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Facile Phenylphosphinidene Transfer Reactions from Carbene-Phosphinidene Zinc Complexes

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DOI

[10.1002/anie.201703672](https://doi.org/10.1002/anie.201703672)

[10.1002/ange.201703672](https://doi.org/10.1002/ange.201703672)

Publication date

2017

Document Version

Other version

Published in

Angewandte Chemie, International Edition

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Citation for published version (APA):

Krachko, T., Bispinghoff, M., Tondreau, A. M., Stein, D., Baker, M., Ehlers, A. W., Slootweg, J. C., & Grutzmacher, H. (2017). Facile Phenylphosphinidene Transfer Reactions from Carbene-Phosphinidene Zinc Complexes. *Angewandte Chemie, International Edition*, 56(27), 7948-7951. <https://doi.org/10.1002/anie.201703672>, <https://doi.org/10.1002/ange.201703672>

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Supporting Information

Facile Phenylphosphinidene Transfer Reactions from Carbene–Phosphinidene Zinc Complexes

Tetiana Krachko, Mark Bispinghoff, Aaron M. Tondreau, Daniel Stein, Matthew Baker, Andreas W. Ehlers, J. Chris Slootweg, and Hansjörg Grützmacher**

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Supporting Information

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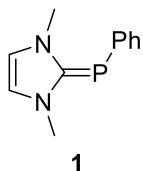
1. Synthetic procedures

All syntheses were carried out under an atmosphere of dry argon employing standard Schlenk-line and glovebox techniques. Solvents were purified using an Innovative Technology PureSolv MD 7 solvent purification system. Deuterated solvents were purchased from Cambridge Isotope Laboratories. THF-*d*₈ and C₆D₆ were distilled from sodium benzophenone, whereas CD₂Cl₂ was dried over 4 Å molecular sieves before use. All reagents were used as received from commercial suppliers unless otherwise stated. The compounds 1,3-dimethylimidazolium iodide,^[1] [DippNHC-H]-[Cl],^[2] diphenylketene^[3] and (PPh)₅^[4] were synthesized according to literature procedures. Zinc chloride was dried by refluxing in thionyl chloride.^[5]

¹H and ¹³C{¹H} NMR spectra were recorded on Bruker Avance 300 or Bruker Avance 500 spectrometers and internally referenced to the residual proton resonances (for CDCl₃, ¹H at δ = 7.26, ¹³C{¹H} at δ = 77.16; for CD₂Cl₂, ¹H at δ = 5.32, ¹³C{¹H} at δ = 53.84; for THF-*d*₈, ¹H at δ = 3.58, 1.72, ¹³C{¹H} at δ = 67.21, 25.31; for C₆D₆, ¹H at δ = 7.16, ¹³C{¹H} at δ = 128.06; for DMF-*d*₇, ¹H at δ = 8.03, 2.92, 2.75, ¹³C{¹H} at δ = 163.15, 34.89, 29.76).^[6] ³¹P{¹H} spectra were recorded on a Bruker Avance 300 or Bruker Avance 250 and externally referenced (85% H₃PO₄). The ¹H and ¹³C resonance signals were assigned by means of 2D HSQC and HMBC experiments. Melting points were measured on samples in sealed capillaries on a Büchi M-560 melting point apparatus and are uncorrected. Elemental analyses were performed at the microanalysis laboratory of ETH Zürich.

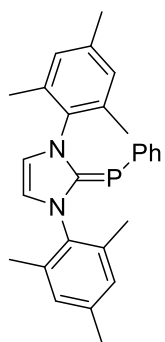
Synthesis of the adduct ^{Me}NHC=PPh (**1**):

A 50 mL round bottom flask was charged with (PPh)₅ (1.00 g, 1.85 mmol, 1.0 eq) and NaOtBu (0.900 g, 9.36 mmol, 5.1 eq) and both were dissolved in THF (20 mL). To the stirring solution, 1,3-dimethylimidazolium iodide ([^{Me}NHC-H]-[I]) (2.07 g, 9.24 mmol, 5.0 eq) was added over the course of 10 minutes, causing the initially pale yellow solution to turn bright orange. The reaction was allowed to stir at 20 °C for 60 minutes. All volatiles were removed under reduced pressure and the residue was extracted into toluene, filtered over Celite, and the solution was concentrated to roughly 10% of the original volume. *n*-hexane (30 mL) was added and the orange precipitate was collected on a glass frit and dried under reduced pressure, yielding 1.80 g of ^{Me}NHC=PPh (95%) as an orange powder.



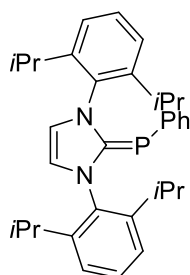
Analysis for C₁₁H₁₃N₂P₁: Calculated: C = 64.70%, H = 6.42%, N = 13.72%. Found: C = 64.0%, H = 6.2%, N = 12.9%. **MP:** 185 °C. **¹H NMR (300.1 MHz, C₆D₆, 293 K):** δ = 7.63 (ddd, ³J_{H,H} = 7.0 Hz, ⁴J_{H,H} = 1.2 Hz, ³J_{H,P} = 5.9 Hz, 2H; *o*-PhH), 7.09 (td, ³J_{H,H} = 7.4 Hz, ⁴J_{H,P} = 2.0 Hz, 2H; *m*-PhH), 6.95 (tt, ³J_{H,H} = 7.3 Hz, ⁴J_{H,H} = ⁵J_{H,P} = 1.2 Hz, 1H; *p*-PhH), 5.64 (s, 2H; NCH), 2.83 (d, ⁴J_{H,P} = 0.8 Hz, 6H; NCH₃). **¹³C{¹H} NMR (75.5 MHz, C₆D₆, 293 K):** δ = 170.1 (d, ¹J_{C,P} = 99.6 Hz; NCN), 147.0 (d, ¹J_{C,P} = 46.5 Hz; *ipso*-PhC), 133.4 (d, ²J_{C,P} = 17.8 Hz; *o*-PhC), 127.5 (d, ³J_{C,P} = 5.3 Hz; *m*-PhC), 122.9 (s; *p*-PhC), 119.0 (d, ³J_{C,P} = 3.2 Hz; NCH), 36.2 (d, ³J_{C,P} = 9.8 Hz; NCH₃). **³¹P{¹H} NMR (121.5 MHz, C₆D₆, 293 K):** δ = -49.1 (s).

Synthesis of the adduct ^{Mes}NHC=PPh:



A 50 mL round bottom flask was charged with (PPh)₅ (1.00 g, 1.85 mmol, 1.0 eq) and NaOtBu (0.900 g, 9.36 mmol, 5.1 eq) and both were dissolved in THF (20 mL). To the stirring solution, [^{Mes}NHC-H]-[Cl] (3.15 g, 9.24 mmol, 5.0 eq) was added over the course of 10 minutes, causing the initially pale yellow solution to turn bright orange. The reaction was allowed to stir at 20 °C for 60 minutes. All volatiles were removed under reduced pressure and the residue was extracted into toluene, filtered over Celite, and the solution was concentrated to roughly 10% of the original volume. *n*-hexane (30 mL) was added and the orange precipitate was collected on a glass frit and dried under reduced pressure, yielding 3.54 g of ^{Mes}NHC=PPh (93%) as an orange powder. This sample was spectroscopically identical to a previously reported sample.^[7]

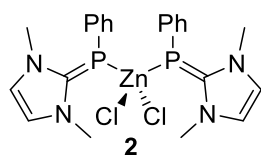
Synthesis of the adduct ^{Dipp}NHC=PPh:



A 50 mL round bottom flask was charged with (PPh)₅ (1.00 g, 1.85 mmol, 1.0 eq) and NaOtBu (0.900 g, 9.36 mmol, 5.1 eq) and both were dissolved in THF (20 mL). To the stirring solution, [^{Dipp}NHC-H]-[Cl] (3.93 g, 9.24 mmol, 5.0 eq) was added over the course of 10 minutes, causing the initially pale yellow solution to turn bright orange. The reaction was allowed to stir at 20 °C for 60 minutes. All volatiles were removed under reduced pressure and the residue was extracted into toluene, filtered over Celite, and the solution was concentrated to roughly 10% of the original volume. *n*-hexane (30 mL) was added and the orange precipitate was collected on a glass frit and dried under reduced pressure, yielding 3.99 g of ^{Dipp}NHC=PPh (87%) as an orange powder. This sample was spectroscopically identical to a previously reported sample.^[8]

- Synthesis of ZnCl₂ complexes

Synthesis of bis(phosphinidene) zinc complex 2:

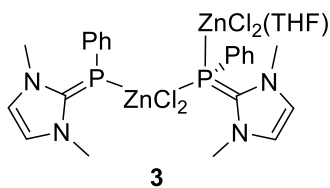


A solution of ZnCl₂ (0.066 g, 0.484 mmol, 1.0 eq) in THF (2 mL) was added dropwise to a solution of ^{Me}NHC=PPh (0.200 g, 0.980 mmol, 2.0 eq) in THF (1 mL) and the reaction mixture was allowed to stir for 10 min. Next, the pale yellow precipitate was collected on a glass frit, washed with THF (2 mL) and dried *in vacuo* to give [(^{Me}NHC=PPh)₂ZnCl₂] (**2**) as a pale yellow solid (0.200 g, 0.366 mmol, 76%). Single crystals suitable for X-ray crystallography were obtained from the reaction mixture in DME at 20 °C.

MP: >200 °C (decomposition). Due to the poor solubility of **2** in common organic solvents its structure is only evidenced from X-ray crystallographic data (Scheme 2).

Synthesis of the phosphinidene zinc complex **3**:

A solution of $^{\text{Me}}\text{NHC}=\text{PPh}$ (1.00 g, 4.90 mmol, 1.0 eq) in DME (10 mL) was added dropwise to a suspension of ZnCl_2 (0.734 g, 5.35 mmol, 1.1 eq) in DME (60 mL). Upon vigorous stirring for 15 minutes, the initially yellow suspension turned colorless. Next, this suspension was filtered through a teflon cannula equipped with a glassfiber filter to remove the excess ZnCl_2 and the solution was left standing at 20 °C. The product that precipitated overnight was collected on a glass frit and dried under reduced pressure to yield **3** as a white powder (1.21 g). The filtrate was concentrated to roughly 10% of the original volume and cooled to -35 °C overnight. Collection of the precipitate on a glass frit and subsequent drying under reduced pressure afforded a second batch of **3** (0.250 g). Combined yield 87% (n=1, 1.46 g, 4.29 mmol). Single crystals suitable for X-ray crystallography were obtained from a saturated THF solution at -35 °C. One THF molecule completes Zn four-coordination in the crystal structure, however after drying *in vacuo* complex **3** does not contain any solvent coordinated; the following analyses were performed on the solvent-free product $\{^{\text{Me}}\text{NHC}=\text{PPhZnCl}_2\}_n$, which is used in the synthesis of **4** and **10**:



Analysis for $\text{C}_{11}\text{H}_{13}\text{Cl}_2\text{N}_2\text{P}_1\text{Zn}_1$: Calculated: C = 38.8%, H = 3.9%, N = 8.2%. Found: C = 38.3%, H = 3.9%, N = 7.9%. **MP:** >147 °C (decomposition). **^1H NMR (300.1 MHz, THF- d_8 , 293K):** δ = 7.54 (ddd, $^3J_{\text{H,H}} = 6.6$ Hz, $^4J_{\text{H,H}} = 1.4$ Hz, $^3J_{\text{H,P}} = 7.4$ Hz, 2H; *o*-PhH), 7.38 (s, 2H; NCH), 7.16 (td, $^3J_{\text{H,H}} = 7.1$ Hz, $^4J_{\text{H,P}} = 1.8$ Hz, 2H; *m*-PhH), 7.12 (td, $^3J_{\text{H,H}} = 7.0$ Hz, $^4J_{\text{H,H}} = 1.4$ Hz, 1H; *p*-PhH), 3.60 (s, 6H; NCH₃). **$^{13}\text{C}\{^1\text{H}\}$ NMR (75.5 MHz, THF- d_8 , 293 K):** δ = 156.9 (d, $^1J_{\text{C,P}} = 67.7$ Hz; NCN), 136.6 (d, $^1J_{\text{C,P}} = 18.0$ Hz; *ipso*-PhC), 134.7 (d, $^2J_{\text{C,P}} = 14.2$ Hz; *o*-PhC), 128.9 (d, $^3J_{\text{C,P}} = 5.0$ Hz, *m*-PhC), 126.9 (s; *p*-PhC), 124.2 (d, $^3J_{\text{C,P}} = 1.5$ Hz; NCH), 37.6 (d, $^3J_{\text{C,P}} = 8.0$ Hz; NCH₃). **$^{31}\text{P}\{^1\text{H}\}$ NMR (121.5 MHz, THF- d_8 , 293 K):** δ = -88.1 (s).

Reaction of **2** with ZnCl_2

In an NMR tube, ZnCl_2 powder (0.004 g, 0.029 mmol, 1.1 eq) was slowly added to a yellow suspension of **2** (0.015 g, 0.027 mmol, 1.0 eq) in THF (0.6 mL) at 20 °C. The resulting colorless solution was analyzed by $^{31}\text{P}\{^1\text{H}\}$ NMR spectroscopy, indicating the formation of **3**.

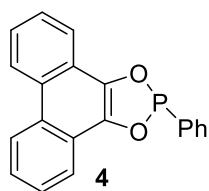
- **Reactions of the phosphinidene zinc complex **3** with organic electrophiles**

Addition of organic electrophiles was performed to both in situ prepared $^{\text{Me}}\text{NHC}=\text{PPh-ZnCl}_2$ complex and isolated compound **3**. Both methods lead to the same products, meanwhile requiring different amounts of solvent. Herein we report the optimal procedures for each electrophile.

Reaction of the phosphinidene zinc complex **3** with 9,10-phenanthrenequinone

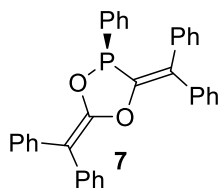
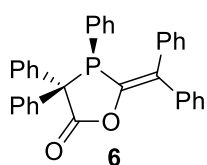
A solution of 9,10-phenanthrenequinone (0.320 g, 1.54 mmol, 1.05 eq.) in THF (15 mL) was added dropwise to a solution of **3** (n=1, 0.500 mg, 1.47 mmol, 1.0 eq) in THF (25 mL) at -78 °C to give a green solution and a small amount of a yellow precipitate. The reaction mixture was stirred for 10 min, the precipitate filtered off and the filtrate evaporated to dryness. Extraction into toluene (3 x 10 mL) and recrystallization from toluene at 60 °C gave phosphonite **4**^[9] as a pale green crystalline solid in 46% yield (0.214 g, 0.677 mmol). Crystals

suitable for X-ray crystallography were obtained from a saturated toluene solution at 20 °C. The residue, which was insoluble in toluene, contained $[\text{MeNHC}\cdot\text{ZnCl}_2]_n$ together with some unidentified by-products.



Analysis for $\text{C}_{20}\text{H}_{13}\text{O}_2\text{P}$: Calculated: C = 76.0%, H = 4.1%, N = 0.0%. Found: C = 75.7%, H = 3.9%, N = 0.1%. **MP:** 142 °C. **$^1\text{H NMR}$ (300.1 MHz, C_6D_6 , 293 K):** δ = 8.32 (d, $^3J_{\text{H,H}}$ = 8.3 Hz, 2H; *o*- C_6H_4), 8.21 (dd, $^3J_{\text{H,H}}$ = 8.0 Hz, $^4J_{\text{H,H}}$ = 0.9 Hz, 2H; *o*- C_6H_4), 7.46 (t, $^3J_{\text{H,H}}$ = 6.6 Hz, 2H; *m*- C_6H_4), 7.37 (t, $^3J_{\text{H,H}}$ = 7.5 Hz, 2H; *m*- C_6H_4), 7.28 (ddd, $^3J_{\text{H,H}}$ = 6.6 Hz, $^4J_{\text{H,H}}$ = 1.4 Hz, $^3J_{\text{H,P}}$ = 7.9 Hz, 2H; *o*-PPhH), 6.87-6.70 (m, 3H; *m*-PPhH, *p*-PPhH). **$^{13}\text{C}\{^1\text{H}\}$ NMR (75.5 MHz, CD_2Cl_2 , 293 K):** δ = 142.4 (d, $^1J_{\text{C,P}}$ = 48.5 Hz; *ipso*-PPhC), 138.2 (d, $^2J_{\text{C,P}}$ = 6.8 Hz; *ipso*-phenanthreneOC), 131.9 (s; *p*-PPhC), 128.9 (d, $^3J_{\text{C,P}}$ = 6.5 Hz; *m*-PPhC), 128.7 (d, $^2J_{\text{C,P}}$ = 23.4 Hz; *o*-PPhC), 128.2 (s; *ipso*-phenanthreneC), 127.7 (s; *m*- C_6H_4), 125.9 (s; *m*- C_6H_4), 123.7 (s; *ipso*-phenanthreneC), 123.6 (s; *o*- C_6H_4), 121.2 (s; *o*- C_6H_4). **$^{31}\text{P}\{^1\text{H}\}$ NMR (121.5 MHz, C_6D_6 , 293 K):** δ = 183.3 (s).

Reaction of the phosphinidene zinc complex 3 with 2 equivalents of diphenylketene

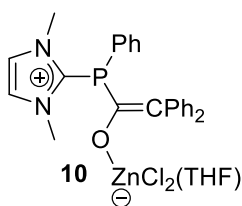


To a stirring solution of $\text{MeNHC}=\text{PPh}$ (0.100 g, 0.490 mmol, 1.0 eq) in THF (4 mL), ZnCl_2 (0.070 g, 0.514 mmol, 1.05 eq) was added over the course of 5 minutes as a solid at 20 °C. The resulting colorless solution was stirred for 5 minutes after which diphenylketene (0.200 g, 1.03 mmol, 2.1 eq) in THF (6 mL) was added dropwise. The reaction mixture was stirred for 10 min and the volatiles removed under reduced pressure. The residue was extracted into refluxing *n*-hexane (2 x 20 mL), giving a mixture of **6** and **7** in approximately 2:3 ratio (determined by the integration of the signals in the $^{31}\text{P}\{^1\text{H}\}$ NMR spectra). The ^{13}C and ^{31}P NMR signals of the heterocycle **7** correspond to literature values,^[10] while heterocycle **6** was identical to the one obtained in the reaction of $\text{MeNHC}=\text{PPh}$ with diphenylketene without ZnCl_2 (see below). The residue, which was insoluble in *n*-hexane, contained $[\text{MeNHC}\cdot\text{ZnCl}_2]_n$.

6: $^{31}\text{P}\{^1\text{H}\}$ NMR (121.5 MHz, $\text{THF-}d_8$, 293 K): δ = -2.6 (s).

7: $^{31}\text{P}\{^1\text{H}\}$ NMR (121.5 MHz, $\text{THF-}d_8$, 293 K): δ = 90.9 (s). $^{13}\text{C}\{^1\text{H}\}$ NMR (75.5 MHz, $\text{THF-}d_8$, 293 K): δ = 157.1 (d, $^2J_{\text{C,P}}$ = 11.9 Hz; OCO), 96.4 (s; $\text{Ph}_2\text{C}=\text{CO}_2$). From the mixture, these characteristic signals of **7** were identified; the other carbon signals overlap with the ones of **6**.

Reaction of the phosphinidene zinc complex 3 with 1 equivalent of diphenylketene



A solution of diphenylketene (0.120 g, 0.618 mmol, 1.05 eq) in THF (2 mL) was added dropwise to a stirring solution of **3** ($n=1$, 0.200 g, 0.587 mmol, 1.0 eq) in THF (10 mL) at 20 °C. The resulting pale yellow solution was evaporated to dryness and the crude product was washed with toluene (2 x 10 mL) and diethyl ether (2 x 5 mL) to give **10** as an off-white powder in 82% yield (0.300 g, 0.480 mmol). Due to its extreme sensitivity, compound **10** could not be obtained analytically pure. Based on $^{31}\text{P}\{^1\text{H}\}$ NMR spectroscopy, it

contained traces of **3**, and heterocycles **6** and **7** (Figure S1). Crystallization from DME at $-35\text{ }^{\circ}\text{C}$ afforded single crystals suitable for X-ray diffraction.

$^{31}\text{P}\{^1\text{H}\}$ NMR (121.5 MHz, THF, 293 K): $\delta = -16.6$ (s).

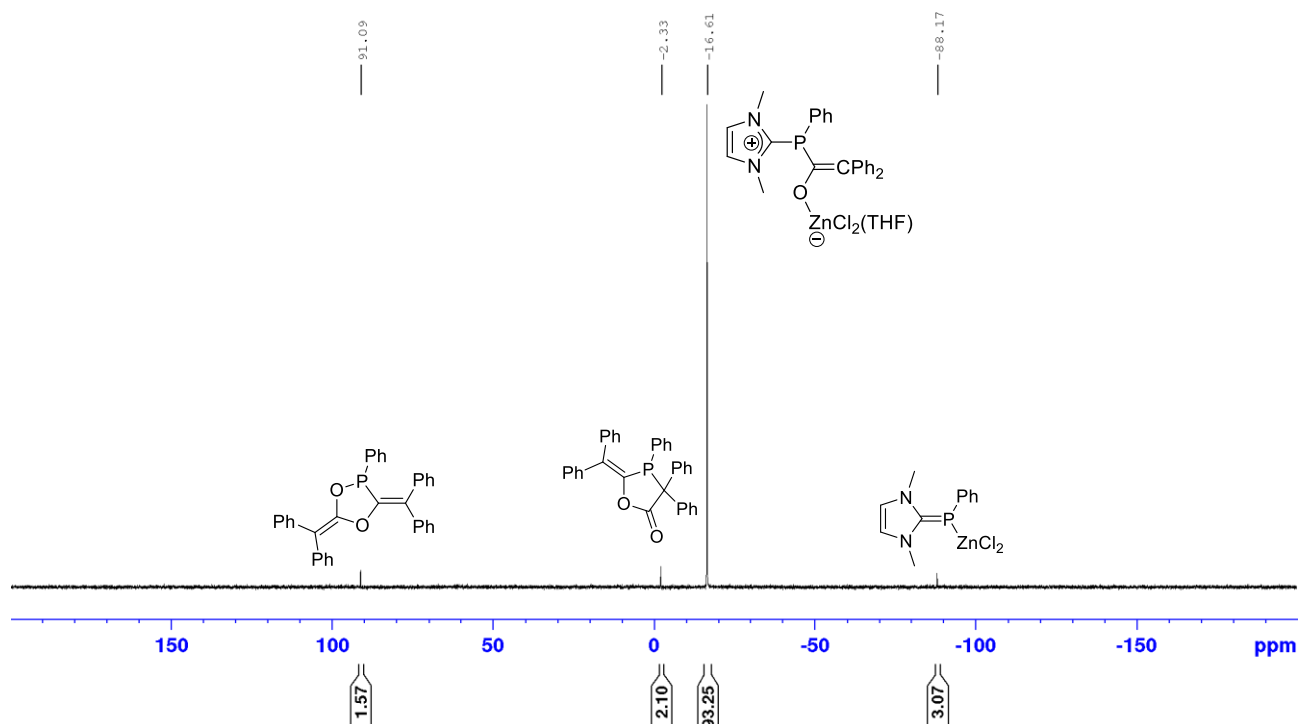


Figure S1. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **10** with structures of impurities.

Reaction of **10** with diphenylketene

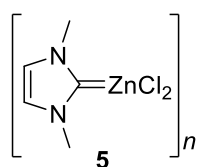
To a stirring solution of **10** (0.100 g, 0.160 mmol, 1.0 eq) in THF (2 mL) diphenylketene (0.034 g, 0.176 mmol, 1.1 eq) in THF (1 mL) was added at $20\text{ }^{\circ}\text{C}$. The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of the resulting yellow solution showed signals at -2.3 ppm and 91.1 ppm in a ratio of 2:3, corresponding to the heterocycles **6** and **7**, confirming the intermediacy of **10** in the formation of **6** and **7**.

Reaction of the phosphinidene zinc complex **3** with *trans*-chalcone

$[\text{MeNHC}\cdot\text{ZnCl}_2]_n$ (**5**)

To a stirring solution of $\text{MeNHC}=\text{PPh}$ (0.500 g, 2.45 mmol, 1.0 eq) in THF (7 mL), ZnCl_2 (0.350 g, 2.57 mmol, 1.05 eq) was added as a solid over the course of 5 minutes. After stirring the resulting colorless solution for 5 minutes, *trans*-chalcone (0.535 g, 2.57 mmol, 1.05 eq) was added as a solid over a period of 5 minutes. The reaction mixture was stirred for another 10 minutes before it was cooled to $-35\text{ }^{\circ}\text{C}$ overnight. The resulting precipitate was collected on a glass frit, washed with diethyl ether (3 x 5 mL) and dried under reduce pressure to give $[\text{MeNHC}\cdot\text{ZnCl}_2]_n$ as a white powder in 83% yield (0.470 g, 2.02 mmol). Crystallization from a saturated THF solution at $20\text{ }^{\circ}\text{C}$ afforded single crystals suitable for X-ray diffraction.

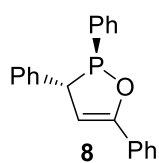
Analysis for $\text{C}_5\text{H}_8\text{Cl}_2\text{N}_2\text{Zn}$: Calculated: C = 25.8%, H = 3.5%, N = 12.1%. Found: C = 26.4%, H = 3.3%, N = 11.8%. **MP**: $>260\text{ }^{\circ}\text{C}$ (decomposition). ^1H NMR (300.1 MHz, $\text{DMF-}d_7$, 293K): $\delta =$



7.49 (s, 2H; NCH), 3.99 (s, 6H; NCH₃). ¹³C{¹H} NMR (75.5 MHz, DMF-*d*₇, 293 K): δ = 172.3 (s; NCN), 123.4 (s; NCH), 37.0 (s; NCH₃).

Oxo-3-phospholene 8:

After removal of [MeNHC·ZnCl₂]_{*n*}, the filtrate was evaporated to dryness and the residue was dissolved in diethyl ether (3 x 15 mL) and filtered over Celite. Removal of the solvent under reduced pressure and subsequent recrystallization from toluene at 60 °C afforded **8** as a white, crystalline solid in 80% yield (0.620 g, 1.96 mmol). Crystals suitable for X-ray crystallography were grown from a saturated toluene solution at 20 °C.



Analysis for C₂₁H₁₇OP: Calculated: C = 79.7%, H = 5.4%, N = 0.0%. Found: C = 78.8%, H = 5.2%, N = 0.1%. **MP:** 123–124 °C. ¹H NMR (300.1 MHz, C₆D₆, 293K): δ = 7.73 (dd, ³J_{H,H} = 8.2 Hz, ⁴J_{H,H} = 1.4 Hz, 2H; *o*-CH=C(PhH)), 7.51–7.16 (m, 2H; *o*-P(PhH)), 7.26–6.93 (m, 11H; PhH), 5.47 (dd, ³J_{H,P} = 8.8 Hz, ³J_{H,H} = 3.9 Hz, 1H; CH=CPh), 4.08 (dd, ³J_{H,H} = 3.4 Hz, ²J_{H,P} = 3.4 Hz, 1H; PCHPh). ¹³C{¹H} NMR (75.5 MHz, CD₂Cl₂, 293 K): δ = 159.5 (d, ²J_{C,P} = 12.6 Hz; CH=CPh), 143.1 (d, ¹J_{C,P} = 35.2 Hz; *ipso*-P(C₆H₅)), 142.5 (d, ²J_{C,P} = 18.9 Hz; *ipso*-PCH(C₆H₅)), 132.0 (s; *ipso*-CH=C(C₆H₅)), 129.9 (s; C_{Ph}H), 129.5 (s; C_{Ph}H), 129.3 (d, J_{C,P} = 1.7 Hz; C_{Ph}H), 129.1 (s; *p*-CH=C(C₆H₅)), 129.0 (s; C_{Ph}H), 128.0 (d, ²J_{C,P} = 8.7 Hz; *o*-P(C₆H₅)), 127.8 (d, ³J_{C,P} = 5.4 Hz; *o*-PCH(C₆H₅)), 127.2 (d, J_{C,P} = 2.6 Hz; C_{Ph}H), 126.1 (s; *o*-CH=C(C₆H₅)), 102.0 (s; CH=CPh), 59.4 (d, ¹J_{C,P} = 23.4 Hz; PCHPh). ³¹P{¹H} NMR (121.5 MHz, C₆D₆, 293 K): δ = 133.9 (s).

- **Screening of the reaction of different Lewis acids with MeNHC=PPh (1)**

Reaction of 1 with ZnCl₂:

In an NMR tube, ZnCl₂ powder (0.007 g, 0.051 mmol, 1.1 eq) was slowly added to an orange solution of **1** (0.010 g, 0.049 mmol, 1.0 eq) in THF (0.6 mL) at 20 °C. The resulting colorless solution was analyzed by ³¹P{¹H} NMR spectroscopy (Figure S2), indicating formation of **3**.

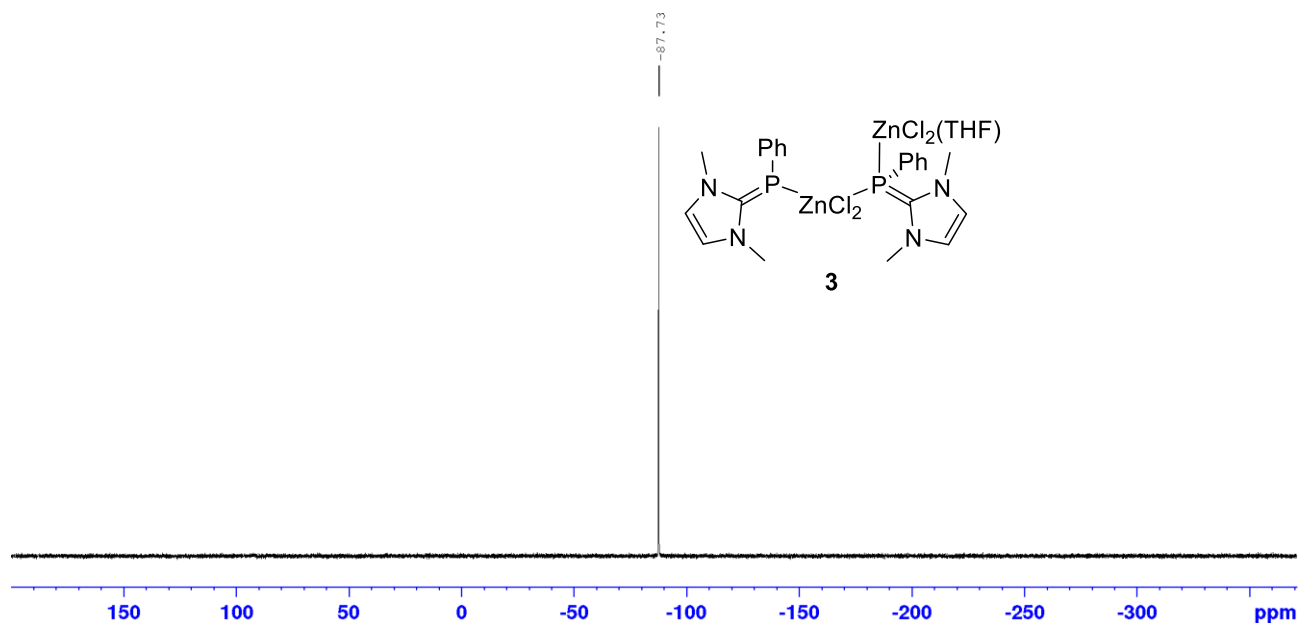


Figure S2. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum recorded directly after mixing $^{\text{Me}}\text{NHC}=\text{PPh}$ with ZnCl_2 in THF at RT.

Reaction of **1** with MgCl_2 :

In an NMR tube, MgCl_2 powder (0.005 g, 0.052 mmol, 1.1 eq) was slowly added to an orange solution of **1** (0.010 g, 0.049 mmol, 1.0 eq) in THF (0.6 mL) at 20 °C. The resulting yellow suspension was analyzed by $^{31}\text{P}\{^1\text{H}\}$ NMR spectroscopy. The obtained spectrum is presented in Figure S3.

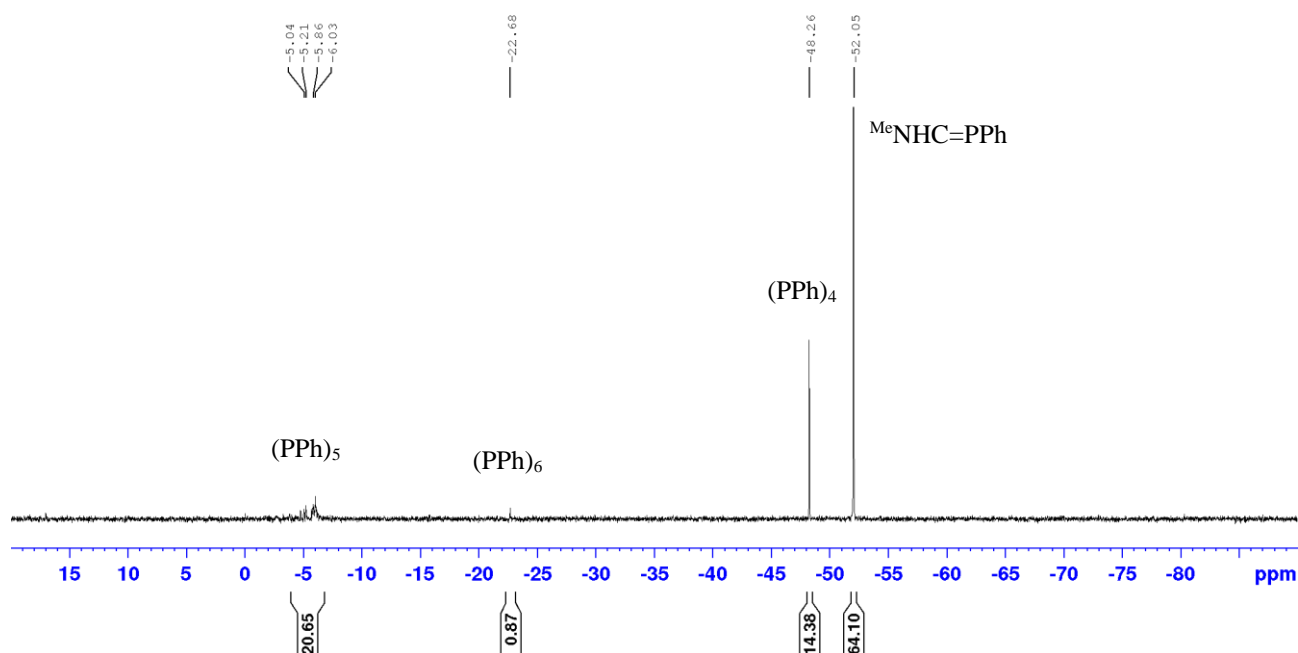


Figure S3. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum recorded directly after mixing $^{\text{Me}}\text{NHC}=\text{PPh}$ with MgCl_2 in THF at RT.

The main signal ($\delta = -52.05$ ppm) in the spectrum originates from unreacted $^{\text{Me}}\text{NHC}=\text{PPh}$, which is due to the poor solubility of MgCl_2 in THF. However, new products are also formed. The signals could be assigned by comparison with literature values^[11] to $(\text{PPh})_5$ (m , $\delta = -5$ to -6 ppm), $(\text{PPh})_6$ ($\delta = -22.7$ ppm), $(\text{PPh})_4$ ($\delta = -48.3$ ppm).

Reaction of **1** with AlCl₃:

In an NMR tube, AlCl₃ powder (0.014 g, 0.052 mmol, 1.1 eq) was slowly added to an orange solution of **1** (0.010 g, 0.049 mmol, 1.0 eq) in THF (0.6 mL) at 20 °C. The resulting colorless solution was analyzed by ³¹P{¹H} NMR spectroscopy (Figure S4), indicating the formation of (PPh)₅, (PPh)₆, (PPh)₄ and (PPh)₃^[12].

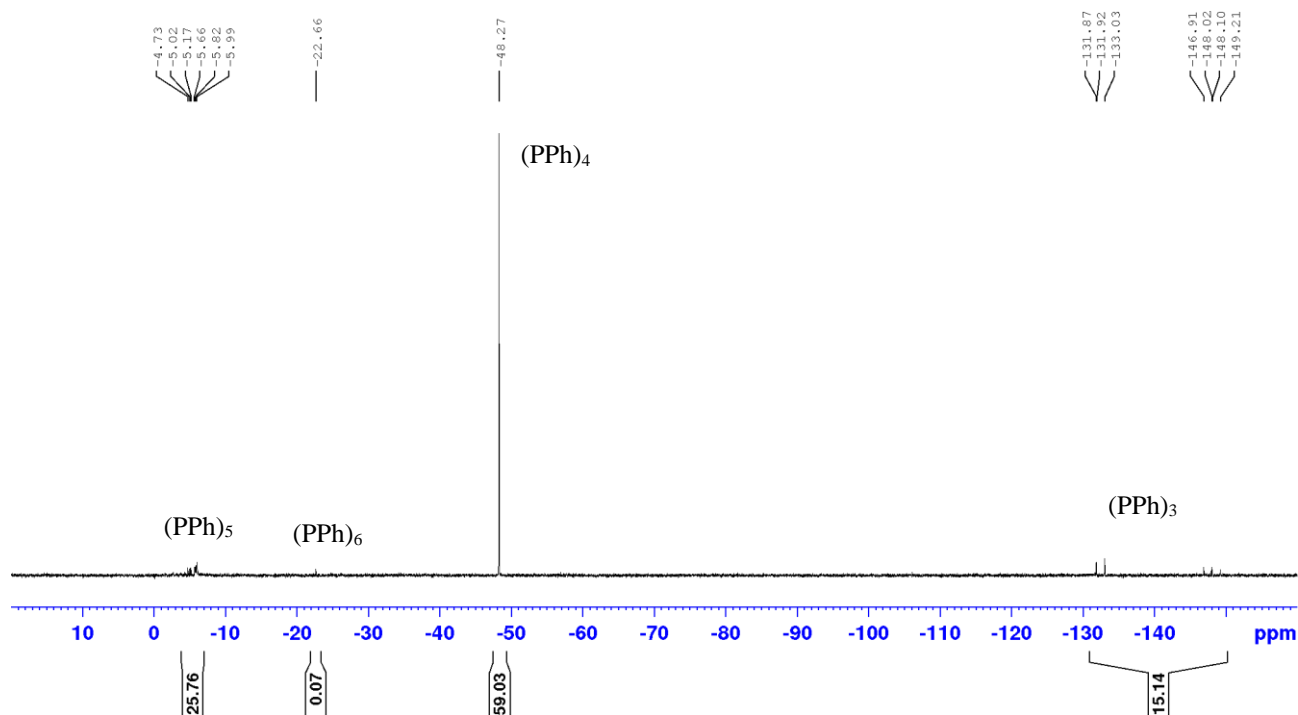


Figure S4. ³¹P{¹H} NMR spectrum recorded directly after mixing ^{Me}NHC=PPh with AlCl₃ in THF at RT.

Reaction of **1** with BPh₃:

In an NMR tube, BPh₃ powder (0.013 g, 0.054 mmol, 1.1 eq) was slowly added to an orange solution of **1** (0.010 g, 0.049 mmol, 1.0 eq) in THF (0.6 mL) at 20 °C. The resulting yellowish suspension was analyzed by ³¹P{¹H} NMR spectroscopy (Figure S5), indicating the formation of (PPh)₅, (PPh)₄ and new product ($\delta = -36.2$ ppm) assigned to the Lewis adduct ^{Me}MHC=P(Ph)BPh₃. After 1h, however, the signal at -36.2 ppm disappeared, and only signals corresponding to cyclopolyphosphines and unreacted **1** were found in the spectrum (Figure S6).

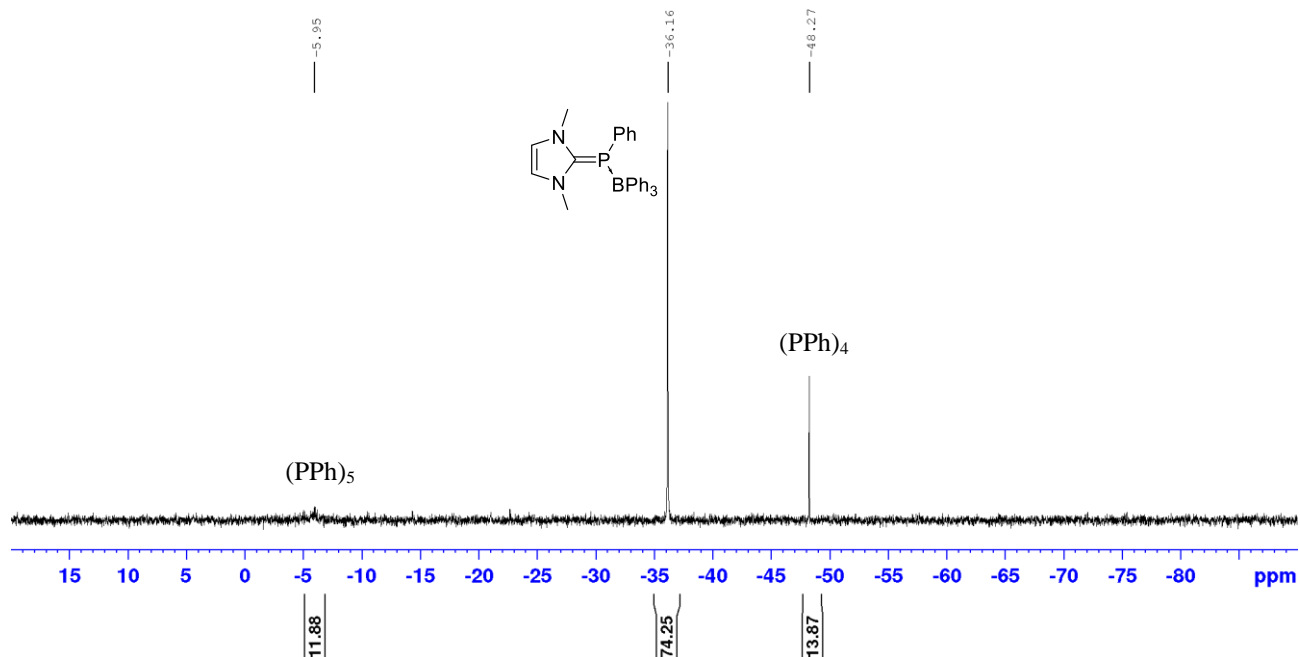


Figure S5. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum recorded directly after mixing $\text{MeNHC}=\text{PPh}$ with BPh_3 in THF at RT.

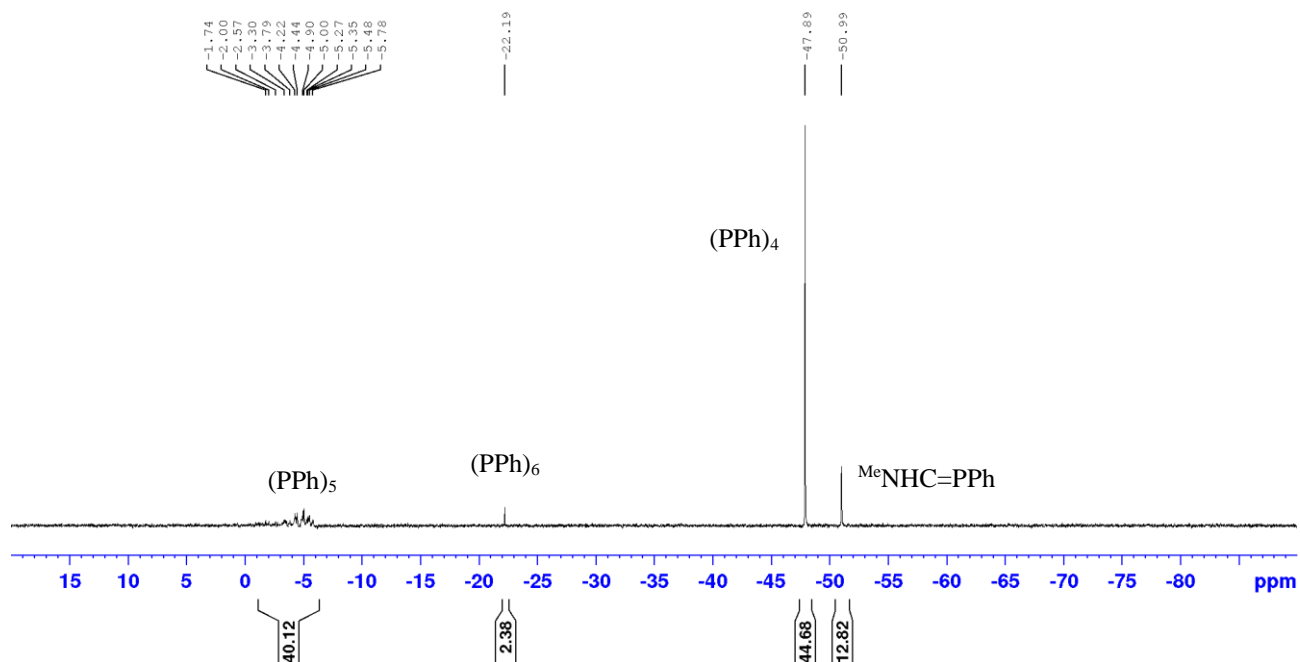


Figure S6. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum recorded after 1h after mixing $\text{MeNHC}=\text{PPh}$ with BPh_3 in THF at RT

Reaction of 1 with $\text{Zn}(\text{OAc})_2$:

In an NMR tube, $\text{Zn}(\text{OAc})_2$ powder (0.010 g, 0.054 mmol, 1.1 eq) was slowly added to an orange solution of **1** (0.010 g, 0.049 mmol, 1.0 eq) in THF (0.6 mL) at 20 °C. The resulting yellow suspension was analyzed by $^{31}\text{P}\{^1\text{H}\}$ NMR spectroscopy (Figure S7), indicating the formation of $(\text{PPh})_5$, $(\text{PPh})_6$, $(\text{PPh})_4$ and an unidentified product (br, $\delta = -60.7$).

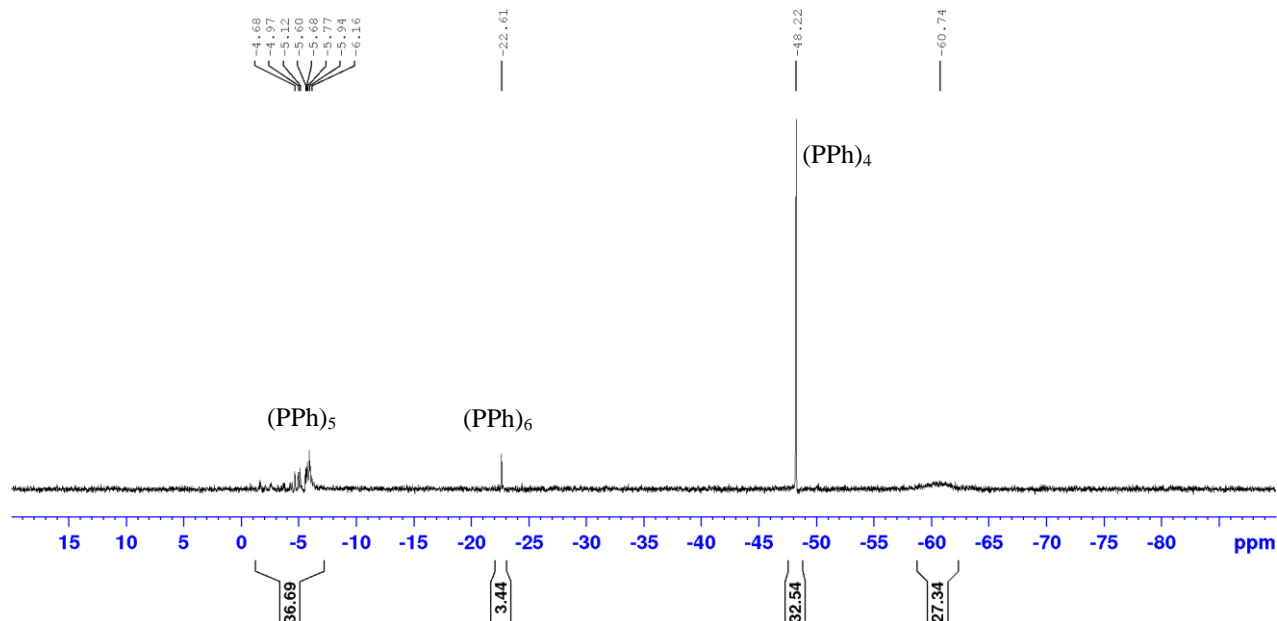
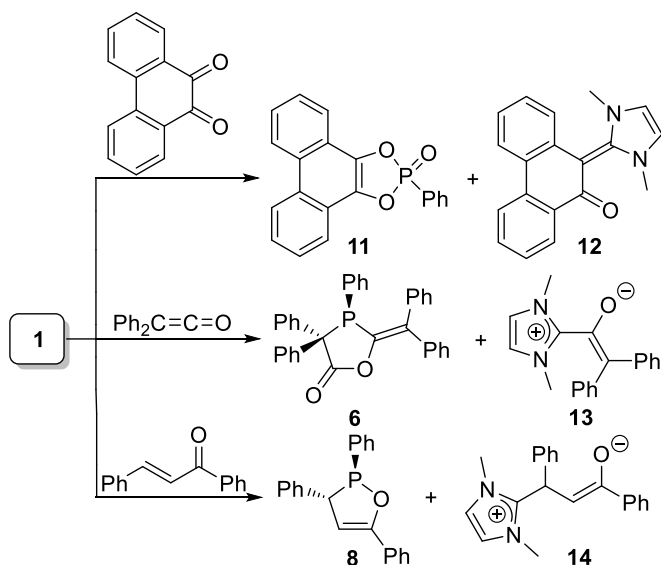


Figure S7. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum recorded directly after mixing $^{\text{Me}}\text{NHC}=\text{PPh}$ with $\text{Zn}(\text{OAc})_2$ in THF at RT.

- **Reactions of $^{\text{Me}}\text{NHC}=\text{PPh}$ with organic electrophiles**

The reactivity of **1** towards electron-poor heterodienes was also studied (Scheme S1). The substrates revealed diverse reactivity, albeit of low selectivity, likely due to the highly reactive free carbene being released. The reaction of **1** with two equivalents of 9,10-phenanthrenequinone resulted in formation of the dioxypyphosphineoxide **11** and the quinone-methide **12**. Addition of *trans*-chalcone to **1** led to an intractable mixture of products, among which the oxo-3-phospholene **8** was also formed in low yield. In fact, the desired phosphinidene transfer was only observed in the case of diphenylketene. However, together with the formation of the 1,3-oxaphospholan-5-one **6** as the sole phosphorus-containing product, the additional equivalent of ketene was consumed to trap the carbene to the carbene-ketene adduct **13**.



Scheme S1. Reactivity of $^{\text{Me}}\text{NHC}=\text{PPh}$ (**1**) towards *ortho*-quinone, diphenylketene and *trans*-chalcone.

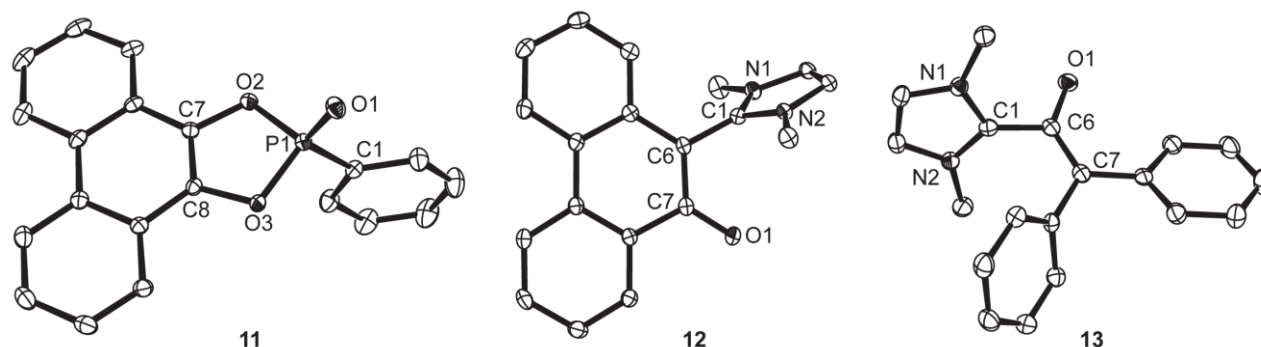
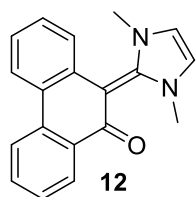


Figure S8. Molecular structures of **11** (disordered THF solvent molecules omitted), **12** (THF solvent molecule omitted, one crystallographic independent molecule is shown) and **13** (one crystallographic independent molecule is shown). Selected bond lengths [Å] and angles [°] for **11** (values for the second molecule in square brackets): P1–C1 1.7699(14), P1–O1 1.4598(10), P1–O2 1.6245(11), P1–O3 1.6251(10), C7–C8 1.3459(19); **12**: N1–C1 1.353(2) [1.351(2)], N2–C1 1.3470(19) [1.3502(19)], C1–C6 1.460(2) [1.459(2)], C6–C7 1.406(2) [1.408(2)], C7–O1 1.2733(17) [1.2741(17)]; **13**: N1–C1 1.3458(17) [1.3429(18)], N2–C1 1.3418(17) [1.3460(18)], C1–C6 1.5009(19) [1.507(2)], C6–O1 1.2889(16) [1.2852(17)], C6–C7 1.3768(19) [1.381(2)].*

Reaction of ^{Me}NHC=PPh with phenanthrene-9,10-quinone

Quinone-methide **12**:

To a stirring solution of ^{Me}NHC=PPh (0.200 g, 0.980 mmol, 1.0 eq) in THF (8 mL) was added phenanthrene-9,10-quinone (0.410 g, 1.970 mmol, 2.0 eq) as a solid over the course of 20 minutes at 20 °C. Next, the solution was cooled to –35 °C overnight, which resulted in the precipitation of **12**. The precipitate was collected on a glass frit, washed with THF (2 mL) and dried under reduced pressure, yielding light orange crystals of **12** (0.268 g, 0.930 mmol, 95%). The compound co-crystallizes with half an equivalent of THF. Crystals suitable for single-crystal X-ray crystallography were obtained from THF at –35 °C (Figure S8).

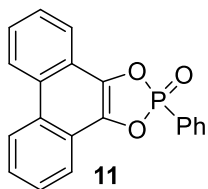


Analysis for C₄₂H₄₀N₄O₃: Calculated: C = 77.75%, H = 6.21%, N = 8.64%. Found: C = 77.75%, H = 6.07% N = 8.48%. **MP:** >220 °C (decomposition). **¹H NMR (300.1 MHz, CD₂Cl₂, 293K):** δ = 8.55 (dd, ³J_{H,H} = 7.9 Hz, ⁴J_{H,H} = 1.6 Hz, 1H; *o*-C₆H₄), 8.51 (dd, ³J_{H,H} = 8.2 Hz, ⁴J_{H,H} = 0.4 Hz, 1H; *o*-C₆H₄), 8.42 (dd, ³J_{H,H} = 8.1 Hz, ⁴J_{H,H} = 0.6 Hz, 1H; *o*-C₆H₄), 7.63 (ddd, ³J_{H,H} = 8.3 Hz, ³J_{H,H} = 7.0 Hz, ⁴J_{H,H} = 1.6 Hz, 1H; *m*-C₆H₄), 7.52 (ddd, ³J_{H,H} = 8.0 Hz, ³J_{H,H} = 7.0 Hz, ⁴J_{H,H} = 1.2 Hz, 1H; *m*-C₆H₄), 7.26 (s, 2H; HC=CH), 7.25 (ddd, ³J_{H,H} = 8.0 Hz, ³J_{H,H} = 7.0 Hz, ⁴J_{H,H} = 1.3 Hz, 1H; *m*-C₆H₄), 7.07 (ddd, ³J_{H,H} = 8.2 Hz, ³J_{H,H} = 7.0 Hz, ⁴J_{H,H} = 1.2 Hz, 1H; *m*-C₆H₄), 6.51 (dd, ³J_{H,H} = 8.1 Hz, ⁴J_{H,H} = 0.8 Hz, 1H; *o*-C₆H₄), 3.65 (s, 6H; NCH₃). **¹³C{¹H} NMR (CDCl₃):** δ = 186.86 (s; C=O), 150.60, 134.48, 133.46, 132.70, 127.82, 126.93, 125.51, 125.43, 121.85, 120.83, 118.79, 118.37, 88.99, 35.11 (s; CH₃).

* CCDC 1523938 (**11**), 1523940 (**12**) and 1523937 (**13**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. For the experimental details of the X-ray crystal structure determinations, see the Supporting Information.

Dioxyphosphineoxide **11**:

After removal of **12**, the volume of the filtrate was reduced to approximately 3 mL and the solution was cooled to $-35\text{ }^{\circ}\text{C}$ for 24 hours. The crystalline precipitate was collected on a glass frit and dried under reduced pressure to yield **11** as a pale green solid in 84% yield (0.275 g, 0.828 mmol).

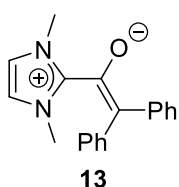


Analysis for $\text{C}_{20}\text{H}_{13}\text{O}_3\text{P}_1$: Calculated: C = 72.29%, H = 3.94%. Found: C = 72.22%, H = 3.79%. **MP**: 184–187 $^{\circ}\text{C}$. **^1H NMR (300.1 MHz, CD_2Cl_2 , 293K)**: δ = 8.79–8.72 (m, 2H; *o*-phenanthreneH), 8.12–8.05 (m, 2H; *o*-phenanthreneH), 7.92 (ddd, $^3J_{\text{H,P}}$ = 14.9 Hz, $^3J_{\text{H,H}}$ = 7.2 Hz, $^4J_{\text{H,H}}$ = 1.4 Hz, 2H; *o*-PPhH), 7.76–7.67 (m, 5H; *m*-phenanthreneH, *p*-PPhH), 7.55 (td, $^3J_{\text{H,H}}$ = 7.8, $^4J_{\text{H,P}}$ = 5.1 Hz, 2H; *m*-PPhH). **$^{13}\text{C}\{^1\text{H}\}$ NMR (75.5 MHz, CD_2Cl_2 , 293 K)**: δ = 137.4 (d, $J_{\text{C,P}}$ = 0.9 Hz; *ipso*-phenanthreneC), 135.1 (d, $^4J_{\text{C,P}}$ = 3.3 Hz, *p*-PPhC), 132.9 (d, $^2J_{\text{C,P}}$ = 11.7 Hz; *o*-PPhC), 129.5 (d, $^3J_{\text{C,P}}$ = 16.5 Hz; *m*-PPhC), 128.2 (s; *m*-phenanthreneC), 128.1 (s; *ipso*-phenanthreneC), 126.8 (s; *m*-phenanthreneC), 126.3 (br. s., *ipso*-PPhC), 123.8 (s; *o*-phenanthreneC), 122.0 (d, $J_{\text{C,P}}$ = 8.9 Hz; *ipso*-phenanthreneC), 121.1 (s; *o*-phenanthreneC). **$^{31}\text{P}\{^1\text{H}\}$ NMR (121.5 MHz, CD_2Cl_2 , 293 K)**: δ = 38.6 (s).

Reaction of $^{\text{Me}}\text{NHC}=\text{PPh}$ with diphenylketene

Carbene-ketene adduct **13**:

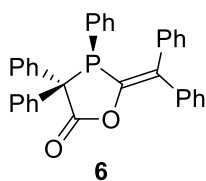
A solution of diphenylketene (0.310 g, 1.60 mmol, 3.1 eq) in THF (2 mL) was slowly added to a stirring solution of $^{\text{Me}}\text{NHC}=\text{PPh}$ (0.100 g, 0.490 mmol, 1.0 eq) in THF (3 mL). The reaction mixture was stirred for 1 hour at 20 $^{\circ}\text{C}$ and then cooled to $-35\text{ }^{\circ}\text{C}$ for 16 hours. The yellow-green precipitate was collected on a glass frit, washed with THF (2 mL) at $-20\text{ }^{\circ}\text{C}$ and dried under reduced pressure yielding a light green powder of **13** (0.100 g, 0.344 mmol, 70%).



MP: $>130\text{ }^{\circ}\text{C}$ (decomposition). **^1H NMR (300.0 MHz, CDCl_3 , 293K)**: δ = 7.84 (d, $^3J_{\text{H,H}}$ = 7.3 Hz, 2H; *o*-PhH), 7.21 (t, $^3J_{\text{H,H}}$ = 7.7 Hz, 2H; *m*-PhH), 7.09 (t, $^3J_{\text{H,H}}$ = 7.2 Hz, 2H; *m*-PhH), 7.00 (m, 2H; *p*-PhH), 6.91 (d, $^3J_{\text{H,H}}$ = 6.9 Hz, 2H; *o*-PhH), 6.71 (s, 2H; NCH), 3.56 (s, 6H; NCH₃). **$^{13}\text{C}\{^1\text{H}\}$ NMR (75.5 MHz, CDCl_3 , 293K)**: δ = 151.9 (s; NCN), 148.1 (s; CO), 143.0 (s; *ipso*-PhC), 141.94 (s; *ipso*-PhC), 130.8 (s; *o*-PhC), 128.2 (s; *o*-PhC), 128.1 (s; *m*-PhC), 127.6 (s; *m*-PhC), 125.1 (s; *p*-PhC), 123.6 (s; *p*-PhC), 119.9 (s; NCH), 114.44 (s; =CPh₂), 35.4 (s; NCH₃).

1,3-oxaphospholan-5-one **6**:

Next, the filtrate was evaporated to dryness, the brown residue extracted into refluxing *n*-hexane (3 x 20 mL) and filtered through a teflon cannula equipped with a glassfiber filter. Concentration to roughly 20% of the original volume and cooling to $-35\text{ }^{\circ}\text{C}$ afforded **6** as a white crystalline solid in 83% yield (202.2 mg, 0.407 mmol). Crystals suitable for single-crystal X-ray crystallography were obtained from diethyl ether at 20 $^{\circ}\text{C}$.



Analysis for $\text{C}_{34}\text{H}_{25}\text{O}_2\text{P}_1$: Calculated: C = 82.2%, H = 5.1%, N = 0.0%. Found: C = 82.0%, H = 4.9%, N = 0.1%. **MP**: 167–168 $^{\circ}\text{C}$. **^1H NMR (300.1 MHz, CD_2Cl_2 , 293K)**: δ = 7.73 (dd, $^3J_{\text{H,H}}$ = 7.5 Hz, $^4J_{\text{H,H}}$ = 2.2, 2H; *o*-PhH), 7.51–6.95 (m, 21H; PhH), 6.75 (d, $^3J_{\text{H,H}}$ = 7.2 Hz, 2H; *o*-PhH). **$^{13}\text{C}\{^1\text{H}\}$ NMR (75.5 MHz, CD_2Cl_2 , 293K)**: δ = 174.1 (d, $^2J_{\text{C,P}}$ = 3.5 Hz; C=O), 143.8 (d, $^1J_{\text{C,P}}$ = 23.2 Hz; PC=CPh₂), 139.5 (d, $J_{\text{C,P}}$ = 2.3 Hz; C_q), 139.4 (d, $J_{\text{C,P}}$ = 8.7 Hz;

C_q), 138.1 (d, $J_{C,P} = 3.7$ Hz; C_q), 137.7 (d, $J_{C,P} = 4.4$ Hz; C_q), 135.1 (d, $J_{C,P} = 20.7$ Hz; C_q), 133.6 (d, $J_{C,P} = 19.0$ Hz; C_{PhH}), 132.5 (d, $J_{C,P} = 21.3$ Hz; C_q) 130.2 (s; C_{PhH}), 130.2 (d, $J_{C,P} = 9.5$ Hz; C_{PhH}), 129.4 (d, $J_{C,P} = 1.7$ Hz; C_{PhH}), 129.3 (d, $J_{C,P} = 7.1$ Hz; C_{PhH}), 129.2 (d, $J_{C,P} = 17.3$ Hz; C_{PhH}), 128.9 (d, $J_{C,P} = 1.7$ Hz; C_{PhH}), 128.7 (d, $J_{C,P} = 21.6$ Hz; C_{PhH}), 128.6 (d, $J_{C,P} = 15.0$ Hz; C_{PhH}), 128.0 (s), 126.9 (d, $J_{C,P} = 1.3$ Hz; C_{PhH}), 62.7 (d, $J_{C,P} = 15.2$ Hz; PCPh₂). ³¹P{¹H} NMR (121.5 MHz, CD₂Cl₂, 293 K): $\delta = 0.0$ (s).

Reaction of ^{Me}NHC=PPh with *trans*-chalcone

A solution of *trans*-chalcone (0.428 g, 2.06 mmol, 2.1 eq) in THF (8 mL) was slowly added to a stirring solution of ^{Me}NHC=PPh (0.200 g, 0.979 mmol, 1.0 eq) in THF (5 mL) at -78 °C to give a dark green suspension. The reaction mixture was stirred for 2 hours at 20 °C and was analyzed using ³¹P NMR spectroscopy (see Figure S9). Since the spectrum still contained the signal corresponding to starting material ($\delta = -51.4$ (16.33%)), an additional equivalent of *trans*-chalcone (0.204 g, 0.979 mmol, 1 eq) was added as a solid. The resulting reaction mixture was stirred for 2 hours and again was analyzed by ³¹P NMR spectroscopy (see Figure S10). The spectrum shows formation of **8** ($\delta = 133.9$ (39.56%)) together with some unidentified products ($\delta = 135.7$ (23.80%), 135.6 (23.80%), 126.1 (5.08%), 42.7 (3.61%), 32.3 (4.15%)), but it was impossible to purify the compounds from the mixture. However, single crystals of **8** were obtained from the mixture and confirmed the identity of this phosphorus heterocycle. In addition, low quality single crystals of **14** were obtained from the precipitation and allowed us to identify **14** as the zwitterionic carbene-chalcone species.

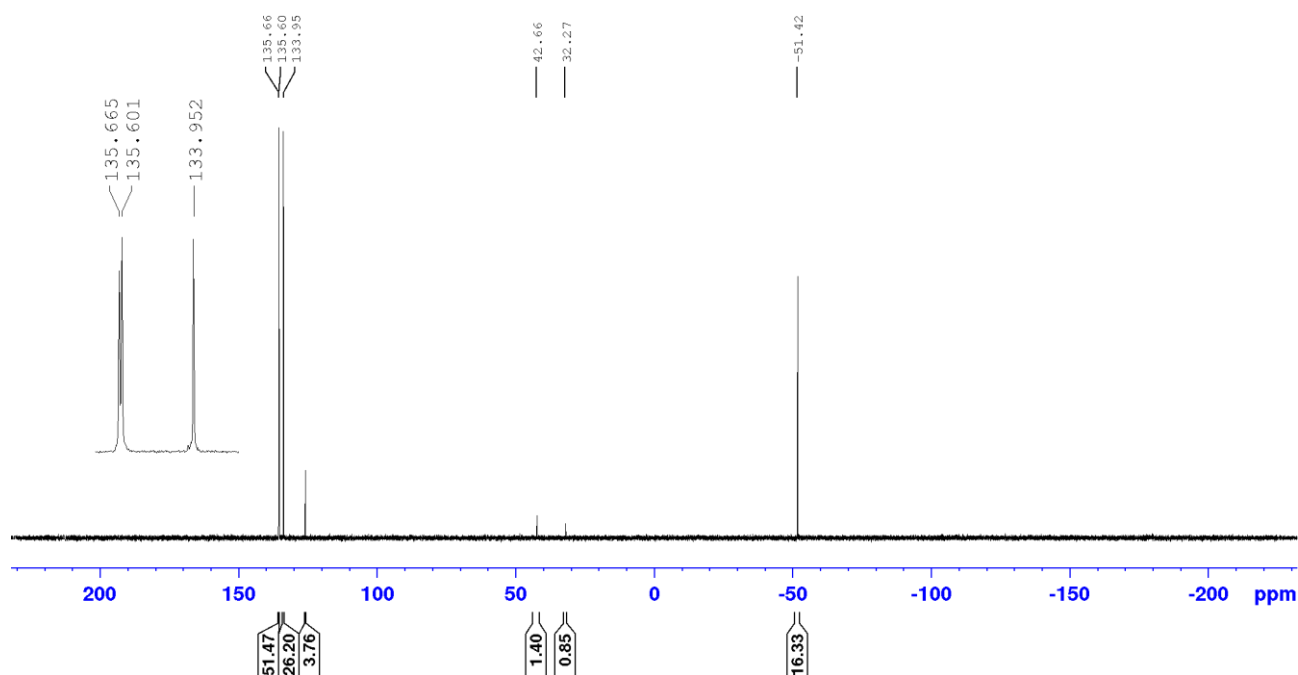


Figure S9. ³¹P{¹H} NMR spectrum recorded after mixing ^{Me}NHC=PPh with *trans*-chalcone (2.1 eq).

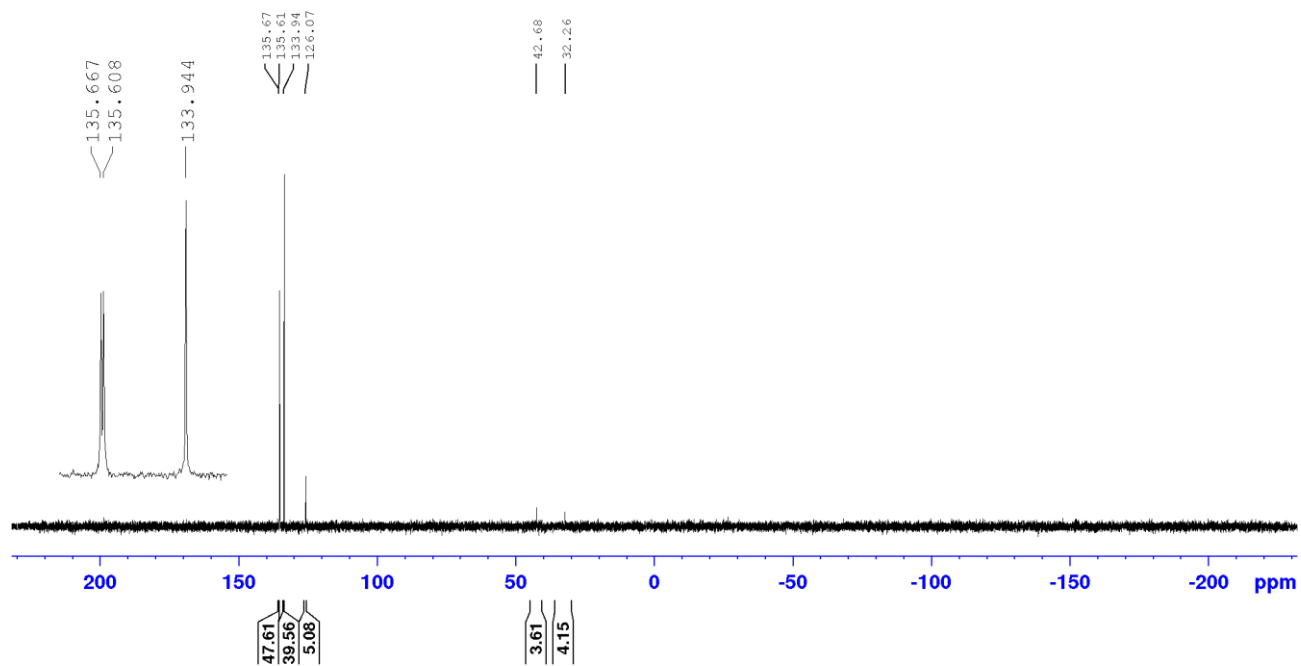


Figure S10. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum recorded after mixing $^{\text{Me}}\text{NHC}=\text{PPh}$ with *trans*-chalcone (3.1 eq.)

2. Computational details

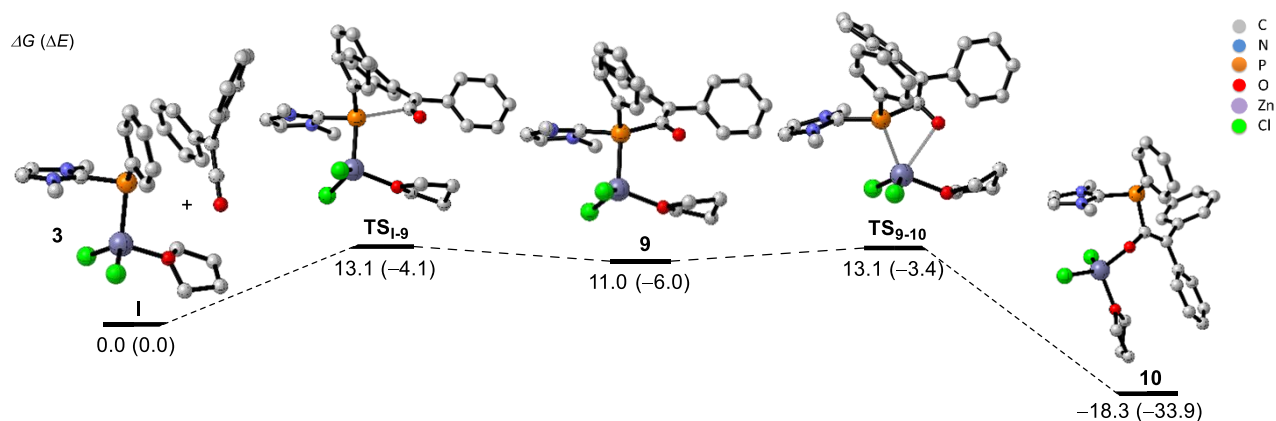
Density functional calculations were performed with the Gaussian09 suite of software, revision D.01,^[13] using the ω B97X-D functional,^[14] the 6-31G** basis set.^[15-17] All geometries have been computed and optimized in the gas phase. The stationary points were characterized by full vibration frequencies calculations as minima (no imaginary frequency) or transition states (one single imaginary frequency). When necessary, final proof for the position of the transition state was obtained by an IRC calculation. All coordinates are reported in angstroms, energies in kcal·mol⁻¹.

Reaction of the phosphinidene zinc complex 3 with 1 equivalent of diphenylketene

In principle, two different reaction pathways for the formation of **10** can be envisioned, i.e. the direct nucleophilic attack of the phosphorus atom at the ketene's carbonyl carbon atom (**A**, Scheme S2) or the initial coordination of the ketene to **3** by Zn–O bond formation, followed by nucleophilic attack of the phosphorus atom (**B**, Scheme S3).

A: Direct nucleophilic attack

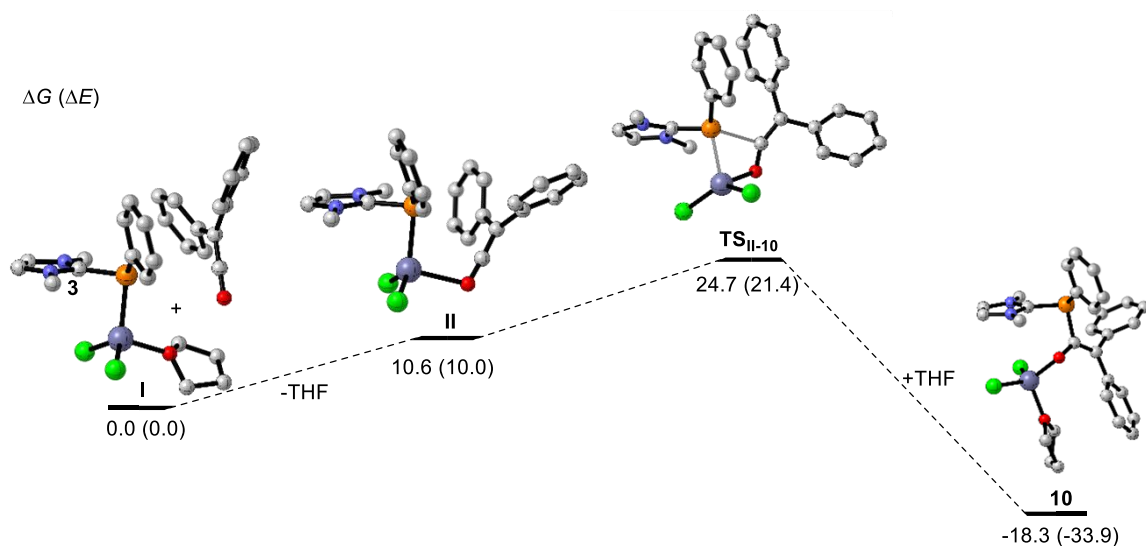
Calculations reveal that direct nucleophilic attack of the phosphorus atom of **3** at the ketene's carbonyl carbon indeed is possible. After formation of adduct **9** ($\Delta G = 11.0$ kcal·mol⁻¹; $\Delta G_a = 13.1$ kcal·mol⁻¹), **10** is formed by ZnCl₂ transfer from P to O ($\Delta G = -18.3$ kcal·mol⁻¹; $\Delta G_a = 13.1$ kcal·mol⁻¹).



Scheme S2. Relative energies for the pathway **A** (direct nucleophilic attack) leading from **3** and diphenylketene to **10**.

B: Nucleophilic attack on a ZnCl₂ coordinated ketene

Alternatively, replacing THF with the ketene in **3** by Zn–O bond formation could lead to formation of an intermediate **II** ($\Delta G = 10.6$ kcal·mol⁻¹). However, subsequent nucleophilic attack by the phosphorus atom at the carbonyl carbon has a significantly higher barrier ($\Delta G_a = 24.7$ kcal·mol⁻¹) than the direct attack (Pathway **A**).



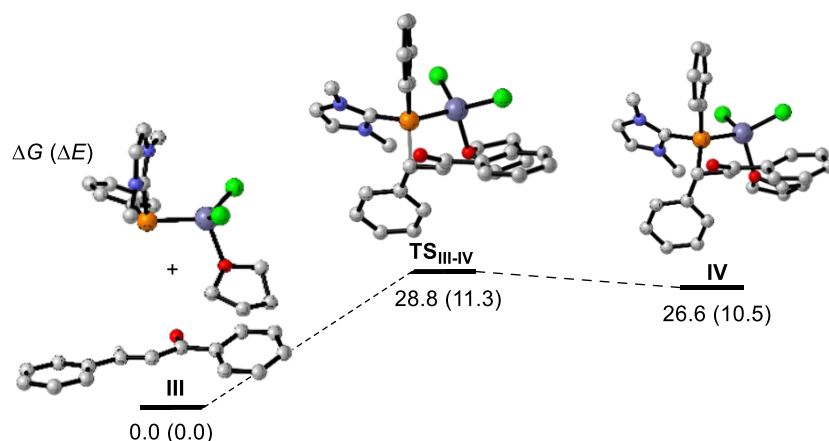
Scheme S3. Relative energies for the pathway **B** leading from **3** and diphenylketene to **10**.

Reaction of the phosphinidene zinc complex 3 with trans-chalcone

The reaction mechanism of the phosphinidene zinc complex **3** and *trans*-chalcone was envisioned to involve the P–Zn insertion intermediate **VII** akin to **10** (Scheme S5). To form **VII**, two possible reaction pathways have been evaluated, i.e. the direct nucleophilic attack by the phosphorus atom at the carbonyl carbon (**A**, Scheme S4) or initial coordination of *trans*-chalcone to **3** by Zn–O bond formation, followed by nucleophilic attack with phosphorus atom (**B**, Scheme S5).

A: Direct nucleophilic attack

In contrast to the ketene, the direct nucleophilic attack on *trans*-chalcone is highly disfavored due to the repulsion between the carbonyl substituent and the coordinated THF. Therefore, P–C bond formation has an activation barrier of 28.8 kcal·mol⁻¹ (ΔG_a) (Scheme S4).

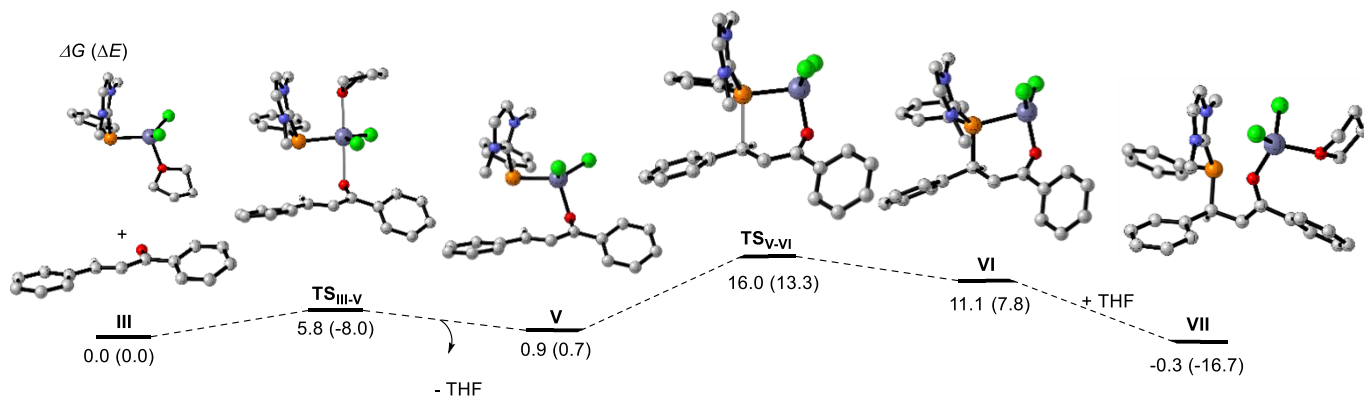


Scheme S4. Relative energies of products resulting from the addition of *trans*-chalcone to complex **3** (Pathway **A**).

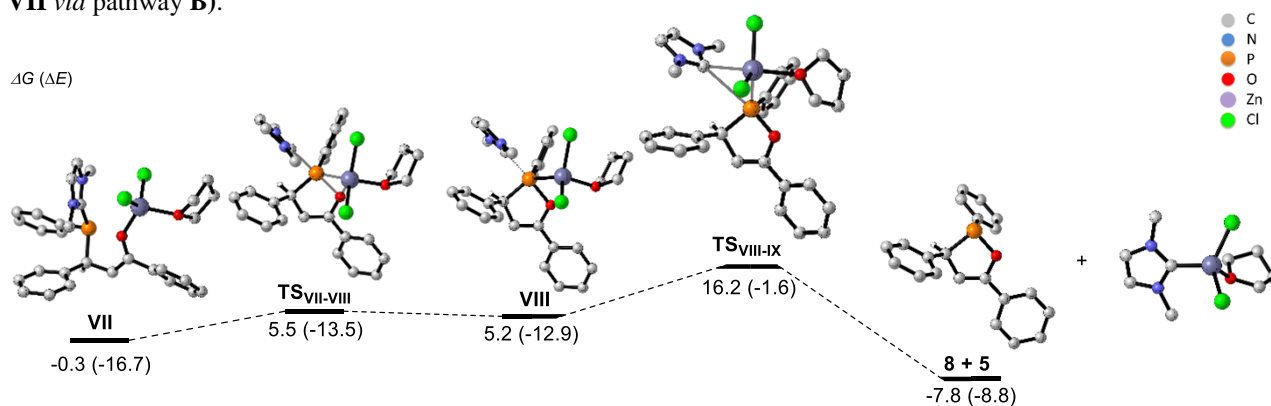
B: Nucleophilic attack on a ZnCl₂ activated trans-chalcone

Coordination of *trans*-chalcone to **3** by Zn–O bond formation (**V**: $\Delta G = 0.9$ kcal·mol⁻¹; $\Delta G_a = 5.8$ kcal·mol⁻¹) activates *trans*-chalcone towards nucleophilic attack. This attack *via* a low energy transition state ($\Delta G_a = 16.0$ kcal·mol⁻¹) leads to the formation of a six-membered ring **VI** ($\Delta G = 11.1$ kcal·mol⁻¹), which after subsequent

ring-opening in the presence of THF yields **VII** ($\Delta G = -0.3 \text{ kcal}\cdot\text{mol}^{-1}$). Afterwards, nucleophilic attack of the oxygen atom at P takes place from the backside of the P–C_{carbene} bond (at σ^* MO of the P–C_{carbene} bond), while simultaneously transferring ZnCl₂ to P, leads to the formation of intermediate **VIII** ($\Delta G = 5.2 \text{ kcal}\cdot\text{mol}^{-1}$; $\Delta G_a = 5.5 \text{ kcal}\cdot\text{mol}^{-1}$). The former intermediate **VIII** eliminating (NHC)Zn complex **5** yields product **8** ($\Delta G = -7.8 \text{ kcal}\cdot\text{mol}^{-1}$; $\Delta G_a = 16.2 \text{ kcal}\cdot\text{mol}^{-1}$). The magnitude of all activation barriers in this pathway is fully consistent with mild experimental conditions of the reaction.



Scheme S5. Relative energies of products resulting from the addition of *trans*-chalcone to complex **3** (to the intermediate **VII** via pathway **B**).

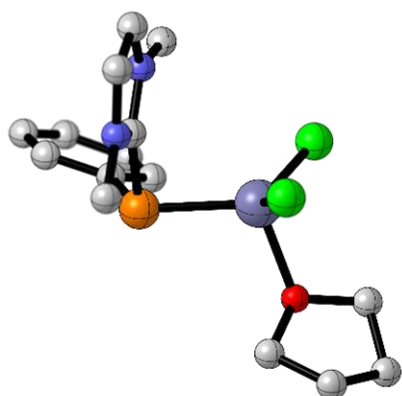


Scheme S6. Relative energies of products resulting from the addition of *trans*-chalcone to complex **3** (to form **8** and **5**).

Optimized structures

(MeNHC=PPh)ZnCl₂THF (**3**):

Structure



Cartesian Coordinates

Element	X	Y	Z
C	-1.68643200	-3.68654490	0.22976400
H	-1.56824994	-4.75114679	0.11716500
C	-2.31982398	-2.95650411	1.17618895
H	-2.87620401	-3.26058197	2.04718995
C	-1.40230203	-1.52652597	-0.27387300
P	-0.73743099	-0.07546200	-1.14845300
Zn	1.00384295	0.12673500	0.46121499
C	-2.07500911	1.14700496	-0.84472698
C	-3.35676503	0.91269302	-1.36241698
C	-1.83473694	2.35069990	-0.17348200
C	-4.37942123	1.83817196	-1.18129897
H	-3.55395103	-0.00686600	-1.90759504
C	-2.85289001	3.28709698	-0.01305000
H	-0.86009401	2.54236102	0.26459399
C	-4.12808609	3.03205395	-0.50814700
H	-5.36872196	1.63492894	-1.58027995
H	-2.64891911	4.21284199	0.51583803
H	-4.92172289	3.76059604	-0.37432599
N	-2.13211894	-1.62702501	0.86276001
N	-1.14232194	-2.79434896	-0.66605002
C	-0.30409500	-3.16083694	-1.79791498
H	0.74629200	-3.07872295	-1.50769401
H	-0.54196501	-4.18485117	-2.08728600
H	-0.51120901	-2.47808599	-2.62390709
C	-2.57346201	-0.52061200	1.70638704
H	-3.40936995	0.00500500	1.24243605
H	-2.87854290	-0.93743497	2.66580009
H	-1.74476397	0.17233799	1.86837602
Cl	2.01944089	-1.90119302	0.58078802
Cl	0.63390201	1.29377604	2.33018899
O	2.55306101	1.16116095	-0.42846900
C	3.06381702	0.65404999	-1.68080103
C	3.64620304	1.47495604	0.47176999
C	4.53466797	0.36399201	-1.42199004
H	2.48684907	-0.23240501	-1.95326602
H	2.92159510	1.43001902	-2.44081497
C	4.89315987	1.44675303	-0.40050799
H	3.42718601	2.43891311	0.93171400
H	3.68360090	0.70473802	1.24882901
H	5.13303185	0.41010499	-2.33448911
H	4.64019823	-0.62897003	-0.97483999
H	5.04257679	2.41166306	-0.89606899
H	5.78940201	1.21315205	0.17777100

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	15.3743	35.0121	46.4679
Red. masses	--	7.1211	5.2619	5.1630
Frc consts	--	0.0010	0.0038	0.0066
IR Inten	--	3.7538	3.2486	1.5366

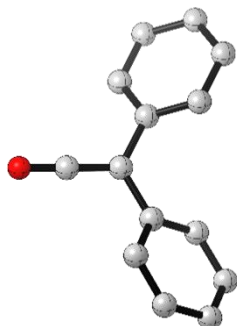
Thermochemistry

Sum of electronic and zero-point Energies = -3809.358710
 Sum of electronic and thermal Energies = -3809.333956
 Sum of electronic and thermal Enthalpies = -3809.333012
 Sum of electronic and thermal Free Energies = -3809.416163

HF = -3809.70840034

Diphenylketene:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	0.00001700	0.84366000	0.00009700
C	-0.00023800	2.16980410	0.00003800
O	-0.00041100	3.33665991	-0.00007200
C	-1.31059599	0.14357901	-0.03480200
C	-1.44392800	-1.06239200	-0.73447102
C	-2.43492699	0.67439002	0.60821301
C	-2.66915107	-1.71644795	-0.78550398
H	-0.58063501	-1.48506296	-1.23842204
C	-3.66452909	0.02867900	0.53563303
H	-2.34415293	1.59617198	1.17665505
C	-3.78643489	-1.17228305	-0.15649000
H	-2.75311899	-2.65324306	-1.32765198
H	-4.52616501	0.46001300	1.03551304
H	-4.74327707	-1.68202996	-0.20324899
C	1.31062102	0.14367799	0.03497800
C	2.43487501	0.67455101	-0.60821003
C	1.44418395	-1.06219697	0.73470002
C	3.66448808	0.02891600	-0.53583199
H	2.34401393	1.59639394	-1.17654395
C	2.66946411	-1.71622205	0.78550500
H	0.58104002	-1.48493898	1.23884904
C	3.78659105	-1.17207003	0.15627100
H	4.52601719	0.46029499	-1.03586197
H	2.75348902	-2.65299010	1.32769501
H	4.74347019	-1.68175900	0.20283601

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	30.9919	52.5518	82.4304
Red. masses	--	4.4161	4.0449	4.5246
Frc consts	--	0.0025	0.0066	0.0181
IR Inten	--	0.6846	0.3036	0.0138

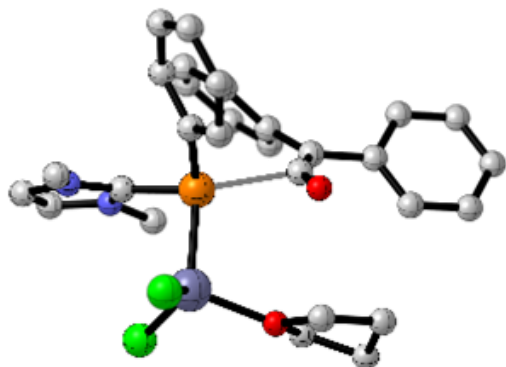
Thermochemistry

Sum of electronic and zero-point Energies = -614.304182
Sum of electronic and thermal Energies = -614.292380
Sum of electronic and thermal Enthalpies = -614.291435
Sum of electronic and thermal Free Energies = -614.343873

HF = -614.502942854

TS_{I-9}:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	-2.47071004	2.83157301	-2.37167311
H	-2.36513805	3.36853504	-3.29947901
C	-3.53393102	2.67193007	-1.54953897
H	-4.53889418	3.05523300	-1.61242998
C	-1.83346403	1.51987505	-0.69056100
P	-0.83801597	0.31231400	0.25514501
Zn	-1.84578001	-1.62913406	-0.70611799
C	-1.37445402	0.67408699	1.96142995
C	-1.51425803	1.98854494	2.43063211
C	-1.55875897	-0.38216999	2.85859609
C	-1.84567201	2.23870707	3.75720191
H	-1.37905896	2.82443094	1.74811804
C	-1.87214005	-0.12823100	4.19102478
H	-1.48373103	-1.40605402	2.51051807
C	-2.01963806	1.17832696	4.64418507
H	-1.96032095	3.26234508	4.10057878
H	-2.01423407	-0.95995897	4.87345791
H	-2.27050209	1.37132096	5.68229103
N	-3.13366795	1.85011995	-0.51906198
N	-1.43158305	2.11580491	-1.82684100
C	-0.16451401	1.88822997	-2.50823593
H	-0.36800501	1.39182699	-3.45761895
H	0.35126999	2.83886194	-2.64743590
H	0.45319700	1.23638296	-1.89500403
C	-4.04714584	1.31207502	0.48763099
H	-3.92253089	1.83169305	1.43816400
H	-5.06221724	1.44350302	0.11455700
H	-3.86084390	0.24499300	0.62890297
Cl	-2.12302995	-1.05561602	-2.86763906

Cl	-3.44650888	-2.50288606	0.56234199
O	1.13874900	-1.23187900	1.35501897
C	1.43973196	-0.22554301	0.78702998
C	2.41754699	0.58532500	0.32299301
C	3.79253602	0.01245000	0.42784700
C	4.04425192	-1.34413302	0.19003600
C	4.87747622	0.83194000	0.77038503
C	5.32633495	-1.86886001	0.30252701
H	3.22202992	-1.99618995	-0.08449000
C	6.16203690	0.30953601	0.87061298
H	4.70804405	1.88687801	0.96144402
C	6.39499092	-1.04394400	0.64129001
H	5.49085522	-2.92604303	0.11603300
H	6.98442316	0.96513999	1.14103401
H	7.39721918	-1.45154202	0.72682798
C	2.23684812	1.96222699	-0.16880500
C	1.36321998	2.86416292	0.45224300
C	2.97299910	2.41460896	-1.27532697
C	1.18029404	4.14862394	-0.05290200
H	0.84602600	2.55544090	1.35363603
C	2.81400895	3.70657110	-1.76142395
H	3.67245603	1.73784494	-1.75641704
C	1.90369403	4.57766819	-1.16251802
H	0.49264100	4.82687521	0.44436800
H	3.39538598	4.03290510	-2.61856103
H	1.77562499	5.58518887	-1.54589200
C	0.78412300	-2.83371902	-1.62786102
O	-0.36133999	-3.00413895	-0.77408803
C	-0.09144500	-3.93531895	0.29749900
C	1.38428998	-4.29478884	0.15407801
C	1.65788603	-4.04412079	-1.33362401
H	0.41831699	-2.77174091	-2.65377402
H	1.28385901	-1.89224899	-1.36752796
H	-0.32049200	-3.44472003	1.24478102
H	-0.75849003	-4.79030895	0.16007200
H	1.98816895	-3.62846088	0.77571499
H	1.58418298	-5.32555914	0.45369801
H	2.71186996	-3.85089207	-1.54809594
H	1.33535397	-4.89895582	-1.93582404

Harmonic Frequencies

		1	2	2
		A	A	A
Frequencies	--	-107.4554	22.6343	26.7228
Red. masses	--	9.3253	6.4809	6.0564
Frc consts	--	0.0634	0.0020	0.0025
IR Inten	--	90.2705	1.8411	1.5192

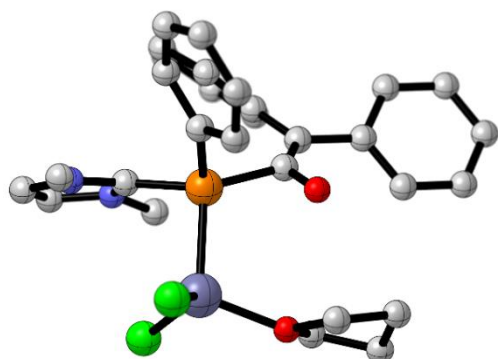
Thermochemistry

Sum of electronic and zero-point Energies	=	-4423.669225
Sum of electronic and thermal Energies	=	-4423.632802
Sum of electronic and thermal Enthalpies	=	-4423.631858
Sum of electronic and thermal Free Energies	=	-4423.739108

HF = -4424.22060274

9:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	-1.91056705	3.06748700	-2.32558393
H	-1.72669101	3.57743096	-3.25637603
C	-2.98758292	3.06733990	-1.50620496
H	-3.93059492	3.58337593	-1.57754898
C	-1.46670794	1.70049000	-0.63300902
P	-0.73064703	0.27499801	0.29743499
Zn	-1.98791206	-1.48342597	-0.77281398
C	-1.20410800	0.66497397	2.01377797
C	-1.25176203	1.97022796	2.51839995
C	-1.46516299	-0.40581000	2.87174892
C	-1.55930495	2.19992995	3.85429597
H	-1.06357396	2.81805897	1.86518598
C	-1.76314402	-0.17304200	4.21077919
H	-1.44523203	-1.41890204	2.48999405
C	-1.81193805	1.12595296	4.70468092
H	-1.59592104	3.21685004	4.23207998
H	-1.96652603	-1.01328194	4.86616898
H	-2.04757309	1.30369198	5.74902678
N	-2.70975995	2.20720100	-0.46779001
N	-0.98944199	2.20935893	-1.77859998
C	0.20933400	1.78068101	-2.49068904
H	-0.09920400	1.41206503	-3.46923709
H	0.90559202	2.61532807	-2.56885791
H	0.68039501	0.96492398	-1.94628096
C	-3.71551204	1.80253100	0.51795298
H	-3.55263400	2.30976701	1.46842098
H	-4.69113398	2.06641102	0.11193000
H	-3.68719697	0.72061700	0.66631800
Cl	-2.16419196	-0.74859601	-2.88649893
Cl	-3.72311711	-1.97934902	0.51473701
O	0.89792502	-1.34714901	1.06843400
C	1.12820995	-0.23281400	0.55862600
C	2.28687191	0.43462199	0.23604999
C	3.57126403	-0.29399100	0.41234201
C	3.69323611	-1.66257405	0.13229500
C	4.71757078	0.37902299	0.86139500
C	4.90194321	-2.32812500	0.29362601
H	2.82187796	-2.20773196	-0.20827200
C	5.92965698	-0.28405401	1.01808000

H	4.65357924	1.43796694	1.09248805
C	6.03084612	-1.64335597	0.73622900
H	4.96323919	-3.38952303	0.06928800
H	6.79811001	0.26449400	1.37097895
H	6.97614622	-2.16198993	0.86179298
C	2.33775711	1.84712696	-0.17472900
C	1.52896595	2.82313895	0.42218801
C	3.21404004	2.26935196	-1.19292104
C	1.51565397	4.13854790	-0.03773800
H	0.93640101	2.54588199	1.28551602
C	3.22912312	3.58658695	-1.62931097
H	3.87793803	1.54152298	-1.64932001
C	2.35900092	4.52778482	-1.07271504
H	0.86677200	4.86796284	0.43952999
H	3.91401601	3.88207507	-2.41872001
H	2.36529994	5.55543995	-1.42234600
C	0.40729600	-3.01832700	-1.70803404
O	-0.76294202	-3.07436395	-0.86650199
C	-0.55387098	-3.95691609	0.26283300
C	0.90178400	-4.39913702	0.16527399
C	1.20552099	-4.25678492	-1.33088803
H	0.06062900	-2.99252605	-2.74200201
H	0.95718801	-2.09761190	-1.48339999
H	-0.76444000	-3.40145993	1.17743802
H	-1.26475298	-4.78118610	0.16011100
H	1.52490997	-3.71904492	0.75027502
H	1.04365504	-5.41810417	0.53157198
H	2.27089190	-4.13156319	-1.53870404
H	0.84421599	-5.12709808	-1.88743198

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	17.9520	25.7368	39.8614
Red. masses	--	5.7535	6.0937	6.0421
Frc consts	--	0.0011	0.0024	0.0057
IR Inten	--	2.1192	1.1906	0.2442

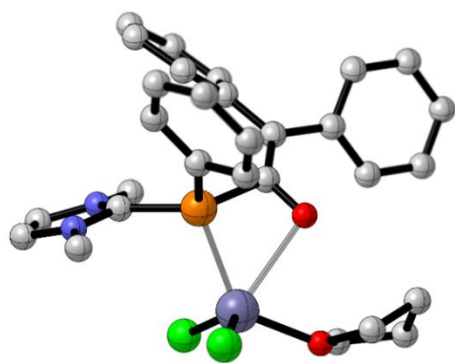
Thermochemistry

Sum of electronic and zero-point Energies	=	-4423.672505
Sum of electronic and thermal Energies	=	-4423.635828
Sum of electronic and thermal Enthalpies	=	-4423.634883
Sum of electronic and thermal Free Energies	=	-4423.742528

HF = -4424.22434355

TS₉₋₁₀:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	-3.10912704	1.79226303	-2.73658490
H	-3.12559891	2.31893206	-3.67618895
C	-4.10009909	1.19727898	-2.03107190
H	-5.15462494	1.10350001	-2.23091292
C	-2.19743609	0.90974098	-0.91621798
P	-1.01664305	0.03020300	0.18972600
Zn	-0.69213802	-2.23854303	-0.60449803
C	-1.69241405	0.34476501	1.85152900
C	-2.47273707	1.45836401	2.18356204
C	-1.38931096	-0.59765297	2.83902407
C	-2.94685292	1.62472498	3.48004794
H	-2.71783400	2.20052600	1.42797303
C	-1.85403299	-0.41898701	4.13799715
H	-0.79825503	-1.47112596	2.58824611
C	-2.63469696	0.68653297	4.46081877
H	-3.55378890	2.49064898	3.72503209
H	-1.61269701	-1.15613401	4.89642382
H	-3.00343204	0.81659901	5.47323084
N	-3.52333999	0.64235198	-0.91223598
N	-1.94084895	1.59443295	-2.04061890
C	-0.62787801	1.95540702	-2.56626296
H	-0.59753799	1.66652703	-3.61663890
H	-0.46171400	3.02576900	-2.44158792
H	0.13668200	1.39377797	-2.03455400
C	-4.23322678	-0.23997100	0.01676100
H	-4.42167282	0.26958901	0.96176302
H	-5.17536306	-0.52033103	-0.45208001
H	-3.64929795	-1.14796102	0.19668099
Cl	-0.77624100	-1.65013194	-2.79707789
Cl	-2.19964600	-3.41462302	0.56457001
O	1.12461400	-0.89572102	0.71757299
C	0.84948200	0.29679900	0.37603399
C	1.64794004	1.40267098	0.23699300
C	3.11419106	1.23205698	0.41760501
C	3.79370093	0.10265900	-0.05877600
C	3.86707211	2.21677995	1.07326305
C	5.16389894	-0.04259100	0.12130500
H	3.23269010	-0.66925102	-0.57101703
C	5.23938179	2.07529902	1.25002599
H	3.36617708	3.10263395	1.45251501
C	5.89678907	0.94286197	0.77794403
H	5.66347313	-0.92899698	-0.26006901

H	5.79563189	2.85248303	1.76605904
H	6.96700382	0.82903099	0.91944599
C	1.13966894	2.75149608	-0.07003700
C	-0.03027000	3.26441002	0.50503999
C	1.81935704	3.56772804	-0.99352801
C	-0.55348498	4.49413776	0.10976800
H	-0.50868398	2.70912004	1.30172098
C	1.31465101	4.80480480	-1.36879396
H	2.74443412	3.20585704	-1.43152201
C	0.10918300	5.26864815	-0.83688599
H	-1.46639800	4.86144114	0.57087100
H	1.85736501	5.40899277	-2.08988810
H	-0.28964001	6.23268986	-1.13659596
C	2.03339601	-3.14769292	-1.47058904
O	0.94444001	-3.44450593	-0.56618398
C	1.45170999	-3.90175605	0.70781302
C	2.91257811	-3.48168612	0.72279900
C	3.29553199	-3.61636806	-0.75431597
H	1.83304501	-3.65977407	-2.41293311
H	2.03722906	-2.06965494	-1.65254498
H	0.85377699	-3.44069791	1.49443400
H	1.32448900	-4.98865318	0.74694902
H	2.98840690	-2.44080710	1.04614305
H	3.51705694	-4.11195087	1.37887597
H	4.16317987	-3.01090693	-1.02803004
H	3.51485205	-4.65982294	-1.00283897

Harmonic Frequencies

		1	2	3
	A	A	A	A
Frequencies	--	-75.7627	18.1845	21.9901
Red. masses	--	11.5002	6.2317	5.3968
Frc consts	--	0.0389	0.0012	0.0015
IR Inten	--	5.5636	2.7739	0.2933

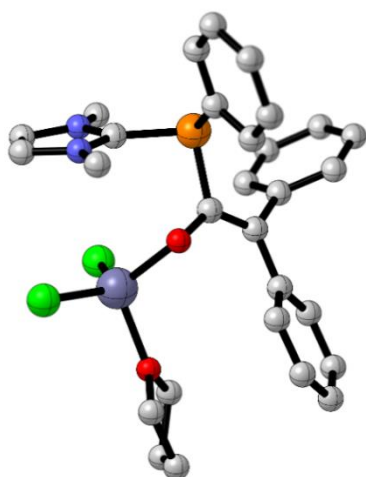
Thermochemistry

Sum of electronic and zero-point Energies	=	-4423.668300
Sum of electronic and thermal Energies	=	-4423.631807
Sum of electronic and thermal Enthalpies	=	-4423.630863
Sum of electronic and thermal Free Energies	=	-4423.739191

HF = -4424.21886235

10:

Structure



Cartesian Coordinates

Element	X	Y	Z
Zn	-1.11035097	-1.65397704	0.33824399
Cl	-0.93963999	-1.05196702	2.50785303
P	2.26831388	0.55427498	0.28568301
Cl	-0.92104799	-3.80085301	-0.28075799
O	0.01500600	-0.53727198	-0.76768202
N	2.38487697	-1.43724096	2.23736811
N	2.24811101	-2.37336302	0.29176399
C	0.47430900	0.57145399	-0.24394900
C	2.30678201	-2.78951812	2.44867492
H	2.27928090	-3.21288490	3.43847799
C	2.23004198	-3.37582588	1.22809398
H	2.11553407	-4.40894318	0.94633400
C	2.32484603	-1.17907500	0.91469902
C	-0.18616401	1.75967503	-0.14064699
C	0.37970200	2.86881590	0.68059200
C	-1.51537895	1.98190296	-0.75760400
C	0.41690600	2.74542403	2.07456589
H	0.02110300	1.83803701	2.52452111
C	2.49100590	0.58943897	-2.54895997
H	1.44322598	0.87184000	-2.56720591
C	-3.16843390	1.52020895	-2.48057294
H	-3.46270990	0.96028101	-3.36436605
C	3.12139606	0.33532801	-1.32846701
C	-2.38167906	2.96189594	-0.24639800
H	-2.07924199	3.53559899	0.62363499
C	-1.93711197	1.26479304	-1.89037299
H	-1.28984404	0.49708399	-2.29595804
C	2.18162203	-2.62221503	-1.15000296
H	3.17715693	-2.53108907	-1.58776402
H	1.49120200	-1.90418100	-1.58668995
H	1.77408397	-3.62203193	-1.28726804
C	4.47285700	-0.02825000	-1.32280099
H	4.98272896	-0.20263401	-0.37809601
C	0.84662098	4.04962587	0.09554300
H	0.80099797	4.15925407	-0.98426503
C	-3.62057304	3.20612097	-0.83129001
H	-4.27208281	3.96508288	-0.40854600
C	4.53065586	0.06252200	-3.73093390
H	5.07258987	-0.05008300	-4.66455412

C	3.19505310	0.45469499	-3.74212289
H	2.69353509	0.64710897	-4.68535995
C	-4.02293110	2.48659396	-1.95290899
H	-4.98591423	2.68031096	-2.41553211
C	2.35936809	-0.44811201	3.30975509
H	2.92518210	-0.84150797	4.15464783
H	1.31844997	-0.27166501	3.58893204
H	2.81189108	0.47782201	2.95620799
C	5.17019701	-0.17786101	-2.51701808
H	6.21513224	-0.47176799	-2.49918604
C	0.94332898	3.76498508	2.86200690
H	0.97027701	3.65397811	3.94211197
C	1.37318003	5.06922102	0.88218403
H	1.74600601	5.97526217	0.41415501
C	1.42758000	4.92709494	2.26709390
H	1.83900404	5.72322607	2.88014603
C	-3.72862792	-1.76277101	-1.22487497
C	-3.90103412	-0.35305300	0.68145502
C	-5.14672518	-1.19665301	-1.15015900
H	-3.69083905	-2.85089803	-1.12922800
H	-3.19623089	-1.46505499	-2.13249493
C	-5.29779911	-0.83989900	0.33258200
H	-3.73862600	0.68375999	0.37081900
H	-3.62075496	-0.47203401	1.72843003
H	-5.22329283	-0.29025599	-1.75729597
H	-5.89187384	-1.91458595	-1.49899304
H	-6.05705404	-0.07540200	0.51060599
H	-5.54986906	-1.72741997	0.92153901
O	-3.03580594	-1.20750594	-0.09030000

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	23.2999	24.4300	27.4451
Red. masses	--	5.9961	5.7961	5.6301
Frc consts	--	0.0019	0.0020	0.0025
IR Inten	--	1.5276	1.9829	0.0868

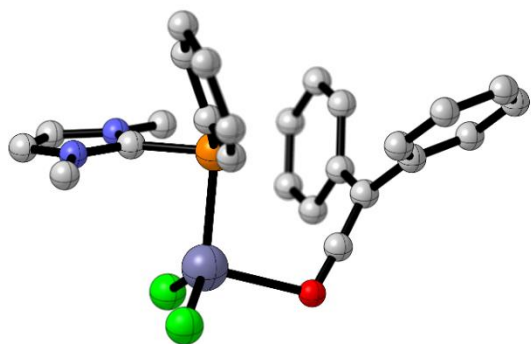
Thermochemistry

Sum of electronic and zero-point Energies	=	-4423.717263
Sum of electronic and thermal Energies	=	-4423.680403
Sum of electronic and thermal Enthalpies	=	-4423.679459
Sum of electronic and thermal Free Energies	=	-4423.789130

HF = -4424.26895883

II:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	2.77408791	-2.80904102	1.97621596
H	2.76084089	-3.80417490	2.38835692
C	3.80605292	-2.00339699	1.63277495
H	4.87090015	-2.15280604	1.70017898
C	1.91352296	-0.91847497	1.15832603
P	0.63919199	0.22242101	0.54483902
Zn	1.11407995	-0.50206000	-1.67266297
C	1.41870999	1.84465098	0.90231800
C	1.74308002	2.18079901	2.22464299
C	1.60161602	2.80744696	-0.09652500
C	2.27186108	3.42906404	2.53347301
H	1.58160996	1.45395303	3.01669788
C	2.10545301	4.06770182	0.21865800
H	1.39091599	2.56327510	-1.13368905
C	2.45011592	4.37968588	1.52986503
H	2.52899694	3.66583991	3.56157494
H	2.24608397	4.79930019	-0.57086998
H	2.85559797	5.35747194	1.77014995
N	3.26536703	-0.84354597	1.12025297
N	1.61569703	-2.12173200	1.69497800
C	0.27266300	-2.67431211	1.82026696
H	-0.02013800	-3.13140988	0.87280899
H	0.27527201	-3.41679001	2.61852503
H	-0.42746800	-1.87178397	2.05791712
C	4.04795408	0.23476100	0.52542198
H	4.06207609	1.10673404	1.18102396
H	5.06061506	-0.13519099	0.36803699
H	3.61719108	0.51252300	-0.43924400
Cl	1.00347197	-2.72673512	-1.69716406
Cl	2.43291402	0.69924200	-2.95946503
O	-0.98578602	-0.19993100	-2.60829806
C	-1.79461002	-0.14649101	-1.75531399
C	-2.64683294	-0.08742600	-0.75515503
C	-3.20572305	1.24869001	-0.40545601
C	-2.37382293	2.36828089	-0.31449100
C	-4.57522202	1.39184296	-0.15814100
C	-2.90434790	3.61518502	0.00078300
H	-1.30483997	2.26202106	-0.47478399
C	-5.09924078	2.63595390	0.17208301
H	-5.22326422	0.52320600	-0.22415400
C	-4.26688194	3.75179505	0.24597600
H	-2.24484992	4.47450876	0.06655900
H	-6.16295385	2.73807192	0.36232600

H	-4.68135881	4.72271299	0.49763700
C	-2.86989307	-1.31529498	0.04886600
C	-3.21201992	-1.20162702	1.40132797
C	-2.68375301	-2.58937693	-0.50007498
C	-3.36705589	-2.34125400	2.18380404
H	-3.34437394	-0.21825100	1.83989501
C	-2.82495093	-3.72395301	0.29071400
H	-2.41643095	-2.70010400	-1.54701698
C	-3.17049694	-3.60637689	1.63488996
H	-3.63492203	-2.23633504	3.23071909
H	-2.66863298	-4.70240211	-0.15173700
H	-3.29246211	-4.49412918	2.24733305

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	19.0236	22.5334	30.2675
Red. masses	--	6.1143	6.0035	8.1088
Frc consts	--	0.0013	0.0018	0.0044
IR Inten	--	0.2689	0.4007	0.6644

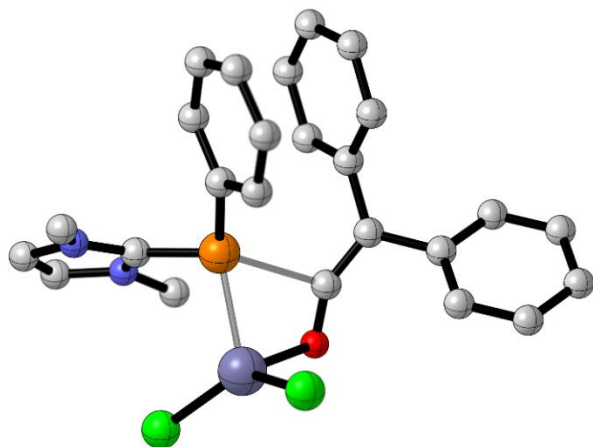
Thermochemistry

Sum of electronic and zero-point Energies	=	-4191.380190
Sum of electronic and thermal Energies	=	-4191.348090
Sum of electronic and thermal Enthalpies	=	-4191.347146
Sum of electronic and thermal Free Energies	=	-4191.447324

HF = -4191.80901653

TS_{II-10}:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	-4.36203623	0.36267999	-2.03950191
H	-4.88250017	0.14698499	-2.95759606
C	-4.80811310	0.85760897	-0.86107302
H	-5.79288721	1.16858494	-0.55370700
C	-2.62330508	0.46595401	-0.64861399
P	-0.97878200	0.12205600	0.00639800
Zn	-1.00956297	-2.22285700	0.54344499

C	-0.62017399	1.46483696	1.16510105
C	-0.87690198	2.80656409	0.86019099
C	0.06223500	1.14490604	2.34478498
C	-0.48597801	3.81125808	1.73705006
H	-1.36029899	3.06631804	-0.07750100
C	0.47297999	2.15785098	3.20609999
H	0.26989701	0.10525300	2.58626604
C	0.19460000	3.48910189	2.90930390
H	-0.68861401	4.84934998	1.49268794
H	1.00421298	1.90218198	4.11734390
H	0.51107901	4.27496386	3.58790112
N	-3.72716403	0.90890801	-0.00594500
N	-3.01131296	0.13888501	-1.89855397
C	-2.15958691	-0.51161897	-2.88501096
H	-2.02614808	-1.56198096	-2.61324406
H	-2.63812590	-0.43218899	-3.86061096
H	-1.19142306	-0.01024100	-2.90475297
C	-3.80119491	1.22581601	1.41372097
H	-3.35900497	2.20211792	1.61722803
H	-4.84944582	1.21584105	1.71012902
H	-3.25722194	0.46382201	1.97542906
Cl	-2.85947490	-3.04018807	-0.34481299
Cl	0.15854500	-2.77307296	2.30778098
O	0.42783099	-2.06194210	-1.15082002
C	0.90429300	-0.95924002	-1.01466298
C	1.94485998	-0.12407800	-0.92090303
C	3.26569104	-0.77356899	-0.66241002
C	3.38818789	-1.83742797	0.23756000
C	4.40938282	-0.30018499	-1.31678605
C	4.62837219	-2.42651296	0.46076700
H	2.51562405	-2.19728088	0.77662098
C	5.64804888	-0.88534099	-1.08160901
H	4.32245302	0.53008997	-2.01109290
C	5.76129723	-1.95417404	-0.19547901
H	4.70647001	-3.24992394	1.16362596
H	6.52666998	-0.50749302	-1.59555995
H	6.72837877	-2.41298699	-0.01493600
C	1.85189402	1.34684205	-1.03359699
C	2.50469995	2.15794492	-0.09667000
C	1.13118196	1.96091795	-2.06232500
C	2.41567492	3.54125309	-0.17404100
H	3.06695890	1.69036102	0.70515299
C	1.03623998	3.34806800	-2.13698506
H	0.66696799	1.34198594	-2.82379103
C	1.67752194	4.14239120	-1.19222796
H	2.91343188	4.15306711	0.57146603
H	0.47694600	3.80722094	-2.94678402
H	1.60846198	5.22416019	-1.25208998

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Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	-169.1290	18.6976	33.0813
Red. masses	--	11.0041	6.1710	5.3972
Frc consts	--	0.1855	0.0013	0.0035
IR Inten	--	127.3982	0.7300	1.7384

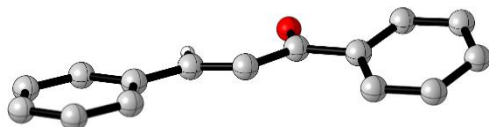
Thermochemistry

Sum of electronic and zero-point Energies = -4191.360750
 Sum of electronic and thermal Energies = -4191.330009
 Sum of electronic and thermal Enthalpies = -4191.329065
 Sum of electronic and thermal Free Energies = -4191.424893

HF = -4191.79005447

Trans-chalcone:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	-1.25967097	-0.81579798	0.11608000
H	-1.21059597	-1.89163697	0.27990499
C	-0.08322700	-0.18374699	-0.00420700
H	-0.03034200	0.88302100	-0.19232599
C	-2.60081792	-0.22922400	0.03818300
C	-3.71058297	-1.08097899	0.11135400
C	-2.82543993	1.14702797	-0.11233900
C	-5.00475597	-0.57900000	0.02966500
H	-3.55075693	-2.14885902	0.23148200
C	-4.11643887	1.64952898	-0.19251600
H	-1.98556495	1.83274198	-0.16292700
C	-5.21106005	0.78819501	-0.12375200
H	-5.85077381	-1.25658798	0.08483000
H	-4.27262878	2.71711397	-0.31002399
H	-6.21930695	1.18482196	-0.18880500
C	1.18072903	-0.95947403	0.07087100
O	1.17198098	-2.17946100	0.14171200
C	2.48632407	-0.22089700	0.03017100
C	3.63692498	-0.95699698	-0.27143300
C	2.60326099	1.14592695	0.29962200
C	4.87728024	-0.33623201	-0.32398701
H	3.52934003	-2.01947403	-0.46108699
C	3.84844995	1.76581097	0.25958201
H	1.73129404	1.73336899	0.56786603
C	4.98477888	1.02818894	-0.05940800
H	5.76305580	-0.91374302	-0.56904602
H	3.93172503	2.82573104	0.47772300
H	5.95418978	1.51520300	-0.09860500

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	21.3746	35.6032	54.6247
Red. masses	--	4.2064	4.0361	4.8915
Frc consts	--	0.0011	0.0030	0.0086
IR Inten	--	0.5612	0.3240	0.2210

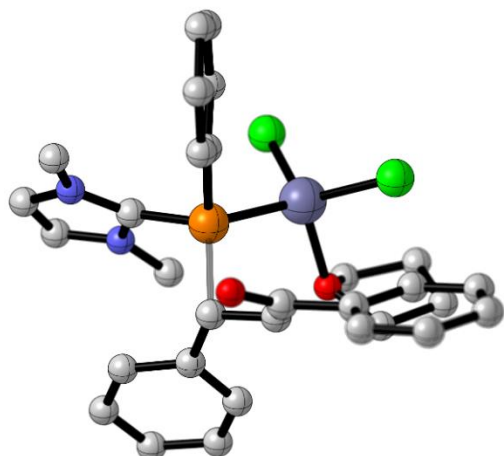
Thermochemistry

Sum of electronic and zero-point Energies = -653.591279
 Sum of electronic and thermal Energies = -653.578288
 Sum of electronic and thermal Enthalpies = -653.577344
 Sum of electronic and thermal Free Energies = -653.633380

HF = -653.819085164

TS_{III-IV}:

Structure



Cartesian Coordinates

Element	X	Y	Z
Zn	0.65129799	1.04729605	-1.44320297
Cl	-1.32242799	1.51001704	-2.31566811
Cl	2.48806405	0.85056001	-2.74221897
O	1.06145799	2.74319601	-0.28337300
C	-0.08633800	3.51536989	0.13160101
C	1.97495401	3.70075488	-0.85434800
C	-0.24723400	4.62558317	-0.91884398
H	-0.93915302	2.83806491	0.18157201
H	0.13037100	3.91876602	1.12731600
C	1.08041406	4.58959484	-1.70914400
H	2.44442701	4.25272799	-0.02985000
H	2.72822690	3.14864397	-1.41629303
H	-0.41141400	5.59176493	-0.43608901
H	-1.09333003	4.41084480	-1.57251298
H	1.51484704	5.57924604	-1.86447597
H	0.93028897	4.11917782	-2.68439889
P	0.60324901	-0.87420398	-0.02773200
C	-0.45230699	-0.68696302	1.79396701
H	-0.58249098	-1.72781098	2.10351491
C	-2.86554193	-0.91815901	1.45989501
C	-4.17408419	-0.27347499	1.09257901
C	-5.34662819	-0.77121598	1.66599095
C	-4.25717878	0.77275997	0.16953200
C	-6.57864189	-0.20847400	1.35469103
H	-5.26711607	-1.60530996	2.35558605
C	-5.49313116	1.32572401	-0.15406100
H	-3.36131597	1.12702096	-0.33300400
C	-6.65449095	0.84465498	0.44443899
H	-7.48300695	-0.59465200	1.81599903

H	-5.54759121	2.12535405	-0.88671601
H	-7.61718416	1.28152895	0.19532301
C	0.57806998	0.03023300	2.61949492
C	1.63764799	-0.68487197	3.18938994
C	0.52028900	1.40908301	2.83390594
C	2.63225102	-0.03959300	3.91602302
H	1.68438804	-1.76331306	3.05200505
C	1.51734805	2.06101704	3.55397010
H	-0.32309601	1.96889699	2.44820094
C	2.58238101	1.34217501	4.09036684
H	3.44275689	-0.61602998	4.35204983
H	1.45341003	3.13410211	3.70753193
H	3.35641503	1.85081804	4.65647984
O	-2.86414099	-2.12873411	1.77572501
C	-1.70306396	-0.10297400	1.46029794
H	-1.78539002	0.95170599	1.22790504
C	-0.15277000	-2.12912297	-1.11622202
C	0.39057100	-2.28795195	-2.39967489
C	-1.22848296	-2.92379403	-0.71136999
C	-0.11156600	-3.26555395	-3.25166702
H	1.20239699	-1.64860201	-2.73798490
C	-1.73446596	-3.88639998	-1.58169794
H	-1.68694103	-2.80314398	0.26895699
C	-1.17372000	-4.06878901	-2.84207201
H	0.31907201	-3.38643098	-4.24046803
H	-2.57644391	-4.49295187	-1.26404095
H	-1.57167006	-4.82471704	-3.51210403
C	2.28605199	-1.55835104	0.20511800
C	4.41736412	-1.64353502	0.86412001
C	3.97911906	-2.91755390	0.73489898
H	5.37878990	-1.25205600	1.15205705
H	4.48339176	-3.85764790	0.88622397
N	3.36649704	-0.81902802	0.54473603
N	2.66154194	-2.85576105	0.34128699
C	3.45342803	0.63789201	0.59164298
H	4.26069689	0.90170300	1.27380502
H	3.64459896	1.01875997	-0.41321999
H	2.52701712	1.05787599	0.98254800
C	1.82620597	-4.04060507	0.16368601
H	1.58307505	-4.18457508	-0.88946801
H	2.38369608	-4.89779186	0.54012603
H	0.90126199	-3.93453503	0.72954100

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	-206.9488	18.6559	22.7442
Red. masses	--	7.9681	5.9522	5.6408
Frc consts	--	0.2011	0.0012	0.0017
IR Inten	--	389.4737	0.3581	0.9740

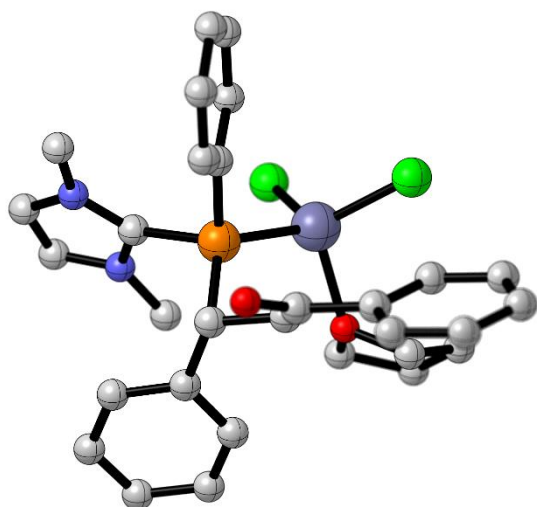
Thermochemistry

Sum of electronic and zero-point Energies	=	-4462.931632
Sum of electronic and thermal Energies	=	-4462.894161
Sum of electronic and thermal Enthalpies	=	-4462.893217
Sum of electronic and thermal Free Energies	=	-4463.003633

HF = -4463.51156913

IV:

Structure



Cartesian Coordinates

Element	X	Y	Z
Zn	-0.29974401	-0.84463799	-1.68313503
Cl	1.60122502	-0.78241903	-2.78870296
Cl	-2.22141194	-0.84056997	-2.85636711
O	-0.22247399	-2.61595201	-0.60525799
C	1.05894899	-3.27092695	-0.48016199
C	-1.21929204	-3.64449191	-0.80263197
C	0.97908199	-4.38123608	-1.51043797
H	1.83444405	-2.53053308	-0.67614198
H	1.15376103	-3.65577793	0.54336202
C	-0.47017100	-4.87232924	-1.35399699
H	-1.68961704	-3.84265709	0.16735800
H	-1.95975494	-3.24065304	-1.49587905
H	1.71674097	-5.16743517	-1.33873200
H	1.14622998	-3.95108008	-2.50186110
H	-0.52427202	-5.70155716	-0.64353901
H	-0.89453202	-5.21101093	-2.30054092
P	-0.58884001	0.81323701	0.02756200
C	-0.02625000	0.50922197	1.74237394
H	0.08554200	1.46127295	2.27475595
C	2.43538809	0.84926301	1.72645402
C	3.80730104	0.37939301	1.32362998
C	4.88070393	0.65444303	2.17351294
C	4.04530001	-0.29228300	0.12144700
C	6.16450787	0.23041201	1.84990895
H	4.68319416	1.20733297	3.08617592
C	5.33327007	-0.70523697	-0.20929600
H	3.23213005	-0.44913501	-0.58189601
C	6.39391279	-0.45415601	0.65750402
H	6.99001884	0.43955800	2.52443409
H	5.50732803	-1.20922303	-1.15552998
H	7.39829588	-0.77795303	0.39968899
C	-0.93569702	-0.41884300	2.51235795
C	-2.07907891	0.08950100	3.13774896
C	-0.69243503	-1.79150403	2.58128905
C	-2.97259593	-0.75273299	3.79158401

H	-2.26581597	1.16124296	3.11320305
C	-1.58642006	-2.63935399	3.23002911
H	0.21120100	-2.18644595	2.13148689
C	-2.73409796	-2.12565398	3.82940698
H	-3.84994698	-0.33773899	4.27877092
H	-1.37960899	-3.70437288	3.27987409
H	-3.42642498	-2.78663206	4.34133291
O	2.34012008	1.89169896	2.41938710
C	1.33078897	0.08665600	1.29737604
H	1.47354102	-0.89763600	0.87012601
C	0.11780200	2.33870602	-0.65136099
C	-0.18496899	2.60190201	-1.99382699
C	0.90650600	3.22998691	0.08001100
C	0.26528001	3.77548003	-2.58963799
H	-0.77026999	1.89704597	-2.58098602
C	1.35704505	4.39666510	-0.53065097
H	1.21201503	3.00492501	1.10056496
C	1.03017199	4.67824602	-1.85477304
H	0.03379500	3.97169995	-3.63131499
H	1.98131096	5.08057499	0.03511300
H	1.39024305	5.58974314	-2.32159710
C	-2.43490696	1.31106305	0.10656700
C	-4.62785101	1.03733802	0.42213199
C	-4.38132620	2.36777806	0.39670900
H	-5.54723787	0.48952901	0.54681802
H	-5.04633999	3.21050096	0.49113300
N	-3.42245889	0.40401599	0.25281999
N	-3.02606201	2.52436495	0.21416400
C	-3.30680203	-1.05184102	0.28229499
H	-3.83751297	-1.41795194	1.16220105
H	-3.70795298	-1.46170795	-0.64395797
H	-2.26277709	-1.33305895	0.38487899
C	-2.38833809	3.84149194	0.18824500
H	-1.97151899	4.04627705	-0.79735702
H	-3.15190196	4.57966423	0.43098500
H	-1.59239697	3.88820291	0.92912000

Harmonic Frequencies

		1	2	2
		A	A	A
Frequencies	--	16.4031	21.2842	26.5073
Red. masses	--	4.8352	5.7282	3.1689
Frc consts	--	0.0008	0.0015	0.0013
IR Inten	--	3.1760	1.6024	1.4793

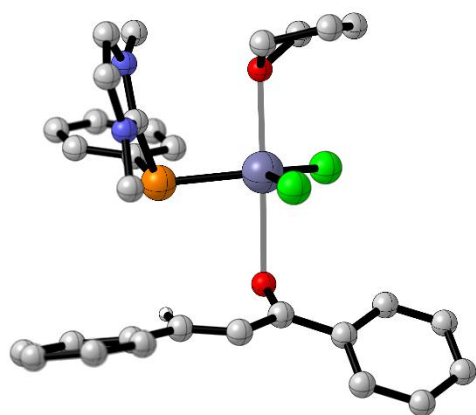
Thermochemistry

Sum of electronic and zero-point Energies	=	-4462.933552
Sum of electronic and thermal Energies	=	-4462.895475
Sum of electronic and thermal Enthalpies	=	-4462.894531
Sum of electronic and thermal Free Energies	=	-4463.007161

HF = -4463.51417401

TS_{III-v}:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	2.42557812	2.29950809	2.66854692
H	2.17173910	2.87922311	3.54040599
C	3.57341790	1.67663300	2.31833100
H	4.52229309	1.60622799	2.82393193
C	2.08338690	1.30645800	0.68837798
P	1.14049006	0.81347102	-0.78231901
C	2.49717903	0.49034101	-1.97644997
C	3.33552408	1.54369295	-2.36851001
C	2.66630292	-0.76058602	-2.58127308
C	4.35131788	1.34131503	-3.29720211
H	3.19250894	2.52961993	-1.93292105
C	3.66906595	-0.95568800	-3.52841091
H	2.01804304	-1.58905494	-2.30703402
C	4.52122593	0.08698400	-3.87994289
H	5.00007486	2.16570091	-3.57845306
H	3.78609610	-1.93271601	-3.98700595
H	5.30564785	-0.07171300	-4.61354780
N	3.35097790	1.05797601	1.10392106
N	1.52061200	2.07223511	1.65559602
C	0.15634599	2.58337212	1.61194599
H	-0.55702102	1.75986195	1.70574903
H	0.02456200	3.28818202	2.43270206
H	-0.00205000	3.09403896	0.66076100
C	4.31865978	0.17617600	0.46561801
H	4.83211279	0.68469298	-0.35196200
H	5.03663778	-0.13584501	1.22491300
H	3.79785705	-0.69889700	0.08308100
Cl	-1.14376104	-0.84943497	1.82091701
Cl	0.29690099	-3.19878602	-0.99747598
C	-2.79367304	-0.43053100	-0.97923702
C	-3.82082009	-1.49597597	-0.81743401
C	-3.41397691	-2.82958794	-0.93336701
C	-5.16717100	-1.20027304	-0.58218902
C	-4.34488916	-3.85107207	-0.79799801
H	-2.36558008	-3.04596710	-1.11587298
C	-6.09862089	-2.22549200	-0.46364301
H	-5.49909401	-0.16882300	-0.51377499
C	-5.68606901	-3.55176806	-0.56546998
H	-4.02303123	-4.88455391	-0.87630397
H	-7.14447212	-1.99151301	-0.29178801
H	-6.41260004	-4.35267115	-0.46537200

O	-1.72656095	-0.67335403	-1.53557897
C	-2.43999290	3.35051489	-0.38463500
C	-1.79069495	4.36503983	-1.10050905
C	-3.09209108	3.68767190	0.81038702
C	-1.80322599	5.67987490	-0.64668500
H	-1.26757002	4.11078215	-2.01814604
C	-3.10253906	4.99990988	1.26506603
H	-3.57244897	2.91273594	1.39956605
C	-2.45998597	6.00118017	0.53776902
H	-1.29688704	6.45293713	-1.21616697
H	-3.60825706	5.24281120	2.19447303
H	-2.46782303	7.02537584	0.89744502
C	-3.07469296	0.92484301	-0.44851601
H	-3.84618902	1.02707803	0.30731401
C	-2.35523891	1.97043896	-0.87488502
H	-1.60842800	1.77782094	-1.64224303
Zn	0.22062799	-1.21931803	0.04761900
C	2.63401294	-3.05074692	1.34468603
O	2.06888795	-1.73523998	1.38066006
C	2.00076699	-1.40897095	2.77122998
C	1.54391301	-2.69798589	3.46847391
C	1.88785505	-3.80569506	2.44322705
H	2.48173404	-3.45238304	0.34423599
H	3.71010208	-2.97126102	1.56382895
H	3.00324106	-1.10185897	3.10570002
H	1.30242705	-0.58010900	2.88657808
H	2.05593610	-2.83575010	4.42424011
H	0.46876901	-2.65763211	3.65097904
H	2.49022508	-4.61174583	2.86866212
H	0.97691000	-4.23758411	2.02268291

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	-64.6238	7.3639	15.4768
Red. masses	--	16.0700	5.7777	6.1291
Frc consts	--	0.0395	0.0002	0.0009
IR Inten	--	42.8851	0.4151	0.7017

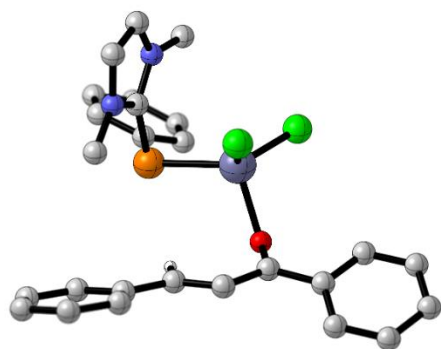
Thermochemistry

Sum of electronic and zero-point Energies	=	-4462.963485
Sum of electronic and thermal Energies	=	-4462.924950
Sum of electronic and thermal Enthalpies	=	-4462.924006
Sum of electronic and thermal Free Energies	=	-4463.040333

HF = -4463.54246357

V:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	2.41229796	1.63702500	3.11124301
H	2.21176600	2.38399911	3.86076188
C	3.12159491	0.48685101	3.17053604
H	3.67467093	0.03988500	3.97976804
C	2.27275801	0.64890802	1.11224997
P	1.68202603	0.34237000	-0.58045202
C	3.13520002	-0.53022599	-1.28660703
C	4.38170195	0.11052500	-1.32762694
C	3.01674390	-1.80184495	-1.85766602
C	5.48860788	-0.51832801	-1.88800001
H	4.48628283	1.10796797	-0.90780699
C	4.12015390	-2.42002702	-2.44089699
H	2.07010293	-2.33118296	-1.81082904
C	5.35891914	-1.78679097	-2.45057893
H	6.44978094	-0.01296700	-1.89765298
H	4.00968885	-3.40940809	-2.87362289
H	6.21991014	-2.27570510	-2.89577603
N	3.02358794	-0.11903400	1.93626404
N	1.91196096	1.73374104	1.83302796
C	0.97697401	2.75316691	1.38418102
H	-0.04412200	2.38485193	1.51372004
H	1.13329399	3.65737891	1.97305906
H	1.15546000	2.96157908	0.32856199
C	3.54119110	-1.45019305	1.63767695
H	4.40578604	-1.38828003	0.97526401
H	3.82244110	-1.91681302	2.58119607
H	2.76127791	-2.05185294	1.16463101
Cl	-0.79839301	-0.26466101	2.14833498
Cl	0.52428699	-3.37212205	0.27817500
C	-2.68930197	-0.55539697	-0.70253497
C	-3.86638999	-1.41263103	-0.44705999
C	-3.64031601	-2.75677705	-0.12301600
C	-5.17647123	-0.92632198	-0.52722102
C	-4.71586514	-3.59654498	0.13110600
H	-2.61968493	-3.12266803	-0.06186400
C	-6.24951792	-1.77523899	-0.28770599
H	-5.36350822	0.10737200	-0.79988700
C	-6.01849318	-3.10785198	0.04671400
H	-4.53839016	-4.63393879	0.39379701
H	-7.26445293	-1.39880598	-0.36252099
H	-6.85749197	-3.76846290	0.24281999
O	-1.60309005	-1.09325600	-0.97282898
C	-1.67107296	3.12675405	-0.97761798

C	-0.61735100	3.74727297	-1.66348600
C	-2.52069712	3.91691089	-0.19004899
C	-0.42245501	5.12084103	-1.57441998
H	0.05881300	3.13594604	-2.25502300
C	-2.32445192	5.28808880	-0.10025400
H	-3.32681608	3.45410800	0.37022600
C	-1.27609801	5.89411592	-0.79237998
H	0.39860401	5.58626795	-2.11014390
H	-2.98507094	5.88810921	0.51729000
H	-1.12332904	6.96595383	-0.71550798
C	-2.79982495	0.90496498	-0.61123699
H	-3.67363000	1.32486296	-0.12649700
C	-1.80072904	1.67373800	-1.07638299
H	-0.97281599	1.16543496	-1.56672204
Zn	0.04646900	-1.19155705	0.25742200

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	4.5528	20.6132	28.7556
Red. Masses	--	7.1961	6.1658	5.9846
Frc consts	--	0.0001	0.0015	0.0029
IR Inten	--	1.4861	0.4024	0.4687

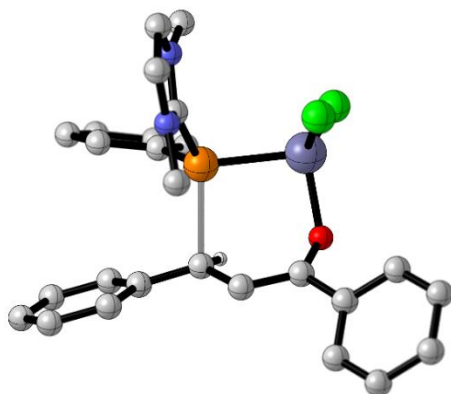
Thermochemistry

Sum of electronic and zero-point Energies	=	-4230.681962
Sum of electronic and thermal Energies	=	-4230.648837
Sum of electronic and thermal Enthalpies	=	-4230.647892
Sum of electronic and thermal Free Energies	=	-4230.752277

HF = -4231.14065401

TS_{v-vj}:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	0.76212299	-1.28321695	3.87659788
H	0.32230201	-1.11288702	4.84487200
C	1.59011102	-2.26201200	3.43625212
H	2.02096605	-3.10575604	3.94929290
C	1.16387403	-0.91204500	1.72221100
P	0.90735799	-0.32750201	0.03313300

C	2.56812501	-0.35242501	-0.68240303
C	3.66507411	0.21857800	-0.02065600
C	2.72965598	-0.83441800	-1.98775005
C	4.90616512	0.28267199	-0.64215201
H	3.54004788	0.62843901	0.97798097
C	3.97050500	-0.74427801	-2.61389589
H	1.89528501	-1.31066406	-2.49646902
C	5.05856895	-0.19172700	-1.94421995
H	5.75050783	0.72088099	-0.11919700
H	4.08791685	-1.12469399	-3.62349391
H	6.02514601	-0.13063900	-2.43427110
N	1.82706404	-2.02501607	2.10069394
N	0.52075303	-0.45124701	2.80868411
C	-0.42810401	0.65235001	2.77657199
H	-1.30546200	0.35454300	2.19421101
H	-0.72307599	0.88464701	3.79926300
H	0.05146100	1.52146900	2.32586408
C	2.51746988	-2.93414807	1.19180202
H	3.44204712	-2.48273492	0.82970500
H	2.73576999	-3.85364509	1.73317897
H	1.86623502	-3.15995312	0.34257600
Cl	-1.86158204	-2.26818204	1.18215895
Cl	-0.11317500	-3.20664406	-2.21708894
C	-2.27462792	0.83162600	-0.87187803
C	-3.73552990	0.99452698	-0.62881303
C	-4.54069805	-0.14661001	-0.56595200
C	-4.31938410	2.25522304	-0.46744201
C	-5.90397692	-0.02732100	-0.32425800
H	-4.08268213	-1.12155998	-0.68846798
C	-5.68528414	2.37300611	-0.23714200
H	-3.70769691	3.14838290	-0.55388999
C	-6.47898817	1.23070598	-0.16029900
H	-6.51877213	-0.91966897	-0.26388299
H	-6.13298512	3.35570097	-0.12568100
H	-7.54547787	1.32288504	0.02130700
O	-1.89503205	-0.19207700	-1.53643894
C	0.96677899	2.75097299	-0.26660699
C	2.15064812	2.90709400	-0.99822402
C	0.73545998	3.61112094	0.81475103
C	3.08430600	3.87573099	-0.64702898
H	2.34534192	2.25500488	-1.84435999
C	1.66739404	4.57976198	1.16605306
H	-0.18747699	3.53601694	1.38133502
C	2.84906292	4.71209621	0.43970001
H	3.99823689	3.97288489	-1.22403800
H	1.46744001	5.23911619	2.00489497
H	3.57694507	5.46827316	0.71563703
C	-1.37055397	1.76794100	-0.35130900
H	-1.73265803	2.51125789	0.34767300
C	0.00289100	1.69420004	-0.66222501
H	0.21909399	1.24761701	-1.63514602
Zn	-0.88762599	-1.70954394	-0.78487700

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	-201.7199	6.1216	27.3902
Red. Masses	--	10.1574	6.7672	5.3731

Frc consts	--	0.2435	0.0001	0.0024
IR Inten	--	337.2915	1.3862	0.2003

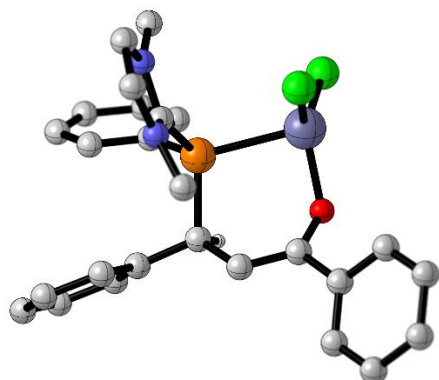
Thermochemistry

Sum of electronic and zero-point Energies	=	-4230.660736
Sum of electronic and thermal Energies	=	-4230.628690
Sum of electronic and thermal Enthalpies	=	-4230.627746
Sum of electronic and thermal Free Energies	=	-4230.728196

HF = -4231.11877314

VI:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	0.55573797	-0.57604301	3.88501596
H	0.07057600	-0.31482199	4.81067514
C	1.49711895	-1.50364399	3.60500002
H	2.00940490	-2.20699096	4.24021006
C	0.95501399	-0.48379201	1.70121706
P	0.80664599	-0.32783100	-0.12407400
C	2.53794003	-0.38214499	-0.66616201
C	3.55064201	0.37864399	-0.06730500
C	2.83195710	-1.19208598	-1.76776397
C	4.84933186	0.31211400	-0.55569202
H	3.32253408	1.02869701	0.77270800
C	4.13357306	-1.23995304	-2.26176190
H	2.05247998	-1.80711699	-2.21261001
C	5.14019394	-0.49529099	-1.65510404
H	5.63231993	0.89965200	-0.08725600
H	4.35950708	-1.87166095	-3.11442709
H	6.15469790	-0.54301000	-2.03847790
N	1.73127198	-1.44710100	2.25065303
N	0.22294401	0.04015300	2.70038700
C	-0.96513999	0.88290602	2.59304309
H	-1.17508602	1.10261095	1.54457796
H	-1.81097198	0.31714800	2.98568392
H	-0.81580001	1.80448401	3.15881395
C	2.50897002	-2.46164894	1.53641999
H	3.44990301	-2.04865098	1.17459095
H	2.69963598	-3.27594304	2.23382998
H	1.92416000	-2.84782410	0.69821203
Cl	-1.74173200	-2.33701992	1.37703800

Cl	-0.05574200	-3.47990298	-1.94681394
C	-2.19929600	0.71726900	-0.96957099
C	-3.64275408	1.02691102	-0.73971999
C	-4.51083279	-0.01407300	-0.39806199
C	-4.14888811	2.32560301	-0.84549600
C	-5.85253286	0.24464899	-0.14264800
H	-4.11818600	-1.02233303	-0.31995100
C	-5.49393320	2.58241296	-0.59916902
H	-3.48857307	3.13267493	-1.14958298
C	-6.34879684	1.54272497	-0.24252300
H	-6.51441002	-0.57039100	0.13384400
H	-5.87832594	3.59324789	-0.69874102
H	-7.39924908	1.74121499	-0.05229500
O	-1.93087602	-0.42980999	-1.53672898
C	1.14535606	2.48867512	-0.45226100
C	2.10541105	2.89829111	-1.38047504
C	1.10419703	3.13262296	0.78737003
C	3.00812101	3.91241503	-1.07584202
H	2.15664291	2.40528607	-2.34696198
C	2.00733304	4.14373302	1.09798002
H	0.35396501	2.84745193	1.51605296
C	2.96688890	4.53513908	0.16754299
H	3.74685502	4.21244192	-1.81206799
H	1.95750105	4.63111210	2.06681800
H	3.67260098	5.32347679	0.40902001
C	-1.24141002	1.60132396	-0.56323802
H	-1.52104497	2.54572392	-0.11091600
C	0.21701200	1.34610295	-0.78309602
H	0.37132600	1.07006395	-1.83995795
Zn	-1.04182899	-1.91304803	-0.73413801

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	20.7490	24.0442	34.1205
Red. Masses	--	7.4417	4.8753	5.6452
Frc consts	--	0.0019	0.0017	0.0039
IR Inten	--	1.6996	0.9136	0.3928

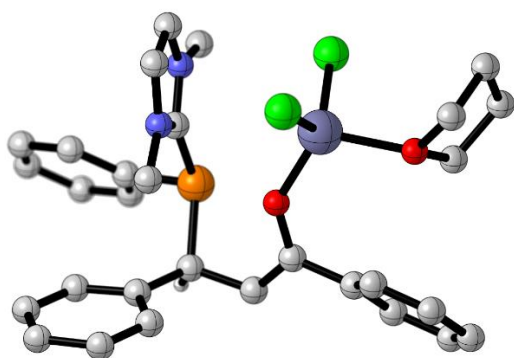
Thermochemistry

Sum of electronic and zero-point Energies	=	-4230.669548
Sum of electronic and thermal Energies	=	-4230.637518
Sum of electronic and thermal Enthalpies	=	-4230.636574
Sum of electronic and thermal Free Energies	=	-4230.735987

HF = -4231.12898809

VII:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	0.45980799	2.13637304	-1.18305397
C	-0.67044801	1.58032000	-0.69137102
H	0.40371400	3.07417011	-1.72474504
O	-0.63406599	0.48991200	0.05093600
C	-1.99130404	2.23141098	-0.92842001
C	-2.36657095	2.66983509	-2.20105505
C	-2.87234211	2.42095590	0.14068501
C	-3.59821296	3.28620410	-2.40301204
H	-1.68940699	2.50735593	-3.03419089
C	-4.10167885	3.03805494	-0.05944300
H	-2.58950901	2.07787991	1.13198698
C	-4.46981478	3.47106910	-1.33242500
H	-3.88024807	3.61568594	-3.39855909
H	-4.77536917	3.18088508	0.77996498
H	-5.43148518	3.95044088	-1.48835695
C	-4.92718506	-0.91121501	0.72033000
C	-5.15003204	-1.53801203	-1.57633698
C	-5.37135983	-2.07782698	-0.14965899
H	-4.58213282	-1.17729402	1.72011399
H	-5.69736719	-0.13154700	0.79090399
H	-6.07915401	-1.15056705	-2.00328708
H	-4.76600599	-2.31479192	-2.23955488
H	-4.71678782	-2.93297100	0.03554100
H	-6.40623999	-2.37154603	0.03971200
O	-3.80504107	-0.37559199	0.00836500
C	-4.12607813	-0.40069601	-1.39559996
H	-3.19495606	-0.56975901	-1.93765795
H	-4.52968693	0.58087999	-1.66346502
C	1.83036995	1.58721697	-0.89557803
H	2.46034908	1.78696203	-1.77614403
C	2.54040790	2.23724103	0.28810599
C	3.91457295	2.06957603	0.49320301
C	1.83493495	3.05438495	1.17472804
C	4.54725409	2.64476895	1.59148598
H	4.49960899	1.48695695	-0.20960200
C	2.46668601	3.63734794	2.26874399
H	0.77590197	3.21745706	1.00404596
C	3.82360196	3.42276502	2.49190402
H	5.61243582	2.49169302	1.73668897
H	1.89332998	4.26049614	2.94826388
H	4.31672192	3.87223506	3.34819102
P	1.78256500	-0.29068601	-1.10719705

C	1.55509305	-1.31772196	0.41313100
C	1.12039304	-2.28837991	2.36680102
C	1.23739004	-3.26932001	1.44260800
H	0.85378402	-2.32446599	3.40915895
H	1.10596800	-4.33482599	1.52239299
C	3.57909489	-0.67620301	-1.34297395
C	4.09177780	-0.48420700	-2.63201904
C	4.44479895	-1.14684296	-0.34796599
C	5.43270493	-0.72680497	-2.91333604
H	3.43112612	-0.14286900	-3.42564893
C	5.78184986	-1.40828097	-0.63138700
H	4.08177280	-1.29221702	0.66546398
C	6.28155899	-1.19235301	-1.91290796
H	5.81232405	-0.56338900	-3.91703200
H	6.43808794	-1.76961505	0.15436500
H	7.32640791	-1.38909805	-2.13066792
N	1.32958698	-1.09247100	1.72062099
N	1.51064897	-2.65853190	0.24487500
C	1.63422704	-3.36637998	-1.02308404
H	0.91529202	-2.95208693	-1.73103905
H	2.65344191	-3.27955103	-1.40478301
H	1.38825703	-4.41208506	-0.84691000
C	1.26742601	0.19749600	2.39907789
H	0.84227598	0.03017900	3.38678503
H	2.26507807	0.63185501	2.47200990
H	0.59699202	0.83891898	1.83243406
Zn	-1.89467001	-0.85151500	0.57886499
Cl	-2.02506804	-0.90692300	2.82315111
Cl	-1.66877103	-2.77142000	-0.59164000

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	11.7456	18.6884	28.9906
Red. Masses	--	5.7356	5.4264	10.8818
Frc consts	--	0.0005	0.0011	0.0054
IR Inten	--	0.1262	0.0582	2.4075

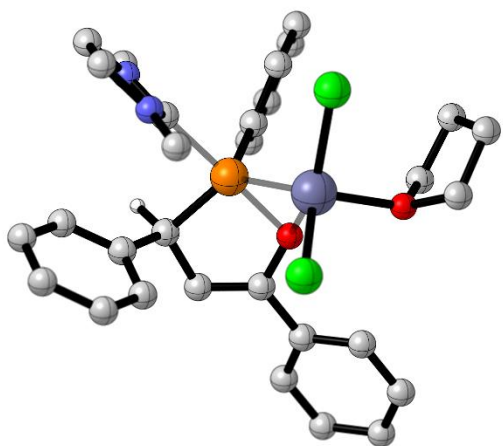
Thermochemistry

Sum of electronic and zero-point Energies	=	-4462.976536
Sum of electronic and thermal Energies	=	-4462.938868
Sum of electronic and thermal Enthalpies	=	-4462.937924
Sum of electronic and thermal Free Energies	=	-4463.049980

HF = -4463.55813809

TS_{VII-VIII}:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	0.28878799	2.28927207	1.52381802
C	1.39160800	1.62539697	1.11974394
H	0.30562600	3.31641889	1.86550105
O	1.23438799	0.39725700	0.63978797
C	2.77324891	2.15372801	1.11844802
C	3.18741107	3.13096094	2.02747893
C	3.68334794	1.66755497	0.17415699
C	4.48589420	3.62630105	1.98505402
H	2.49284410	3.49095106	2.78076601
C	4.97994614	2.16792607	0.13236400
H	3.35564303	0.91056699	-0.53137398
C	5.38572407	3.14727092	1.03576601
H	4.79860306	4.38191509	2.69927502
H	5.67638493	1.79545105	-0.61279702
H	6.39895391	3.53601909	1.00162005
C	2.96530604	-1.98956299	-2.46650100
C	2.71094394	-3.44762897	-0.53620100
C	2.96869898	-3.47408795	-2.05986691
H	2.33338904	-1.76169705	-3.32555795
H	3.97693706	-1.61277604	-2.65501809
H	3.38509107	-4.09876585	0.02498200
H	1.68081903	-3.74426198	-0.32490900
H	2.17529106	-4.01654005	-2.57550406
H	3.92719793	-3.93876696	-2.30462193
O	2.43911409	-1.27244496	-1.33407998
C	2.90043497	-1.98077297	-0.17055200
H	2.32629895	-1.62383699	0.68188798
H	3.95811892	-1.72716200	-0.01925800
C	-1.02359295	1.60544395	1.27860403
H	-1.55990803	1.39676797	2.21711993
C	-1.95417404	2.39349794	0.37417299
C	-3.31815505	2.49390411	0.65504301
C	-1.45841897	2.98958611	-0.78878999
C	-4.17792320	3.15614200	-0.21689500
H	-3.71330595	2.03950906	1.56126499
C	-2.31524801	3.65298891	-1.66068196
H	-0.40153199	2.90534592	-1.02357399
C	-3.67757797	3.73469305	-1.38057601
H	-5.23663807	3.22480106	0.01478500
H	-1.91400397	4.09351206	-2.56753492

H	-4.34493589	4.25291920	-2.06222796
C	-2.57792497	-0.51749003	0.36231101
C	-4.71644592	-1.07906795	0.74607599
C	-4.59404421	-0.78747898	-0.56910902
H	-5.56894016	-1.39237595	1.32631004
H	-5.32118320	-0.78974098	-1.36407995
N	-3.47047091	-0.90249401	1.30709100
N	-3.28152704	-0.44348300	-0.78469902
C	-2.79502511	-0.01864000	-2.09888601
H	-2.03439498	0.75108099	-1.98976004
H	-2.37917995	-0.87621701	-2.63011003
H	-3.63709211	0.41011000	-2.64157701
C	-3.21630812	-1.11243403	2.72788501
H	-4.16694498	-1.03004599	3.25537491
H	-2.77520895	-2.09583592	2.89874911
H	-2.53385091	-0.35324800	3.10366797
Zn	0.48665100	-0.59711498	-1.54109395
Cl	0.65542603	1.03778803	-3.03185391
Cl	-0.46614200	-2.60490608	-2.16970110
P	-0.63759702	-0.07003200	0.48632300
C	-0.33299199	-1.35375404	1.75231004
C	0.18973900	-1.01430404	3.00328994
C	-0.58750898	-2.69478393	1.45234597
C	0.41841900	-2.00030899	3.95648789
H	0.42565399	0.02336800	3.22464991
C	-0.34363800	-3.68124509	2.40600395
H	-0.95928901	-2.96799898	0.46740800
C	0.14830300	-3.33582902	3.66189408
H	0.81991398	-1.72819495	4.92771006
H	-0.53446400	-4.72178411	2.16235805
H	0.33363399	-4.10487080	4.40531111

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	-14.6829	20.8269	29.5115
Red. Masses	--	8.9739	5.7864	4.8980
Frc consts	--	0.0011	0.0015	0.0025
IR Inten	--	3.4801	0.2358	2.2576

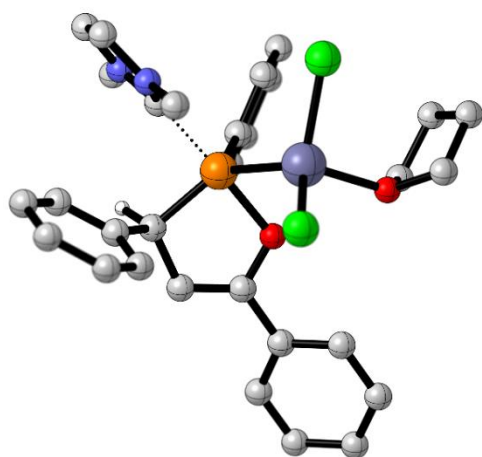
Thermochemistry

Sum of electronic and zero-point Energies	=	-4462.970499
Sum of electronic and thermal Energies	=	-4462.933754
Sum of electronic and thermal Enthalpies	=	-4462.932810
Sum of electronic and thermal Free Energies	=	-4463.040737

HF = -4463.55169526

VIII:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	0.44067299	2.36802197	1.44693398
C	1.51118004	1.65291595	1.04552102
H	0.49628401	3.40534997	1.75100696
O	1.30061603	0.41790599	0.60536098
C	2.91147494	2.12511396	1.00135195
C	3.37882304	3.11353493	1.87141395
C	3.78432393	1.57461298	0.05719300
C	4.69378996	3.55759001	1.79012895
H	2.71238708	3.52232695	2.62520003
C	5.09759903	2.02442193	-0.02422300
H	3.41278100	0.80885702	-0.61683798
C	5.55659103	3.01563907	0.84030199
H	5.04808712	4.32235289	2.47460794
H	5.76565123	1.60291195	-0.76924700
H	6.58300686	3.36365294	0.77521002
C	2.69718504	-2.19208503	-2.54688191
C	2.47921896	-3.58052802	-0.56197000
C	2.65361691	-3.66320992	-2.09598589
H	2.04405499	-1.95959997	-3.38874006
H	3.71637297	-1.86646199	-2.78382397
H	3.15941310	-4.23801804	-0.01578400
H	1.45219898	-3.83384395	-0.28784701
H	1.80877995	-4.18072510	-2.55217600
H	3.57475710	-4.17988491	-2.37710500
O	2.24604201	-1.42184603	-1.41680098
C	2.73858809	-2.11066103	-0.25477600
H	2.22319889	-1.70682800	0.61383599
H	3.81085491	-1.89212406	-0.16346000
C	-0.89160901	1.71186304	1.24192798
H	-1.42299294	1.55187702	2.19217801
C	-1.81009603	2.48789406	0.31571800
C	-3.16738510	2.63926911	0.60583198
C	-1.31100404	3.02237511	-0.87535697
C	-4.01724195	3.29227304	-0.28271401
H	-3.56606889	2.23043799	1.53203499
C	-2.15767097	3.67551708	-1.76446199
H	-0.25982901	2.89880610	-1.11719501
C	-3.51342392	3.80995989	-1.47342598
H	-5.07076693	3.40133905	-0.04302000
H	-1.75426805	4.06650686	-2.69273806

H	-4.17311096	4.32037783	-2.16830707
C	-2.53117394	-0.40595800	0.50952798
C	-4.65712404	-0.90642899	1.03792799
C	-4.60810423	-0.66104501	-0.29065800
H	-5.47828913	-1.18236601	1.67920005
H	-5.37964201	-0.67300099	-1.04249096
N	-3.37591410	-0.73831803	1.51785195
N	-3.30377698	-0.35235500	-0.59415102
C	-2.90224504	0.03930600	-1.94553196
H	-2.06829596	0.73564798	-1.90583801
H	-2.61826801	-0.84616399	-2.51614809
H	-3.74518895	0.55288702	-2.40773392
C	-3.05191398	-0.90167600	2.93063498
H	-3.97163391	-0.77324301	3.50207090
H	-2.62933898	-1.88995099	3.11817098
H	-2.33279705	-0.14794099	3.24312091
Zn	0.30374700	-0.70929098	-1.58203900
Cl	0.48918799	0.84096003	-3.15794110
Cl	-0.76511401	-2.68717790	-2.05176497
P	-0.55131298	-0.00696300	0.51849300
C	-0.24483100	-1.25877702	1.81674695
C	0.34612000	-0.89861798	3.03111696
C	-0.56292802	-2.59796309	1.57558799
C	0.58134198	-1.86084902	4.00670624
H	0.62646401	0.13645400	3.20773506
C	-0.30858001	-3.56202602	2.54912710
H	-0.99613303	-2.88898706	0.62125498
C	0.25320700	-3.19469905	3.76897597
H	1.03406894	-1.57202697	4.95016003
H	-0.54605198	-4.60216808	2.34869790
H	0.44648600	-3.94604897	4.52828312

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	18.8659	30.7673	35.7626
Red. masses	--	7.4249	5.8636	4.8742
Frc consts	--	0.0016	0.0033	0.0037
IR Inten	--	1.4946	0.2430	0.9232

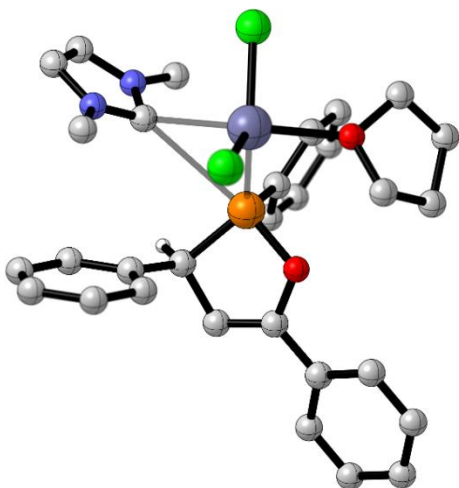
Thermochemistry

Sum of electronic and zero-point Energies	=	-4462.970102
Sum of electronic and thermal Energies	=	-4462.932737
Sum of electronic and thermal Enthalpies	=	-4462.931793
Sum of electronic and thermal Free Energies	=	-4463.041322

HF = -4463.55177557

TS_{VIII-IX}:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	1.62983799	1.96348000	1.33591604
C	2.43724608	1.18884695	0.60010701
H	1.96697295	2.84117293	1.87150002
O	1.82556403	0.18459600	-0.11025800
C	3.89036798	1.29113197	0.39873499
C	4.68630314	2.03873706	1.27375305
C	4.49300194	0.64677000	-0.68594402
C	6.05321884	2.15231705	1.05772305
H	4.23628521	2.52085209	2.13583994
C	5.86243916	0.76111001	-0.89846599
H	3.88002491	0.06404400	-1.36378396
C	6.64618111	1.51536500	-0.03069100
H	6.65976620	2.73551893	1.74322498
H	6.31717014	0.26173499	-1.74809897
H	7.71472502	1.60539806	-0.19786200
C	0.45689499	-3.61850190	-2.00315404
C	2.64320397	-2.59493804	-1.75535095
C	1.86088598	-3.89560294	-1.44436395
H	-0.37332201	-3.97310996	-1.39249206
H	0.33833399	-4.02260399	-3.01645994
H	3.56380010	-2.77635694	-2.31509304
H	2.90009594	-2.07363105	-0.83034998
H	1.82226598	-4.07243681	-0.36668900
H	2.30554795	-4.77593422	-1.91406703
O	0.37046999	-2.19345093	-2.06936502
C	1.64206600	-1.75591302	-2.55390692
H	1.71125996	-0.68115199	-2.38897204
H	1.69781601	-1.95874095	-3.63099694
C	0.15643600	1.64749706	1.22202396
H	-0.31339601	1.48204195	2.19677305
C	-0.58242702	2.75825000	0.50644100
C	-1.59068894	3.46684194	1.15980995
C	-0.22068299	3.12875390	-0.79032600
C	-2.22260690	4.53622007	0.53208601
H	-1.88522804	3.17587399	2.16449094
C	-0.86300403	4.18585587	-1.42556703
H	0.55138099	2.57483506	-1.31643701
C	-1.85973799	4.89776278	-0.76267999
H	-3.00276089	5.08270502	1.05331802

H	-0.58956200	4.44370985	-2.44313097
H	-2.35555601	5.72803402	-1.25580299
C	-2.74962902	0.20120300	0.77155697
C	-4.71992302	-0.05184100	1.88928294
C	-4.93771219	0.82425201	0.88464999
H	-5.38343096	-0.44224000	2.64445710
H	-5.82917118	1.34973598	0.58175802
N	-3.38749790	-0.40914401	1.80858505
N	-3.73162699	0.96774602	0.22699501
C	-3.60379004	1.76019502	-0.98347998
H	-2.55234003	1.93255401	-1.19536495
H	-4.04474401	1.22962105	-1.83069396
H	-4.10009909	2.72239089	-0.84393001
C	-2.79704189	-1.43810403	2.64395189
H	-3.49822402	-1.68999696	3.44139910
H	-2.59697390	-2.32878709	2.04528689
H	-1.86631298	-1.08559000	3.08914208
Zn	-1.21636295	-0.85048401	-1.41095805
Cl	-1.12248802	0.55435401	-3.12736797
Cl	-2.68292499	-2.49435210	-1.05974197
P	0.20182000	-0.00165500	0.35629901
C	0.41786399	-1.21600294	1.69917500
C	0.95598799	-0.90504700	2.95412302
C	0.08183900	-2.54278398	1.41620004
C	1.13892305	-1.90240097	3.90609908
H	1.24268997	0.11404800	3.19010091
C	0.26730499	-3.54015493	2.36801696
H	-0.37383899	-2.78961205	0.46371299
C	0.79391301	-3.22075796	3.61554098
H	1.55558097	-1.65071201	4.87615204
H	-0.01187100	-4.56294298	2.13595104
H	0.93430299	-3.99573112	4.36259508

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	-86.7666	24.2342	30.2528
Red. masses	--	9.0532	5.8693	5.3356
Frc consts	--	0.0402	0.0020	0.0029
IR Inten	--	12.3968	0.3990	0.7798

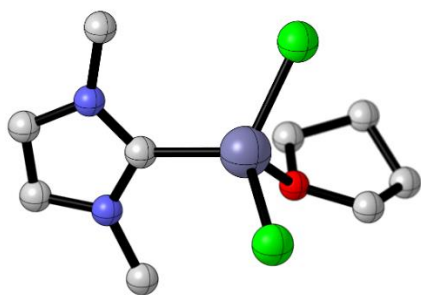
Thermochemistry

Sum of electronic and zero-point Energies	=	-4462.952196
Sum of electronic and thermal Energies	=	-4462.914804
Sum of electronic and thermal Enthalpies	=	-4462.913860
Sum of electronic and thermal Free Energies	=	-4463.023726

HF = -4463.53192277

^{Me}NHC=ZnCl₂THF (5):

Structure



Cartesian Coordinates

Element	X	Y	Z
C	-2.77556801	0.90155399	-0.02855300
C	-3.75411296	0.67750502	-1.17259204
C	-3.03489304	-0.39718199	-1.99296606
C	-1.58647895	0.05984000	-1.90270495
H	-2.78258395	1.90626395	0.39526299
H	-2.92331100	0.17340399	0.77496803
H	-3.88357306	1.59270096	-1.75985801
H	-4.73358393	0.35805300	-0.81135303
H	-3.38647008	-0.46626699	-3.02460790
H	-3.13861990	-1.37477696	-1.51341403
H	-1.34499097	0.81438297	-2.66081309
H	-0.86948198	-0.76206499	-1.96118999
Zn	-0.13066299	-0.24077700	0.74706501
Cl	-0.95731503	-2.32382202	0.60289198
Cl	-0.35542601	1.04237998	2.55071211
O	-1.46172905	0.67702597	-0.60391003
C	1.62349606	0.06260400	-0.19201300
C	3.34851098	1.18667102	-1.09894502
C	3.67912698	-0.12770200	-1.08452404
H	3.89211798	2.04943490	-1.44849896
H	4.56821489	-0.63803297	-1.41772294
N	2.08744693	1.27842402	-0.55076700
N	2.60800791	-0.79539698	-0.52709597
C	2.57069397	-2.23490310	-0.30245000
H	2.81748199	-2.75439906	-1.23045897
H	3.28918195	-2.50833988	0.47310299
H	1.56509602	-2.51704192	0.01351000
C	1.34778297	2.51731110	-0.33202401
H	1.22709501	2.68980694	0.73913002
H	1.89573503	3.34083200	-0.79025000
H	0.35849100	2.43229198	-0.78407300

Harmonic Frequencies

	1	2	3
	A	A	A
Frequencies	-- 25.3373	40.4711	47.3660
Red. masses	-- 4.6512	4.2211	3.7046
Frc consts	-- 0.0018	0.0041	0.0049
IR Inten	-- 2.2893	0.4788	0.5604

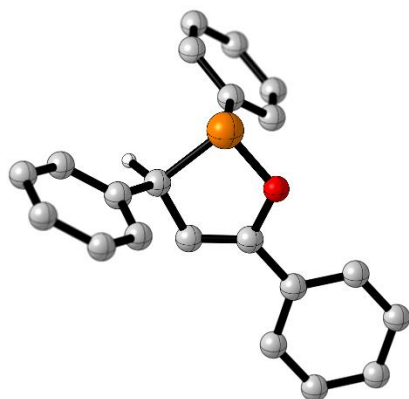
Thermochemistry

Sum of electronic and zero-point Energies	= -3236.540618
Sum of electronic and thermal Energies	= -3236.522165
Sum of electronic and thermal Enthalpies	= -3236.521220
Sum of electronic and thermal Free Energies	= -3236.589829

HF = -3236.79511104

8:

Structure



Cartesian Coordinates

Element	X	Y	Z
C	-1.33416498	-0.08230400	0.47213799
C	-0.09884700	0.66026700	0.90909398
C	0.86494601	0.75818801	-0.01425900
H	-1.57693803	-0.89304900	1.16860604
H	-0.03007500	1.10822999	1.89178300
O	0.62703401	0.12313000	-1.21534503
P	-0.73566997	-0.87486601	-1.13794601
C	-2.55735612	0.79228503	0.28717700
C	-3.81600499	0.33125401	0.67752701
C	-2.45837307	2.05377293	-0.30560201
C	-4.95243216	1.11056399	0.48234001
H	-3.90703392	-0.64738297	1.14269400
C	-3.59295201	2.83369899	-0.50381702
H	-1.48317206	2.42673397	-0.60630798
C	-4.84390783	2.36531806	-0.11008200
H	-5.92248011	0.73722702	0.79617000
H	-3.49875402	3.81098104	-0.96719199
H	-5.72894907	2.97477293	-0.26311201
C	0.02297600	-2.38694406	-0.41240299
C	-0.83059800	-3.45261097	-0.10777800
C	1.39279699	-2.52437210	-0.18072900
C	-0.32727900	-4.62703419	0.44185099
H	-1.89870596	-3.36653709	-0.29967099
C	1.89664805	-3.70377111	0.36093301
H	2.06631088	-1.70847404	-0.42346901
C	1.03960598	-4.75431585	0.67683297
H	-1.00079799	-5.44425678	0.68083400
H	2.96311092	-3.80130601	0.53912997
H	1.43621004	-5.67150211	1.10080099
C	2.16445088	1.44455600	0.06571700
C	3.14821410	1.19207203	-0.89570498
C	2.44115305	2.34765506	1.09920001
C	4.38882303	1.81637502	-0.81354398
H	2.92938209	0.50605297	-1.70632601
C	3.68103600	2.96687603	1.17943597

H	1.67927504	2.57788110	1.83687198
C	4.66082716	2.70226407	0.22407199
H	5.14399815	1.60967100	-1.56530905
H	3.88154793	3.66645098	1.98475003
H	5.62849188	3.18969893	0.28730100

Harmonic Frequencies

		1	2	3
		A	A	A
Frequencies	--	25.7680	32.8395	34.3899
Red. masses	--	3.9551	4.0506	4.9795
Frc consts	--	0.0015	0.0026	0.0035
IR Inten	--	0.0071	0.0669	0.1375

Thermochemistry

Sum of electronic and zero-point Energies	= -1226.422523
Sum of electronic and thermal Energies	= -1226.404073
Sum of electronic and thermal Enthalpies	= -1226.403129
Sum of electronic and thermal Free Energies	= -1226.472199

HF = -1226.74600487

3. X-ray structure determination

Single crystals suitable for X-ray diffraction were coated with Polybutene oil ($M_n \approx 920 \text{ g mol}^{-1}$) in a glovebox and transferred to a Nylon loop. Diffraction studies were performed on an *Rigaku Oxford Diffraction XCalibur S* or a *Bruker X8 APEX2* diffractometer, both equipped with a molybdenum X-ray tube ($\lambda = 0.7107 \text{ \AA}$). Preliminary data was collected to determine the crystal system. The data was processed using the corresponding diffractometer software (CrysAlisPro v38.41 and Apex2 v.2014.1) and corrected for absorption with a multi-scan method.

The structures were solved using direct methods (ShelXS) or intrinsic phasing (ShelXT) and refined using least square procedures (ShelXL) on Olex2 v1.2.8.

Table S1: Crystal data and structure refinement details.

Compound	^{Me} NHC=PPh (1)	[^{Me} NHC=PPh)ZnCl ₂] ₂ ·THF (3)
CCDC Number	923521	1523907
Empirical formula	C ₂₅ H ₂₉ N ₄ P ₂	C ₃₀ H ₄₂ Cl ₄ N ₄ O ₂ P ₂ Zn ₂
Formula weight	447.46	825.15
Temperature/K	200(2)	102(2)
Crystal system	monoclinic	monoclinic
Space group	P2 ₁ /c	I2/a
a/Å	15.2973(7)	18.8804(6)
b/Å	8.6624(4)	11.6134(4)
c/Å	19.6907(9)	34.4262(13)
α/°	90.00	90
β/°	110.4090(10)	97.364(4)
γ/°	90.00	90
Volume/Å ³	2445.45(19)	7486.2(5)
Z	4	8
ρ _{calc} /cm ³	1.215	1.464
μ/mm ⁻¹	0.197	1.685
F(000)	948.0	3392.0
Crystal size/mm ³	0.53 × 0.49 × 0.44	0.12 × 0.1 × 0.06
Radiation	MoKα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2θ range for data collection/°	2.84 to 52.74	5.598 to 56.558
Reflections collected	15480	14978
Independent reflections	4988	14978
Data/restraints/parameters	4988/0/384	14978/30/402
Goodness-of-fit on F ²	1.042	0.872
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0382, wR ₂ = 0.1052	R ₁ = 0.0460, wR ₂ = 0.0919
Final R indexes [all data]	R ₁ = 0.0434, wR ₂ = 0.1102	R ₁ = 0.0997, wR ₂ = 0.0996
Largest diff. peak/hole / e Å ⁻³	0.28/-0.25	0.62/-0.64
Compound	[^{Me} NHC=PPh) ₂ ZnCl ₂] (2)	Phosphonite 4
CCDC Number	1523933	1523934
Empirical formula	C ₂₆ H ₃₆ Cl ₂ N ₄ O ₂ P ₂ Zn	C ₂₀ H ₁₃ O ₂ P
Formula weight	634.80	316.27
Temperature/K	106(3)	100(2)
Crystal system	monoclinic	orthorhombic
Space group	P2 ₁ /c	Pna2 ₁
a/Å	14.5447(9)	15.6734(4)
b/Å	14.2504(7)	17.0441(5)
c/Å	14.6202(9)	5.44464(17)
α/°	90	90
β/°	97.634(6)	90
γ/°	90	90
Volume/Å ³	3003.4(3)	1454.47(7)
Z	4	4
ρ _{calc} /cm ³	1.404	1.444
μ/mm ⁻¹	1.132	0.196
F(000)	1320.0	656.0
Crystal size/mm ³	0.1 × 0.04 × 0.04	0.23 × 0.1 × 0.07
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/°	5.652 to 50.698	5.722 to 52.742
Reflections collected	14599	15306
Independent reflections	5490	2968
Data/restraints/parameters	5490/0/340	2968/1/208
Goodness-of-fit on F ²	1.054	1.055
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0585, wR ₂ = 0.0900	R ₁ = 0.0338, wR ₂ = 0.0735
Final R indexes [all data]	R ₁ = 0.0884, wR ₂ = 0.0987	R ₁ = 0.0365, wR ₂ = 0.0750
Largest diff. peak/hole / e Å ⁻³	0.62/-0.48	0.21/-0.21

Compound	[^{Me}NHC·ZnCl₂]_n (5)	1,3-oxaphospholan-5-one 6
CCDC Number	1523939	1523936
Empirical formula	C ₅ H ₈ Cl ₂ N ₂ Zn	C ₃₄ H ₂₅ O ₂ P
Formula weight	232.40	496.51
Temperature/K	106(5)	107.9(7)
Crystal system	monoclinic	monoclinic
Space group	P2 ₁ /m	P2 ₁ /n
a/Å	8.2392(6)	9.6497(5)
b/Å	7.0629(5)	22.1091(9)
c/Å	15.0722(11)	12.4703(6)
α/°	90	90
β/°	94.933(7)	101.655(5)
γ/°	90	90
Volume/Å ³	873.84(11)	2605.6(2)
Z	4	4
ρ _{calc} /cm ³	1.767	1.266
μ/mm ⁻¹	3.350	0.135
F(000)	464.0	1040.0
Crystal size/mm ³	0.28 × 0.28 × 0.15	0.3 × 0.16 × 0.07
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/°	5.858 to 52.742	5.672 to 52.746
Reflections collected	10679	11780
Independent reflections	1936	5321
Data/restraints/parameters	1936/0/122	5321/0/334
Goodness-of-fit on F ²	1.151	1.032
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0469, wR ₂ = 0.1057	R ₁ = 0.0541, wR ₂ = 0.0919
Final R indexes [all data]	R ₁ = 0.0519, wR ₂ = 0.1082	R ₁ = 0.0824, wR ₂ = 0.1030
Largest diff. peak/hole / e Å ⁻³	1.38/-0.41	0.24/-0.28
Compound	Oxo-3-phospholene 8	Intermediate 10
CCDC Number	1523935	1523941
Empirical formula	C ₂₁ H ₁₇ OP	C _{32.5} H ₃₇ Cl ₂ N ₂ O ₃ PZn
Formula weight	316.32	670.88
Temperature/K	296(2)	105(2)
Crystal system	Monoclinic	triclinic
Space group	P2 ₁ /c	P-1
a/Å	5.6130(4)	11.1677(4)
b/Å	9.8000(7)	11.2291(5)
c/Å	30.332(2)	14.6507(9)
α/°	90.00	105.078(5)
β/°	93.187(4)	109.008(4)
γ/°	90.00	97.307(3)
Volume/Å ³	1665.9(2)	1631.45(15)
Z	4	2
ρ _{calc} /cm ³	1.261	1.366
μ/mm ⁻¹	0.167	1.000
F(000)	664.0	698.0
Crystal size/mm ³	0.35 × 0.10 × 0.10	0.13 × 0.06 × 0.06
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/°	4.36 to 54.2	5.682 to 51.362
Reflections collected	16598	15519
Independent reflections	3653	6189
Data/restraints/parameters	3653/0/276	6189/63/434
Goodness-of-fit on F ²	0.924	1.080
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0455, wR ₂ = 0.1249	R ₁ = 0.0534, wR ₂ = 0.0978
Final R indexes [all data]	R ₁ = 0.0771, wR ₂ = 0.1431	R ₁ = 0.0740, wR ₂ = 0.1053
Largest diff. peak/hole / e Å ⁻³	0.21/-0.26	0.43/-0.35

Compound	Dioxyphosphineoxide 11	Quinone-methide 12
CCDC Number	1523938	1523940
Empirical formula	C ₂₃ H ₂₀ O ₃ P	C ₄₂ H ₄₀ N ₄ O ₃
Formula weight	382.96	648.81
Temperature/K	100(2)	296(2)
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
a/Å	9.5508(8)	11.537(3)
b/Å	9.7315(7)	12.270(4)
c/Å	11.9454(9)	13.264(4)
α/°	67.401(2)	80.535(11)
β/°	69.018(2)	64.747(7)
γ/°	85.756(2)	76.809(9)
Volume/Å ³	954.43(13)	1648.7(8)
Z	2	2
ρ _{calc} /cm ³	1.332	1.307
μ/mm ⁻¹	0.164	0.083
F(000)	401.8	688.0
Crystal size/mm ³	0.50 × 0.20 × 0.10	0.50 × 0.20 × 0.20
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/°	3.96 to 59.14	3.4 to 55.76
Reflections collected	17234	33022
Independent reflections	5324	7813
Data/restraints/parameters	5324/0/291	7813/0/446
Goodness-of-fit on F ²	1.047	1.396
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0409, wR ₂ = 0.1101	R ₁ = 0.0483, wR ₂ = 0.1685
Final R indexes [all data]	R ₁ = 0.0488, wR ₂ = 0.1166	R ₁ = 0.0579, wR ₂ = 0.1800
Largest diff. peak/hole / e Å ⁻³	0.51/-0.34	0.84/-0.52
Compound	Carbene-ketene adduct 13	
CCDC Number	1523937	
Empirical formula	C ₁₉ H ₁₈ N ₂ O	
Formula weight	290.35	
Temperature/K	100(2)	
Crystal system	Triclinic	
Space group	P-1	
a/Å	10.0918(5)	
b/Å	10.9642(6)	
c/Å	15.4584(8)	
α/°	98.511(2)	
β/°	108.481(2)	
γ/°	96.238(2)	
Volume/Å ³	1582.15(14)	
Z	4	
ρ _{calc} /cm ³	1.219	
μ/mm ⁻¹	0.076	
F(000)	616.0	
Crystal size/mm ³	0.19 × 0.17 × 0.08	
Radiation	MoKα (λ = 0.71073)	
2θ range for data collection/°	5.16 to 50.04	
Reflections collected	17236	
Independent reflections	5532	
Data/restraints/parameters	5532/0/541	
Goodness-of-fit on F ²	1.058	
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0363, wR ₂ = 0.0829	
Final R indexes [all data]	R ₁ = 0.0473, wR ₂ = 0.0918	
Largest diff. peak/hole / e Å ⁻³	0.20/-0.27	

4. References

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