0.726269	1.622667	-0.029192
C	-0.959835	1.030445	-0.015763
O	-2.011683	1.684989	0.040087
N	0.786789	-0.917620	1.328493
N	-0.392243	-1.071193	1.302203
C	-2.548675	-0.993085	-0.092530
H	-2.599374	-2.078490	-0.218391
H	-3.018992	-0.708998	0.851057
H	-3.101575	-0.506812	-0.899517
N	2.853980	-0.165912	-0.105309
H	3.189386	0.248094	0.758113
H	3.159866	-1.134399	-0.155190

IIIaD

N	-0.998970	1.452833	0.007685
C	-1.550293	0.244848	-0.016234

IIIbD

N	0.336201	-1.644241	0.022665
C	1.209247	-0.666118	-0.029876
C	-1.526181	-0.216226	0.003366
N	-1.014871	-1.432118	0.034411
C	-3.046651	-0.198081	-0.008125
H	-3.414192	-1.226230	0.062710
H	-3.453140	0.384445	0.828329
H	-3.437692	0.253027	-0.929363
P	-0.704242	1.375461	-0.011044
C	0.995704	0.802939	-0.004144
O	2.003808	1.551786	0.042653
N	2.557155	-1.014859	-0.113089
H	3.133637	-0.237038	0.193004
H	2.762442	-1.916966	0.294522

TSIaE

C	0.820618	-0.074910	0.000030
C	3.153426	-1.035223	0.000338
C	3.374960	1.425643	-0.000496
N	1.224895	-0.785837	1.190460
N	2.446299	-1.174702	1.174282
N	2.446345	-1.175337	-1.173571
C	1.207059	0.618826	-0.003127
N	0.349997	1.613358	-0.004595
C	2.667428	1.005866	-0.002233
H	2.757954	2.095214	-0.007095
H	3.181306	0.593819	0.874783
H	3.184627	0.586360	-0.873811
P	-0.791492	-1.372962	-0.026806
C	0.938964	-0.832604	0.008634
O	1.890953	-1.642413	0.032785
N	-2.961367	0.291367	-0.069080
H	-3.401697	-0.467093	0.437751
H	-3.284018	1.200902	0.247868

IE

N	1.936697	-0.888701	-0.798477
C	1.316132	-0.000311	-0.004780
C	3.885135	-0.002399	-0.001538
N	3.258041	-0.896703	-0.786532
C	5.381884	-0.002384	0.009584
H	5.762254	0.989109	-0.252918
H	5.751947	-0.235869	1.012788
H	5.759791	-0.741139	-0.697441
C	-0.163788	-0.000146	-0.002585

N	1.224957	-0.786467	-1.190011	C	-0.890559	1.194505	-0.090003
P	1.738556	1.820810	-0.000553	C	-0.890149	-1.194999	0.087110
O	4.555604	1.578573	-0.000533	C	-2.282275	1.202792	-0.089934
C	4.598966	-1.417250	0.000468	C	-2.281813	-1.203078	0.091974
H	4.830190	-2.003204	0.895322	C	-2.978739	-0.000154	0.002257
H	4.830166	-2.003951	-0.893904	F	-0.258649	2.364651	-0.214368
H	5.239489	-0.524726	0.000085	F	-2.951017	2.354990	-0.190759
C	-0.702439	0.039702	-0.000041	F	-4.311544	-0.000361	0.004467
C	-1.423528	-1.170559	-0.000153	F	-2.950367	-2.355223	0.194918
C	-1.489936	1.195487	0.000173	F	-0.257859	-2.365080	0.209065
C	-2.814593	-1.226170	-0.000190	N	3.255197	0.897869	0.780348
C	-2.886840	1.161036	0.000146	N	1.938061	0.892413	0.789685
C	-3.556952	-0.051951	-0.000042				
F	-0.964509	2.431759	0.000436		**TSIbE**		
F	-3.585383	2.311404	0.000327	C	-3.380666	-0.277801	-0.374081
F	-4.900234	-0.092683	-0.000075	C	-0.879638	-0.292006	-0.325739
F	-3.447872	-2.413135	-0.000327	N	-2.743480	-1.579126	-0.163342
F	-0.797845	-2.351489	-0.000189	N	-1.482056	-1.548012	-0.090585
				N	-1.451362	0.408279	-1.421126
	IIaE			N	-2.710974	0.380978	-1.497874
C	-0.815523	-0.037682	-0.164916	C	-4.861710	-0.456036	-0.671658
C	-3.291273	-0.057459	-0.571846	H	-5.336056	0.514749	-0.839040
C	-3.191581	0.103533	1.044379	H	-4.984596	-1.065333	-1.573102

N	-1.333605	1.074531	-1.016038	H	-5.359187	-0.960253	0.161158
N	-2.564420	1.062691	-1.200135	C	0.599169	-0.227887	-0.264199
N	-2.583120	-1.290939	-0.962357	C	1.236210	1.019088	-0.407910
N	-1.351836	-1.285362	-0.776754	C	1.450533	-1.309425	0.021710
P	-1.515123	0.147036	1.635581	C	2.615046	1.179132	-0.311854
O	-4.266487	0.172963	1.641620	C	2.833089	-1.161063	0.128813
C	0.694462	-0.032423	-0.136369	C	3.424017	0.084249	-0.037055
C	1.420035	1.170729	-0.108206	P	-3.209858	0.811902	1.242652
C	1.462321	-1.204217	-0.038209	C	-1.491535	0.838796	1.349076
C	2.812849	1.206121	-0.063918	O	-0.529626	1.213875	1.953758
C	2.856706	-1.182736	0.006164	F	0.993735	-2.559035	0.183181
C	3.540358	0.024874	-0.009662	F	0.527034	2.128294	-0.650915
C	-4.732381	-0.092521	-1.036648	F	3.170655	2.395097	-0.468050
H	-5.247278	-0.938100	-0.577498	F	4.758551	0.226545	0.059965
H	-5.240973	0.823040	-0.730336	F	3.606995	-2.234880	0.381264
H	-4.776078	-0.187381	-2.125571				
F	0.905152	-2.418740	0.035337		**IIbE**		
F	3.544975	-2.336754	0.080878	C	-3.398087	0.230002	-0.424008
F	4.883700	0.051132	0.033962	C	-0.908038	0.171073	-0.141369
F	3.458011	2.386833	-0.055669	C	-1.470852	-0.622499	1.229903
F	0.810174	2.361688	-0.102384	N	-2.653807	-0.514147	-1.466122
				N	-1.415830	-0.548660	-1.334731
	TSIIaE			N	-1.491161	1.519913	-0.156420

C	0.785094	-0.138334	-0.170791	N	-2.731352	1.543599	-0.293922
C	3.278869	0.588040	-0.139323	C	-4.844378	0.417072	-0.848115
N	2.485843	1.004921	-1.232541	H	-5.384081	0.993174	-0.092237
N	1.248578	0.682037	-1.226505	H	-4.896687	0.953797	-1.801760
P	1.701847	-1.742919	0.152591	H	-5.328807	-0.555535	-0.966563
C	3.304622	-0.955414	0.099646	P	-3.238095	-0.707124	1.249982
O	4.419344	-1.484085	0.224966	O	-0.604415	-1.017487	2.002539
N	1.315148	0.917440	1.255587	C	0.598647	0.165237	-0.143713
N	2.466490	1.177354	1.197220	C	1.256798	-1.067554	-0.280497
C	4.649052	1.225315	-0.142803	C	1.425519	1.278232	0.054385
H	4.571751	2.290237	-0.378339	C	2.642650	-1.187287	-0.270043
H	5.123158	1.094702	0.831787	C	2.818464	1.173775	0.070402
H	5.276162	0.730706	-0.887733	C	3.433146	-0.058923	-0.091023
C	-0.714926	-0.102350	-0.101626	F	0.947327	2.516421	0.236604
C	-1.556557	-1.223974	-0.090670	F	3.572071	2.276298	0.245325
C	-1.372363	1.141113	-0.049549	F	4.773863	-0.160871	-0.079004
C	-2.946163	-1.121805	-0.017953	F	3.224165	-2.391486	-0.418826
C	-2.757160	1.262943	0.026052	F	0.564592	-2.200849	-0.438174
C	-3.553718	0.124740	0.040042				
F	-0.682010	2.288794	-0.050551	**TSIIbE**			
F	-3.331597	2.478071	0.085247	C	-3.441395	-0.333214	-0.339608
F	-4.891606	0.230112	0.110543	C	-0.885639	-0.211329	-0.000295
F	-3.704449	-2.233365	-0.017897	N	-1.434989	-1.471706	-0.263424

F	-1.075499	-2.471731	-0.163873	N	-2.703811	-1.532967	-0.434847
				C	-4.860494	-0.504565	-0.843223
	IIIaE			H	-4.868280	-1.064247	-1.783872
N	-2.737408	0.908482	1.324285	H	-5.448967	-1.060262	-0.107299
C	-3.655185	0.380116	0.540558	H	-5.329009	0.470299	-1.000289
C	-0.942374	0.040105	0.113444	P	-3.265017	0.657877	1.236643
N	-1.402845	0.758691	1.132994	C	-1.482145	0.592166	1.213438
P	-1.782796	-0.830704	-1.178068	O	-0.676372	1.076013	2.019663
C	-3.482153	-0.451352	-0.663777	N	-2.638000	0.626209	-1.544376
O	-4.477304	-0.865978	-1.291378	N	-1.468913	0.721482	-1.423369
C	-5.086784	0.666831	0.922264	C	0.611741	-0.169891	-0.051726
H	-5.611612	1.170808	0.102213	C	1.447241	-1.284519	0.106475
H	-5.634613	-0.266637	1.096860	C	1.261289	1.065092	-0.205871
H	-5.112224	1.288481	1.820096	C	2.838739	-1.181274	0.059830
C	0.559804	0.019419	0.068664	C	2.646687	1.183916	-0.254234
C	1.303003	-1.144269	0.286710	C	3.444362	0.054081	-0.119859
C	1.290501	1.186800	-0.179678	F	0.562977	2.197667	-0.339253
C	2.696473	-1.156004	0.253974	F	3.222234	2.388573	-0.423409
C	2.682829	1.199313	-0.217909	F	4.784424	0.157121	-0.166693
C	3.390148	0.021754	0.001094	F	3.601406	-2.282043	0.205493
F	3.377443	-2.295084	0.479954	F	0.970089	-2.515312	0.330202
F	0.691126	-2.306692	0.561760				
F	4.734856	0.022641	-0.033877	**IIIbE**			

F	3.352229	2.339258	-0.472562	N	1.570404	-0.950115	-0.931654
F	0.662460	2.345351	-0.420847	C	1.035355	-0.076671	-0.097848
				C	3.772983	-0.399951	-0.384379
	IF			N	2.894895	-1.123678	-1.087754
N	0.442588	0.970173	0.000050	P	3.502630	0.852069	0.826308
C	0.856594	-0.299532	0.000036	C	1.682666	0.860137	0.834015
C	-1.671653	0.106731	-0.000008	O	1.015056	1.600225	1.579917
N	-0.870148	1.176462	0.000002	C	5.214907	-0.747784	-0.714556
C	-3.154479	0.325717	0.000003	H	5.919752	-0.158216	-0.120619
H	-3.609171	-0.137165	-0.881061	H	5.401257	-1.811887	-0.528295
H	-3.609183	-0.137342	0.880967	H	5.415721	-0.568696	-1.777411
H	-3.371183	1.394403	0.000105	C	-0.460105	-0.077231	-0.089405
N	-1.231348	-1.174810	-0.000050	C	-1.199519	1.078202	-0.364997
N	0.060287	-1.392797	-0.000036	C	-1.194668	-1.231290	0.199232
O	2.158437	-0.574957	0.000132	C	-2.591471	1.090687	-0.352021
C	3.069145	0.537773	-0.000100	C	-2.588325	-1.244054	0.209961
H	4.061711	0.088839	-0.000861	C	-3.291009	-0.076591	-0.063448
H	2.925948	1.157109	-0.888932	F	-0.581812	2.216388	-0.706069
H	2.927089	1.156482	0.889370	F	-3.270678	2.218518	-0.638101
				F	-4.637389	-0.076847	-0.056722
	TSIbF			F	-3.261497	-2.375500	0.498705
C	1.575902	-0.388728	-0.067985	F	-0.575136	-2.380362	0.509843
C	-0.866646	-0.626903	0.279997				

C	-0.492685	1.554912	0.073683
N	0.853339	-1.068991	-1.115958
N	-0.414629	-1.117313	-0.928724
N	-0.104097	-0.952125	1.390197
N	1.161508	-0.898256	1.222603
C	3.078118	-0.536406	-0.254623
H	3.614333	-0.006667	0.537371
H	3.350744	-1.596502	-0.213266
H	3.382350	-0.135005	-1.225086
P	1.189928	1.598329	-0.165108
O	-1.575647	2.049816	0.187418
O	-2.216295	-0.646500	0.524677
C	-3.044889	-0.587068	-0.624423
H	-2.754849	0.232769	-1.289159
H	-3.019018	-1.525028	-1.193163
H	-4.058590	-0.409077	-0.253534

IIbF

C	1.501933	-0.522637	0.000053
C	-0.948302	-0.041369	-0.000005
C	-0.286196	1.464115	-0.000052
N	0.757015	-0.999414	-1.190414
N	-0.470514	-0.766854	-1.185683

TSIaF

C	1.050800	-0.289087	0.249673
C	-1.370559	-0.804102	-0.071351
C	-1.208814	1.383983	-0.051041
N	0.709515	-0.950750	-0.983925
N	-0.542047	-1.130432	-1.150000
N	-0.839624	-1.144723	1.182011
N	0.408272	-0.966957	1.351794
P	0.459931	1.628605	0.206872
O	-2.314099	1.821048	-0.202826
C	-2.839264	-1.048563	-0.261073
H	-3.007679	-1.613348	-1.183407
H	-3.236150	-1.612117	0.588974
H	-3.382864	-0.097743	-0.332078
O	2.431375	-0.282221	0.494159
C	3.240039	0.024926	-0.628323
H	2.939614	0.971239	-1.099405
H	4.261781	0.124129	-0.247622
H	3.202096	-0.764756	-1.386669

IIaF

C	-1.081075	0.199568	0.000145
C	1.236669	-0.728883	-0.000041

N	-0.470700	-0.766769	1.185648	C	1.474031	0.893196	-0.000007
N	0.756842	-0.999418	1.190369	N	-0.728923	-0.614908	1.184181
C	2.905540	-1.102962	0.000087	N	0.433105	-1.073138	1.188473
H	3.447362	-0.770983	0.889469	N	0.433118	-1.073103	-1.188445
H	2.868695	-2.198501	0.000410	N	-0.728910	-0.614957	-1.184226
H	3.447243	-0.771498	-0.889558	P	-0.045376	1.815351	-0.000039
P	1.494593	1.404525	-0.000018	O	2.653022	1.252222	-0.000020
O	-1.082872	2.394566	0.000037	C	2.551452	-1.480051	0.000014
O	-2.329347	0.086252	-0.000038	H	3.132072	-1.208233	-0.883296
C	-3.035705	-1.143881	-0.000009	H	3.131205	-1.209518	0.884297
H	-4.099985	-0.888456	0.000792	H	2.371780	-2.559587	-0.000813
H	-2.808877	-1.738391	-0.893938	O	-2.438774	0.525369	0.000136
H	-2.807701	-1.739007	0.893206	C	-3.319558	-0.590306	-0.000113
				H	-4.334278	-0.180932	0.001331
	TSIIbF			H	-3.181877	-1.209677	-0.894783
C	-1.551217	-0.462203	0.142511	H	-3.180086	-1.211447	0.893045
C	0.976432	0.008713	0.070706				
N	0.521106	-0.871893	1.048168		**TSIIaF**		
N	-0.739786	-1.129833	1.076454	C	-1.107032	0.252609	0.073482
C	-2.953726	-1.035570	0.096292	C	1.283878	-0.684175	0.119946
H	-3.452078	-0.743263	-0.831757	N	0.386807	-1.160222	1.095124
H	-2.922627	-2.128422	0.158872	N	-0.813793	-0.702352	1.049385
H	-3.541611	-0.658481	0.939025	P	-0.069398	1.808019	0.009363

P	-1.458991	1.411736	0.083054
C	0.329114	1.439038	0.027509
O	1.096966	2.404220	-0.023248
N	-0.788910	-0.956876	-1.355920
N	0.375604	-0.747653	-1.395833
O	2.340656	0.076233	-0.047924
C	3.036527	-1.145382	0.145345
H	4.067815	-0.957646	-0.169343
H	3.021796	-1.465816	1.192204
H	2.611718	-1.949826	-0.469689

IIIbF

N	0.506666	-1.266697	-0.000019
C	1.014640	-0.068314	-0.000022
C	-1.714495	-0.545741	0.000024
N	-0.834458	-1.533065	-0.000105
P	-1.458004	1.219438	0.000327
C	0.353200	1.260994	-0.000134
O	1.018237	2.310853	-0.000365
C	-3.156264	-1.030738	-0.000176
H	-3.702373	-0.670922	0.880520
H	-3.701674	-0.672466	-0.881969
H	-3.164423	-2.124761	0.000697
C	1.456176	0.877925	0.056423
O	2.621460	1.303090	0.051341
N	-0.616936	-0.662126	-1.385222
N	0.504662	-1.047448	-1.333660
C	2.598154	-1.431005	0.125297
H	3.143228	-1.231327	-0.799478
H	3.216158	-1.084193	0.956654
H	2.421402	-2.505765	0.225504
O	-2.449679	0.520358	-0.075193
C	-3.332981	-0.571924	0.144805
H	-3.396594	-0.842097	1.203938
H	-4.313133	-0.242575	-0.213577
H	-3.018703	-1.457460	-0.421777

IIIaF

N	0.409404	1.572496	0.000324
C	1.439757	0.761559	0.000053
C	-1.170186	-0.145871	0.000028
N	-0.883760	1.138018	0.000152
P	-0.130330	-1.594455	0.000513
C	1.457199	-0.717926	-0.000203
O	2.551600	-1.321612	-0.000645
C	2.797772	1.421778	0.000013

O	2.386302	0.031108	0.000046	H	3.381973	1.109620	0.873872
C	3.101917	-1.190771	0.000118	H	3.381611	1.110235	-0.874307
H	2.870918	-1.799867	-0.882160	H	2.679651	2.508318	0.000405
H	4.161090	-0.913653	0.000193	O	-2.516835	-0.456492	-0.000343
H	2.870783	-1.799844	0.882376	C	-3.427370	0.633472	-0.000273
				H	-3.301847	1.270356	-0.883093
	IG			H	-4.424803	0.181581	-0.000675
N	0.979009	1.191098	-0.002755	H	-3.302302	1.269861	0.882959
C	0.342701	0.003171	-0.001881				
C	2.927619	0.003542	0.000114		**TSIaG**		
N	2.298166	1.191449	-0.001741	C	-0.102403	-0.266325	0.000359
C	4.425431	-0.002268	0.004563	C	2.343111	-0.838516	0.001416
H	4.801421	-0.509391	0.898571	C	2.225836	1.406122	-0.002395
H	4.806869	-0.549615	-0.862681	N	0.397919	-0.934478	1.184500
H	4.800355	1.021410	-0.016160	N	1.653974	-1.143785	1.176938
C	-1.134081	0.000793	-0.000705	N	1.654066	-1.147624	-1.173153
C	-1.840391	-1.213118	-0.000043	N	0.398011	-0.938291	-1.181510
C	-1.843351	1.213008	-0.000045	P	0.541516	1.661715	-0.002738
C	-3.232662	-1.210571	0.001268	O	3.355277	1.800425	-0.003053
C	-3.235486	1.207191	0.001244	C	3.821387	-1.091781	0.001881
C	-3.933760	-0.002574	0.001905	H	4.102775	-1.655862	0.896533
N	2.296368	-1.187409	-0.001818	H	4.102798	-1.659070	-0.890733
N	0.981343	-1.187994	-0.002756	H	4.377580	-0.145325	0.000189

H	-1.287730	-2.145320	-0.000598
H	-3.771831	-2.153066	0.001781
H	-5.019845	-0.003860	0.002920
H	-3.776917	2.148389	0.001729
H	-1.292641	2.146399	-0.000591

TSIbG

C	2.490200	-0.489326	-0.000075
C	-0.017182	-0.419880	-0.000077
C	0.625037	1.578453	0.000195
N	1.828203	-1.035316	-1.188141
N	0.567847	-0.930608	-1.180618
N	0.567840	-0.930985	1.180306
N	1.828195	-1.035730	1.187798
C	3.964777	-0.862634	-0.000148
H	4.458404	-0.464987	0.890861
H	4.068383	-1.952976	0.000011
H	4.458232	-0.465252	-0.891369
P	2.348036	1.462034	0.000332
O	-0.322488	2.308269	0.000138
C	-1.495808	-0.340600	-0.000048
C	-2.211603	-0.272438	1.205558
C	-2.211625	-0.271902	-1.205612
C	-1.609050	-0.171544	0.000374
C	-2.319497	-0.107614	1.206254
C	-2.319654	-0.114291	-1.205764
C	-3.709843	0.009544	1.205318
H	-1.765176	-0.165969	2.136230
C	-3.710001	0.002916	-1.205345
H	-1.765335	-0.177801	-2.135416
C	-4.412531	0.065600	-0.000135
H	-4.246507	0.056574	2.150300
H	-4.246784	0.044721	-2.150506
H	-5.496227	0.158188	-0.000316

IIaG

C	0.119550	-0.149455	-0.000050
C	-2.354520	-0.594416	-0.000337
C	-2.281506	1.034395	0.000660
N	-0.404659	-0.860331	-1.191040
N	-1.631115	-1.084179	-1.190213
N	-1.631153	-1.085734	1.188802
N	-0.404669	-0.861851	1.189958
P	-0.612487	1.652991	0.001007
O	-3.368989	1.615036	0.001081
C	1.625764	-0.122216	-0.000066

C	-3.601020	-0.163575	1.204537	C	2.339409	-0.085961	-1.205711
H	-1.659654	-0.319967	2.137945	C	2.339447	-0.087924	1.205615
C	-3.601041	-0.163080	-1.204525	C	3.732945	-0.018995	-1.204906
H	-1.659692	-0.318987	-2.138032	C	3.732987	-0.020966	1.204878
C	-4.306314	-0.110270	0.000025	C	4.437685	0.013647	0.000002
H	-4.136594	-0.116994	2.150337	C	-3.787286	-1.085753	-0.000709
H	-4.136631	-0.116113	-2.150297	H	-4.306447	-0.711108	0.883184
H	-5.390220	-0.021405	0.000056	H	-4.306188	-0.710423	-0.884465
				H	-3.812434	-2.179644	-0.001153
	IIbG			H	1.787317	-0.123548	2.137979
C	-2.507762	-0.482490	0.000394	H	4.270113	0.004669	2.150307
C	-0.010331	-0.203171	0.000123	H	5.523888	0.067284	0.000022
C	-0.583682	1.385341	-0.001183	H	4.270045	0.008193	-2.150308
N	-1.800708	-1.010805	1.189788	H	1.787247	-0.120062	-2.138115
N	-0.560864	-0.865266	1.191170				
N	-0.560784	-0.867422	-1.189580		**TSIIaG**		
N	-1.800659	-1.012954	-1.187999	C	-0.149364	-0.086650	0.162887
C	-3.951550	-0.953810	0.000801	C	2.383269	-0.572483	-0.117577
H	-4.466861	-0.583149	-0.889123	N	1.615016	-1.498346	0.620167
H	-3.996617	-2.048787	0.001554	N	0.358863	-1.267488	0.724250
H	-4.466784	-0.581944	0.890272	P	0.663905	1.527931	0.653818
P	-2.358127	1.436380	-0.001260	C	2.318147	0.908136	0.384330
O	0.275310	2.256909	-0.001983	O	3.401736	1.489578	0.548186

C	1.493278	-0.227421	0.000173	N	0.437145	-0.325184	-1.565506
C	2.206735	-0.212369	1.204683	N	1.602413	-0.518525	-1.614780
C	2.206794	-0.215517	-1.204335	C	3.790677	-1.061206	-0.371763
C	3.601407	-0.200564	1.204994	H	4.386009	-0.945808	0.536856
C	3.601468	-0.203704	-1.204613	H	3.778546	-2.113455	-0.669131
C	4.306832	-0.197678	0.000203	H	4.258427	-0.460364	-1.154110
H	1.654425	-0.221798	2.137700	C	-1.645577	-0.064013	0.085990
H	4.139112	-0.191235	2.150455	C	-2.428019	-1.062074	0.686985
H	5.394397	-0.186389	0.000219	C	-2.296338	0.963864	-0.613857
H	4.139217	-0.196848	-2.150070	C	-3.819482	-1.023301	0.602465
H	1.654513	-0.227398	-2.137342	H	-1.920309	-1.859692	1.217044
				C	-3.687516	0.998442	-0.702812
	TSIIbG			H	-1.694265	1.734601	-1.084777
C	-2.544225	-0.484378	-0.034331	C	-4.457743	0.006123	-0.092936
C	0.022941	-0.104627	0.135008	H	-4.408911	-1.801990	1.081744
N	-0.522005	-1.213141	0.793164	H	-4.171471	1.803168	-1.251405
N	-1.784780	-1.414825	0.702186	H	-5.542877	0.033719	-0.160167
C	-3.947786	-0.986897	-0.305432				
H	-3.926945	-2.039725	-0.605106		**IIIaG**		
H	-4.555999	-0.898729	0.599933	N	-1.754435	1.598902	-0.156986
H	-4.415960	-0.396747	-1.097510	C	-2.683637	0.669492	-0.064930
P	-2.407115	1.309255	0.464194	C	0.059633	0.108187	-0.022218
C	-0.618603	1.291786	0.472339	N	-0.427093	1.343113	-0.151994

O	0.144230	2.238426	0.712589	P	-0.825202	-1.424977	0.166463
N	-1.724270	-0.552811	-1.583920	C	-2.518335	-0.785983	0.066210
N	-0.561612	-0.357712	-1.543225	O	-3.518542	-1.531550	0.126694
C	1.520099	-0.143246	0.062364	C	-4.110332	1.160267	-0.095308
C	2.254637	-1.143720	0.713860	H	-4.656466	0.713540	-0.934823
C	2.215425	0.813944	-0.692574	H	-4.647148	0.847155	0.808075
C	3.646010	-1.185413	0.617884	H	-4.124493	2.249531	-0.179910
H	1.712402	-1.884205	1.290378	C	1.560312	0.069790	-0.019158
C	3.604916	0.766885	-0.793901	C	2.279167	-1.116660	-0.246531
H	1.657369	1.598326	-1.187659	C	2.297740	1.245849	0.213588
C	4.328974	-0.231052	-0.137712	C	3.673694	-1.131024	-0.230477
H	4.197392	-1.969259	1.132786	C	3.690629	1.232232	0.226821
H	4.125458	1.517535	-1.384129	C	4.390763	0.043050	0.006959
H	5.413505	-0.263692	-0.214793	H	1.732158	-2.033577	-0.443646
				H	4.201939	-2.064553	-0.411801
	IIIbG			H	5.478263	0.032261	0.017856
N	-0.613135	-1.274831	0.000142	H	4.234862	2.156066	0.412464
C	-0.054954	-0.066089	0.000026	H	1.740144	2.161339	0.374405
C	-2.840813	-0.582368	0.000077				
N	-1.919773	-1.554001	0.000151				
P	-2.604196	1.154945	-0.000044				
C	-0.782906	1.221138	-0.000112				
O	-0.228278	2.341532	-0.000275				

C	-4.263078	-1.115714	0.000047
H	-4.998588	-0.305433	0.000026
H	-4.435239	-1.745469	-0.881123
H	-4.435259	-1.745504	0.881185
C	1.444846	-0.116759	0.000005
C	2.261456	1.033039	0.000238
C	2.096483	-1.370643	-0.000240
C	3.654484	0.925169	0.000267
C	3.483264	-1.470543	-0.000226
C	4.279572	-0.320531	0.000036
H	1.775631	1.999098	0.000339
H	4.254531	1.833307	0.000470
H	5.364824	-0.398111	0.000044
H	3.948624	-2.454636	-0.000434
H	1.474863	-2.258053	-0.000409

Table S?. Cartesian coordinates for all optimized species at B3LYP/6-311G(d,p) level of theory

IB				**TSIB**			
N	-0.660923	1.188152	0.000046	C	-1.358468	-0.250223	0.000017
C	-1.286965	0.005539	0.000006	C	1.074835	-0.850255	-0.000023
C	1.286965	0.005541	0.000014	C	0.952909	1.407423	0.000001

N	0.660925	1.188153	0.000049
N	0.656434	-1.183648	0.000049
N	-0.656436	-1.183649	0.000047
C	2.783590	-0.003282	-0.000070
H	3.159506	1.018452	0.000213
H	3.158294	-0.532057	0.879647
H	3.158185	-0.531486	-0.880184
C	-2.783592	-0.003279	-0.000068
H	-3.158198	-0.531479	-0.880179
H	-3.158289	-0.532064	0.879647
H	-3.159493	1.018458	0.000229

IIB

C	-1.383911	-0.175980	0.000052
C	1.091559	-0.574855	0.000002
C	0.980965	1.049525	0.000011
N	-0.848364	-0.883899	1.188746
N	0.377037	-1.083352	1.190171
N	0.376990	-1.083293	-1.190215
N	-0.848396	-0.883870	-1.188791
C	-2.899137	-0.236775	0.000034
H	-3.293098	0.259430	-0.889230
H	-3.235458	-1.278660	-0.000140
N	-0.865986	-0.929643	1.181280
N	0.385111	-1.149081	1.173634
N	0.385053	-1.149176	-1.173623
N	-0.866043	-0.929723	-1.181215
C	-2.876867	-0.197398	0.000046
H	-3.239831	0.318837	-0.891572
H	-3.271015	-1.217649	0.000073
H	-3.239795	0.318868	0.891662
P	-0.729139	1.649479	-0.000072
O	2.073996	1.801310	0.000041
C	2.551223	-1.104279	-0.000024
H	2.828230	-1.669783	-0.893692
H	3.110565	-0.161228	0.000105
H	2.828235	-1.669960	0.893537

TSIIB

C	1.416367	-0.103712	-0.141760
C	-1.134409	-0.522392	-0.139943
N	-0.374721	-1.141750	-1.142507
N	0.890949	-0.950077	-1.129234
C	2.923188	-0.197825	-0.046828
H	3.245174	-1.231180	-0.202745
H	3.389309	0.428732	-0.812289

H	-3.293065	0.259130	0.889479
P	-0.701962	1.622951	-0.000017
O	2.046491	1.659059	0.000038
C	2.530952	-1.039989	-0.000012
H	3.042348	-0.658094	-0.883904
H	3.042807	-0.656759	0.883040
H	2.570549	-2.132453	0.000804

IIIB

N	-0.364302	1.607357	-0.000133
C	-1.225608	0.618343	-0.000009
C	1.536381	0.241137	0.000052
N	0.982348	1.444283	-0.000092
C	3.056512	0.281807	0.000066
H	3.377266	1.325844	0.001159
H	3.469982	-0.220701	0.881010
H	3.469865	-0.218622	-0.882141
P	0.766268	-1.357220	0.000037
C	-0.965430	-0.832433	-0.000032
O	-1.912428	-1.641267	-0.000110
C	-2.682434	1.014342	0.000133
H	-3.197016	0.599080	-0.873010
H	-3.196750	0.599453	0.873632
H	3.261943	0.142385	0.934029
C	-2.560790	-1.010145	-0.093919
H	-2.985470	-0.828617	0.894742
H	-3.160934	-0.455461	-0.817619
H	-2.597496	-2.077285	-0.323773
P	0.697946	1.612987	-0.003283
C	-0.988160	1.024940	-0.016232
O	-2.032332	1.684156	0.053699
N	0.801605	-0.928896	1.322993
N	-0.360722	-1.092395	1.317234

H -2.760798 2.102729 -0.000015

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