Electronic Supplementary Material (ESI) for Nanoscale.

Unraveling Aminophosphine Redox Mechanisms for Glovebox-free InP Quantum Dot Syntheses Supporting Information

Geoffry Laufersky,[†,‡] Siobhan Bradley,[†,‡] Elian Frécaut,[¶,‡] Matthias Lein,[†,§] and Thomas Nann[*,†,‡]

†*School of Chemical and Physical Sciences (SCPS), Victoria University of Wellington, New Zealand*

‡*The MacDiarmid Institute for Advanced Materials and Nanotechnology*

¶*Établissement Public à Caractère Scientifique, Culturel et Professionnel (EPCSCP), SIGMA Clermont, France*

§*Centre for Theoretical Chemistry and Physics (CTCP), New Zealand Institute for Advanced Study, Massey University Auckland*

E-mail: thomas.nann@vuw.ac.nz

Supporting Information

Experimental Details

List of Chemicals Indium chloride (Sigma-Aldrich, anhydrous 99.999%), zinc chloride (Sigma-Aldrich, anhydrous 97%), zinc bromide (Sigma-Aldrich, anhydrous 98%), and zinc iodide (Sigma-Aldrich, 98%) were stored in a common air-desiccator. Tris(diethylamino) phosphine (Sigma-Aldrich, 97%) and trioctylphosphine (Sigma-Aldrich, 97%) were stored under nitrogen with septa and accessed with Schlenk techniques. Oleylamine (Sigma-Aldrich, 70%), 1-octadecene (Sigma-Aldrich, 90%), myristic acid (Merck, 98%), zinc undecylenate (Merck), sulfur (BDA, sublimed), toluene (ROMIL, 99.9%), and ethanol (Fisher, 99.99%) were used as received and stored under ambient conditions.

1-pot synthesis of InP cores Nanoparticles were synthesized using a modification of literature methods.[1] Typically, 100 mg (0.45 mmol) $InCl_3$, 2.2 mmol of zinc halide (300 mg $ZnCl_2$, 495 mg $ZnBr_2$, or 702 mg ZnI_2), and 5.0 mL (15 mmol) of oleylamine were degassed at 120 °C under vacuum for 1 hour before flushed with nitrogen atmosphere and heated to 180 °C. 0.45 mL (1.6 mmol) tris(diethylamino) phosphine was injected and allowed to stir for 30 minutes before rapidly cooling to 70 °C. The reaction solution was diluted with toluene and centrifuged (5 min, 10,000 rpm) to separate any solid precipitate. The supernatant was cleaned twice with toluene/ethanol precipitations and centrifugations (10 min, 10,000 rpm). The resulting nanoparticle precipitate was dispersed in toluene for further analysis.

2-pot synthesis of InP cores 100 mg (0.45 mmol) $InCl_3$ and 10.0 mL (30 mmol) of oleylamine were degassed at 120 °C under vacuum for 1 hour before being put under nitrogen atmosphere and raised to 180 °C. Separately, 2.2 mmol of zinc halide (300 mg $ZnCl_2$, 495 mg $ZnBr_2$, or 702 mg ZnI_2) and 3.0 mL (9.0 mmol) oleylamine were degassed at 120 °C under vacuum for 30 minutes. The zinc solution was put under nitrogen atmosphere and the temperature increased to 150 °C. 0.45 mL (1.6 mmol) tris(diethylamino) phosphine was injected and the solution stirred for 30 minutes. 1.0 mL (3.0 mmol) of additional oleylamine

was introduced and briefly allowed to mix before loading the zinc-phosphorus solution into a syringe and quickly injecting into the hot indium-oleylamine solution. The reaction was allowed to react for 30 minutes before rapidly cooling to 70 °C. The solution was cleaned and prepared as above.

Non-coordinating synthesis of InP cores (ODE-3MA) 100 mg (0.45 mmol) $InCl_3$, 338 mg (1.35 mmol) myristic acid (MA), and 10.0 mL (31 mmol) of 1-octadecene (ODE) were degassed at 120 °C under vacuum for 1 hour before being put under nitrogen atmosphere and raised to 180 °C. Separately, 2.2 mmol of zinc halide (300 mg $ZnCl_2$, 495 mg $ZnBr_2$, or 702 mg ZnI_2) and 3.0 mL (9.0 mmol) oleylamine were degassed at 120 °C under vacuum for 30 minutes. The zinc solution was put under nitrogen atmosphere and the temperature increased to 150 °C. 0.45 mL (1.6 mmol) tris(diethylamino) phosphine was injected and the solution stirred for 30 minutes. 1.0 mL (3.1 mmol) of additional ODE was introduced and briefly allowed to mix before loading the zinc-phosphorus solution into a syringe and quickly injecting into the hot In-ODE solution. The reaction was allowed to react for 30 minutes before rapidly cooling to 70 °C. The solution was cleaned and prepared as above.

Adapted synthesis of InP cores (ODE-1MA) 100 mg (0.45 mmol) $InCl_3$, 113 mg (0.45 mmol) myristic acid, 0.3 mL (0.9 mmol) oleylamine, and 10.0 mL (31 mmol) of 1-octadecene (ODE) were degassed at 120 °C under vacuum for 1 hour before being put under nitrogen atmosphere and raised to 180 °C. Separately, 2.2 mmol of zinc halide (300 mg $ZnCl_2$, 495 mg $ZnBr_2$, or 702 mg ZnI_2) and 3.0 mL (9.0 mmol) oleylamine were degassed at 120 °C under vacuum for 30 minutes. The zinc solution was put under nitrogen atmosphere and the temperature increased to 150 °C. 0.45 mL (1.6 mmol) tris(diethylamino) phosphine was injected and the solution was stirred for 30 minutes. 1.0 mL (3.1 mmol) of additional ODE was introduced and briefly allowed to mix before loading the zinc-phosphorus solution into a syringe and quickly injecting into the hot In-ODE solution. The reaction was allowed to react for 30 minutes before rapidly cooling to 70 °C. The solution was cleaned and prepared as above.

Synthesis of InP/ZnS core/shell materials A literature method was used to grow a shell of zinc sulfide in situ.[1] The core syntheses were carried out as above, however after 20 minutes of core growth, 1 mL saturated TOP-S (2.2 M) was slowly injected into the reaction solution. At 60 minutes, the temperature was increased to 200 °C. At 120 minutes, 0.7 g of zinc (undecylenate)$_2$ in 1.0 mL TOP and 3.0 mL ODE was slowly injected while the temperature was increased to 220 °C. At 150 minutes, 0.7 mL saturate TOP-S was slowly injected while the temperature was increased to 240 °C. At 180 minutes, 0.35 g Zn(undecylenate)$_2$ in 0.5 mL TOP and 1.5 mL ODE was slowly injected while the temperature was increased to 260 °C. At 210 minutes, the reaction was rapidly cooled to 70 °C and the solution was cleaned and prepared as above.

Instrumentation

Absorption UV-Vis absorption spectra were obtained with the use of a quartz cuvette loaded in a Cary® Bio-50 spectrometer equipped with a Xenon flash lamp. Samples were scanned from 300nm-800nm with a 0.1s dwell time and background-subtracted with a toluene blank.

Emission Photoluminescent data were obtained with the use of a quartz cuvette loaded in an Edinburgh Instruments FLS980 spectrophotometer equipped with a continuous Xenon lamp, single-grating excitation and emission monochrometers, and a Hamamatsu R928P thermoelectrically-cooled photomultiplier tube detector. Typical emission spectra resulted from 5 scans of 0.2s dwell time each, utilizing moderate excitation ($\Delta\lambda$ = 1-4 nm) and fine emission ($\Delta\lambda$ <0.5 nm) bandwidths, optimizing peak signal to $\sim$ 300,00 counts per second (cps) with sample optical density <0.1 au at excitation wavelength. Integrating sphere measurements were performed with a direct excitaiton geometry and 5 scans of 0.2 s dwell time each, utilizng broad excitation ($\Delta\lambda$ = 10-12 nm) and fine emission ($\Delta\lambda$ <0.5 nm) bandwidths, optimizing detected excitation peak signal to $\sim$ 750,000 cps with sample optical density <0.1 au at excitation wavelength. Care was taken to preserve bandwidths

and emission intensity between sample and blank measurements for accurate quantum yield calculations.

TEM Transmission electron microscope (TEM) images were obtained using a JEOL 2100F FEG TEM operated at 200 kV. InP QD samples were initially purified using either centrifuge separation followed by two washing steps with toluene/ethanol as solvent/anti-solvent or via size-exclusion column with BioRad S-X1 beads and toluene as eluent. A drop of purified QD solution was allowed to dry on a holey carbon TEM substrate (ProSciTech, 200 mesh Cu grid) which was then left in a desiccator overnight to dry completely before any imaging.

Synthesis

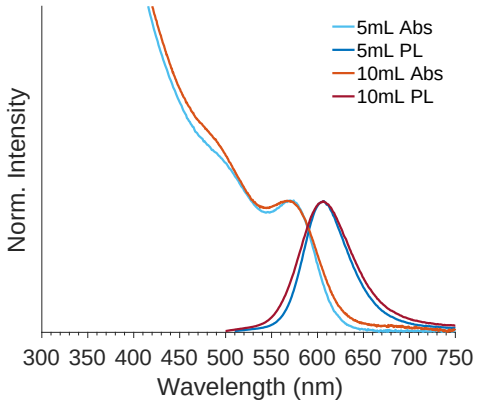


Figure S1: Absorption and emission profiles of 1-pot $ZnCl_2$ materials synthesized in 5mL and 10mL oleylamine.

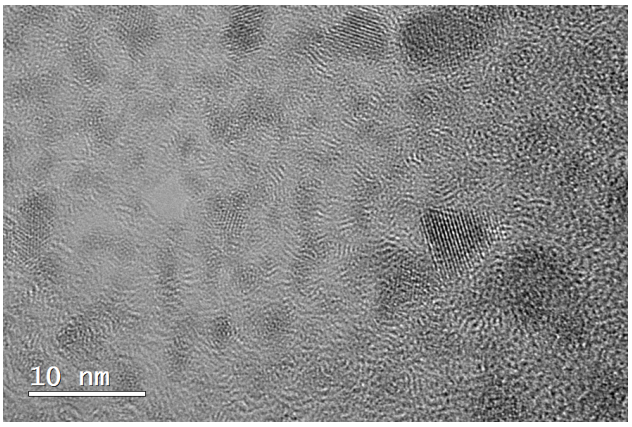


Figure S2: Transmission electron microscope image of InP OA cores after cleaning.

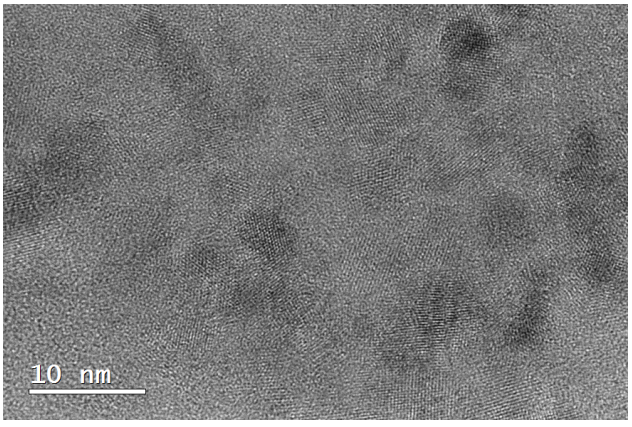


Figure S3: Transmission electron microscope image of InP ODE-1MA cores after cleaning.

Spectroscopy

FWHM

Absorption FWHM were determined from examining the min and max values of 1^{st} derivative of each sample's excition absorption peak according to a literature method.[1]

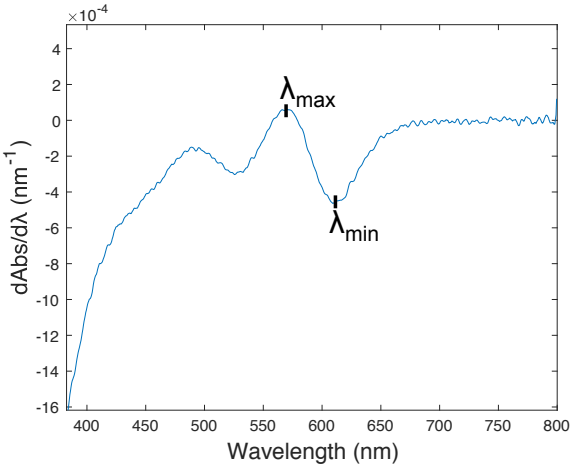


Figure S4: Example first derivative absorption used to determine FWHM.

$$FWHM = \sqrt{2\ ln(2)}\ (\lambda_{max} - \lambda_{min}) \tag{S1}$$

Quantum Yield

Quantum yields (QY^{True}) were calculated using an integrating sphere and correcting the observed QY for self-absorption effects with a standard 90°, 1 cm path length, <0.1 au OD emission scan ($PL_{90°}$) according to a literature method.[2] The fraction, a, of self-absorbed light due to the increased path length of an integrating sphere was determined by tail-matching a background-subtracted integrating sphere emission scan to that of $PL_{90°}$, as outlined in Figure S6 and Equation S3 below.

$$QY^{Obs} = \frac{\int_c^d (PL_{sphere} - blank_{sphere})}{\int_a^b (blank_{sphere} - PL_{sphere})} * 100\% \tag{S2}$$

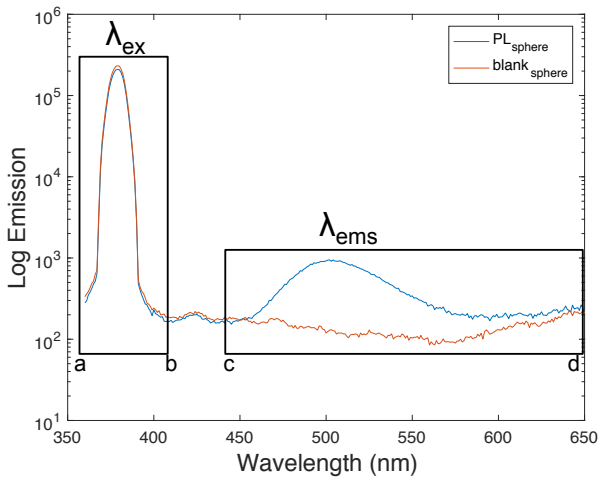


Figure S5: Scattering and emission peaks with a toluene blank and InP/ZnS sample with λ_{ex} = 380nm, $\Delta\lambda_{ex}$= 12 nm.

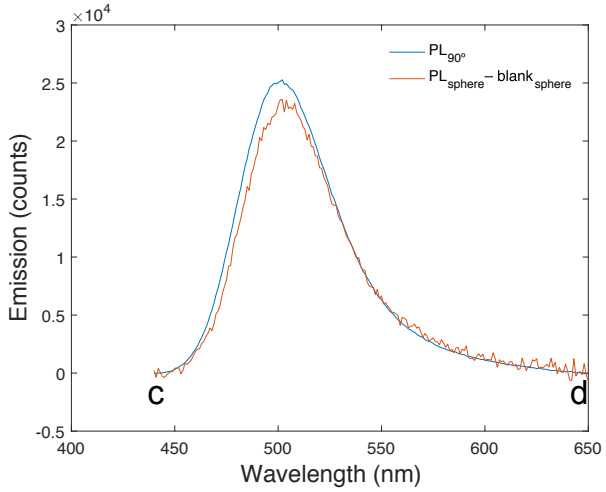


Figure S6: Blank-subtracted integrating sphere emission scaled to tail-match a standard PL_{90° spectrum.

$$a = \frac{\int_c^d PL_{90^\circ} - (PL_{sphere} - blank_{sphere})}{\int_c^d PL_{90^\circ}} \tag{S3}$$

$$QY^{True} = \frac{QY^{Obs}}{(1 - a + a * \frac{QY^{Obs}}{100})} \tag{S4}$$

Lifetimes

Photoluminescent lifetimes were determined through time correlated single photon counting (TCSPC) for each sample using a 380nm picosecond pulsed laser and an Edinburgh Instruments FLS980 spectrophotometer. Samples were excited and emission monochrometers were set to peak maxima from PL_{90° spectra with $\Delta\lambda$=20 nm, ensuring laser intensity resulted in emission <1% of laser pulse cps. Signals were collected from 1 or 2 μs pulse rates divided across 8192 time bins until one bin registered 10,000 counts. Instrument response functions (IRF) were recorded for each sample using a scattering solution at the same pulse rates with λ_{Ems}=380 nm, $\Delta\lambda$=20 nm, 10,000 max counts, and ∼1,000 cps laser intensity. The IRF was subtracted from each sample and the tail was fit to a number of decay functions (Equations S5 – S10) using randomly selected initial parameters which were analytically minimized to optimize probabilistic likelihood. These random fits were performed 10 times each, with the best of each of the 5 models kept to compare across all of the samples. Random fitting also included a horizontal baseline fit corresponding to signal detected outside the general characteristic decay. As excitons stuck in trap states can spontaneously emit through phenomena such as phonon coupling, the fraction of this baseline that accounts for total decay signal is presented as "dark counts" and can correspond to trap or dark exciton states. Although the triexponential was frequently found to fit the data the best, the model can generate equivalently good fits for drastically different parameters so was rejected. The log-normal distribution was the next best fit, and so was chosen for sample comparisons as is an apt model due to the heterogeneity inherent in nanoparticle syntheses.[3]

$$Monoexponential: \quad f(t;\tau) = \mathrm{e}^{-t/\tau} \tag{S5}$$

$$Biexponential: \quad f(t;\theta_i,\tau_i) = \theta_1\mathrm{e}^{-t/\tau_1} + \theta_2\mathrm{e}^{-t/\tau_2} \tag{S6}$$

$$Triexponential: \quad f(t;\theta_i,\tau_i) = \theta_1\mathrm{e}^{-t/\tau_1} + \theta_2\mathrm{e}^{-t/\tau_2} + \theta_3\mathrm{e}^{-t/\tau_3} \tag{S7}$$

$$Stretched: \quad f(t;\tau,\beta) = \mathrm{e}^{(-t/\tau)^\beta} \tag{S8}$$

$$Lognormal: \quad g(\tau;\mu,\sigma) = \frac{1}{\tau\sigma\sqrt{2\pi}}\exp\left(-\frac{(log\tau-\mu)^2}{2\sigma^2}\right) \tag{S9}$$

$$f(t;\mu,\sigma) = \int_0^\infty g(\tau;\mu,\sigma)\frac{1}{\tau}\mathrm{e}^{(-t/\tau)}d\tau \tag{S10}$$

ZnCl2 1-pot

	Mono	Bi		Tri			Stretch	Lognormal
R2	0.9619	0.9966			0.9994		0.9721	0.9987
loglikelihood	-10315924	-10260841.9636			-10257653.4824		-10277069.7193	-10259465.3729
dark photons	0.080285	0.0410			0.0311		0.0575	0.0383
Tau	52.3611	32.51597	147.9778	20.46535	58.97293	253.5658	52.8882	69.9674
theta		0.69767	0.30233	0.31805	0.53912	0.14282		0.9721
beta							0.8128	
mu								3.9154
sigma								0.8157

Figure S7: Example of the parameters of one sample fit with each decay function. Dark photons presented as the fraction of total counts existing as the baseline. Theta for the lognormal distribution is the spread (standard deviation divided by the mean) of the distribution.

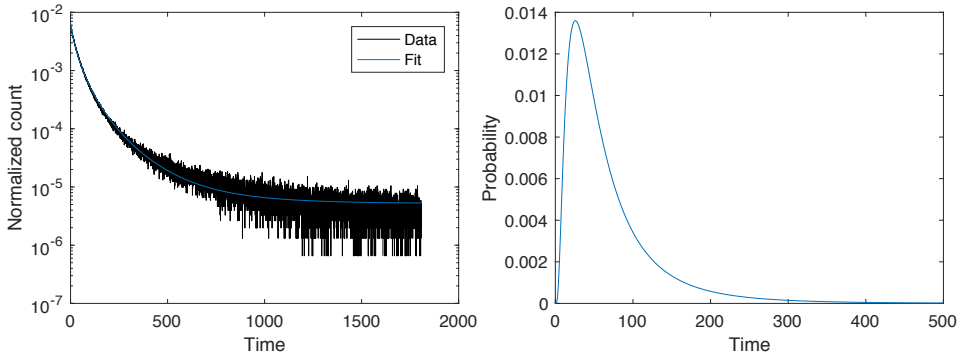


Figure S8: Example of a fit(left) using a lognormal distribution of lifetimes(right).

Supporting Calculations

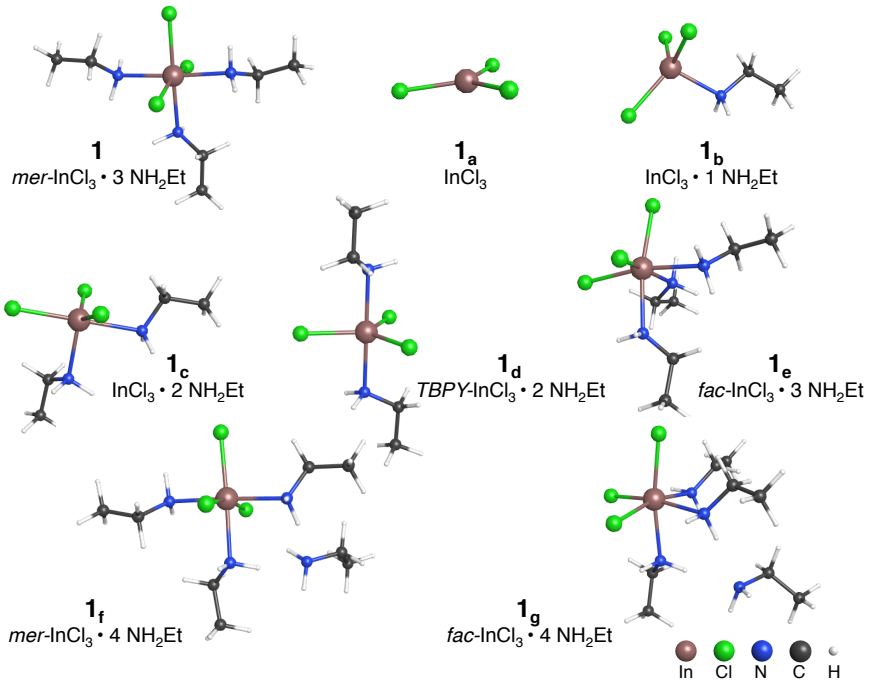


Figure S9: Geometries of $InCl_3$ solvation complexes at the PBE0-D3/def2-TZVP/PCM_{OA} level of theory.

Table S1: Difference in electronic, internal, enthalpic, and free energies as compared to **1**. Energies calculated as the sum of $InCl_3 \cdot N$ NH_2Et and $4 - N$ free NH_2Et as determined at the PBE0-D3/def2-TZVP/PCM_{OA} level of theory.

	ΔE	ΔU	ΔH	ΔG
1	0.00	0.00	0.00	0.00
$\mathbf{1_a}$	68.07	63.78	66.48	15.90
$\mathbf{1_b}$	33.20	29.53	31.33	-0.94
$\mathbf{1_c}$	20.93	19.44	20.34	3.41
$\mathbf{1_d}$	11.55	10.16	11.06	-6.70
$\mathbf{1_e}$	3.93	3.72	3.72	4.88
$\mathbf{1_f}$	-10.30	-8.73	-9.63	6.28

Table S2: Difference in electronic, internal, enthalpic, and free energies of In·**2** conformers as compared to **3** at the PBE0-D3/def2-TZVP/PCM_{OA} level of theory.

	ΔE	ΔU	ΔH	ΔG
3	0.00	0.00	0.00	0.00
$\mathbf{3_a}$	0.42	0.28	0.28	0.71
$\mathbf{3_b}$	4.10	3.49	3.49	5.40
$\mathbf{3_c}$	7.63	7.03	7.04	9.06

Table S3: Difference in electronic, internal, enthalpic, and free energies of In·P ligand exchange geometries as compared to $\mathbf{4_I}$ at the PBE0-D3/def2-TZVP/PCM_{OA} level of theory.

	ΔE	ΔU	ΔH	ΔG
$\mathbf{4_I}$	0.00	0.00	0.00	0.00
$\mathbf{4}^{\ddagger}$	14.26	13.37	13.36	19.99
$\mathbf{4_{II}}$	-1.18	-1.09	-1.09	1.86
$\mathbf{4_{aI}}$	-0.09	-0.34	-0.34	1.89
$\mathbf{4}^{\ddagger}_{\mathbf{a}}$	12.07	11.29	11.28	17.45
$\mathbf{4_{aII}}$	-0.25	-0.23	-0.24	3.66

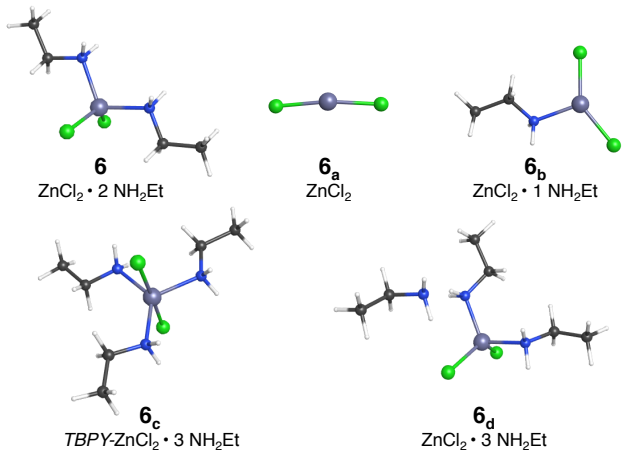


Figure S10: Geometries of $ZnCl_2$ solvation complexes at the PBE0-D3/def2-TZVP/PCM_{OA} level of theory.

Table S4: Difference in electronic, internal, enthalpic, and free energies as compared to **6**. Energies calculated as the sum of $ZnCl_2 \cdot N$ NH_2Et and $3 - N$ free NH_2Et as determined at the PBE0-D3/def2-TZVP/PCM_{OA} level of theory.

	ΔE	ΔU	ΔH	ΔG
6	0.00	0.00	0.00	0.00
$\mathbf{6_a}$	42.92	39.90	41.70	14.25
$\mathbf{6_b}$	20.54	18.98	19.88	5.27
$\mathbf{6_c}$	-10.53	-9.00	-9.90	6.71
$\mathbf{6_d}$	-9.49	-8.00	-8.90	7.73

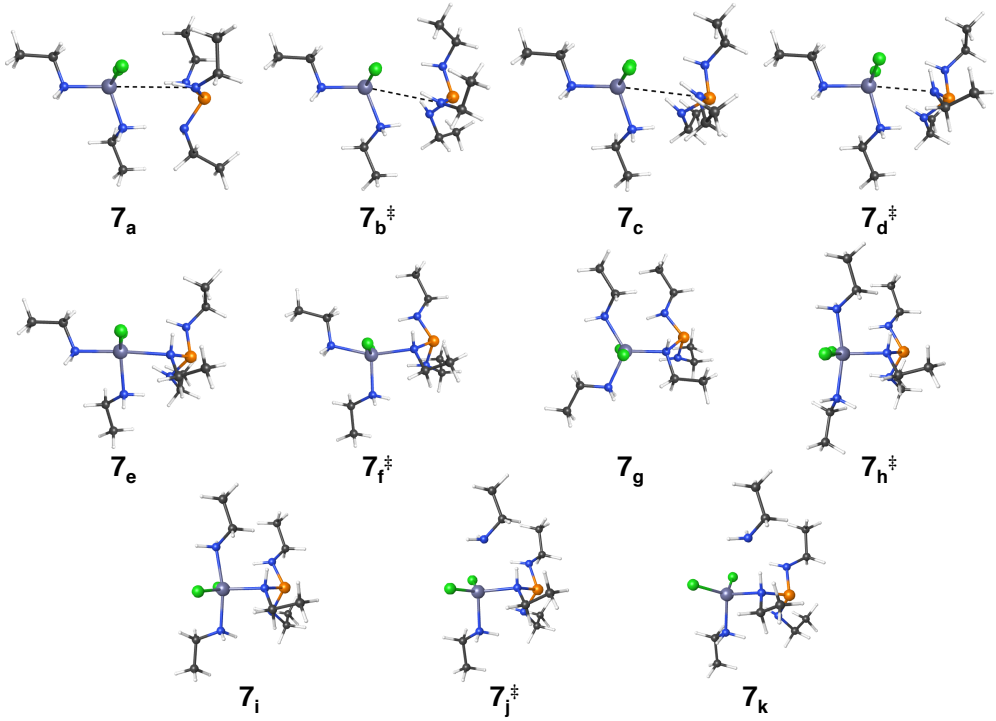


Figure S11: Zinc activation geometries.

Table S5: Difference in electronic, internal, enthalpic, and free energies of In·P ligand exchange geometries as compared to $\mathbf{7_a}$ at the PBE0-D3/def2-TZVP/PCM_{OA} level of theory.

	ΔE	ΔU	ΔH	ΔG
$\mathbf{7_a}$	0.00	0.00	0.00	0.00
$\mathbf{7_b^‡}$	0.88	0.14	0.14	4.25
$\mathbf{7_c}$	0.62	0.66	0.66	1.16
$\mathbf{7_d^‡}$	1.05	0.47	0.47	3.10
$\mathbf{7_e}$	1.06	0.88	0.88	4.25
$\mathbf{7_f^‡}$	3.39	2.35	2.35	8.37
$\mathbf{7_g}$	0.80	0.55	0.55	2.62
$\mathbf{7_h^‡}$	0.82	-0.17	-0.17	5.95
$\mathbf{7_i}$	-0.44	-0.66	-0.66	2.74
$\mathbf{7_j^‡}$	1.66	1.12	1.12	4.14
$\mathbf{7_k}$	-0.71	-0.48	-0.48	-0.11

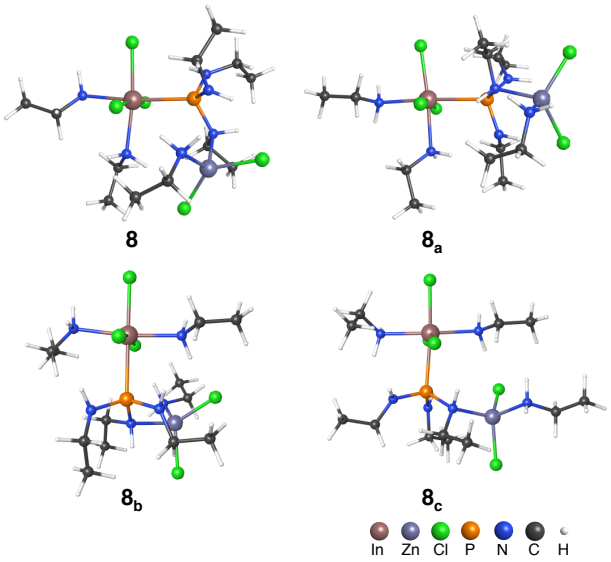


Figure S12: Various In·ZnP conformers at the PBE0-D3/def2-TZVP/PCM_{OA} level of theory.

Table S6: Difference in electronic, internal, enthalpic, and free energies of the structures of Figure S12 as compared to **8**

	ΔE	ΔU	ΔH	ΔG
8	0.00	0.00	0.00	0.00
$\mathbf{8_a}$	3.64	3.54	3.54	2.56
$\mathbf{8_b}$	6.87	6.72	6.72	7.30
$\mathbf{8_c}$	6.57	6.24	6.24	7.53

Table S7: Difference in electronic, internal, enthalpic, and free energies of the zinc-activated ligand exchange as compared to $\mathbf{9_I}$

	ΔE	ΔU	ΔH	ΔG
$\mathbf{9_I}$	0.00	0.00	0.00	0.00
$\mathbf{9}^{\ddagger}$	15.02	14.78	14.78	16.37
$\mathbf{9_{II}}$	-3.29	-2.90	-2.90	-3.97

Table S8: Thermodynamic calculations for the zinc-free (top) and zinc-bound (bottom) disproportionation reactions including the highest occupied molecular orbital energies. Electronic, internal, enthalpic, and free energies presented as deviation from each minima (*).

	ΔE [a]	ΔU [a]	ΔH [a]	ΔG [a]	C_v [b]	S [b]	HOMO[c]
$\mathbf{5_I}$*	0.00	0.00	0.00	0.00	220.88	373.04	-5.96
$\mathbf{5}^{\ddagger}$	61.50	61.21	61.21	64.01	220.50	366.87	-4.14
$\mathbf{5_{II}}$	0.01	-0.61	-0.61	3.60	220.39	363.75	-5.36
$\mathbf{10_I}$*	0.00	0.00	0.00	0.00	263.06	434.72	-6.10
$\mathbf{10}^{\ddagger}$	52.56	51.95	51.96	55.13	261.90	427.71	-4.90
$\mathbf{10_{II}}$	-8.43	-8.47	-8.47	-9.03	262.74	435.97	-5.90

[a]kcal/mol [b]cal/mol-K [c]eV

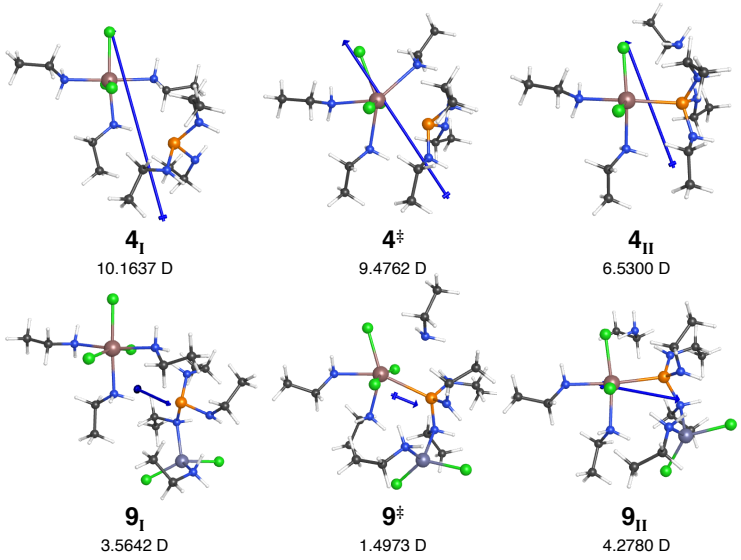


Figure S13: Dipole moments in Debye (D) about the zinc-free and zinc-activated ligand exchanges. The net horizontal moment can be attributed to the P$\cdots$In interaction, while the vertical moment corresponds to the In–Cl electron-withdrawing environments. The dipole of $\mathbf{4_{II}}$ suggests an In$\rightarrow$P instead of P$\rightarrow$In dative environment, which would reduce the ability of the aminophosphine to passivate the indium center. Conversely, the zinc activated series is initially neutral vertically, with the In–Cl and Zn–Cl moments effectively canceling each other. This then progresses to a strong P$\rightarrow$In bond as the reaction proceeds, which increases the effective passivation and is likely responsible for lowering ΔE. These differences already highlight the preference of the activated pathway and will serve to electronically stabilize the disproportionation reaction.

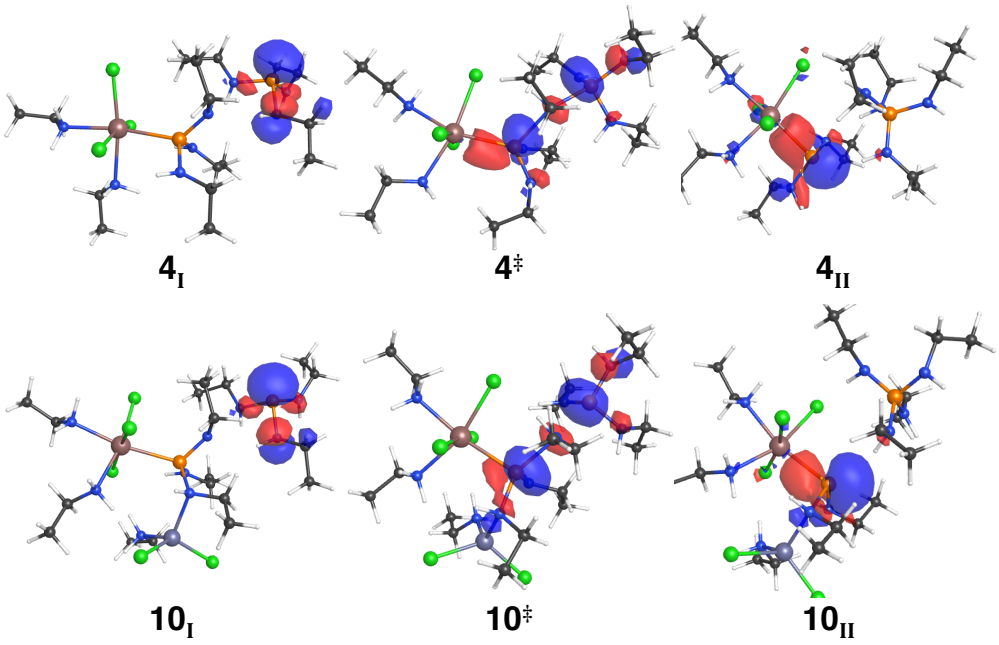


Figure S14: 0.050 au isosurfaces of the highest occupied molecular orbitals of the disproportionations.

References

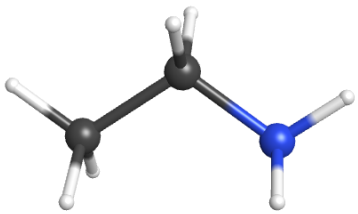
1. Tessier, M. D.; Dupont, D.; De Nolf, K.; De Roo, J.; Hens, Z. Economic and Size-Tunable Synthesis of InP/ZnE (E = S, Se) Colloidal Quantum Dots. *Chemistry of Materials* **2015**, *27*, 4893–4898.

2. Ahn, T.-S.; Al-Kaysi, R. O.; Mller, A. M.; Wentz, K. M.; Bardeen, C. J. Self-absorption correction for solid-state photoluminescence quantum yields obtained from integrating sphere measurements. *Review of Scientific Instruments* **2007**, *78*, 086105.

3. Roding, M.; Bradley, S. J.; Nyden, M.; Nann, T. Fluorescence Lifetime Analysis of Graphene Quantum Dots. *The Journal of Physical Chemistry C* **2014**, *118*, 30282–30290.

DFT Geometries

Cartesian coordinates, three lower frequencies, and thermochemistry of NH_2Et.

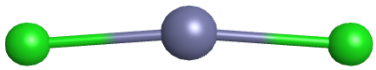


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.009606	0.004850	0.000763
2	6	0	-0.002452	-0.001268	1.515643
3	1	0	1.014041	-0.011151	1.915730
4	1	0	-0.520008	0.880607	1.900139
5	1	0	-0.518751	-0.887529	1.897433
6	7	0	-1.351165	0.055546	-0.521968
7	1	0	-1.339815	0.054035	-1.534939
8	1	0	-1.857080	-0.777365	-0.241374
9	1	0	0.581822	-0.864473	-0.359350
10	1	0	0.538171	0.894669	-0.355545

	1	2	3
	A	A	A
Frequencies --	242.4759	282.1096	418.6863
Red. masses --	1.0656	1.1249	2.3032
Frc consts --	0.0369	0.0527	0.2379
IR Inten --	37.5337	16.6229	12.2348

Sum of electronic and zero-point Energies=	-134.970194
Sum of electronic and thermal Energies=	-134.961490
Sum of electronic and thermal Enthalpies=	-134.960055
Sum of electronic and thermal Free Energies=	-135.012673

Cartesian coordinates, three lower frequencies, and thermochemistry of $ZnCl_2$.

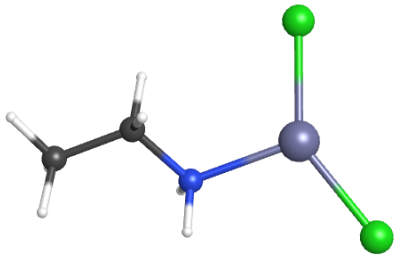


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	0.002496	0.000000	0.000176
2	17	0	-0.000341	0.000000	2.118015
3	17	0	0.297633	0.000000	-2.096998

	1	2	3
	A1	A1	B2
Frequencies --	159.7188	320.3305	461.3115
Red. masses --	45.8102	34.9693	45.7784
Frc consts --	0.6885	2.1141	5.7398
IR Inten --	25.9783	0.1334	114.8030

Sum of electronic and zero-point Energies= -2699.404156
Sum of electronic and thermal Energies= -2699.397291
Sum of electronic and thermal Enthalpies= -2699.395855
Sum of electronic and thermal Free Energies= -2699.447859

Cartesian coordinates, three lower frequencies, and thermochemistry of $ZnCl_2 \cdot$ 1 NH_2Et.

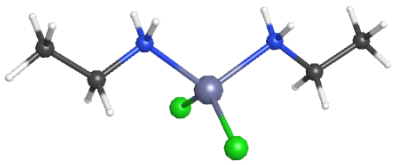


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.003617	-0.028085	0.007334
2	30	0	0.074110	-0.052884	2.087393
3	17	0	2.069744	-0.651775	2.744650
4	17	0	-1.877298	0.549810	2.864199
5	6	0	1.276973	0.352740	-0.637395
6	6	0	1.217733	0.324372	-2.148550
7	1	0	2.186855	0.601230	-2.568417
8	1	0	0.967332	-0.674886	-2.514538
9	1	0	0.472468	1.026707	-2.530602
10	1	0	1.537179	1.349841	-0.276559
11	1	0	2.041995	-0.325267	-0.256186
12	1	0	-0.278049	-0.949297	-0.319076
13	1	0	-0.739952	0.602535	-0.281093

	1	2	3
	A	A	A
Frequencies --	30.7219	63.4147	79.1794
Red. masses --	1.7230	4.8241	4.8914
Frc consts --	0.0010	0.0114	0.0181
IR Inten --	0.9707	4.6836	13.5818

Sum of electronic and zero-point Energies=	-2834.410010
Sum of electronic and thermal Energies=	-2834.392119
Sum of electronic and thermal Enthalpies=	-2834.390684
Sum of electronic and thermal Free Energies=	-2834.474847

Cartesian coordinates, three lower frequencies, and thermochemistry of $ZnCl_2 \cdot 2\,NH_2Et$.



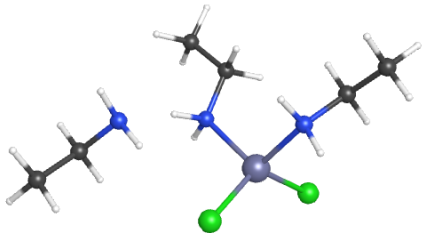
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	0.138432	-0.000001	0.062082
2	17	0	0.170468	-0.035481	2.303613
3	17	0	1.832953	0.035478	-1.405598
4	7	0	-0.940962	-1.713847	-0.484505
5	6	0	-0.200233	-2.924447	-0.078348
6	6	0	-0.915182	-4.213055	-0.421798
7	1	0	-0.324484	-5.072852	-0.098985
8	1	0	-1.887493	-4.269084	0.075475
9	1	0	-1.075137	-4.301425	-1.499809
10	1	0	0.777084	-2.874249	-0.562722
11	1	0	-0.026746	-2.843614	0.996602
12	1	0	-1.860687	-1.720028	-0.053113
13	1	0	-1.091496	-1.729356	-1.489009
14	7	0	-0.987834	1.713848	-0.379919
15	6	0	-0.191746	2.924446	-0.097271
16	6	0	-0.923866	4.213055	-0.402405
17	1	0	-0.289827	5.072851	-0.176287
18	1	0	-1.199685	4.269085	-1.459095
19	1	0	-1.834992	4.301428	0.195543
20	1	0	0.097033	2.874249	0.954572
21	1	0	0.726100	2.843611	-0.683082
22	1	0	-1.277839	1.720029	-1.353515
23	1	0	-1.837822	1.729359	0.176148

	1	2	3
	A	A	A
Frequencies --	8.0042	32.9948	47.1309

Red. masses --	2.9517	3.7916	4.0672
Frc consts --	0.0001	0.0024	0.0053
IR Inten --	0.0876	1.2985	1.7260

Sum of electronic and zero-point Energies=	-2969.412939
Sum of electronic and thermal Energies=	-2969.383861
Sum of electronic and thermal Enthalpies=	-2969.382426
Sum of electronic and thermal Free Energies=	-2969.495921

Cartesian coordinates, three lower frequencies, and thermochemistry of $ZnCl_2 \cdot 3\ NH_2Et$.



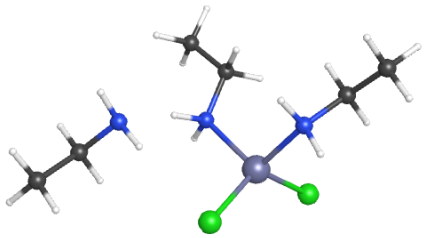
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	0.129892	-0.139552	-0.008895
2	7	0	0.030272	-0.080454	2.100514
3	6	0	1.302942	0.039574	2.830339
4	6	0	1.157172	-0.106525	4.330209
5	1	0	2.129457	-0.014131	4.818905
6	1	0	0.498474	0.662774	4.742881
7	1	0	0.743617	-1.084533	4.590273
8	1	0	1.976020	-0.715331	2.420721
9	1	0	1.735641	1.009752	2.577264
10	1	0	-0.618491	0.641974	2.399248
11	1	0	-0.419827	-0.960144	2.340839
12	7	0	0.375015	1.801324	-0.694987
13	6	0	1.288606	2.651929	0.078805
14	6	0	1.529905	4.005538	-0.557600
15	1	0	2.201330	4.608450	0.057836
16	1	0	1.988125	3.895149	-1.544057
17	1	0	0.591809	4.553334	-0.677210

18	1	0	0.853699	2.776437	1.074408
19	1	0	2.230050	2.111756	0.206590
20	1	0	0.717113	1.725381	-1.648931
21	1	0	-0.563862	2.238626	-0.743629
22	17	0	-1.987035	-0.791402	-0.489500
23	17	0	2.030607	-1.246540	-0.470480
24	7	0	-2.445376	2.588338	-0.824396
25	6	0	-2.770356	2.640347	-2.247116
26	6	0	-4.235868	2.414202	-2.574675
27	1	0	-4.411409	2.459741	-3.652863
28	1	0	-4.560000	1.432220	-2.220060
29	1	0	-4.863898	3.172522	-2.097986
30	1	0	-2.442606	3.609858	-2.635413
31	1	0	-2.162488	1.881736	-2.749995
32	1	0	-2.711201	1.677511	-0.456331
33	1	0	-2.975777	3.287302	-0.316999

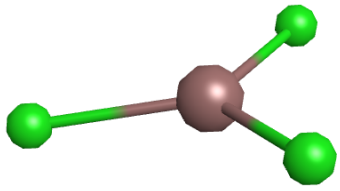
	1	2	3
	A	A	A
Frequencies --	13.6407	25.0545	42.4643
Red. masses --	4.3400	3.4661	2.7546
Frc consts --	0.0005	0.0013	0.0029
IR Inten --	1.4496	0.7326	0.4710

Sum of electronic and zero-point Energies= -3104.398252
Sum of electronic and thermal Energies= -3104.358093
Sum of electronic and thermal Enthalpies= -3104.356658
Sum of electronic and thermal Free Energies= -3104.496272

Cartesian coordinates, three lower frequencies, and thermochemistry of pyramidal $ZnCl_2 \cdot 3\ NH_2Et$.



Cartesian coordinates, three lower frequencies, and thermochemistry of $InCl_3$.

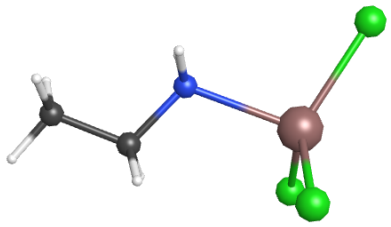


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	0.000271	-0.000003	0.000137
2	17	0	-0.000831	-0.000001	2.299305
3	17	0	1.992125	0.000002	-1.146777
4	17	0	-1.990221	-0.000121	-1.147069

	1	2	3
	A	A	A
Frequencies --	82.6116	85.7683	95.9447
Red. masses --	39.8606	39.9760	52.3497
Frc consts --	0.1603	0.1733	0.2839
IR Inten --	13.9248	14.4514	19.3574

Sum of electronic and zero-point Energies=	-1570.483006
Sum of electronic and thermal Energies=	-1570.472732
Sum of electronic and thermal Enthalpies=	-1570.471297
Sum of electronic and thermal Free Energies=	-1570.538667

Cartesian coordinates, three lower frequencies, and thermochemistry of $InCl_3 \cdot 1\ NH_2Et$.

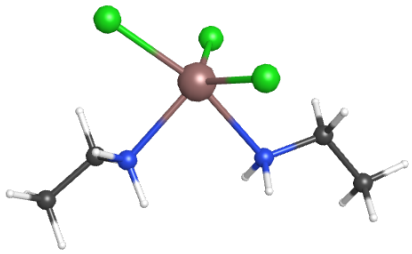


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000778	0.000804	-0.015696
2	7	0	-0.009130	0.015180	1.466345
3	1	0	0.946250	0.016600	1.817049
4	1	0	-0.432390	-0.841102	1.817598
5	49	0	-1.095564	1.762053	2.348551
6	17	0	-0.870699	1.401049	4.648770
7	17	0	-3.234547	1.447554	1.451649
8	17	0	0.131939	3.541541	1.451203
9	6	0	0.739136	-1.188807	-0.583455
10	1	0	0.717368	-1.154532	-1.674130
11	1	0	1.785623	-1.191662	-0.268543
12	1	0	0.279485	-2.128741	-0.267931
13	1	0	-1.042256	0.010374	-0.342916
14	1	0	0.450644	0.939204	-0.343517

	1	2	3
	A	A	A
Frequencies --	-30.5295	34.1683	52.9035
Red. masses --	1.6400	4.7744	8.4047
Frc consts --	0.0009	0.0033	0.0139
IR Inten --	0.2970	0.3802	0.0215

Sum of electronic and zero-point Energies= -1705.508757
Sum of electronic and thermal Energies= -1705.488804
Sum of electronic and thermal Enthalpies= -1705.487369
Sum of electronic and thermal Free Energies= -1705.578182

Cartesian coordinates, three lower frequencies, and thermochemistry of $InCl_3 \cdot 2\ NH_2Et$.

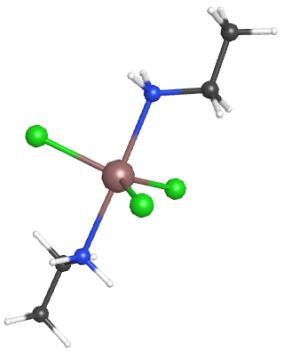


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	-0.094193	-0.192822	-0.093387
2	7	0	-0.055382	-0.079817	2.191560
3	6	0	1.280219	0.266859	2.722150
4	6	0	1.363684	0.156639	4.228707
5	1	0	2.365607	0.422401	4.570925
6	1	0	0.652025	0.827886	4.716980
7	1	0	1.155949	-0.864322	4.558350
8	1	0	1.996849	-0.401561	2.241019
9	1	0	1.515896	1.280301	2.389924
10	1	0	-0.761913	0.517859	2.611234
11	1	0	-0.282417	-1.034217	2.462472
12	17	0	-2.199693	-0.687785	-1.099045
13	17	0	0.728655	-2.450297	0.250141
14	17	0	1.848074	0.806106	-1.045539
15	7	0	-0.955497	2.001759	0.104068
16	6	0	-1.107223	2.712188	-1.180432
17	6	0	-1.727464	4.085297	-1.032507
18	1	0	-1.812423	4.568111	-2.008218
19	1	0	-2.730606	4.022994	-0.602008
20	1	0	-1.117992	4.729401	-0.392579
21	1	0	-0.115509	2.774869	-1.630195
22	1	0	-1.716845	2.076958	-1.825568
23	1	0	-1.867152	1.926421	0.547888
24	1	0	-0.370099	2.555749	0.723454

	1	2	3
	A	A	A
Frequencies --	31.9916	43.4554	46.6424
Red. masses --	5.5869	4.3837	9.3802
Frc consts --	0.0034	0.0049	0.0120
IR Inten --	0.6498	1.5667	0.7372

Sum of electronic and zero-point Energies=	-1840.498505
Sum of electronic and thermal Energies=	-1840.466376
Sum of electronic and thermal Enthalpies=	-1840.464941
Sum of electronic and thermal Free Energies=	-1840.583918

Cartesian coordinates, three lower frequencies, and thermochemistry of pyramidal $InCl_3$ · 2 NH_2Et.



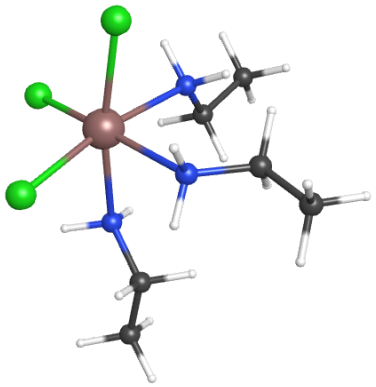
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	0.020208	0.043201	0.000717
2	7	0	0.024301	-0.022234	2.300110
3	6	0	1.337001	0.051534	2.965172
4	6	0	1.242911	-0.028134	4.474015
5	1	0	0.646538	0.794589	4.877090
6	1	0	2.238675	0.029937	4.918306
7	1	0	0.787453	-0.969747	4.792050
8	1	0	1.805144	0.985449	2.649039
9	1	0	1.944086	-0.764212	2.567795
10	1	0	-0.450762	-0.883361	2.558310
11	1	0	-0.575449	0.734870	2.617557

12	17	0	1.144800	2.153515	0.005932
13	17	0	-2.375774	-0.043674	0.072845
14	17	0	1.284120	-1.993961	-0.076690
15	7	0	-0.031647	0.018963	-2.298899
16	6	0	-0.701044	1.152316	-2.960967
17	6	0	-0.711379	1.035762	-4.470310
18	1	0	0.304995	1.001189	-4.871297
19	1	0	-1.217552	1.896427	-4.912305
20	1	0	-1.238234	0.133841	-4.793088
21	1	0	-0.187632	2.060473	-2.640108
22	1	0	-1.717588	1.199720	-2.565627
23	1	0	-0.481033	-0.854562	-2.561376
24	1	0	0.931905	-0.055509	-2.614653

	1	2	3
	A	A	A
Frequencies --	38.4873	41.5155	47.8197
Red. masses --	4.2064	3.9282	1.6267
Frc consts --	0.0037	0.0040	0.0022
IR Inten --	4.6271	2.2395	2.5205

Sum of electronic and zero-point Energies=	-1840.513455
Sum of electronic and thermal Energies=	-1840.481159
Sum of electronic and thermal Enthalpies=	-1840.479724
Sum of electronic and thermal Free Energies=	-1840.600038

Cartesian coordinates, three lower frequencies, and thermochemistry of *fac*-$InCl_3 \cdot 3$ NH_2Et.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	-0.047492	0.000968	0.032880
2	7	0	0.013283	-0.083757	2.387212
3	6	0	1.271612	0.036711	3.131681
4	6	0	1.078018	0.204544	4.625143
5	1	0	2.042828	0.291629	5.129263
6	1	0	0.501693	1.107139	4.842080
7	1	0	0.548430	-0.650444	5.053586
8	1	0	1.871315	-0.853928	2.924391
9	1	0	1.802120	0.899418	2.721466
10	1	0	-0.561321	0.739585	2.551738
11	1	0	-0.530892	-0.868288	2.732667
12	7	0	-0.426605	-2.321092	-0.024366
13	6	0	-0.828469	-3.076869	1.167365
14	6	0	-1.227650	-4.507967	0.870548
15	1	0	-1.522836	-5.021354	1.788033
16	1	0	-2.073141	-4.539213	0.179256
17	1	0	-0.399540	-5.063721	0.423159
18	1	0	0.004462	-3.055023	1.876399
19	1	0	-1.664545	-2.536791	1.618502
20	1	0	0.335693	-2.789410	-0.504847
21	1	0	-1.195641	-2.299508	-0.690319
22	7	0	2.262631	-0.415790	0.015898
23	6	0	2.836072	-1.765323	0.035366
24	6	0	4.350790	-1.778770	0.061218
25	1	0	4.726090	-2.804193	0.072308
26	1	0	4.759811	-1.277283	-0.818839
27	1	0	4.730724	-1.270228	0.951272
28	1	0	2.436183	-2.290911	0.907300
29	1	0	2.471396	-2.284776	-0.853930
30	1	0	2.488724	0.043009	-0.863413
31	1	0	2.676871	0.161626	0.741690
32	17	0	0.106829	-0.267929	-2.402224
33	17	0	-2.468946	0.146773	0.388668
34	17	0	0.652161	2.330537	0.331579

	1	2	3
	A	A	A
Frequencies --	18.6852	42.1203	52.3985
Red. masses --	3.2275	4.1309	3.4216
Frc consts --	0.0007	0.0043	0.0055
IR Inten --	2.2154	2.4626	0.3345

```
Sum of electronic and zero-point Energies=          -1975.495793
Sum of electronic and thermal Energies=             -1975.452910
Sum of electronic and thermal Enthalpies=           -1975.451475
Sum of electronic and thermal Free Energies=        -1975.594256
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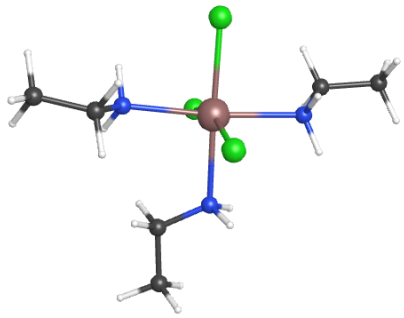
Cartesian coordinates, three lower frequencies, and thermochemistry of *mer*-$InCl_3 \cdot 3\ NH_2Et$.



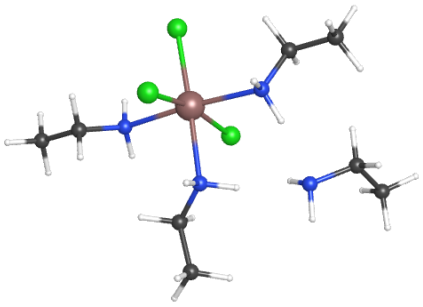
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	-0.080956	-0.031936	-0.012012
2	7	0	-0.038656	0.118983	2.290955
3	6	0	1.250439	-0.107471	2.965278
4	6	0	1.212500	0.216945	4.443680
5	1	0	2.189389	0.034322	4.896297
6	1	0	0.956320	1.266516	4.610034
7	1	0	0.478545	-0.401262	4.968297
8	1	0	1.532133	-1.147338	2.793323
9	1	0	1.990058	0.506228	2.448281
10	1	0	-0.328332	1.087512	2.407720
11	1	0	-0.767960	-0.439642	2.724851
12	7	0	0.008171	0.002264	-2.312533
13	6	0	-0.987624	0.778067	-3.068040
14	6	0	-0.686637	0.840714	-4.550543
15	1	0	-1.447845	1.427979	-5.068325
16	1	0	0.283344	1.309946	-4.733996
17	1	0	-0.671783	-0.158511	-4.994489
18	1	0	-1.966139	0.331728	-2.882446

19	1	0	-1.018477	1.776706	-2.629616
20	1	0	0.083551	-0.942953	-2.676935
21	1	0	0.929171	0.419418	-2.429018
22	7	0	-1.417677	-1.958634	0.107901
23	6	0	-1.655825	-2.677803	-1.150027
24	6	0	-2.504786	-3.921248	-0.983901
25	1	0	-2.648522	-4.417599	-1.945971
26	1	0	-2.025782	-4.633014	-0.306626
27	1	0	-3.490119	-3.673411	-0.581110
28	1	0	-2.136546	-1.979798	-1.840171
29	1	0	-0.676500	-2.936419	-1.559911
30	1	0	-0.963839	-2.583010	0.768430
31	1	0	-2.301219	-1.657301	0.510116
32	17	0	1.738322	-1.716590	-0.123502
33	17	0	-2.294053	1.091185	0.127119
34	17	0	1.315870	1.989865	-0.065305

	1	2	3
	A	A	A
Frequencies --	31.5656	39.2573	43.1989
Red. masses --	3.0290	2.9266	3.1901
Frc consts --	0.0018	0.0027	0.0035
IR Inten --	0.4638	1.7259	1.7486

Sum of electronic and zero-point Energies= -1975.502058
Sum of electronic and thermal Energies= -1975.458838
Sum of electronic and thermal Enthalpies= -1975.457403
Sum of electronic and thermal Free Energies= -1975.602028

Cartesian coordinates, three lower frequencies, and thermochemistry of *mer*-$InCl_3 \cdot 4$ NH_2Et.



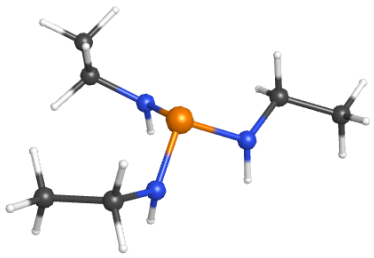
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	0.058901	0.019979	-0.014461
2	17	0	-0.029154	0.018386	2.497376
3	17	0	0.727440	0.002733	-2.421243
4	17	0	-2.360621	0.084987	-0.383610
5	7	0	0.256983	-2.257830	-0.031676
6	6	0	-0.926867	-3.037772	0.362039
7	6	0	-0.746085	-4.529400	0.169775
8	1	0	-1.644177	-5.063348	0.487827
9	1	0	-0.569438	-4.769111	-0.882253
10	1	0	0.097073	-4.910797	0.751329
11	1	0	-1.138052	-2.794179	1.405486
12	1	0	-1.774143	-2.671976	-0.219309
13	1	0	0.523940	-2.479939	-0.987490
14	1	0	1.049692	-2.486500	0.577142
15	7	0	-0.031436	2.315004	0.157107
16	6	0	0.303783	3.155019	-1.001626
17	6	0	0.097643	4.633020	-0.745039
18	1	0	0.357000	5.212326	-1.633711
19	1	0	-0.944831	4.847349	-0.496135
20	1	0	0.724296	4.983175	0.080045
21	1	0	1.339747	2.947071	-1.276908
22	1	0	-0.306508	2.809385	-1.837072
23	1	0	0.491003	2.599425	0.980914
24	1	0	-1.014179	2.429839	0.395283
25	7	0	2.386614	0.023997	0.282628
26	6	0	3.030312	1.133354	0.993548
27	6	0	4.524618	0.953778	1.172757
28	1	0	4.953547	1.811234	1.695846

29	1	0	4.745670	0.058957	1.760456
30	1	0	5.028023	0.859627	0.207235
31	1	0	2.832091	2.049244	0.430572
32	1	0	2.532151	1.229807	1.960988
33	1	0	2.580842	-0.856873	0.760097
34	1	0	2.749622	-0.056142	-0.663595
35	7	0	2.330254	-2.441587	2.302370
36	6	0	1.873182	-3.696520	2.900080
37	6	0	2.184733	-3.842722	4.378593
38	1	0	1.815637	-4.796023	4.765700
39	1	0	3.263387	-3.802728	4.555981
40	1	0	1.716223	-3.039424	4.953278
41	1	0	0.792184	-3.760960	2.747316
42	1	0	2.317530	-4.523949	2.338372
43	1	0	3.320731	-2.326845	2.492736
44	1	0	1.849927	-1.665272	2.755090

	1	2	3
	A	A	A
Frequencies --	22.8209	30.8445	38.2416
Red. masses --	3.5987	3.6552	4.0911
Frc consts --	0.0011	0.0020	0.0035
IR Inten --	0.6555	1.0885	1.7772

Sum of electronic and zero-point Energies=	-2110.488664
Sum of electronic and thermal Energies=	-2110.434241
Sum of electronic and thermal Enthalpies=	-2110.432806
Sum of electronic and thermal Free Energies=	-2110.604693

Cartesian coordinates, three lower frequencies, and thermochemistry of $P_{Am}(III)$, $P(NH_2Et)_3$.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.053714	0.033653	0.010040
2	6	0	0.013174	0.017525	1.528860
3	1	0	1.050505	0.025359	1.874810
4	1	0	-0.495431	0.888284	1.950105
5	1	0	-0.467598	-0.879949	1.929541
6	7	0	-1.395468	-0.033733	-0.536165
7	15	0	-2.291846	1.372597	-0.829665
8	7	0	-3.171880	0.809439	-2.171834
9	6	0	-4.238002	1.645032	-2.693962
10	6	0	-4.635908	1.219030	-4.093184
11	1	0	-5.429459	1.861161	-4.482832
12	1	0	-3.781165	1.269177	-4.770951
13	1	0	-5.009090	0.190366	-4.096172
14	1	0	-5.121835	1.651302	-2.039833
15	1	0	-3.868570	2.676374	-2.710001
16	1	0	-3.415041	-0.174043	-2.150309
17	7	0	-3.532902	1.477574	0.335707
18	6	0	-3.279941	2.114340	1.613198
19	6	0	-4.540367	2.714677	2.206208
20	1	0	-4.330030	3.192457	3.166517
21	1	0	-4.965983	3.460161	1.531040
22	1	0	-5.296546	1.942677	2.376270
23	1	0	-2.829231	1.420822	2.339042
24	1	0	-2.537487	2.901622	1.442463
25	1	0	-4.160623	0.683901	0.401760
26	1	0	-1.901161	-0.866920	-0.261389
27	1	0	0.535589	-0.798414	-0.391971
28	1	0	0.408121	0.949038	-0.370874

	1	2	3
	A	A	A
Frequencies --	26.7905	46.7312	56.0035
Red. masses --	2.9333	2.6111	2.2659
Frc consts --	0.0012	0.0034	0.0042
IR Inten --	0.1974	0.7560	0.6837

Sum of electronic and zero-point Energies= -744.424253
Sum of electronic and thermal Energies= -744.394562

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Sum of electronic and thermal Enthalpies=            -744.393127
Sum of electronic and thermal Free Energies=         -744.500767
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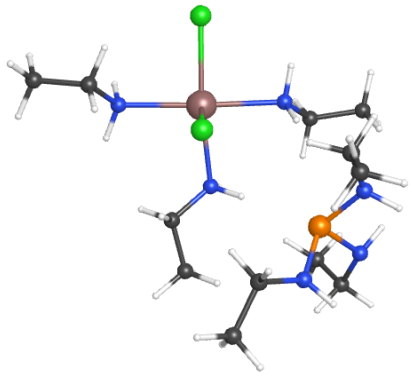
Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}_I$, the starting geometry of the ligand exchange of the aminophosphine P_{Am}(III) onto *mer*- $InCl_3$, replacing an outer ligand.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	17	0	3.409718	-1.498096	1.483883
3	17	0	2.552916	-1.484080	-2.116346
4	17	0	0.793130	1.134794	1.711212
5	7	0	3.450172	1.208441	-0.505353
6	6	0	4.022513	1.971690	0.615906
7	6	0	5.198482	2.833076	0.206438
8	1	0	5.587591	3.377153	1.069687
9	1	0	6.010320	2.224517	-0.200695
10	1	0	4.909151	3.567372	-0.550726
11	1	0	4.312170	1.246472	1.378201
12	1	0	3.217808	2.571465	1.043033
13	1	0	4.159569	0.618166	-0.933582
14	1	0	3.137671	1.841252	-1.235557
15	7	0	0.197771	0.539780	-1.391090
16	6	0	0.241130	1.958070	-1.759887
17	6	0	-0.943782	2.387432	-2.602788
18	1	0	-0.892461	3.455495	-2.825422
19	1	0	-0.966807	1.844165	-3.551063
20	1	0	-1.882577	2.194430	-2.077978

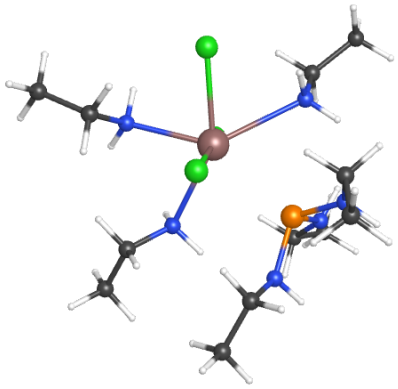
21	1	0	1.170217	2.139390	-2.307249
22	1	0	0.289188	2.530704	-0.830657
23	1	0	-0.684416	0.345803	-0.900208
24	1	0	0.229361	-0.041270	-2.224540
25	7	0	0.281228	-1.972841	0.518499
26	6	0	-0.319896	-2.819261	-0.521333
27	6	0	-1.239625	-3.882527	0.042214
28	1	0	-1.678915	-4.473080	-0.765116
29	1	0	-0.693186	-4.565256	0.697982
30	1	0	-2.049629	-3.425947	0.617843
31	1	0	-0.873692	-2.163917	-1.197998
32	1	0	0.493645	-3.256839	-1.101157
33	1	0	0.789931	-2.543146	1.189987
34	1	0	-0.447895	-1.490364	1.038594
35	15	0	-2.927004	-0.096850	0.194019
36	7	0	-3.200644	-1.035824	1.573059
37	6	0	-2.412377	-0.832978	2.779601
38	6	0	-3.089358	0.048964	3.813760
39	1	0	-2.461783	0.151105	4.702169
40	1	0	-3.277053	1.047062	3.411715
41	1	0	-4.047126	-0.378113	4.124974
42	1	0	-2.174743	-1.806091	3.225029
43	1	0	-1.460952	-0.372639	2.491831
44	1	0	-4.171202	-1.265564	1.759003
45	7	0	-4.101281	-0.916911	-0.752735
46	6	0	-4.250585	-0.554998	-2.155782
47	6	0	-3.146229	-1.061907	-3.069379
48	1	0	-3.335820	-0.777528	-4.107499
49	1	0	-2.177786	-0.646762	-2.780195
50	1	0	-3.072047	-2.152264	-3.027127
51	1	0	-5.216868	-0.936215	-2.501278
52	1	0	-4.312208	0.534881	-2.209522
53	1	0	-3.997642	-1.917841	-0.636838
54	7	0	-3.701109	1.395352	0.235688
55	6	0	-3.017265	2.587492	0.703084
56	6	0	-3.505854	3.837368	-0.002363
57	1	0	-4.572820	3.995013	0.178514
58	1	0	-3.355746	3.763240	-1.081513
59	1	0	-2.972255	4.718287	0.362527
60	1	0	-3.129190	2.716851	1.788077
61	1	0	-1.945671	2.442880	0.532387
62	1	0	-4.700990	1.388700	0.401766

1	2	3

	A	A	A
Frequencies --	3.0529	19.7713	30.8289
Red. masses --	2.4338	3.8595	4.2535
Frc consts --	0.0000	0.0009	0.0024
IR Inten --	0.3232	0.4755	0.5224

Sum of electronic and zero-point Energies=	-2719.949542
Sum of electronic and thermal Energies=	-2719.874154
Sum of electronic and thermal Enthalpies=	-2719.872718
Sum of electronic and thermal Free Energies=	-2720.095816

Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}^{\ddagger}$, the transition state geometry of the zinc-free ligand exchange, replacing an outer ligand.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	-0.747922	-0.478322	-0.026677
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3	17	0	-0.510225	-1.102999	2.368490
4	17	0	-1.134174	0.651909	-2.189262
5	7	0	-3.037187	-0.209675	0.606766
6	6	0	-4.036180	0.097435	-0.422291
7	6	0	-5.463597	-0.001862	0.077056
8	1	0	-6.167291	0.232795	-0.725034
9	1	0	-5.683764	-1.011911	0.432742
10	1	0	-5.646798	0.695716	0.899780
11	1	0	-3.860252	-0.596079	-1.245642
12	1	0	-3.825794	1.095642	-0.810204
13	1	0	-3.182115	-1.157625	0.943934

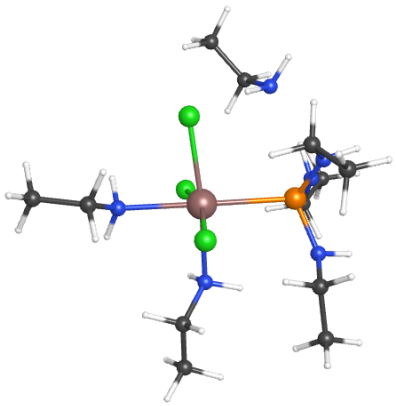
14	1	0	-3.148924	0.398350	1.411834
15	7	0	-0.837359	1.802221	1.092394
16	6	0	-1.765375	2.865507	0.709912
17	6	0	-1.838923	4.007189	1.706863
18	1	0	-2.525226	4.782848	1.358636
19	1	0	-2.194324	3.653820	2.678809
20	1	0	-0.858614	4.466488	1.857954
21	1	0	-2.757682	2.430199	0.577141
22	1	0	-1.466680	3.225544	-0.276464
23	1	0	0.113808	2.166070	1.098559
24	1	0	-1.019846	1.481289	2.039496
25	7	0	1.047253	-2.488581	-0.375230
26	6	0	1.135644	-3.478680	0.693816
27	6	0	1.854533	-4.753676	0.292044
28	1	0	1.895362	-5.457561	1.127513
29	1	0	1.338766	-5.245164	-0.537464
30	1	0	2.881360	-4.545746	-0.024265
31	1	0	1.630017	-3.011242	1.549400
32	1	0	0.116412	-3.696489	1.016551
33	1	0	0.528564	-2.884025	-1.153202
34	1	0	1.973085	-2.246663	-0.713177
35	15	0	1.884707	0.504287	-0.179871
36	7	0	2.793951	-0.192889	-1.393664
37	6	0	2.274650	-0.586698	-2.696675
38	6	0	2.494045	0.440015	-3.790306
39	1	0	2.155950	0.045404	-4.751281
40	1	0	1.930547	1.351749	-3.584800
41	1	0	3.552991	0.697131	-3.883782
42	1	0	2.740878	-1.536434	-2.980784
43	1	0	1.204304	-0.773939	-2.590385
44	1	0	3.785154	0.013835	-1.372490
45	7	0	2.904777	0.134592	1.120902
46	6	0	2.645436	0.675982	2.457580
47	6	0	3.616475	0.079243	3.453637
48	1	0	3.453481	0.506085	4.445052
49	1	0	3.476216	-1.002705	3.532753
50	1	0	4.650782	0.271266	3.158591
51	1	0	2.772232	1.759829	2.418938
52	1	0	1.618448	0.473136	2.782377
53	1	0	3.048530	-0.867498	1.159426
54	7	0	2.053236	2.181183	-0.099678
55	6	0	1.485112	3.029545	-1.142249
56	6	0	1.345718	4.462394	-0.673517
57	1	0	2.318275	4.884631	-0.405471
58	1	0	0.698054	4.531570	0.202541

59	1	0	0.918626	5.081931	-1.464961
60	1	0	2.101978	3.002686	-2.049413
61	1	0	0.514153	2.612856	-1.421733
62	1	0	2.990716	2.466833	0.164934

	1	2	3
	A	A	A
Frequencies --	-56.6834	21.3029	27.2884
Red. masses --	6.9765	2.5723	3.5479
Frc consts --	0.0132	0.0007	0.0016
IR Inten --	6.1435	0.0885	0.1201

Sum of electronic and zero-point Energies=	-2719.926824
Sum of electronic and thermal Energies=	-2719.852855
Sum of electronic and thermal Enthalpies=	-2719.851420
Sum of electronic and thermal Free Energies=	-2720.063967

Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}_{II}$, the final geometry of the zinc-free ligand exchange, replacing an outer ligand.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	0.662773	-0.548149	0.040477
2	17	0	-0.483911	-2.148053	1.561896
3	17	0	-0.583626	-1.404455	-2.026626
4	17	0	2.384050	0.281326	1.642468
5	7	0	2.009105	-2.358367	-0.496932
6	6	0	2.951636	-2.872065	0.506755

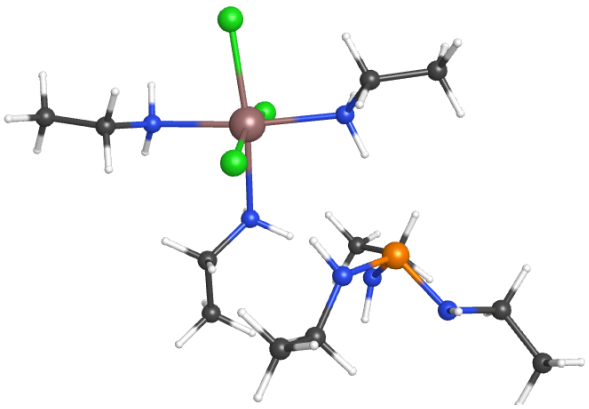
7	6	0	3.571189	-4.197975	0.116318
8	1	0	4.259864	-4.538526	0.892645
9	1	0	2.805308	-4.967066	-0.014391
10	1	0	4.133229	-4.114446	-0.818230
11	1	0	2.399220	-2.958979	1.444112
12	1	0	3.713855	-2.108326	0.664992
13	1	0	1.274093	-3.040384	-0.669914
14	1	0	2.473916	-2.225236	-1.390252
15	7	0	1.713227	0.731539	-1.658992
16	6	0	3.163656	0.944059	-1.675392
17	6	0	3.659013	1.649429	-2.921872
18	1	0	4.742956	1.778301	-2.883037
19	1	0	3.418809	1.075409	-3.820783
20	1	0	3.207361	2.639748	-3.023227
21	1	0	3.646224	-0.031735	-1.576758
22	1	0	3.424196	1.498801	-0.773055
23	1	0	1.219047	1.621996	-1.658574
24	1	0	1.400357	0.242032	-2.494173
25	15	0	-1.041741	1.452265	0.367414
26	7	0	-1.648312	1.504912	1.899232
27	6	0	-0.982223	1.076201	3.118089
28	6	0	-0.430911	2.223859	3.941666
29	1	0	0.005459	1.848052	4.870209
30	1	0	0.349769	2.755496	3.393345
31	1	0	-1.217070	2.938475	4.202010
32	1	0	-1.692556	0.491134	3.710123
33	1	0	-0.177752	0.392699	2.845754
34	1	0	-2.481334	2.065270	2.023260
35	7	0	-2.461767	1.450968	-0.500595
36	6	0	-2.503593	1.647150	-1.948302
37	6	0	-3.942683	1.650276	-2.422712
38	1	0	-3.986563	1.810808	-3.502087
39	1	0	-4.423631	0.693350	-2.205855
40	1	0	-4.516309	2.438797	-1.929736
41	1	0	-2.033921	2.602127	-2.194662
42	1	0	-1.943405	0.864765	-2.472412
43	1	0	-3.020175	0.627463	-0.204322
44	7	0	-0.351506	2.876551	-0.203636
45	6	0	0.839567	3.427950	0.434744
46	6	0	1.561070	4.393018	-0.482716
47	1	0	0.917010	5.233680	-0.755028
48	1	0	1.875803	3.903362	-1.407445
49	1	0	2.448939	4.795286	0.009442
50	1	0	0.581551	3.936210	1.372281
51	1	0	1.495316	2.597475	0.711095

52	1	0	-1.042548	3.589737	-0.412992
53	7	0	-3.676823	-1.079171	0.397782
54	6	0	-4.110648	-1.938839	-0.698717
55	6	0	-4.281116	-3.402203	-0.328139
56	1	0	-4.596457	-3.994699	-1.191676
57	1	0	-3.336854	-3.813252	0.038976
58	1	0	-5.032009	-3.524062	0.458431
59	1	0	-5.051067	-1.539386	-1.092971
60	1	0	-3.367556	-1.846865	-1.495561
61	1	0	-2.806440	-1.439397	0.786069
62	1	0	-4.354330	-1.102884	1.151933

	1	2	3
	A	A	A
Frequencies --	28.4077	33.7157	38.3302
Red. masses --	3.3828	4.1998	3.0738
Frc consts --	0.0016	0.0028	0.0027
IR Inten --	0.4167	0.8028	0.3626

Sum of electronic and zero-point Energies=	-2719.951429
Sum of electronic and thermal Energies=	-2719.875886
Sum of electronic and thermal Enthalpies=	-2719.874451
Sum of electronic and thermal Free Energies=	-2720.092849

Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}_{A_I}$, the starting geometry of the zinc-free ligand exchange, replacing the middle ligand.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

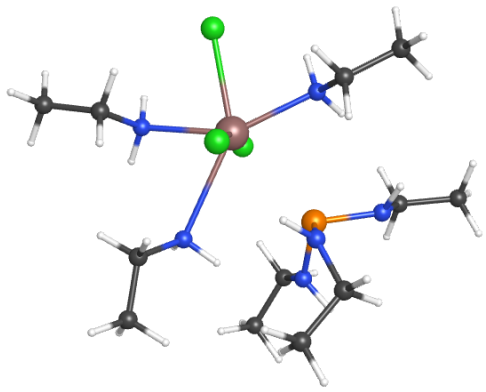
1	49	0	1.736959	-0.472573	-0.004109
2	17	0	1.066052	0.746910	2.045442
3	17	0	3.420081	-1.934425	1.047400
4	17	0	1.997242	-1.407234	-2.341210
5	7	0	0.414576	1.051869	-1.194761
6	6	0	0.531221	2.490934	-0.931528
7	6	0	-0.237437	3.339103	-1.925150
8	1	0	-0.142774	4.399227	-1.680240
9	1	0	0.137690	3.190748	-2.941314
10	1	0	-1.299693	3.083513	-1.919091
11	1	0	0.190657	2.665029	0.089691
12	1	0	1.589368	2.762973	-0.951154
13	1	0	0.714660	0.839826	-2.143768
14	1	0	-0.575537	0.787578	-1.158612
15	7	0	3.566177	0.852054	-0.499252
16	6	0	4.097955	1.710882	0.569937
17	6	0	5.403216	2.383019	0.199886
18	1	0	5.284391	3.027699	-0.675568
19	1	0	5.759781	3.001330	1.026389
20	1	0	6.175553	1.642803	-0.024194
21	1	0	3.330565	2.446164	0.818683
22	1	0	4.218445	1.079408	1.451929
23	1	0	3.443409	1.377722	-1.359590
24	1	0	4.236012	0.116598	-0.713547
25	7	0	0.095577	-2.033392	0.268609
26	6	0	0.005901	-2.691701	1.584167
27	6	0	-1.014161	-3.810856	1.604078
28	1	0	-1.057994	-4.265695	2.596112
29	1	0	-2.010370	-3.436180	1.355683
30	1	0	-0.752054	-4.594414	0.887694
31	1	0	1.000750	-3.057506	1.840673
32	1	0	-0.246400	-1.916745	2.310269
33	1	0	-0.826375	-1.638471	0.056211
34	1	0	0.303216	-2.714740	-0.458042
35	15	0	-2.854902	-0.185991	0.321616
36	7	0	-4.520675	0.103510	0.641899
37	6	0	-5.490925	-0.783143	0.014347
38	6	0	-6.905617	-0.359761	0.353025
39	1	0	-7.079896	-0.409814	1.431632
40	1	0	-7.089592	0.666670	0.028203
41	1	0	-7.632387	-1.014830	-0.132410
42	1	0	-5.346997	-0.731568	-1.068294
43	1	0	-5.342323	-1.836240	0.299523
44	1	0	-4.667435	0.150976	1.644862

45	7	0	-2.726021	0.295103	-1.312405
46	6	0	-2.812517	-0.711436	-2.367990
47	6	0	-1.868777	-0.436953	-3.523490
48	1	0	-2.052048	-1.140869	-4.338764
49	1	0	-2.013738	0.573852	-3.914673
50	1	0	-0.824870	-0.547627	-3.222268
51	1	0	-2.575543	-1.681674	-1.918330
52	1	0	-3.838362	-0.795035	-2.746859
53	1	0	-3.208166	1.153674	-1.557499
54	7	0	-2.242507	1.066828	1.236218
55	6	0	-2.618160	2.469101	1.140889
56	6	0	-2.236030	3.218417	2.401461
57	1	0	-2.504900	4.274009	2.318805
58	1	0	-2.744684	2.796471	3.270933
59	1	0	-1.159012	3.155240	2.579397
60	1	0	-2.146106	2.953184	0.274254
61	1	0	-3.696921	2.521232	0.980486
62	1	0	-1.293063	0.914716	1.562194

	1	2	3
	A	A	A
Frequencies --	18.2232	24.5353	27.8258
Red. masses --	3.5887	3.3496	3.6326
Frc consts --	0.0007	0.0012	0.0017
IR Inten --	0.2083	0.1641	0.0081

Sum of electronic and zero-point Energies= -2719.949677
Sum of electronic and thermal Energies= -2719.874700
Sum of electronic and thermal Enthalpies= -2719.873265
Sum of electronic and thermal Free Energies= -2720.092802

Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}_A^{\ddagger}$, the transition state geometry of the zinc-free ligand exchange, replacing the middle ligand.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	-1.031732	-0.613682	0.181213
2	17	0	-1.189839	-0.104068	-2.207305
3	17	0	-2.742087	-2.606807	0.105971
4	17	0	-0.647467	-0.636225	2.609122
5	7	0	-0.738400	2.253832	0.356589
6	6	0	-1.462124	3.149269	-0.543725
7	6	0	-0.912229	4.563940	-0.592238
8	1	0	-1.484154	5.184054	-1.287345
9	1	0	-0.950754	5.036442	0.393527
10	1	0	0.129905	4.560614	-0.924464
11	1	0	-1.440243	2.698390	-1.539260
12	1	0	-2.512289	3.172273	-0.237926
13	1	0	-0.857675	2.551998	1.319990
14	1	0	0.258632	2.337824	0.175112
15	7	0	-3.061960	0.363166	0.696469
16	6	0	-4.037915	0.581956	-0.377536
17	6	0	-5.360889	1.121491	0.126713
18	1	0	-5.231081	2.083881	0.630885
19	1	0	-6.054580	1.268450	-0.704080
20	1	0	-5.823774	0.427451	0.833096
21	1	0	-3.587403	1.258776	-1.104081
22	1	0	-4.170762	-0.376915	-0.880314
23	1	0	-2.889096	1.219066	1.211832
24	1	0	-3.425210	-0.319875	1.356273
25	7	0	0.270886	-2.546864	-0.005528
26	6	0	0.618925	-2.999935	-1.354861
27	6	0	1.442320	-4.271802	-1.366993
28	1	0	1.673248	-4.568864	-2.392361

29	1	0	2.389174	-4.138349	-0.834671
30	1	0	0.900956	-5.092760	-0.890473
31	1	0	-0.320454	-3.136458	-1.893353
32	1	0	1.145131	-2.185903	-1.860884
33	1	0	1.094997	-2.466224	0.581544
34	1	0	-0.359657	-3.214036	0.433076
35	15	0	1.815440	0.275838	-0.139691
36	7	0	3.159005	-0.778712	-0.027073
37	6	0	3.579367	-1.297668	1.265546
38	6	0	4.805803	-2.173568	1.119207
39	1	0	4.593750	-3.041933	0.488205
40	1	0	5.626635	-1.616012	0.663041
41	1	0	5.133388	-2.542910	2.092869
42	1	0	3.808255	-0.447903	1.913227
43	1	0	2.785810	-1.863013	1.780206
44	1	0	3.144818	-1.487759	-0.750051
45	7	0	2.358840	1.606031	0.741692
46	6	0	2.030125	1.833652	2.143763
47	6	0	2.023534	3.313114	2.473566
48	1	0	1.776401	3.469115	3.526126
49	1	0	3.005284	3.759436	2.291179
50	1	0	1.294781	3.850777	1.862519
51	1	0	1.053547	1.384524	2.335643
52	1	0	2.732049	1.317323	2.810955
53	1	0	3.291281	1.922668	0.500557
54	7	0	1.929042	0.661788	-1.744757
55	6	0	3.015737	1.377515	-2.388677
56	6	0	2.736482	2.862640	-2.550747
57	1	0	3.569345	3.363339	-3.051126
58	1	0	1.837619	3.020597	-3.152571
59	1	0	2.577981	3.336183	-1.579358
60	1	0	3.922625	1.215670	-1.799473
61	1	0	3.207367	0.926824	-3.368191
62	1	0	1.030383	0.688469	-2.212223

	1	2	3
	A	A	A
Frequencies --	-59.2060	23.2375	29.9833
Red. masses --	4.8938	4.1765	4.7640
Frc consts --	0.0101	0.0013	0.0025
IR Inten --	5.4915	1.9809	5.3974

Sum of electronic and zero-point Energies= -2719.930310
Sum of electronic and thermal Energies= -2719.856170

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Sum of electronic and thermal Enthalpies=           -2719.854735
Sum of electronic and thermal Free Energies=        -2720.068013
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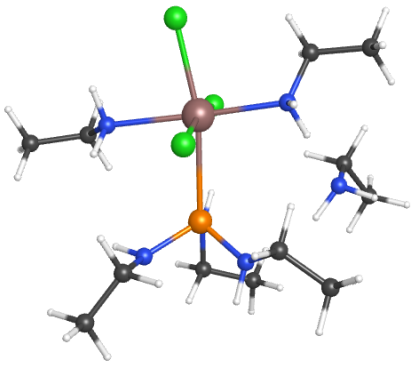
Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}_{A_{II}}$, the final geometry of the zinc-free ligand exchange, replacing the middle ligand.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	0.390886	-1.307306	0.087705
2	17	0	-0.551421	-1.172779	-2.239901
3	17	0	0.811723	-3.743408	0.011345
4	17	0	1.297241	-1.009730	2.417823
5	7	0	-1.694873	-1.560791	0.939064
6	6	0	-2.496430	-2.688610	0.438332
7	6	0	-3.854457	-2.777924	1.105353
8	1	0	-4.434995	-1.865655	0.945031
9	1	0	-4.423230	-3.617022	0.698588
10	1	0	-3.754337	-2.931845	2.183347
11	1	0	-2.598006	-2.553210	-0.640176
12	1	0	-1.925230	-3.605425	0.588145
13	1	0	-2.215731	-0.681367	0.762675
14	1	0	-1.553575	-1.649561	1.942198
15	7	0	2.601583	-1.138981	-0.629647
16	6	0	2.917944	-0.711821	-1.996837
17	6	0	4.405067	-0.582380	-2.254754
18	1	0	4.588297	-0.261685	-3.282637
19	1	0	4.859695	0.154965	-1.586183
20	1	0	4.915408	-1.536657	-2.102586
21	1	0	2.460102	-1.434156	-2.673766

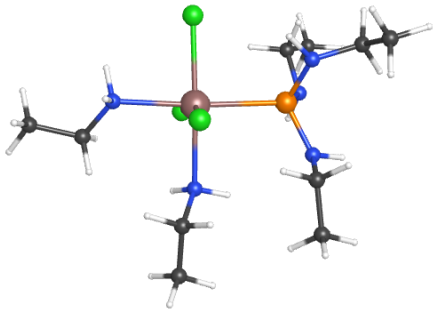
22	1	0	2.405927	0.236149	-2.181221
23	1	0	3.077169	-0.563081	0.059226
24	1	0	2.914906	-2.093925	-0.472539
25	15	0	0.484263	1.433550	0.039459
26	7	0	2.011669	2.146562	0.186153
27	6	0	2.763961	2.169010	1.430939
28	6	0	3.773065	3.299118	1.434068
29	1	0	4.490054	3.187301	0.615521
30	1	0	3.276741	4.265138	1.317457
31	1	0	4.335937	3.306841	2.370027
32	1	0	2.053265	2.297476	2.250150
33	1	0	3.266778	1.213532	1.626477
34	1	0	2.586447	2.026287	-0.636896
35	7	0	-0.375202	2.316329	1.175458
36	6	0	-0.892561	1.778214	2.427476
37	6	0	-1.976176	2.673566	2.990920
38	1	0	-2.370508	2.255249	3.919329
39	1	0	-1.583745	3.669329	3.216095
40	1	0	-2.801297	2.791294	2.284867
41	1	0	-1.292527	0.784984	2.228790
42	1	0	-0.096826	1.640065	3.167883
43	1	0	-0.069077	3.279351	1.257605
44	7	0	0.099054	1.915347	-1.488839
45	6	0	0.030334	3.276278	-1.989645
46	6	0	-1.391263	3.795333	-2.107587
47	1	0	-1.400894	4.813612	-2.504245
48	1	0	-1.976879	3.165359	-2.781641
49	1	0	-1.882767	3.800509	-1.132049
50	1	0	0.614965	3.911678	-1.319440
51	1	0	0.525675	3.322439	-2.965211
52	1	0	-0.321687	1.185020	-2.052903
53	7	0	-3.229198	0.848378	0.159196
54	6	0	-3.830416	0.552869	-1.138852
55	6	0	-4.721817	1.649158	-1.694571
56	1	0	-5.131331	1.365703	-2.667733
57	1	0	-5.561399	1.848399	-1.022086
58	1	0	-4.164039	2.580557	-1.820941
59	1	0	-3.015513	0.327980	-1.831805
60	1	0	-4.405200	-0.373565	-1.040615
61	1	0	-3.946342	1.108798	0.827764
62	1	0	-2.596545	1.639694	0.087807

1	2	3
A	A	A

Frequencies --	24.9318	32.9755	41.9090
Red. masses --	3.3032	3.3094	3.2246
Frc consts --	0.0012	0.0021	0.0033
IR Inten --	0.2353	0.3924	0.7547

Sum of electronic and zero-point Energies=	-2719.949937
Sum of electronic and thermal Energies=	-2719.874528
Sum of electronic and thermal Enthalpies=	-2719.873093
Sum of electronic and thermal Free Energies=	-2720.089981

Cartesian coordinates, three lower frequencies, and thermochemistry of **L**, the phosphorus-bound conformer of the zinc-free ligand exchange, replacing an outer ligand.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	-0.753104	-0.402637	-0.307213
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3	17	0	-0.012354	-2.396440	-1.609137
4	17	0	-0.994304	-1.567912	1.935667
5	7	0	-1.513446	1.391001	1.060419
6	6	0	-2.225130	2.566909	0.546568
7	6	0	-2.747456	3.475316	1.641088
8	1	0	-3.258698	4.339154	1.210663
9	1	0	-3.457954	2.948375	2.283857
10	1	0	-1.933520	3.844913	2.270553
11	1	0	-3.042517	2.215663	-0.086079
12	1	0	-1.545593	3.099296	-0.119414
13	1	0	-2.071941	0.897725	1.752616
14	1	0	-0.673185	1.680848	1.556878

15	7	0	-2.887335	-1.097393	-0.788733
16	6	0	-4.009522	-0.854173	0.125659
17	6	0	-5.295728	-1.521524	-0.316048
18	1	0	-6.097834	-1.312713	0.395146
19	1	0	-5.611438	-1.160853	-1.298406
20	1	0	-5.171462	-2.605780	-0.373838
21	1	0	-4.149711	0.227032	0.196646
22	1	0	-3.703398	-1.210518	1.111156
23	1	0	-2.748836	-2.096195	-0.924468
24	1	0	-3.074949	-0.704461	-1.707844
25	15	0	1.732292	0.155960	0.282475
26	7	0	2.668575	-0.170924	-1.024179
27	6	0	4.114584	-0.061289	-1.101794
28	6	0	4.559011	0.716590	-2.324509
29	1	0	5.649004	0.779565	-2.363641
30	1	0	4.215824	0.229083	-3.240298
31	1	0	4.150826	1.729371	-2.308968
32	1	0	4.461126	0.433050	-0.190278
33	1	0	4.568943	-1.059040	-1.102646
34	1	0	2.199108	-0.655888	-1.776954
35	7	0	2.426299	-0.663920	1.575443
36	6	0	2.589995	-2.115436	1.456152
37	6	0	3.454562	-2.640904	2.581955
38	1	0	3.588294	-3.720254	2.483744
39	1	0	4.438365	-2.166028	2.575655
40	1	0	2.989257	-2.451303	3.553307
41	1	0	1.618380	-2.621440	1.453165
42	1	0	3.060573	-2.318622	0.491912
43	1	0	1.959887	-0.423352	2.443740
44	7	0	1.936764	1.708455	0.863000
45	6	0	1.615795	2.845209	0.005545
46	6	0	1.283369	4.077795	0.819544
47	1	0	1.045816	4.916444	0.161822
48	1	0	0.425567	3.901354	1.472683
49	1	0	2.126596	4.372697	1.449771
50	1	0	2.443488	3.061815	-0.680542
51	1	0	0.770491	2.561755	-0.628429
52	1	0	2.776429	1.834302	1.416504

	1	2	3
	A	A	A
Frequencies --	23.7212	28.4874	31.5382
Red. masses --	4.6983	2.6442	2.9486
Frc consts --	0.0016	0.0013	0.0017

```
IR Inten    --      1.9549                  0.1890                  0.5993

Sum of electronic and zero-point Energies=          -2584.969307
Sum of electronic and thermal Energies=             -2584.904719
Sum of electronic and thermal Enthalpies=           -2584.903284
Sum of electronic and thermal Free Energies=        -2585.097848
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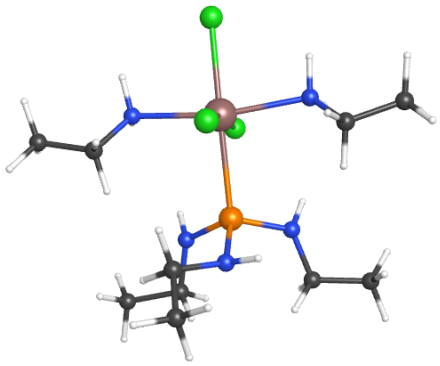
Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}_A$, the phosphorus-bound conformer of the zinc-free ligand exchange, replacing the middle ligand.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	17	0	-0.913203	-0.077207	-2.642682
3	17	0	-3.576964	-1.260148	-0.334562
4	17	0	-1.148889	-0.518963	2.365210
5	7	0	-0.637769	-2.608997	-0.408466
6	6	0	0.395788	-3.226298	0.433283
7	6	0	0.593774	-4.701066	0.149699
8	1	0	1.365512	-5.113783	0.803340
9	1	0	-0.328185	-5.262404	0.321600
10	1	0	0.905187	-4.866270	-0.885388
11	1	0	0.104486	-3.061598	1.472344
12	1	0	1.322975	-2.673707	0.268470
13	1	0	-1.530905	-3.081090	-0.286197
14	1	0	-0.406902	-2.693863	-1.395136
15	7	0	-2.273377	1.685531	-0.085189
16	6	0	-1.939500	2.679436	0.944749
17	6	0	-2.791437	3.929321	0.864432

18	1	0	-2.511055	4.631924	1.652355
19	1	0	-2.664264	4.433877	-0.097396
20	1	0	-3.851332	3.692100	0.986938
21	1	0	-0.881600	2.924315	0.829722
22	1	0	-2.050888	2.186637	1.911927
23	1	0	-3.249272	1.405866	-0.008934
24	1	0	-2.166455	2.073155	-1.019013
25	15	0	1.219404	0.541121	-0.143200
26	7	0	1.147064	2.117281	-0.684522
27	6	0	2.301171	2.987855	-0.896903
28	6	0	1.912610	4.445764	-0.759396
29	1	0	2.777771	5.091518	-0.925903
30	1	0	1.146839	4.717567	-1.490996
31	1	0	1.515892	4.647826	0.238049
32	1	0	3.054439	2.725285	-0.152402
33	1	0	2.746316	2.808749	-1.883173
34	1	0	0.443894	2.206427	-1.408600
35	7	0	2.176465	-0.491013	-1.030345
36	6	0	3.599857	-0.306574	-1.293429
37	6	0	4.283941	-1.637187	-1.532963
38	1	0	5.348865	-1.492721	-1.728033
39	1	0	4.176545	-2.290294	-0.663786
40	1	0	3.851284	-2.148618	-2.396887
41	1	0	3.754847	0.355323	-2.154138
42	1	0	4.036323	0.193604	-0.426420
43	1	0	1.660949	-0.871199	-1.815418
44	7	0	2.140607	0.745010	1.242461
45	6	0	2.524417	-0.416741	2.042710
46	6	0	3.392051	0.015164	3.205181
47	1	0	3.695852	-0.851920	3.794917
48	1	0	4.289951	0.529264	2.854621
49	1	0	2.845807	0.691877	3.868095
50	1	0	1.641950	-0.953300	2.411076
51	1	0	3.078116	-1.101889	1.396968
52	1	0	1.746769	1.480730	1.817032

	1	2	3
	A	A	A
Frequencies --	23.4254	31.0036	39.0811
Red. masses --	3.7552	3.9396	2.7613
Frc consts --	0.0012	0.0022	0.0025
IR Inten --	0.1419	0.2707	0.2911

Sum of electronic and zero-point Energies= -2584.968631

```
Sum of electronic and thermal Energies=             -2584.904278
Sum of electronic and thermal Enthalpies=           -2584.902843
Sum of electronic and thermal Free Energies=        -2585.096722
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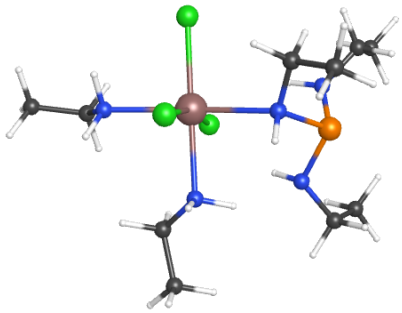
Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}_B$, the nitrogen-bound conformer of the zinc-free ligand exchange, replacing an outer ligand.



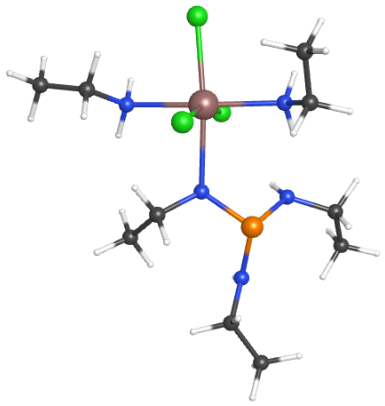
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	-0.991408	-0.421135	-0.104829
2	17	0	-1.928935	-1.184187	-2.316643
3	17	0	-0.960717	-2.581311	1.030037
4	17	0	-0.207567	0.851490	1.905501
5	7	0	-1.007654	1.646229	-1.169284
6	6	0	-1.782890	2.761869	-0.614107
7	6	0	-1.551739	4.070253	-1.342606
8	1	0	-2.149534	4.867937	-0.896410
9	1	0	-0.500780	4.365949	-1.285708
10	1	0	-1.826758	3.990158	-2.397355
11	1	0	-1.512445	2.852104	0.439586
12	1	0	-2.840400	2.488530	-0.654483
13	1	0	-0.013341	1.888263	-1.202633
14	1	0	-1.306241	1.440876	-2.119324
15	7	0	-3.212159	-0.262790	0.498939
16	6	0	-3.597485	0.328138	1.788823
17	6	0	-5.075166	0.188889	2.088829
18	1	0	-5.310087	0.638373	3.055968
19	1	0	-5.683050	0.687533	1.328899
20	1	0	-5.370820	-0.862719	2.125933

21	1	0	-3.296200	1.377009	1.776171
22	1	0	-2.992820	-0.156100	2.557066
23	1	0	-3.450553	-1.252256	0.488140
24	1	0	-3.735166	0.153336	-0.266350
25	7	0	1.097495	-0.703511	-1.159496
26	6	0	1.328020	-2.144029	-1.442429
27	6	0	2.109410	-2.387667	-2.717690
28	1	0	2.244347	-3.460569	-2.870176
29	1	0	1.565306	-1.995883	-3.581798
30	1	0	3.095493	-1.919635	-2.690205
31	1	0	1.834962	-2.565093	-0.572261
32	1	0	0.357332	-2.636140	-1.503359
33	1	0	0.858209	-0.265560	-2.049055
34	15	0	2.616744	0.081166	-0.591958
35	7	0	2.729728	-0.546622	0.938343
36	6	0	3.769638	-1.473174	1.341933
37	6	0	4.486514	-1.016914	2.598516
38	1	0	5.251018	-1.740652	2.891805
39	1	0	4.965348	-0.047940	2.439881
40	1	0	3.783368	-0.914899	3.429200
41	1	0	3.350048	-2.475002	1.497078
42	1	0	4.479200	-1.556550	0.512990
43	1	0	1.957793	-0.437014	1.586346
44	7	0	1.961239	1.640563	-0.430367
45	6	0	2.877329	2.765785	-0.613685
46	6	0	3.779681	3.038448	0.576673
47	1	0	4.403473	3.917408	0.396004
48	1	0	3.187878	3.219722	1.477909
49	1	0	4.434513	2.186343	0.773896
50	1	0	3.478336	2.563940	-1.504966
51	1	0	2.278805	3.655105	-0.837639
52	1	0	1.402908	1.743013	0.417121

	1	2	3
	A	A	A
Frequencies --	17.9718	29.7826	33.0942
Red. masses --	4.2243	3.5486	3.3023
Frc consts --	0.0008	0.0019	0.0021
IR Inten --	1.7124	0.4596	0.0374

Sum of electronic and zero-point Energies= -2584.962768
Sum of electronic and thermal Energies= -2584.899159
Sum of electronic and thermal Enthalpies= -2584.897724
Sum of electronic and thermal Free Energies= -2585.089238

Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}_C$, the nitrogen-bound conformer of the zinc-free ligand exchange, replacing the middle ligand.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	17	0	-3.565102	-1.184897	0.483638
4	17	0	-1.428351	0.167508	-2.287446
5	7	0	0.865197	0.882921	0.042652
6	6	0	0.785731	2.187614	-0.650915
7	6	0	1.190880	3.350158	0.231280
8	1	0	1.072820	4.293671	-0.305254
9	1	0	0.574494	3.402485	1.134542
10	1	0	2.231922	3.263711	0.547974
11	1	0	-0.225751	2.325089	-1.037074
12	1	0	1.425102	2.147294	-1.538506
13	1	0	0.882932	1.033691	1.051461
14	15	0	2.298616	-0.014455	-0.477840
15	7	0	2.217779	-1.164244	0.763247
16	6	0	3.225286	-2.217339	0.807272
17	6	0	4.438287	-1.890375	1.660236
18	1	0	5.131861	-2.734613	1.677943
19	1	0	4.139441	-1.681598	2.691089
20	1	0	4.964781	-1.017645	1.270447
21	1	0	3.534071	-2.419587	-0.223662
22	1	0	2.754775	-3.136020	1.175064
23	1	0	1.899530	-0.863054	1.679135

```
   24          7           0        3.598875    0.967349   -0.085261
   25          6           0        4.389032    1.663838   -1.082639
   26          1           0        4.157116    2.737098   -1.086436
   27          1           0        4.085303    1.279465   -2.061106
   28          6           0        5.878581    1.460043   -0.882494
   29          1           0        6.194905    1.824583    0.098799
   30          1           0        6.447851    2.003982   -1.640025
   31          1           0        6.135357    0.400481   -0.949121
   32          1           0        3.749430    1.262979    0.870572
   33          7           0       -0.397674   -2.333908   -0.076496
   34          6           0       -0.290258   -3.010144   -1.380911
   35          6           0       -1.636811   -3.484734   -1.876942
   36          1           0       -1.522646   -3.981288   -2.842242
   37          1           0       -2.084811   -4.198025   -1.179766
   38          1           0       -2.325658   -2.648075   -1.999166
   39          1           0        0.402439   -3.854234   -1.293643
   40          1           0        0.142288   -2.295982   -2.084098
   41          1           0       -0.920333   -2.904591    0.582115
   42          1           0        0.533339   -2.170097    0.320360
   43          7           0       -2.217208    1.760596    0.729779
   44          6           0       -3.159103    2.403247   -0.200494
   45          6           0       -3.821775    3.631424    0.386387
   46          1           0       -4.507965    4.075615   -0.337638
   47          1           0       -4.394534    3.379681    1.282686
   48          1           0       -3.080643    4.389186    0.656171
   49          1           0       -2.610004    2.646336   -1.111582
   50          1           0       -3.898403    1.648589   -0.473952
   51          1           0       -2.705909    1.468226    1.573060
   52          1           0       -1.511373    2.424341    1.034348
---------------------------------------------------------------------

                     1                      2                      3
                     A                      A                      A
Frequencies --     20.0565                27.8399                31.4351
Red. masses --      3.5835                 3.5631                 3.4895
Frc consts  --      0.0008                 0.0016                 0.0020
IR Inten    --      0.3137                 0.1376                 0.3526

Sum of electronic and zero-point Energies=          -2584.957148
Sum of electronic and thermal Energies=             -2584.893509
Sum of electronic and thermal Enthalpies=           -2584.892073
Sum of electronic and thermal Free Energies=        -2585.083403
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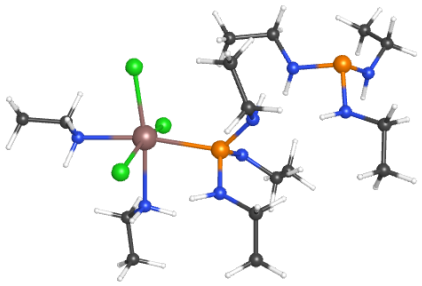
Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{D}_I$, the start-

ing geometry of the zinc-free disproportionation reaction where a second aminophosphine, P_{Am}(III), hydrogen bonds with **L**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	17	0	-1.697553	-1.656779	1.757125
5	7	0	-3.035661	1.359015	1.312389
6	6	0	-3.790619	1.037315	2.527087
7	6	0	-4.026531	2.234514	3.426472
8	1	0	-4.593596	1.943680	4.313613
9	1	0	-3.077726	2.662864	3.761055
10	1	0	-4.587048	3.016009	2.906783
11	1	0	-4.746012	0.602483	2.221925
12	1	0	-3.242772	0.252630	3.051218
13	1	0	-2.169439	1.832506	1.557586
14	1	0	-3.548733	2.011337	0.724507
15	7	0	-4.549484	-1.075096	-0.223276
16	6	0	-4.896362	-2.234955	0.610480
17	6	0	-6.316914	-2.714147	0.397795
18	1	0	-6.477972	-3.015493	-0.640469
19	1	0	-6.526718	-3.576099	1.034646
20	1	0	-7.040338	-1.931031	0.641728
21	1	0	-4.176713	-3.021500	0.377069
22	1	0	-4.723218	-1.958432	1.651676
23	1	0	-4.662112	-1.310076	-1.206978
24	1	0	-5.178702	-0.296712	-0.050167
25	15	0	-0.065429	0.905942	-0.323485

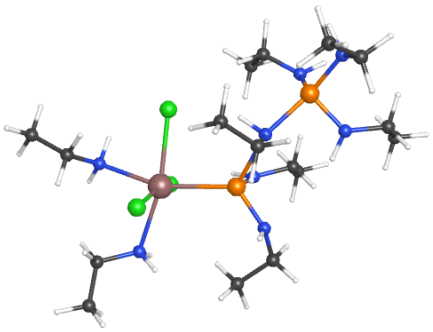
26	7	0	0.635032	0.608816	1.147128
27	6	0	1.565726	1.487590	1.843303
28	6	0	2.124067	0.804672	3.073442
29	1	0	2.813368	1.470370	3.596414
30	1	0	1.326516	0.529115	3.768739
31	1	0	2.665802	-0.105878	2.806632
32	1	0	2.385882	1.736558	1.166135
33	1	0	1.075293	2.426567	2.133139
34	1	0	0.051291	0.028981	1.742494
35	7	0	-0.491067	2.497502	-0.512728
36	6	0	0.431562	3.609849	-0.698476
37	6	0	0.023263	4.819179	0.118383
38	1	0	0.720629	5.644722	-0.042540
39	1	0	-0.975323	5.161358	-0.164583
40	1	0	0.011054	4.579863	1.184376
41	1	0	1.429995	3.277411	-0.408695
42	1	0	0.493129	3.877192	-1.759691
43	1	0	-1.399268	2.606823	-0.953834
44	7	0	1.212203	0.678044	-1.367870
45	6	0	1.097160	0.964476	-2.793518
46	6	0	0.936719	-0.283013	-3.640067
47	1	0	0.028941	-0.825689	-3.368286
48	1	0	1.790418	-0.952819	-3.504098
49	1	0	0.881783	-0.020181	-4.699111
50	1	0	0.246091	1.634121	-2.944707
51	1	0	1.987936	1.520404	-3.109623
52	1	0	1.768074	-0.152931	-1.149355
53	7	0	4.298798	0.843929	-0.321920
54	6	0	5.326798	1.833792	-0.604746
55	6	0	4.832330	3.226499	-0.267717
56	1	0	4.549820	3.291727	0.785897
57	1	0	5.605061	3.972576	-0.466493
58	1	0	3.956456	3.487406	-0.869922
59	1	0	6.202016	1.592871	0.004382
60	1	0	5.657406	1.804692	-1.654412
61	15	0	4.715483	-0.818496	-0.502161
62	7	0	5.673512	-0.933783	0.874551
63	1	0	5.339163	-0.505765	1.728937
64	6	0	6.695070	-1.945003	1.042050
65	6	0	6.246979	-3.160595	1.836687
66	1	0	5.898833	-2.868916	2.831709
67	1	0	7.069866	-3.869437	1.962859
68	1	0	5.426244	-3.674188	1.330232
69	1	0	7.013575	-2.254328	0.041911
70	1	0	7.572343	-1.495445	1.521808

71	7	0	3.127101	-1.367382	-0.193031
72	1	0	2.688044	-0.968398	0.632364
73	6	0	2.829385	-2.787060	-0.335290
74	6	0	1.340600	-3.027633	-0.479845
75	1	0	0.788507	-2.643456	0.382432
76	1	0	0.939902	-2.539524	-1.370145
77	1	0	1.127450	-4.096129	-0.558085
78	1	0	3.213432	-3.365309	0.517075
79	1	0	3.361321	-3.148433	-1.220845
80	1	0	3.444991	1.048636	-0.831594

	1	2	3
	A	A	A
Frequencies --	16.6514	18.5808	21.7280
Red. masses --	3.7748	4.5081	4.1790
Frc consts --	0.0006	0.0009	0.0012
IR Inten --	0.2019	0.9305	0.3681

Sum of electronic and zero-point Energies=	-3329.413121
Sum of electronic and thermal Energies=	-3329.316823
Sum of electronic and thermal Enthalpies=	-3329.315388
Sum of electronic and thermal Free Energies=	-3329.584779

Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{D}^{\ddagger}$, the transition state of the zinc-free disproportionation reaction.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	49	0	-2.189607	-0.170021	0.071683
2	17	0	-0.697358	-1.991700	1.178784
3	17	0	-2.470198	-1.254869	-2.181257
4	17	0	-2.598996	1.263198	2.220749
5	7	0	-3.943484	1.228433	-0.750893
6	6	0	-5.273345	0.658078	-0.984526
7	6	0	-6.217743	1.598273	-1.707159
8	1	0	-7.193304	1.128125	-1.850958
9	1	0	-6.365984	2.520804	-1.139863
10	1	0	-5.824244	1.861910	-2.692471
11	1	0	-5.132712	-0.261413	-1.556780
12	1	0	-5.694521	0.383250	-0.014302
13	1	0	-3.995195	2.008952	-0.102734
14	1	0	-3.570049	1.580095	-1.626833
15	7	0	-3.783869	-1.476418	1.088876
16	6	0	-4.231312	-2.716129	0.442373
17	6	0	-5.125043	-3.558457	1.328975
18	1	0	-6.028908	-3.012661	1.614177
19	1	0	-5.431533	-4.467567	0.806879
20	1	0	-4.603327	-3.854438	2.242801
21	1	0	-4.737612	-2.445460	-0.485330
22	1	0	-3.332637	-3.265250	0.156623
23	1	0	-4.569577	-0.904528	1.381938
24	1	0	-3.263631	-1.696439	1.935208
25	15	0	0.106494	0.892588	-0.499071
26	7	0	0.419292	1.753385	0.886397
27	6	0	1.677627	2.377827	1.245949
28	6	0	1.473505	3.380309	2.362339
29	1	0	2.421541	3.852063	2.630043
30	1	0	0.767478	4.160681	2.067868
31	1	0	1.078284	2.888421	3.255510
32	1	0	2.417752	1.627681	1.546479
33	1	0	2.083627	2.887525	0.365331
34	1	0	-0.297333	1.718973	1.601222
35	7	0	0.380160	2.057160	-1.703525
36	6	0	-0.060178	3.443999	-1.616503
37	6	0	-1.564265	3.643394	-1.633782
38	1	0	-1.815207	4.706960	-1.619058
39	1	0	-2.008676	3.200815	-2.530037
40	1	0	-2.009858	3.182571	-0.749327
41	1	0	0.345953	3.869615	-0.696220
42	1	0	0.404282	3.986376	-2.445516
43	1	0	0.327228	1.678688	-2.638547
44	7	0	1.952436	-0.425818	-0.578759
45	6	0	1.858747	-1.014822	-1.946250

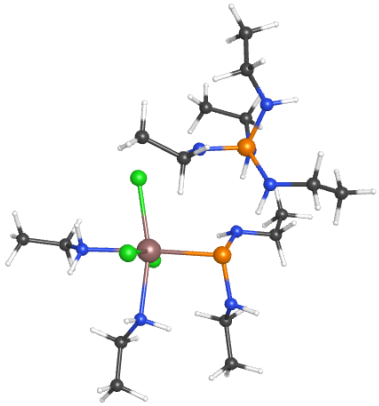
46	6	0	1.347593	-2.437700	-1.963589
47	1	0	0.342905	-2.486421	-1.538778
48	1	0	2.000824	-3.086734	-1.373877
49	1	0	1.308320	-2.819629	-2.986862
50	1	0	1.197609	-0.382518	-2.543058
51	1	0	2.853066	-0.952495	-2.401514
52	1	0	1.446681	-1.044150	0.058443
53	15	0	3.804744	-0.669646	-0.031784
54	7	0	4.226589	0.784740	-0.713923
55	6	0	5.458114	1.530095	-0.540858
56	6	0	5.325829	2.684555	0.438603
57	1	0	5.045504	2.326952	1.432093
58	1	0	6.270457	3.228291	0.520833
59	1	0	4.559543	3.391878	0.110594
60	1	0	6.225481	0.833925	-0.199587
61	1	0	5.785297	1.910019	-1.515323
62	1	0	3.424467	1.341411	-0.967748
63	7	0	5.371915	-1.391899	-0.066359
64	1	0	5.410505	-2.156356	0.597450
65	6	0	5.983358	-1.748033	-1.339215
66	6	0	5.462992	-3.039278	-1.948416
67	1	0	5.633399	-3.884089	-1.275185
68	1	0	5.968015	-3.255527	-2.893188
69	1	0	4.389313	-2.972978	-2.138956
70	1	0	5.819595	-0.915829	-2.028855
71	1	0	7.066649	-1.816976	-1.191253
72	7	0	3.597329	-0.537269	1.621574
73	1	0	4.405544	-0.185692	2.117608
74	6	0	2.770336	-1.437337	2.416845
75	6	0	1.979707	-0.691360	3.472250
76	1	0	2.644384	-0.135473	4.139730
77	1	0	1.287135	0.008871	3.002828
78	1	0	1.394634	-1.389910	4.074044
79	1	0	3.387402	-2.214984	2.884778
80	1	0	2.076912	-1.959804	1.753413

	1	2	3
	A	A	A
Frequencies --	-488.0833	16.4078	27.7317
Red. masses --	9.5112	4.6656	4.0453
Frc consts --	1.3350	0.0007	0.0018
IR Inten --	2317.4536	1.4025	1.1701

Sum of electronic and zero-point Energies= -3329.315122

Sum of electronic and thermal Energies=	-3329.219276
Sum of electronic and thermal Enthalpies=	-3329.217841
Sum of electronic and thermal Free Energies=	-3329.482776

Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{D}_{II}$, the terminal geometry of the zinc-free disproportionation reaction where the oxidized quaternary aminophosphine is separated from the reduced indium-phosphorus compound.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	-1.698473	-0.507385	-0.016314
2	17	0	-0.021650	-2.067011	1.142084
3	17	0	-1.336932	-1.577436	-2.373282
4	17	0	-2.683485	0.337225	2.183582
5	7	0	-3.559776	0.392666	-1.231820
6	6	0	-4.907143	0.463762	-0.669392
7	6	0	-5.948404	1.004775	-1.630185
8	1	0	-6.933151	1.029570	-1.157425
9	1	0	-5.701823	2.021543	-1.945972
10	1	0	-6.018178	0.381159	-2.525530
11	1	0	-5.187070	-0.541548	-0.342441
12	1	0	-4.856073	1.069041	0.237548
13	1	0	-3.215485	1.312186	-1.505455
14	1	0	-3.531577	-0.178343	-2.072499
15	7	0	-2.996171	-2.422690	0.143861
16	6	0	-3.654027	-2.787259	1.402920
17	6	0	-4.297094	-4.158575	1.362148
18	1	0	-3.554204	-4.934584	1.158981

19	1	0	-4.769462	-4.387645	2.320094
20	1	0	-5.066232	-4.213460	0.586177
21	1	0	-2.895778	-2.730465	2.185317
22	1	0	-4.386341	-2.011986	1.632835
23	1	0	-2.273208	-3.101019	-0.083324
24	1	0	-3.649029	-2.447186	-0.633503
25	15	0	-0.270042	1.571393	-0.496819
26	7	0	0.253481	1.931723	1.114671
27	6	0	0.857924	3.236722	1.353256
28	6	0	1.238569	3.405697	2.809952
29	1	0	1.696573	4.382586	2.979836
30	1	0	0.357119	3.329944	3.452494
31	1	0	1.947144	2.635373	3.122469
32	1	0	1.747431	3.317555	0.721136
33	1	0	0.191914	4.059281	1.055854
34	1	0	-0.441209	1.704685	1.822208
35	7	0	-1.458927	2.743513	-0.932700
36	6	0	-2.435803	3.266765	0.012931
37	6	0	-3.440199	4.168039	-0.676254
38	1	0	-4.178094	4.540444	0.037809
39	1	0	-2.946295	5.033431	-1.128186
40	1	0	-3.970261	3.638081	-1.471870
41	1	0	-2.936325	2.422967	0.494136
42	1	0	-1.957123	3.821234	0.832524
43	1	0	-1.064119	3.480335	-1.502600
44	7	0	2.501669	-1.301731	-0.708361
45	6	0	2.303765	-1.837307	-2.054892
46	6	0	2.133438	-3.340527	-2.010756
47	1	0	1.266221	-3.602625	-1.401113
48	1	0	3.014310	-3.831007	-1.588201
49	1	0	1.967106	-3.728720	-3.017587
50	1	0	1.419516	-1.380213	-2.507439
51	1	0	3.167765	-1.562444	-2.665109
52	1	0	1.788054	-1.572805	-0.026078
53	15	0	3.340965	0.034270	-0.369293
54	7	0	2.995473	1.140879	-1.519080
55	6	0	3.899549	2.175581	-1.998198
56	6	0	3.983393	3.412540	-1.120608
57	1	0	4.291961	3.157459	-0.103667
58	1	0	4.704711	4.122933	-1.532131
59	1	0	3.014631	3.913056	-1.061522
60	1	0	4.888139	1.725776	-2.119489
61	1	0	3.569441	2.452880	-3.002565
62	1	0	1.996765	1.374707	-1.552448
63	7	0	4.943049	-0.273811	-0.417444

```
    64          1           0        5.566589    0.481575   -0.176381
    65          6           0        5.580459   -1.561383   -0.656559
    66          6           0        6.362385   -2.053936    0.544470
    67          1           0        7.135011   -1.336558    0.834119
    68          1           0        6.855518   -3.000591    0.312542
    69          1           0        5.702837   -2.211458    1.400406
    70          1           0        4.795705   -2.275184   -0.906800
    71          1           0        6.233723   -1.481592   -1.531102
    72          7           0        2.986063    0.577315    1.125649
    73          1           0        2.032101    0.951983    1.221928
    74          6           0        3.586658    0.080200    2.360693
    75          6           0        3.014661   -1.226301    2.872883
    76          1           0        1.938523   -1.149702    3.032697
    77          1           0        3.180242   -2.036207    2.158148
    78          1           0        3.492928   -1.499685    3.817049
    79          1           0        3.460686    0.864009    3.112134
    80          1           0        4.662018   -0.016899    2.194650
 -------------------------------------------------------------------

                      1                      2                      3
                      A                      A                      A
 Frequencies --     17.4272                26.5044                30.7824
 Red. masses --      3.8517                 3.5899                 2.6442
 Frc consts  --      0.0007                 0.0015                 0.0015
 IR Inten    --      0.8197                 0.8752                 0.3981

 Sum of electronic and zero-point Energies=          -3329.413108
 Sum of electronic and thermal Energies=             -3329.317795
 Sum of electronic and thermal Enthalpies=           -3329.316360
 Sum of electronic and thermal Free Energies=        -3329.579041
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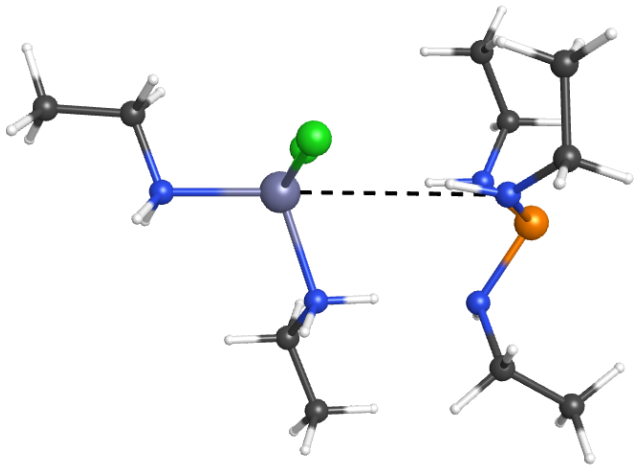
Cartesian coordinates, three lower frequencies, and thermochemistry of the start of the zinc-phosphorus activation, $\mathbf{A}_1$.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	-1.656463	0.055416	-0.151148
2	17	0	-1.089626	-1.282046	-1.869873
3	17	0	-1.542475	-0.436584	2.040264
4	7	0	-0.655369	1.846697	-0.389556
5	1	0	-0.708940	2.154486	-1.356187
6	1	0	0.347107	1.648492	-0.205516
7	6	0	-1.114879	2.915329	0.510148
8	6	0	-0.313083	4.195286	0.394783
9	1	0	-0.707048	4.956337	1.071786
10	1	0	0.734650	4.025885	0.653252
11	1	0	-0.351770	4.596379	-0.621809
12	1	0	-2.169826	3.110090	0.297532
13	1	0	-1.068581	2.516506	1.525907
14	7	0	-3.703483	0.403130	-0.464025
15	6	0	-4.467095	-0.838682	-0.233871
16	6	0	-5.956665	-0.680816	-0.446924
17	1	0	-6.178502	-0.372334	-1.472225
18	1	0	-6.376282	0.064700	0.234024
19	1	0	-6.469083	-1.627589	-0.263911
20	1	0	-4.051166	-1.594320	-0.903540
21	1	0	-4.245191	-1.161583	0.785184
22	1	0	-3.865342	0.731119	-1.411809
23	1	0	-4.046392	1.130885	0.156326
24	7	0	2.273385	-0.846026	-1.059137
25	15	0	2.910473	-0.177450	0.338394
26	7	0	2.248165	1.438669	0.151801

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    27          6           0        2.823328    2.239223   -0.926725
    28          6           0        4.217900    2.774828   -0.649879
    29          1           0        4.584172    3.361725   -1.496118
    30          1           0        4.218613    3.421170    0.232833
    31          1           0        4.919879    1.957644   -0.469092
    32          1           0        2.827110    1.613169   -1.823272
    33          1           0        2.146264    3.075416   -1.138046
    34          1           0        2.352059    1.916494    1.041902
    35          7           0        1.965778   -0.518279    1.688434
    36          6           0        2.270199   -1.654889    2.539238
    37          6           0        1.470909   -2.904296    2.206875
    38          1           0        1.721747   -3.720050    2.890768
    39          1           0        0.400242   -2.702567    2.290328
    40          1           0        1.668914   -3.234242    1.185285
    41          1           0        3.342812   -1.857090    2.452357
    42          1           0        2.090032   -1.375358    3.583974
    43          1           0        0.970859   -0.317537    1.644187
    44          6           0        3.025121   -1.759991   -1.893449
    45          6           0        2.678390   -3.224040   -1.680361
    46          1           0        3.211791   -3.858575   -2.393816
    47          1           0        2.948606   -3.542902   -0.670885
    48          1           0        1.605788   -3.388120   -1.811748
    49          1           0        2.866626   -1.497413   -2.946481
    50          1           0        4.088213   -1.595993   -1.690250
    51          1           0        1.271091   -0.859895   -1.220684
 ---------------------------------------------------------------------

                      1                      2                      3
                      A                      A                      A
 Frequencies --      6.5477                26.6467                35.3304
 Red. masses --      4.3907                 3.6017                 3.7268
 Frc consts  --      0.0001                 0.0015                 0.0027
 IR Inten    --      3.0754                 1.0744                 0.4746

 Sum of electronic and zero-point Energies=          -3713.861491
 Sum of electronic and thermal Energies=             -3713.800809
 Sum of electronic and thermal Enthalpies=           -3713.799374
 Sum of electronic and thermal Free Energies=        -3713.987118
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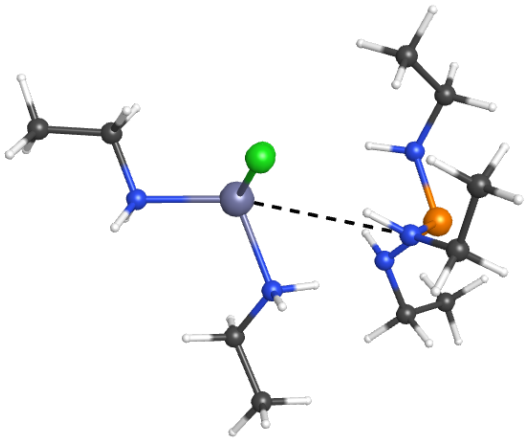
Cartesian coordinates, three lower frequencies, and thermochemistry of the first transition state of the zinc-phosphorus activation, $\mathbf{A}_2^{\ddagger}$.



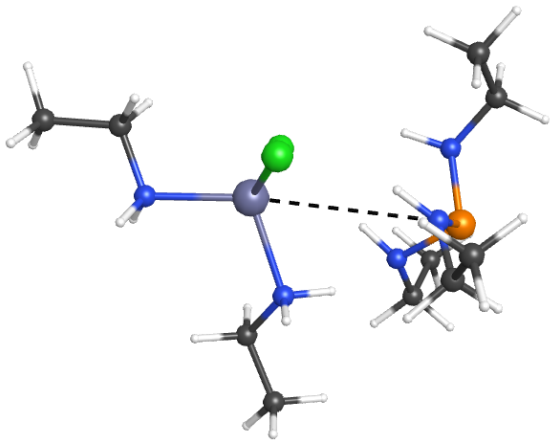
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	-1.556276	0.040780	-0.032073
2	17	0	-1.301728	-1.766687	-1.366965
3	17	0	-1.107009	0.099878	2.176588
4	7	0	-0.492474	1.530183	-0.984830
5	1	0	-0.299888	1.218687	-1.932777
6	1	0	0.421831	1.540820	-0.494578
7	6	0	-1.080137	2.874973	-1.002074
8	6	0	-0.264823	3.876951	-1.794109
9	1	0	-0.733911	4.862953	-1.769543
10	1	0	0.744678	3.969923	-1.387711
11	1	0	-0.180673	3.569394	-2.839870
12	1	0	-2.090323	2.805523	-1.415580
13	1	0	-1.184095	3.196826	0.037187
14	7	0	-3.612567	0.430649	-0.100250
15	6	0	-4.361632	-0.709885	0.462790
16	6	0	-5.862372	-0.520386	0.431687
17	1	0	-6.224322	-0.400143	-0.593069
18	1	0	-6.161862	0.360003	1.006652
19	1	0	-6.363570	-1.389124	0.863459
20	1	0	-4.063042	-1.594881	-0.102576
21	1	0	-4.002510	-0.850202	1.484320
22	1	0	-3.915677	0.596460	-1.055745
23	1	0	-3.833502	1.273410	0.422579
24	7	0	1.995369	-0.534749	-1.190437
25	15	0	2.769584	-0.107427	0.251117
26	7	0	1.946931	1.368214	0.671683
27	6	0	2.722856	2.594944	0.519739

28	6	0	3.776042	2.811366	1.592163
29	1	0	4.318366	3.745906	1.425630
30	1	0	3.313645	2.858880	2.581995
31	1	0	4.496761	1.990193	1.594609
32	1	0	3.192489	2.572114	-0.469231
33	1	0	2.029646	3.443819	0.510635
34	1	0	1.526693	1.316492	1.593362
35	7	0	2.109578	-1.010793	1.518630
36	6	0	2.449110	-2.418202	1.642318
37	6	0	1.361318	-3.351127	1.138150
38	1	0	1.658189	-4.396734	1.257114
39	1	0	0.435789	-3.197130	1.699778
40	1	0	1.139475	-3.167785	0.085733
41	1	0	3.380331	-2.591026	1.091044
42	1	0	2.669005	-2.647341	2.692175
43	1	0	1.142784	-0.817236	1.766720
44	6	0	2.755156	-1.064106	-2.306714
45	6	0	2.767076	-2.581431	-2.383250
46	1	0	3.318390	-2.924841	-3.263053
47	1	0	3.236947	-3.008824	-1.493608
48	1	0	1.747967	-2.972154	-2.446642
49	1	0	2.357705	-0.653933	-3.243074
50	1	0	3.779020	-0.687781	-2.214582
51	1	0	1.033288	-0.861623	-1.167269

	1	2	3
	A	A	A
Frequencies --	-24.3628	29.1305	31.8185
Red. masses --	3.5832	3.6409	4.4287
Frc consts --	0.0013	0.0018	0.0026
IR Inten --	1.3956	1.9414	2.0740

Sum of electronic and zero-point Energies=	-3713.860089
Sum of electronic and thermal Energies=	-3713.800586
Sum of electronic and thermal Enthalpies=	-3713.799151
Sum of electronic and thermal Free Energies=	-3713.980353

Cartesian coordinates, three lower frequencies, and thermochemistry of the rotated intermediate of the zinc-phosphorus activation, $\mathbf{A}_3$.



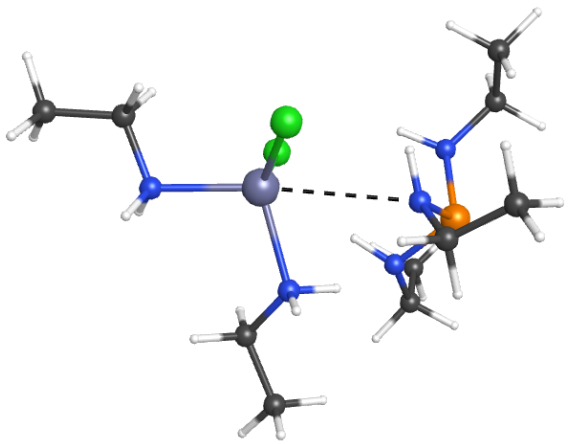
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	1.560482	-0.136735	0.076096
2	17	0	1.370094	-2.102351	1.145860
3	17	0	0.857574	0.206624	-2.045679
4	7	0	0.692463	1.319606	1.263300
5	1	0	0.713550	1.022969	2.234540
6	1	0	-0.298493	1.339407	0.971528
7	6	0	1.240122	2.677511	1.135956
8	6	0	0.519280	3.693970	1.996928
9	1	0	0.944685	4.690069	1.857534
10	1	0	-0.541474	3.737150	1.738717
11	1	0	0.600440	3.437317	3.056561
12	1	0	2.302811	2.645655	1.391277
13	1	0	1.174634	2.950541	0.079621
14	7	0	3.618872	0.228385	-0.056534
15	6	0	4.253988	-0.747113	-0.964529
16	6	0	5.745122	-0.543865	-1.119684
17	1	0	6.260158	-0.641551	-0.160158
18	1	0	5.967720	0.445038	-1.529567
19	1	0	6.160882	-1.289492	-1.800455
20	1	0	4.029622	-1.740208	-0.570021
21	1	0	3.741857	-0.664526	-1.925078
22	1	0	4.049380	0.168868	0.861835
23	1	0	3.794091	1.169993	-0.395639
24	7	0	-1.975312	-0.896541	1.049584
25	15	0	-2.828164	0.069088	-0.043988
26	7	0	-1.818087	1.444703	-0.320611
27	6	0	-2.490925	2.717260	-0.561096

28	6	0	-3.090881	2.860495	-1.949328
29	1	0	-3.560518	3.840283	-2.072479
30	1	0	-2.318936	2.752974	-2.716424
31	1	0	-3.844115	2.089339	-2.126237
32	1	0	-3.273260	2.826890	0.196304
33	1	0	-1.772929	3.526944	-0.385992
34	1	0	-1.098101	1.278898	-1.022992
35	7	0	-2.598195	-0.727737	-1.518734
36	6	0	-3.286867	-1.980477	-1.780683
37	6	0	-2.505612	-3.225443	-1.390012
38	1	0	-3.060963	-4.129857	-1.653996
39	1	0	-1.545695	-3.256158	-1.913340
40	1	0	-2.305331	-3.239280	-0.317340
41	1	0	-4.240047	-1.953055	-1.241944
42	1	0	-3.537238	-2.027061	-2.847084
43	1	0	-1.652998	-0.708827	-1.888890
44	6	0	-2.132652	-0.720585	2.476167
45	6	0	-2.042061	-2.038347	3.222164
46	1	0	-2.153867	-1.886100	4.298941
47	1	0	-2.822613	-2.723425	2.883638
48	1	0	-1.073057	-2.511137	3.042870
49	1	0	-1.391344	-0.019661	2.891473
50	1	0	-3.110939	-0.256066	2.643760
51	1	0	-1.095552	-1.322202	0.778568

	1	2	3
	A	A	A
Frequencies --	21.5417	26.6866	30.1374
Red. masses --	4.4826	3.6750	3.6823
Frc consts --	0.0012	0.0015	0.0020
IR Inten --	2.2396	0.7290	3.6455

Sum of electronic and zero-point Energies=	-3713.860510
Sum of electronic and thermal Energies=	-3713.799765
Sum of electronic and thermal Enthalpies=	-3713.798330
Sum of electronic and thermal Free Energies=	-3713.985268

Cartesian coordinates, three lower frequencies, and thermochemistry of the second transition state of the zinc-phosphorus activation, $\mathbf{A}_4^{\ddagger}$.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	1.502459	-0.210493	0.115498
2	17	0	1.615808	-2.242829	1.063120
3	17	0	0.717274	0.221087	-1.979578
4	7	0	0.817634	1.291479	1.366214
5	1	0	0.914528	1.012916	2.337781
6	1	0	-0.189215	1.312610	1.164847
7	6	0	1.373394	2.635579	1.163548
8	6	0	0.682798	3.697813	1.993793
9	1	0	1.112867	4.682332	1.797602
10	1	0	-0.383106	3.737318	1.756575
11	1	0	0.786266	3.490541	3.062242
12	1	0	2.441719	2.604173	1.393190
13	1	0	1.281726	2.863478	0.098366
14	7	0	3.534921	0.265542	-0.247532
15	6	0	4.158509	-0.779100	-1.080642
16	6	0	5.604301	-0.496892	-1.427580
17	1	0	6.220544	-0.421692	-0.527274
18	1	0	5.700976	0.437047	-1.987906
19	1	0	6.011047	-1.301029	-2.044534
20	1	0	4.056950	-1.719955	-0.536793
21	1	0	3.548651	-0.867892	-1.982113
22	1	0	4.061450	0.373795	0.614151
23	1	0	3.582114	1.157343	-0.731918
24	7	0	-1.427998	-0.753317	0.944485
25	15	0	-2.678254	0.106408	0.135761
26	7	0	-1.832742	1.565388	-0.149711
27	6	0	-2.609544	2.762775	-0.442373

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    28          6           0       -3.109170    2.863123   -1.874411
    29          1           0       -3.652396    3.799103   -2.030950
    30          1           0       -2.272239    2.833982   -2.577797
    31          1           0       -3.771592    2.029018   -2.113702
    32          1           0       -3.456668    2.784073    0.250695
    33          1           0       -1.993599    3.638563   -0.206995
    34          1           0       -1.063390    1.443235   -0.808705
    35          7           0       -2.687926   -0.620276   -1.388035
    36          6           0       -3.566941   -1.739895   -1.672389
    37          6           0       -3.036631   -3.100997   -1.245447
    38          1           0       -3.719164   -3.897668   -1.553929
    39          1           0       -2.061626   -3.297110   -1.700294
    40          1           0       -2.920680   -3.157437   -0.160581
    41          1           0       -4.522532   -1.543470   -1.175091
    42          1           0       -3.774533   -1.750523   -2.747873
    43          1           0       -1.789917   -0.666661   -1.860292
    44          6           0       -1.508180   -0.916692    2.385081
    45          6           0       -2.369692   -2.085752    2.831410
    46          1           0       -2.401634   -2.159875    3.921877
    47          1           0       -3.392792   -1.973965    2.462830
    48          1           0       -1.966190   -3.024229    2.441453
    49          1           0       -0.493239   -1.042660    2.778438
    50          1           0       -1.898111    0.016326    2.807649
    51          1           0       -1.098871   -1.584906    0.473594
---------------------------------------------------------------------

                     1                      2                      3
                     A                      A                      A
Frequencies --    -32.3225               21.9654                30.5899
Red. masses --      5.3300                4.2927                 4.4020
Frc consts  --      0.0033                0.0012                 0.0024
IR Inten    --     18.6824                1.3974                 4.0406

Sum of electronic and zero-point Energies=          -3713.859820
Sum of electronic and thermal Energies=             -3713.800065
Sum of electronic and thermal Enthalpies=           -3713.798630
Sum of electronic and thermal Free Energies=        -3713.982180
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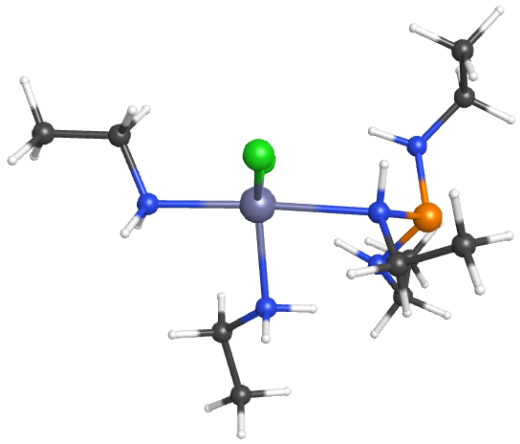
Cartesian coordinates, three lower frequencies, and thermochemistry of the bent intermediate of the zinc-phosphorus activation, $\mathbf{A}_5$.



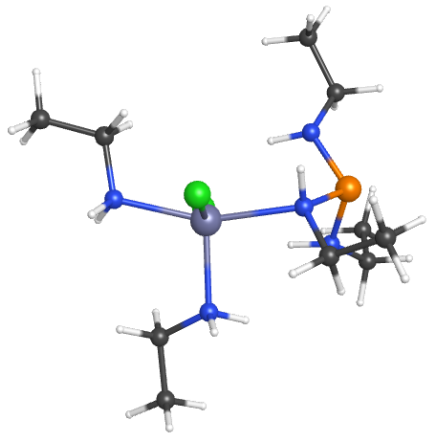
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	1.180676	-0.249056	0.173025
2	17	0	1.727558	-2.236691	1.183649
3	17	0	0.573619	0.285163	-2.006056
4	7	0	0.872627	1.538221	1.273423
5	1	0	1.087838	1.433753	2.259529
6	1	0	-0.144775	1.634381	1.195248
7	6	0	1.503801	2.753194	0.744099
8	6	0	0.975342	4.027986	1.369731
9	1	0	1.467283	4.902831	0.939134
10	1	0	-0.099753	4.126446	1.198752
11	1	0	1.149699	4.038537	2.448934
12	1	0	2.582035	2.673884	0.902777
13	1	0	1.337583	2.756603	-0.336670
14	7	0	3.278105	0.191996	-0.294447
15	6	0	3.875894	-0.805300	-1.193077
16	6	0	5.313729	-0.507943	-1.566478
17	1	0	5.953565	-0.475840	-0.679936
18	1	0	5.397685	0.452967	-2.082137
19	1	0	5.704796	-1.280228	-2.232980
20	1	0	3.790779	-1.772051	-0.694282
21	1	0	3.243036	-0.848426	-2.081924
22	1	0	3.819472	0.245699	0.563047
23	1	0	3.321435	1.106723	-0.732443
24	7	0	-1.068170	-0.755208	0.927991
25	15	0	-2.520951	-0.064847	0.203126
26	7	0	-1.873279	1.489416	-0.042931
27	6	0	-2.804589	2.596863	-0.225128

28	6	0	-3.384037	2.708820	-1.625064
29	1	0	-4.041717	3.578438	-1.704019
30	1	0	-2.586343	2.817000	-2.365183
31	1	0	-3.955150	1.814416	-1.882166
32	1	0	-3.609428	2.475793	0.506339
33	1	0	-2.286231	3.526769	0.034598
34	1	0	-1.138444	1.486752	-0.750760
35	7	0	-2.515575	-0.792871	-1.304347
36	6	0	-3.384526	-1.913503	-1.608942
37	6	0	-2.807506	-3.273204	-1.247041
38	1	0	-3.477833	-4.078128	-1.560391
39	1	0	-1.841320	-3.427432	-1.734925
40	1	0	-2.658917	-3.362441	-0.167291
41	1	0	-4.328550	-1.757514	-1.077012
42	1	0	-3.622223	-1.887167	-2.677559
43	1	0	-1.646609	-0.760739	-1.829213
44	6	0	-1.077259	-0.681643	2.398465
45	6	0	-1.904580	-1.769133	3.055501
46	1	0	-1.895658	-1.662102	4.142850
47	1	0	-2.942196	-1.731461	2.714780
48	1	0	-1.495268	-2.753260	2.811733
49	1	0	-0.044928	-0.746795	2.752908
50	1	0	-1.459194	0.305918	2.679662
51	1	0	-1.000280	-1.730677	0.651653

	1	2	3
	A	A	A
Frequencies --	24.2934	36.3462	37.4422
Red. masses --	3.5636	3.5825	4.0306
Frc consts --	0.0012	0.0028	0.0033
IR Inten --	0.0637	1.8751	3.3754

Sum of electronic and zero-point Energies= -3713.859803
Sum of electronic and thermal Energies= -3713.799407
Sum of electronic and thermal Enthalpies= -3713.797972
Sum of electronic and thermal Free Energies= -3713.980353

Cartesian coordinates, three lower frequencies, and thermochemistry of the third transition state of the zinc-phosphorus activation, $\mathbf{A}_6^{\ddagger}$.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	1.129192	0.043263	0.201729
2	17	0	2.081248	-0.347214	2.352716
3	17	0	0.207241	-0.451673	-1.969627
4	7	0	1.443015	2.096355	-0.174009
5	1	0	1.767853	2.562934	0.667412
6	1	0	0.522896	2.479097	-0.377519
7	6	0	2.353975	2.382094	-1.291926
8	6	0	2.443707	3.852904	-1.640340
9	1	0	3.131097	4.008399	-2.474591
10	1	0	1.466146	4.244614	-1.933876
11	1	0	2.805523	4.438530	-0.791087
12	1	0	3.337686	1.993636	-1.017034
13	1	0	2.000729	1.798378	-2.144700
14	7	0	2.906483	-0.922327	-0.562995
15	6	0	2.795182	-2.386414	-0.511978
16	6	0	4.028039	-3.112039	-1.010129
17	1	0	4.905471	-2.853174	-0.411113
18	1	0	4.239021	-2.859019	-2.052938
19	1	0	3.888115	-4.193850	-0.949426
20	1	0	2.582855	-2.650064	0.526540
21	1	0	1.918719	-2.657562	-1.104865
22	1	0	3.689217	-0.620482	0.008964
23	1	0	3.075364	-0.626386	-1.519239
24	7	0	-0.808879	0.298189	1.339605
25	15	0	-2.423472	0.053447	0.654050
26	7	0	-2.270229	1.184198	-0.589214
27	6	0	-3.463341	1.789373	-1.154867

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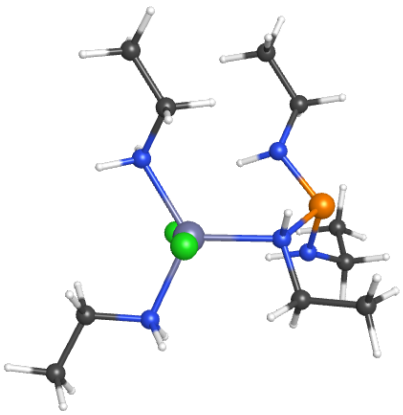
    28          6           0       -4.144955    0.950203   -2.223647
    29          1           0       -5.004359    1.476900   -2.647342
    30          1           0       -3.450729    0.720532   -3.036390
    31          1           0       -4.495864    0.002754   -1.805965
    32          1           0       -4.160858    1.982962   -0.333847
    33          1           0       -3.194590    2.766877   -1.570273
    34          1           0       -1.555133    0.960987   -1.278578
    35          7           0       -2.108965   -1.508825    0.108470
    36          6           0       -3.210299   -2.411126   -0.180276
    37          6           0       -2.772650   -3.859248   -0.076599
    38          1           0       -3.604483   -4.532694   -0.297416
    39          1           0       -1.970512   -4.072491   -0.788541
    40          1           0       -2.401280   -4.079275    0.926712
    41          1           0       -4.010117   -2.208083    0.538701
    42          1           0       -3.632989   -2.230560   -1.179241
    43          1           0       -1.353001   -1.575601   -0.569376
    44          6           0       -0.718379    1.536960    2.139988
    45          6           0       -1.441336    1.463183    3.471072
    46          1           0       -1.336284    2.406685    4.011788
    47          1           0       -2.506066    1.259996    3.339131
    48          1           0       -1.013002    0.671808    4.092062
    49          1           0        0.339161    1.735453    2.323920
    50          1           0       -1.116895    2.348251    1.525242
    51          1           0       -0.641315   -0.486547    1.966959
 ---------------------------------------------------------------------

                     1                      2                      3
                     A                      A                      A
 Frequencies --    -17.6637               27.7427                31.6567
 Red. masses --      4.4390                3.6300                 2.9669
 Frc consts  --      0.0008                0.0016                 0.0018
 IR Inten    --      0.8311                1.2433                 1.4533

 Sum of electronic and zero-point Energies=          -3713.856091
 Sum of electronic and thermal Energies=             -3713.797064
 Sum of electronic and thermal Enthalpies=           -3713.795629
 Sum of electronic and thermal Free Energies=        -3713.973774
```

Cartesian coordinates, three lower frequencies, and thermochemistry of the trigonal bipyramidal geometry of the zinc-phosphorus activation, $\mathbf{A}_7$.



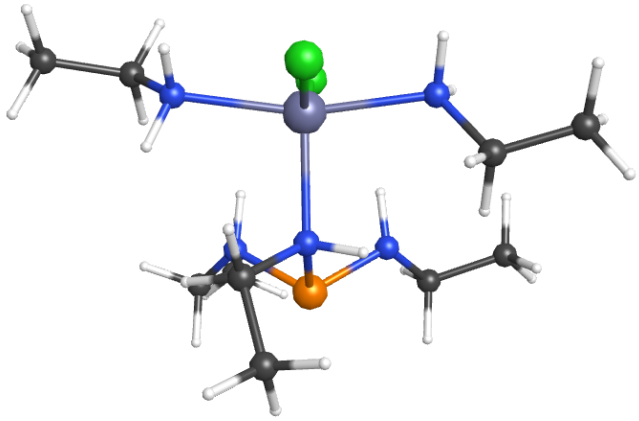
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	-1.123615	-0.037423	0.036634
2	17	0	-2.502486	0.213902	2.029528
3	17	0	-0.058572	-0.269417	-2.238152
4	7	0	-2.354735	-1.619106	-0.563450
5	1	0	-2.695822	-2.096626	0.265462
6	1	0	-1.803165	-2.275067	-1.108276
7	6	0	-3.490104	-1.139000	-1.364530
8	6	0	-4.407614	-2.244311	-1.843488
9	1	0	-5.233002	-1.831433	-2.427714
10	1	0	-3.868575	-2.953292	-2.477458
11	1	0	-4.833858	-2.793419	-0.999793
12	1	0	-4.036885	-0.424829	-0.743763
13	1	0	-3.069400	-0.590729	-2.210826
14	7	0	-1.459504	1.964400	-0.498987
15	6	0	-1.073366	2.985846	0.487912
16	6	0	-1.272193	4.403236	-0.004555
17	1	0	-2.321392	4.595468	-0.245510
18	1	0	-0.675266	4.599062	-0.899831
19	1	0	-0.968528	5.119132	0.762622
20	1	0	-1.657098	2.789904	1.388034
21	1	0	-0.026371	2.804283	0.737743
22	1	0	-2.447159	2.063528	-0.717309
23	1	0	-0.958630	2.097898	-1.373966
24	7	0	0.519389	-0.613558	1.260765
25	15	0	2.227963	-0.350083	0.803697
26	7	0	2.332148	-1.561662	-0.344261
27	6	0	3.586624	-2.243632	-0.596264

28	6	0	4.441784	-1.587405	-1.667306
29	1	0	5.353105	-2.163511	-1.848918
30	1	0	3.891875	-1.513728	-2.609237
31	1	0	4.728482	-0.576318	-1.366111
32	1	0	4.138690	-2.285262	0.348041
33	1	0	3.373634	-3.281073	-0.876849
34	1	0	1.708133	-1.488255	-1.144241
35	7	0	1.940673	1.138181	0.052757
36	6	0	3.076298	2.022803	-0.172201
37	6	0	2.632964	3.462225	-0.344768
38	1	0	3.490509	4.107787	-0.548631
39	1	0	1.937028	3.557429	-1.183154
40	1	0	2.132993	3.827263	0.555030
41	1	0	3.744410	1.938662	0.690389
42	1	0	3.659900	1.714942	-1.051215
43	1	0	1.352666	1.053641	-0.775687
44	6	0	0.230357	-1.966378	1.789127
45	6	0	1.023624	-2.342566	3.024934
46	1	0	0.704157	-3.322733	3.386106
47	1	0	2.095743	-2.387652	2.822764
48	1	0	0.858651	-1.618640	3.827384
49	1	0	-0.837196	-1.986071	2.020468
50	1	0	0.420840	-2.672877	0.980036
51	1	0	0.332491	0.047494	2.015575

	1	2	3
	A	A	A
Frequencies --	11.6235	19.9955	32.8644
Red. masses --	4.3980	3.2229	4.0493
Frc consts --	0.0004	0.0008	0.0026
IR Inten --	3.5060	0.0590	1.4017

Sum of electronic and zero-point Energies= -3713.860215
Sum of electronic and thermal Energies= -3713.799925
Sum of electronic and thermal Enthalpies= -3713.798490
Sum of electronic and thermal Free Energies= -3713.982946

Cartesian coordinates, three lower frequencies, and thermochemistry of the fourth transition state of the zinc-phosphorus activation, $\mathbf{A}_8^{\ddagger}$.



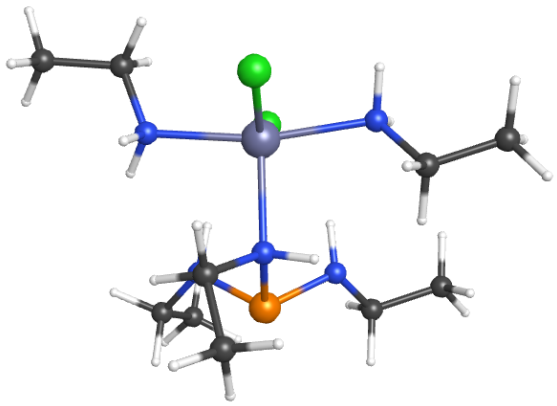
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	-0.368250	1.155936	-0.408943
2	17	0	-0.596983	3.347729	0.481082
3	17	0	-0.368496	-0.207716	-2.348989
4	7	0	-2.543600	1.011286	-0.156009
5	1	0	-2.787521	1.996792	-0.212538
6	1	0	-2.706512	0.754781	0.812789
7	6	0	-3.416622	0.216079	-1.024395
8	6	0	-4.888911	0.361765	-0.694259
9	1	0	-5.496872	-0.248267	-1.366465
10	1	0	-5.095978	0.041025	0.330808
11	1	0	-5.214019	1.400724	-0.796071
12	1	0	-3.213075	0.510097	-2.054709
13	1	0	-3.108381	-0.827429	-0.939508
14	7	0	1.665108	1.771709	-0.983511
15	6	0	2.684265	1.925015	0.056588
16	6	0	3.969737	2.566330	-0.427160
17	1	0	3.781814	3.568512	-0.821393
18	1	0	4.432135	1.969583	-1.218287
19	1	0	4.688090	2.655962	0.391200
20	1	0	2.235769	2.521699	0.855586
21	1	0	2.891958	0.927420	0.453452
22	1	0	1.480002	2.675752	-1.408484
23	1	0	1.990256	1.158857	-1.724465
24	7	0	0.211693	-0.000058	1.326795
25	15	0	0.550033	-1.738048	1.122090
26	7	0	-0.920975	-2.126467	0.405655

27	6	0	-1.431549	-3.485160	0.488979
28	6	0	-0.871757	-4.424836	-0.565848
29	1	0	-1.331433	-5.413933	-0.492538
30	1	0	-1.060300	-4.034754	-1.569601
31	1	0	0.209160	-4.540175	-0.448959
32	1	0	-1.204668	-3.866487	1.489219
33	1	0	-2.523571	-3.449862	0.410529
34	1	0	-1.083874	-1.687727	-0.498238
35	7	0	1.727401	-1.510021	-0.063292
36	6	0	2.746338	-2.524462	-0.280537
37	6	0	4.001152	-1.916158	-0.876272
38	1	0	4.760310	-2.682260	-1.050918
39	1	0	3.781232	-1.439346	-1.835686
40	1	0	4.418712	-1.158797	-0.208689
41	1	0	2.973737	-2.986028	0.685029
42	1	0	2.383722	-3.328562	-0.935780
43	1	0	1.374437	-1.114083	-0.932890
44	6	0	-0.680374	0.288264	2.470246
45	6	0	-0.006317	0.143113	3.820012
46	1	0	-0.713192	0.369574	4.621046
47	1	0	0.371285	-0.870134	3.972500
48	1	0	0.831679	0.840018	3.909327
49	1	0	-1.050118	1.310130	2.349610
50	1	0	-1.532986	-0.391355	2.390567
51	1	0	1.115201	0.425842	1.523325

	1	2	3
	A	A	A
Frequencies --	-72.9935	28.6089	35.3493
Red. masses --	1.6452	3.4024	3.4281
Frc consts --	0.0052	0.0016	0.0025
IR Inten --	0.8020	0.6065	0.7236

Sum of electronic and zero-point Energies= -3713.860191
Sum of electronic and thermal Energies= -3713.801086
Sum of electronic and thermal Enthalpies= -3713.799651
Sum of electronic and thermal Free Energies= -3713.977634

Cartesian coordinates, three lower frequencies, and thermochemistry of the second bent geometry of the zinc-phosphorus activation, $\mathbf{A}_9$.



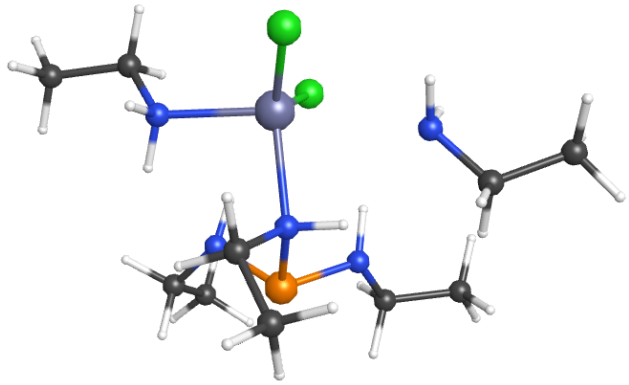
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	1.020699	-0.580109	-0.292294
2	17	0	2.711743	-1.937299	0.631770
3	17	0	0.209273	0.371320	-2.335746
4	7	0	2.324053	1.121691	-0.015721
5	1	0	2.785357	0.966603	0.875296
6	1	0	1.770472	1.968968	0.074538
7	6	0	3.336845	1.269657	-1.066876
8	6	0	4.297067	2.417795	-0.831061
9	1	0	5.027149	2.481626	-1.641288
10	1	0	3.764855	3.372142	-0.783072
11	1	0	4.845699	2.286500	0.105712
12	1	0	3.874637	0.320147	-1.120983
13	1	0	2.803440	1.391225	-2.011033
14	7	0	0.009869	-2.426336	-0.895027
15	6	0	-0.722991	-3.202182	0.107397
16	6	0	-1.198829	-4.554365	-0.385468
17	1	0	-0.355452	-5.175904	-0.697468
18	1	0	-1.875061	-4.443870	-1.237681
19	1	0	-1.735348	-5.086265	0.403810
20	1	0	-0.058070	-3.320580	0.967570
21	1	0	-1.578428	-2.597919	0.422130
22	1	0	0.797649	-2.971271	-1.233903
23	1	0	-0.575593	-2.222439	-1.698870
24	7	0	-0.288250	-0.073081	1.350320
25	15	0	-1.668918	1.005815	1.022182
26	7	0	-0.799383	2.238693	0.269837
27	6	0	-1.290611	3.606377	0.351980

```
    28          6           0       -2.365274    3.942978   -0.667548
    29          1           0       -2.659075    4.993301   -0.594221
    30          1           0       -2.005259    3.760037   -1.683517
    31          1           0       -3.255000    3.327027   -0.510483
    32          1           0       -1.672819    3.762443    1.365290
    33          1           0       -0.440663    4.286633    0.232941
    34          1           0       -0.428101    1.994796   -0.647351
    35          7           0       -2.342772   -0.003487   -0.148468
    36          6           0       -3.759008    0.100850   -0.464927
    37          6           0       -4.280218   -1.197095   -1.049963
    38          1           0       -5.341098   -1.113792   -1.297240
    39          1           0       -3.742384   -1.450922   -1.967817
    40          1           0       -4.151446   -2.019653   -0.342447
    41          1           0       -4.294135    0.338992    0.459166
    42          1           0       -3.958158    0.923832   -1.165194
    43          1           0       -1.765398   -0.118128   -0.979789
    44          6           0        0.516003    0.342354    2.519649
    45          6           0       -0.170994    0.100545    3.848964
    46          1           0        0.474314    0.418873    4.670483
    47          1           0       -1.112237    0.649531    3.919709
    48          1           0       -0.383111   -0.963575    3.985931
    49          1           0        1.458964   -0.209659    2.482479
    50          1           0        0.747954    1.402631    2.390153
    51          1           0       -0.704668   -0.977512    1.561374
 -------------------------------------------------------------------

                     1                      2                      3
                     A                      A                      A
 Frequencies --     21.6058                31.2376                35.8992
 Red. masses --      3.7947                 3.5618                 3.4775
 Frc consts  --      0.0010                 0.0020                 0.0026
 IR Inten    --      0.7167                 2.1047                 0.9911

 Sum of electronic and zero-point Energies=          -3713.862200
 Sum of electronic and thermal Energies=             -3713.801860
 Sum of electronic and thermal Enthalpies=           -3713.800425
 Sum of electronic and thermal Free Energies=        -3713.982750
```

Cartesian coordinates, three lower frequencies, and thermochemistry of the fifth transition state of the zinc-phosphorus activation, $\mathbf{A}_{10}^{\ddagger}$.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	0.517260	-1.235157	-0.341866
2	17	0	0.411484	-3.438231	0.143189
3	17	0	0.320836	-0.165464	-2.333946
4	7	0	2.548794	-0.879779	0.191503
5	1	0	2.803727	-1.561075	0.899579
6	1	0	2.541586	0.039113	0.632315
7	6	0	3.526723	-0.905101	-0.903433
8	6	0	4.927928	-0.527001	-0.470149
9	1	0	5.615238	-0.557108	-1.318553
10	1	0	4.948124	0.485544	-0.056724
11	1	0	5.304481	-1.213272	0.293199
12	1	0	3.509128	-1.908438	-1.334569
13	1	0	3.160955	-0.228862	-1.678915
14	7	0	-2.255301	-1.561461	-0.568820
15	6	0	-3.518170	-1.300394	0.109134
16	6	0	-4.750901	-1.851236	-0.587196
17	1	0	-4.686796	-2.937706	-0.691699
18	1	0	-4.853416	-1.421942	-1.587960
19	1	0	-5.659419	-1.617097	-0.025264
20	1	0	-3.446296	-1.720291	1.118316
21	1	0	-3.611697	-0.216234	0.230354
22	1	0	-2.063233	-2.556119	-0.615020
23	1	0	-2.274778	-1.218164	-1.522613
24	7	0	-0.287585	-0.046667	1.232167
25	15	0	-0.302611	1.718299	1.062971
26	7	0	1.224701	1.890903	0.342149
27	6	0	1.968405	3.128759	0.531340

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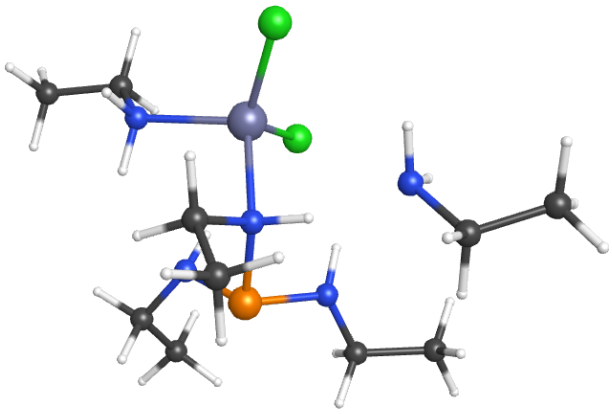
    28          6           0        1.574444    4.246921   -0.417705
    29          1           0        2.202073    5.128322   -0.263314
    30          1           0        1.685470    3.929686   -1.458224
    31          1           0        0.532156    4.538357   -0.264545
    32          1           0        1.821410    3.446961    1.567687
    33          1           0        3.036477    2.910581    0.421939
    34          1           0        1.282126    1.533315   -0.609360
    35          7           0       -1.495105    1.728385   -0.123651
    36          6           0       -2.131262    2.981882   -0.492621
    37          6           0       -3.515266    2.745547   -1.064508
    38          1           0       -3.979458    3.690007   -1.358021
    39          1           0       -3.463602    2.107979   -1.951424
    40          1           0       -4.158727    2.254614   -0.331070
    41          1           0       -2.197727    3.602426    0.406885
    42          1           0       -1.526838    3.544513   -1.217805
    43          1           0       -1.310738    1.128027   -0.923883
    44          6           0        0.249612   -0.503643    2.529756
    45          6           0       -0.719876   -0.322196    3.679705
    46          1           0       -0.272755   -0.668988    4.613770
    47          1           0       -0.997523    0.727287    3.800759
    48          1           0       -1.630938   -0.901615    3.508243
    49          1           0        0.518688   -1.559329    2.430130
    50          1           0        1.175675    0.048365    2.717825
    51          1           0       -1.249807   -0.366725    1.122879
 ---------------------------------------------------------------------

                     1                      2                      3
                     A                      A                      A
 Frequencies --    -72.9827               26.8568                28.4381
 Red. masses --      5.7291                3.2882                 5.2389
 Frc consts  --      0.0180                0.0014                 0.0025
 IR Inten    --     16.5192                0.5197                 3.7245

 Sum of electronic and zero-point Energies=          -3713.858852
 Sum of electronic and thermal Energies=             -3713.799026
 Sum of electronic and thermal Enthalpies=           -3713.797591
 Sum of electronic and thermal Free Energies=        -3713.980517
```

Cartesian coordinates, three lower frequencies, and thermochemistry of the terminal geometry of the zinc-phosphorus activation, $\mathbf{A}_{11}$.



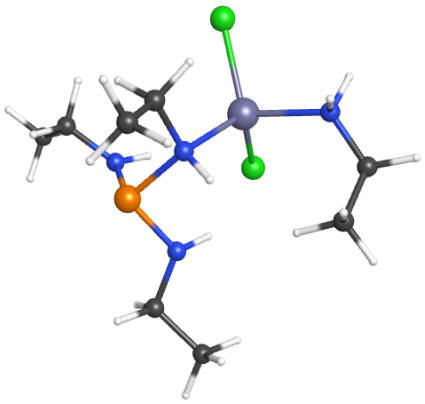
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	0.670318	-1.248819	-0.452348
2	17	0	0.010226	-3.383234	-0.246668
3	17	0	0.696601	-0.098613	-2.396695
4	7	0	2.594980	-1.116736	0.359852
5	1	0	2.729178	-1.851453	1.047575
6	1	0	2.575232	-0.228151	0.860770
7	6	0	3.701529	-1.123598	-0.608216
8	6	0	5.051631	-0.858418	0.023431
9	1	0	5.838541	-0.867160	-0.733722
10	1	0	5.067090	0.119017	0.514015
11	1	0	5.294631	-1.618824	0.770617
12	1	0	3.689043	-2.091713	-1.113203
13	1	0	3.469551	-0.374749	-1.368491
14	7	0	-0.380498	-0.145593	1.000643
15	15	0	-0.254587	1.614059	0.982946
16	7	0	1.387904	1.726897	0.537306
17	6	0	2.151525	2.894998	0.956802
18	6	0	1.962658	4.118706	0.077410
19	1	0	2.602051	4.940476	0.409968
20	1	0	2.215529	3.891590	-0.961972
21	1	0	0.924993	4.461342	0.103345
22	1	0	1.861474	3.124394	1.986454
23	1	0	3.212483	2.622593	0.986654
24	1	0	1.567445	1.470914	-0.431386
25	7	0	-1.216939	1.830700	-0.376436
26	6	0	-1.772819	3.137217	-0.680137
27	6	0	-3.066882	3.013786	-1.460941

```
    28          1           0       -3.473231    4.000098   -1.697527
    29          1           0       -2.900749    2.484962   -2.403447
    30          1           0       -3.812080    2.458097   -0.887122
    31          1           0       -1.954357    3.653350    0.267935
    32          1           0       -1.063609    3.758780   -1.244598
    33          1           0       -0.933648    1.311923   -1.203944
    34          6           0       -0.074664   -0.727250    2.324348
    35          6           0       -1.185509   -0.535269    3.338244
    36          1           0       -0.908386   -0.981799    4.295791
    37          1           0       -1.393977    0.524363    3.501392
    38          1           0       -2.103837   -1.016056    2.993133
    39          1           0        0.115604   -1.795742    2.185588
    40          1           0        0.856605   -0.278574    2.686038
    41          1           0       -1.354668   -0.409207    0.731268
    42          7           0       -2.847657   -1.180484   -0.106280
    43          6           0       -4.172087   -0.880466    0.418965
    44          6           0       -5.328794   -1.379302   -0.430023
    45          1           0       -5.288075   -2.465973   -0.544248
    46          1           0       -5.295467   -0.934825   -1.428909
    47          1           0       -6.290610   -1.121180    0.021569
    48          1           0       -4.237061   -1.306827    1.424805
    49          1           0       -4.241922    0.205113    0.541898
    50          1           0       -2.683862   -2.180761   -0.159669
    51          1           0       -2.754767   -0.824833   -1.052028
 ---------------------------------------------------------------------

                     1                      2                      3
                     A                      A                      A
 Frequencies --     20.6949                23.7036                30.7322
 Red. masses --      3.7346                 3.6448                 3.3189
 Frc consts  --      0.0009                 0.0012                 0.0018
 IR Inten    --      1.3936                 2.0827                 0.4829

 Sum of electronic and zero-point Energies=          -3713.862621
 Sum of electronic and thermal Energies=             -3713.801581
 Sum of electronic and thermal Enthalpies=           -3713.800146
 Sum of electronic and thermal Free Energies=        -3713.987289
```

Cartesian coordinates, three lower frequencies, and thermochemistry of ZnP_{Am}(III), the terminal geometry of the zinc-phosphorus activation ($\mathbf{A}_{11}$) with the free ethylamine removed.



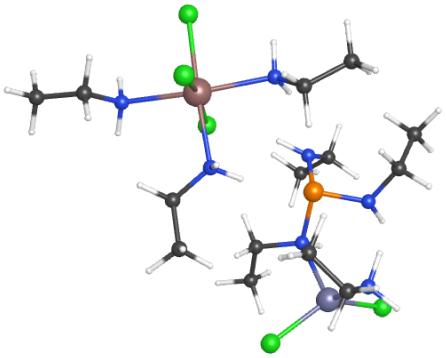
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	0.011111	0.028349	-0.006919
2	17	0	0.006966	0.017073	2.237810
3	17	0	1.992169	0.027608	-1.097398
4	7	0	-0.873367	-1.821065	-0.496592
5	6	0	-0.591286	-2.376036	-1.833839
6	6	0	-1.243454	-1.545794	-2.915732
7	1	0	-0.842776	-0.529594	-2.937182
8	1	0	-2.327393	-1.491029	-2.775212
9	1	0	-1.059747	-1.992572	-3.894061
10	1	0	0.492767	-2.371552	-1.959131
11	1	0	-0.935429	-3.413416	-1.891896
12	1	0	-1.876919	-1.788265	-0.340071
13	1	0	-0.507079	-2.440171	0.221449
14	7	0	-1.323737	1.500683	-0.689683
15	15	0	-0.540554	2.982603	-1.379190
16	7	0	0.769668	3.180505	-0.370353
17	6	0	0.789056	4.134290	0.723883
18	6	0	2.097111	4.898737	0.782869
19	1	0	2.095668	5.602372	1.618839
20	1	0	2.938331	4.214550	0.921778
21	1	0	2.261049	5.455009	-0.142738
22	1	0	-0.045530	4.826627	0.572467
23	1	0	0.610355	3.628639	1.681055
24	1	0	1.465135	2.443655	-0.314581
25	7	0	0.035112	2.180642	-2.740254
26	6	0	0.439419	2.974302	-3.894026
27	6	0	0.454428	2.126929	-5.150335
28	1	0	1.155230	1.293990	-5.046850

29	1	0	-0.536796	1.713085	-5.349353
30	1	0	0.764342	2.720474	-6.013467
31	1	0	-0.273597	3.797226	-4.002880
32	1	0	1.426911	3.430852	-3.743884
33	1	0	0.696240	1.431474	-2.540598
34	6	0	-2.273995	1.849128	0.393493
35	6	0	-3.574884	2.432471	-0.116558
36	1	0	-4.234437	2.672839	0.719885
37	1	0	-3.404650	3.344671	-0.691816
38	1	0	-4.096611	1.716282	-0.758340
39	1	0	-2.462255	0.957643	0.995065
40	1	0	-1.761852	2.546331	1.061404
41	1	0	-1.848024	1.084678	-1.457580

	1	2	3
	A	A	A
Frequencies --	23.3671	30.0468	38.6312
Red. masses --	4.9332	3.4935	3.5124
Frc consts --	0.0016	0.0019	0.0031
IR Inten --	3.3658	0.8373	0.5828

Sum of electronic and zero-point Energies=	-3578.873562
Sum of electronic and thermal Energies=	-3578.824330
Sum of electronic and thermal Enthalpies=	-3578.822895
Sum of electronic and thermal Free Energies=	-3578.979636

Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}_{Zn_I}$, the starting geometry of the ligand exchange of **A** onto *mer*-$InCl_3$, replacing an outer ligand.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	3.151142	0.170752	-0.053354
2	17	0	3.973073	-0.411102	-2.311439
3	17	0	4.982002	1.699327	0.564043
4	17	0	1.961757	0.307264	2.171983
5	7	0	1.362694	-1.172183	-0.675367
6	6	0	1.333540	-2.518562	-0.084798
7	6	0	0.269019	-3.428168	-0.661830
8	1	0	0.336534	-4.419071	-0.207653
9	1	0	-0.740598	-3.054255	-0.479254
10	1	0	0.397905	-3.544790	-1.740966
11	1	0	2.317777	-2.966767	-0.244528
12	1	0	1.199620	-2.394098	0.992554
13	1	0	0.491861	-0.674015	-0.479060
14	1	0	1.455058	-1.240801	-1.685927
15	7	0	4.337297	-1.494185	1.002148
16	6	0	5.302458	-2.306434	0.246047
17	6	0	6.081701	-3.265558	1.120594
18	1	0	5.415625	-3.968759	1.628321
19	1	0	6.783824	-3.844042	0.516637
20	1	0	6.654946	-2.728393	1.880538
21	1	0	4.751197	-2.840897	-0.529778
22	1	0	5.967975	-1.615856	-0.273716
23	1	0	3.698427	-2.084181	1.527541
24	1	0	4.826006	-0.931170	1.695141
25	7	0	2.027547	2.049283	-0.783764
26	6	0	1.450142	2.097743	-2.135581
27	6	0	1.105678	3.503783	-2.580793
28	1	0	2.005720	4.119682	-2.649781
29	1	0	0.635684	3.488415	-3.566689
30	1	0	0.418138	3.987569	-1.882875
31	1	0	2.168088	1.639995	-2.817604
32	1	0	0.560927	1.461207	-2.128831
33	1	0	2.777566	2.732693	-0.696811
34	1	0	1.326458	2.306700	-0.091812
35	15	0	-1.489145	0.972792	0.287770
36	7	0	-2.580059	-0.144081	1.115464
37	6	0	-1.846445	-1.136701	1.932343
38	6	0	-2.750595	-1.761538	2.969809
39	1	0	-3.138534	-1.010257	3.663496
40	1	0	-3.594396	-2.266139	2.496001
41	1	0	-2.195366	-2.499270	3.551463
42	1	0	-1.472699	-1.906569	1.255273

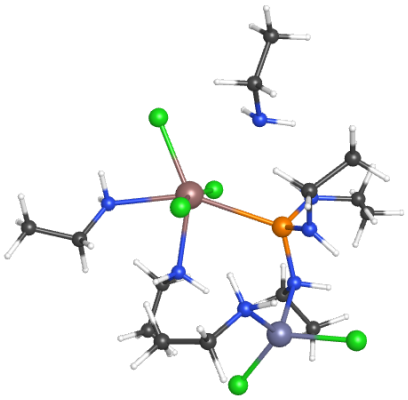
43	1	0	-0.981154	-0.666545	2.413542
44	1	0	-3.211445	0.374843	1.728288
45	30	0	-4.080015	-1.006759	-0.154327
46	17	0	-3.737407	-3.209667	-0.235853
47	17	0	-5.746120	0.321767	0.660845
48	7	0	-4.053667	-0.339135	-2.135346
49	1	0	-3.622923	0.580882	-2.065538
50	1	0	-5.029418	-0.188556	-2.372317
51	6	0	-3.387397	-1.154701	-3.161863
52	6	0	-1.898245	-1.208863	-2.913006
53	1	0	-1.407487	-1.822517	-3.670091
54	1	0	-1.451413	-0.210804	-2.942437
55	1	0	-1.694367	-1.650360	-1.936096
56	1	0	-3.809727	-2.159593	-3.105873
57	1	0	-3.594525	-0.754198	-4.159506
58	7	0	-2.727568	1.863954	-0.428847
59	6	0	-2.428582	2.965136	-1.331098
60	6	0	-2.186793	4.302885	-0.654415
61	1	0	-2.001640	5.080136	-1.399969
62	1	0	-3.058747	4.601463	-0.067237
63	1	0	-1.326717	4.252998	0.015680
64	1	0	-1.552030	2.678974	-1.920633
65	1	0	-3.256548	3.060233	-2.042104
66	1	0	-3.601267	1.964096	0.077533
67	7	0	-0.814037	1.948399	1.464288
68	6	0	-1.522906	2.729574	2.467392
69	6	0	-1.552415	2.075837	3.837305
70	1	0	-2.052040	2.725343	4.559625
71	1	0	-2.083582	1.122114	3.817335
72	1	0	-0.538107	1.885893	4.196261
73	1	0	-1.050354	3.714540	2.542705
74	1	0	-2.539382	2.912174	2.106975
75	1	0	0.100215	1.616016	1.766229

	1	2	3
	A	A	A
Frequencies --	17.7526	26.2915	30.0673
Red. masses --	3.8005	5.4845	6.2880
Frc consts --	0.0007	0.0022	0.0033
IR Inten --	1.0036	2.9265	1.8562

Sum of electronic and zero-point Energies= -5554.396485
Sum of electronic and thermal Energies= -5554.302361
Sum of electronic and thermal Enthalpies= -5554.300926

Sum of electronic and thermal Free Energies= -5554.562225

Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}^{\ddagger}_{Zn}$, the transition state geometry of the zinc-activated aminophosphine ligand exchange, replacing an outer ligand.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	15	0	-0.489847	1.382711	0.312769
3	7	0	-2.030849	0.740156	0.891031
4	6	0	-2.037037	0.263292	2.291839
5	6	0	-3.403229	0.451793	2.911279
6	1	0	-3.690906	1.506920	2.925927
7	1	0	-4.157688	-0.106793	2.354261
8	1	0	-3.400348	0.089111	3.940341
9	1	0	-1.791336	-0.798878	2.301574
10	1	0	-1.268856	0.788978	2.867536
11	1	0	-2.717352	1.495491	0.828480
12	30	0	-3.089713	-0.479602	-0.562597
13	17	0	-3.587937	-2.350953	0.544510
14	17	0	-4.487151	1.216419	-1.174800
15	7	0	-2.056194	-0.840657	-2.324034
16	1	0	-1.055045	-0.667161	-2.212630
17	1	0	-2.399628	-0.092405	-2.919807
18	6	0	-2.252949	-2.142097	-2.995444
19	6	0	-1.479096	-3.240070	-2.300248
20	1	0	-1.645696	-4.192319	-2.806447

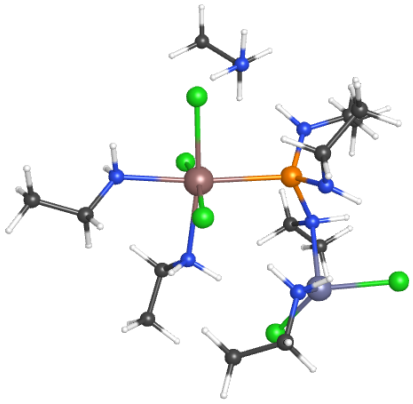
21	1	0	-0.407275	-3.026593	-2.322359
22	1	0	-1.806763	-3.344348	-1.264036
23	1	0	-3.321902	-2.365222	-2.987881
24	1	0	-1.937535	-2.065626	-4.040548
25	7	0	-1.137187	1.929867	-1.117730
26	6	0	-0.354729	2.483494	-2.208523
27	6	0	-0.293677	3.999914	-2.199800
28	1	0	0.284176	4.368617	-3.050742
29	1	0	-1.296692	4.429861	-2.262892
30	1	0	0.171108	4.370622	-1.283627
31	1	0	0.643434	2.049511	-2.153364
32	1	0	-0.790346	2.139264	-3.152603
33	1	0	-2.125622	2.158088	-1.147992
34	7	0	-0.153918	2.659416	1.313429
35	6	0	-0.977486	3.824846	1.578407
36	6	0	-1.379644	3.948320	3.035704
37	1	0	-1.976389	4.849673	3.191857
38	1	0	-1.966617	3.087847	3.361779
39	1	0	-0.496422	4.014466	3.675980
40	1	0	-0.443912	4.730344	1.266717
41	1	0	-1.865798	3.769993	0.941675
42	1	0	0.627197	2.500799	1.936406
43	17	0	1.344173	-0.741824	-2.080318
44	17	0	4.308062	0.187402	-0.022954
45	17	0	1.966704	0.350360	2.619582
46	7	0	0.221943	-1.959326	0.850911
47	6	0	0.366715	-2.646599	2.144677
48	6	0	-0.560946	-3.833085	2.302499
49	1	0	-0.418569	-4.296524	3.281026
50	1	0	-1.605739	-3.529386	2.209640
51	1	0	-0.366584	-4.592483	1.539377
52	1	0	1.409313	-2.951035	2.248645
53	1	0	0.196177	-1.903241	2.923980
54	1	0	-0.719825	-1.584827	0.791367
55	1	0	0.276134	-2.631621	0.090527
56	7	0	3.054188	-2.516954	0.226577
57	6	0	2.549938	-3.766683	-0.350547
58	6	0	3.636127	-4.786585	-0.631388
59	1	0	4.159202	-5.066399	0.286641
60	1	0	3.208489	-5.692344	-1.067045
61	1	0	4.371096	-4.387613	-1.334812
62	1	0	1.815489	-4.194806	0.336633
63	1	0	2.025656	-3.508696	-1.274832
64	1	0	3.477582	-2.688103	1.134617
65	1	0	3.812177	-2.152239	-0.346076

66	7	0	2.439819	2.620198	-0.386585
67	6	0	3.175695	3.004461	-1.584444
68	6	0	4.086609	4.207381	-1.407466
69	1	0	4.841601	4.009625	-0.641465
70	1	0	4.607023	4.448003	-2.338697
71	1	0	3.516854	5.090141	-1.101424
72	1	0	3.757712	2.136040	-1.899343
73	1	0	2.452875	3.204859	-2.380268
74	1	0	3.095948	2.443919	0.367182
75	1	0	1.833003	3.371848	-0.080561

	1	2	3
	A	A	A
Frequencies --	-64.9457	16.4084	26.1245
Red. masses --	6.4285	5.7454	3.3686
Frc consts --	0.0160	0.0009	0.0014
IR Inten --	8.1313	5.6164	0.3056

Sum of electronic and zero-point Energies=	-5554.372552
Sum of electronic and thermal Energies=	-5554.278806
Sum of electronic and thermal Enthalpies=	-5554.277371
Sum of electronic and thermal Free Energies=	-5554.536132

Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}_{Zn_{II}}$, the final geometry of the zinc-activated aminophosphine ligand exchange, replacing an outer ligand.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

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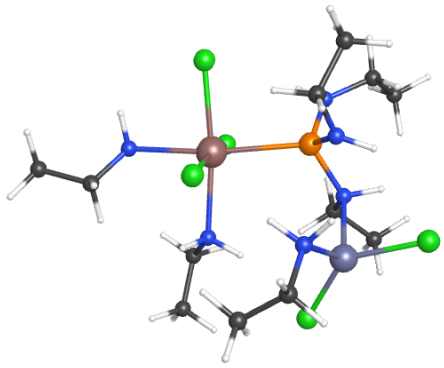
3	7	0	-1.249444	-1.590263	-0.745510
4	6	0	-0.712607	-1.518958	-2.126336
5	6	0	-1.608442	-2.263418	-3.087863
6	1	0	-1.672632	-3.324565	-2.830378
7	1	0	-2.615605	-1.843689	-3.088059
8	1	0	-1.207304	-2.187936	-4.099740
9	1	0	-0.652617	-0.467206	-2.406419
10	1	0	0.304242	-1.922042	-2.147754
11	1	0	-1.688680	-2.504607	-0.616839
12	30	0	-3.066146	-0.439664	-0.376411
13	17	0	-3.252554	0.812337	-2.222369
14	17	0	-4.209497	-2.245225	0.394598
15	7	0	-3.071447	0.743911	1.326655
16	1	0	-2.136527	1.072088	1.586811
17	1	0	-3.316211	0.052046	2.029466
18	6	0	-4.026031	1.869350	1.401646
19	6	0	-3.523431	3.074131	0.638459
20	1	0	-4.244913	3.889631	0.711994
21	1	0	-2.574361	3.422337	1.054039
22	1	0	-3.384524	2.835868	-0.417342
23	1	0	-4.981702	1.528825	0.997125
24	1	0	-4.190965	2.135637	2.450351
25	7	0	-1.042834	-1.543047	1.786633
26	6	0	-0.517992	-1.433133	3.143461
27	6	0	-0.154221	-2.766278	3.767748
28	1	0	0.187520	-2.621779	4.795222
29	1	0	-1.016846	-3.438041	3.789850
30	1	0	0.646966	-3.251262	3.207489
31	1	0	0.357493	-0.779611	3.109620
32	1	0	-1.261551	-0.915088	3.756473
33	1	0	-1.879051	-2.109064	1.685629
34	7	0	1.019327	-2.628649	0.361158
35	6	0	0.662728	-4.034868	0.447805
36	6	0	0.781694	-4.760137	-0.880555
37	1	0	0.547815	-5.820575	-0.759865
38	1	0	0.099007	-4.344322	-1.624320
39	1	0	1.796703	-4.675347	-1.273944
40	1	0	1.311572	-4.513443	1.188483
41	1	0	-0.355941	-4.122857	0.839673
42	1	0	2.032834	-2.452206	0.203450
43	17	0	-0.136039	2.024408	2.129580
44	17	0	2.951772	0.133611	1.970923
45	17	0	2.523768	0.260716	-1.705215

46	7	0	-0.244207	2.107544	-1.036767
47	6	0	0.173660	2.570518	-2.370425
48	6	0	-0.756562	3.619154	-2.943404
49	1	0	-0.415787	3.929761	-3.933315
50	1	0	-1.771011	3.226074	-3.036375
51	1	0	-0.789681	4.507267	-2.305322
52	1	0	1.195294	2.947756	-2.297114
53	1	0	0.226166	1.694234	-3.017160
54	1	0	-1.142970	1.633963	-1.138846
55	1	0	-0.442942	2.903356	-0.434265
56	7	0	2.578395	2.868955	0.302771
57	6	0	2.039415	4.233866	0.363517
58	6	0	3.109648	5.290728	0.547141
59	1	0	3.827667	5.272712	-0.276656
60	1	0	2.660760	6.285621	0.583745
61	1	0	3.655784	5.133338	1.480534
62	1	0	1.486368	4.418638	-0.560491
63	1	0	1.320129	4.262230	1.183892
64	1	0	3.191205	2.754704	-0.500903
65	1	0	3.152349	2.683237	1.122885
66	7	0	3.844388	-2.422233	-0.092703
67	6	0	4.298176	-2.916303	-1.385287
68	6	0	5.704745	-2.491400	-1.770578
69	1	0	6.435025	-2.845091	-1.036950
70	1	0	5.985816	-2.891971	-2.748514
71	1	0	5.773874	-1.401299	-1.818392
72	1	0	4.227440	-4.008975	-1.376587
73	1	0	3.587758	-2.561197	-2.137513
74	1	0	4.435897	-2.766594	0.655032
75	1	0	3.901218	-1.408397	-0.061633

	1	2	3
	A	A	A
Frequencies --	21.1456	31.6353	32.8396
Red. masses --	3.6957	2.9684	3.4136
Frc consts --	0.0010	0.0018	0.0022
IR Inten --	0.6082	0.3868	0.6750

Sum of electronic and zero-point Energies= -5554.401734
Sum of electronic and thermal Energies= -5554.306983
Sum of electronic and thermal Enthalpies= -5554.305548
Sum of electronic and thermal Free Energies= -5554.568548

Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}_{Zn}$, the terminal geometry of the activated aminophosphine ligand exchange ($\mathbf{L}_{Zn_{II}}$) with the free ethylamine removed.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	1.764838	0.451181	-0.027816
2	15	0	-0.720212	1.431484	-0.010077
3	7	0	-1.880682	0.541034	0.922577
4	6	0	-1.524654	0.398469	2.354269
5	6	0	-2.756333	0.121778	3.183660
6	1	0	-3.476254	0.942104	3.110055
7	1	0	-3.244377	-0.799615	2.863010
8	1	0	-2.477569	0.013648	4.232908
9	1	0	-0.818834	-0.427243	2.441075
10	1	0	-1.015688	1.301563	2.702240
11	1	0	-2.790077	1.004103	0.859398
12	30	0	-2.549080	-1.289086	-0.084487
13	17	0	-1.925296	-2.871493	1.373519
14	17	0	-4.543939	-0.333173	-0.624690
15	7	0	-1.766493	-1.624401	-1.970014
16	1	0	-0.796038	-1.308472	-2.051926
17	1	0	-2.313417	-0.980231	-2.533461
18	6	0	-1.883415	-2.987933	-2.529838
19	6	0	-0.817545	-3.902351	-1.969079
20	1	0	-0.920477	-4.901490	-2.395818
21	1	0	0.178495	-3.526175	-2.215393
22	1	0	-0.904168	-3.980196	-0.884192
23	1	0	-2.880916	-3.365551	-2.293590
24	1	0	-1.800352	-2.940786	-3.619990

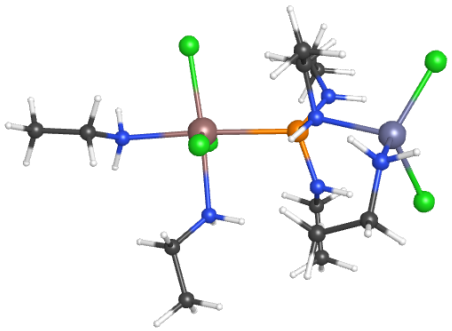
25	7	0	-1.561904	1.433638	-1.433168
26	6	0	-0.982521	1.979885	-2.657004
27	6	0	-1.246577	3.458873	-2.860778
28	1	0	-0.827454	3.787127	-3.814611
29	1	0	-2.319045	3.671048	-2.870354
30	1	0	-0.781695	4.046700	-2.067443
31	1	0	0.092805	1.790125	-2.626875
32	1	0	-1.375421	1.402848	-3.499227
33	1	0	-2.574722	1.398815	-1.398076
34	7	0	-0.585638	2.943402	0.610930
35	6	0	-1.636462	3.938763	0.731565
36	6	0	-2.152161	4.107708	2.148882
37	1	0	-2.903425	4.899830	2.187022
38	1	0	-2.611200	3.188252	2.518427
39	1	0	-1.339982	4.376272	2.828038
40	1	0	-1.256627	4.892300	0.353056
41	1	0	-2.451408	3.650297	0.061037
42	1	0	0.306624	3.157703	1.036172
43	17	0	1.447573	-0.800169	-2.193628
44	17	0	2.507811	2.526087	-1.165477
45	17	0	2.061345	1.347030	2.277390
46	7	0	1.280361	-1.661532	0.848026
47	6	0	1.821313	-2.046994	2.162276
48	6	0	1.675552	-3.526422	2.451349
49	1	0	2.078145	-3.760088	3.439206
50	1	0	0.625413	-3.824093	2.428030
51	1	0	2.218087	-4.128223	1.716658
52	1	0	2.869568	-1.743270	2.200574
53	1	0	1.310488	-1.444737	2.914035
54	1	0	0.276449	-1.856912	0.843326
55	1	0	1.657974	-2.265016	0.120511
56	7	0	4.004749	-0.104693	0.003961
57	6	0	4.511594	-1.415610	-0.424321
58	6	0	6.023482	-1.476493	-0.494821
59	1	0	6.473707	-1.268926	0.479355
60	1	0	6.350037	-2.468397	-0.814086
61	1	0	6.409447	-0.747834	-1.212113
62	1	0	4.136726	-2.164753	0.277137
63	1	0	4.064875	-1.632219	-1.396132
64	1	0	4.328024	0.125289	0.940518
65	1	0	4.366995	0.627689	-0.603817

1	2	3
A	A	A

Frequencies --	24.0947	32.3036	35.6953
Red. masses --	5.1593	4.3658	3.9538
Frc consts --	0.0018	0.0027	0.0030
IR Inten --	3.2339	2.4862	0.7402

Sum of electronic and zero-point Energies=	-5419.415680
Sum of electronic and thermal Energies=	-5419.331653
Sum of electronic and thermal Enthalpies=	-5419.330218
Sum of electronic and thermal Free Energies=	-5419.567881

Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}_{Zn_A}$, a minimum energy conformer of a zinc-activated indium-phosphine complex.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	-2.128840	-0.284023	-0.112880
2	15	0	0.426754	-0.786559	0.582205
3	7	0	1.473890	-0.279063	-0.724886
4	6	0	1.298918	-1.218537	-1.875951
5	6	0	1.798040	-0.609312	-3.164157
6	1	0	1.289176	0.336016	-3.371772
7	1	0	2.879858	-0.460868	-3.136825
8	1	0	1.584007	-1.288240	-3.990948
9	1	0	1.856279	-2.124690	-1.640742
10	1	0	0.240325	-1.478956	-1.977452
11	1	0	1.072294	0.615127	-1.027027
12	30	0	3.572530	0.065097	-0.388234
13	17	0	4.065357	0.804838	1.689827
14	17	0	4.657217	-1.706030	-1.183108

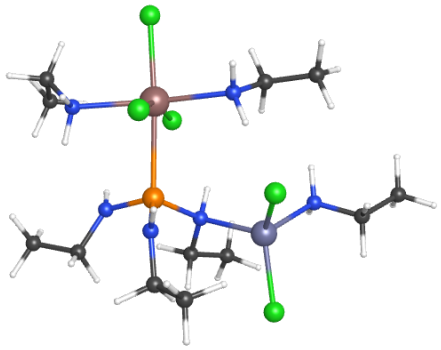
15	7	0	3.881218	1.744666	-1.615287
16	1	0	3.327756	1.663404	-2.463881
17	1	0	4.849819	1.673897	-1.915462
18	6	0	3.649740	3.068598	-1.000332
19	6	0	2.200624	3.247584	-0.606889
20	1	0	2.039087	4.260045	-0.233193
21	1	0	1.527651	3.096909	-1.456004
22	1	0	1.916104	2.555348	0.189345
23	1	0	4.287570	3.127181	-0.117366
24	1	0	3.955721	3.857658	-1.693908
25	7	0	0.909758	-2.296144	0.983314
26	6	0	0.116403	-3.508222	0.809336
27	6	0	-0.173836	-4.190311	2.129142
28	1	0	-0.740640	-5.109079	1.962680
29	1	0	0.752010	-4.453314	2.648012
30	1	0	-0.762626	-3.534803	2.774028
31	1	0	-0.814490	-3.230908	0.310837
32	1	0	0.643685	-4.184402	0.129019
33	1	0	1.851138	-2.429452	1.329777
34	7	0	0.882397	0.318383	1.742439
35	6	0	0.386022	0.089362	3.103924
36	6	0	0.538631	1.336716	3.947735
37	1	0	0.189360	1.150175	4.965079
38	1	0	1.586921	1.640386	3.998894
39	1	0	-0.033212	2.172199	3.536866
40	1	0	-0.661964	-0.222894	3.046173
41	1	0	0.922012	-0.744612	3.571760
42	1	0	1.878437	0.554957	1.748382
43	17	0	-1.134734	1.329735	-1.788442
44	17	0	-2.421940	-2.145124	-1.691108
45	17	0	-3.032012	-1.386375	1.933867
46	7	0	-1.977954	1.593416	1.294389
47	6	0	-2.645644	2.854869	0.951421
48	6	0	-2.257043	4.001540	1.862724
49	1	0	-2.783054	4.914285	1.574842
50	1	0	-2.504624	3.782545	2.904700
51	1	0	-1.183673	4.199679	1.800684
52	1	0	-2.394085	3.082621	-0.085620
53	1	0	-3.724632	2.686969	0.997643
54	1	0	-2.286519	1.262149	2.204445
55	1	0	-0.970767	1.737702	1.359395
56	7	0	-4.305710	0.245940	-0.620236
57	6	0	-4.583442	0.944752	-1.885295
58	6	0	-6.062885	1.063327	-2.183036
59	1	0	-6.580903	1.625218	-1.400915

60	1	0	-6.218994	1.583399	-3.130400
61	1	0	-6.528100	0.077176	-2.259972
62	1	0	-4.109874	1.926168	-1.831120
63	1	0	-4.066928	0.393419	-2.673001
64	1	0	-4.755529	0.716668	0.159586
65	1	0	-4.707110	-0.688823	-0.648953

	1	2	3
	A	A	A
Frequencies --	20.2137	25.7769	29.7691
Red. masses --	5.0796	3.4350	4.6220
Frc consts --	0.0012	0.0013	0.0024
IR Inten --	1.1917	0.2813	1.4476

Sum of electronic and zero-point Energies=	-5419.409881
Sum of electronic and thermal Energies=	-5419.326004
Sum of electronic and thermal Enthalpies=	-5419.324569
Sum of electronic and thermal Free Energies=	-5419.563808

Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}_{Zn_B}$, a minimum energy conformer of a zinc-activated indium-phosphine complex.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	1.996638	-0.926032	0.240585
2	15	0	0.409333	1.284483	0.132221
3	7	0	-0.993926	1.026978	-0.919477
4	6	0	-1.397786	2.120220	-1.842317

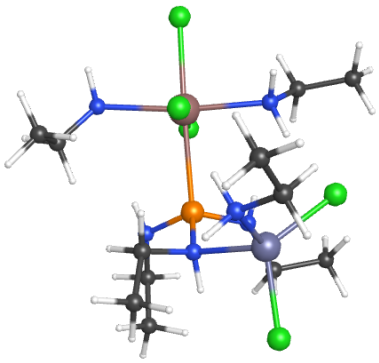
5	6	0	-2.321506	1.608857	-2.924762
6	1	0	-1.866624	0.776406	-3.469785
7	1	0	-3.278547	1.297139	-2.502695
8	1	0	-2.523391	2.405256	-3.643057
9	1	0	-1.900301	2.890656	-1.257357
10	1	0	-0.506596	2.558841	-2.297567
11	1	0	-0.647178	0.265718	-1.514001
12	30	0	-2.692146	0.220037	0.101074
13	17	0	-2.211775	-0.930150	1.972225
14	17	0	-4.242056	1.825672	0.124393
15	7	0	-3.380227	-1.302613	-1.173054
16	1	0	-2.709892	-2.065761	-1.202411
17	1	0	-3.481092	-0.983245	-2.132275
18	6	0	-4.675601	-1.816235	-0.683034
19	6	0	-5.223118	-2.953828	-1.516054
20	1	0	-6.177033	-3.296546	-1.110288
21	1	0	-5.390723	-2.641760	-2.550406
22	1	0	-4.535736	-3.804292	-1.520856
23	1	0	-4.520452	-2.124721	0.352914
24	1	0	-5.365034	-0.970213	-0.660436
25	7	0	1.349626	2.444016	-0.625438
26	6	0	1.254215	3.891672	-0.474975
27	6	0	2.501180	4.561120	-1.012503
28	1	0	2.430136	5.644091	-0.896919
29	1	0	3.389611	4.216517	-0.478252
30	1	0	2.636412	4.347237	-2.076452
31	1	0	0.366553	4.298262	-0.975752
32	1	0	1.149553	4.104410	0.589437
33	1	0	1.685951	2.135217	-1.530978
34	7	0	-0.123396	1.927333	1.533751
35	6	0	-1.078847	3.001992	1.799931
36	6	0	-1.941913	2.674302	2.998015
37	1	0	-2.627383	3.499415	3.198861
38	1	0	-2.526900	1.772483	2.816148
39	1	0	-1.327204	2.517687	3.888785
40	1	0	-0.548473	3.945349	1.966954
41	1	0	-1.718102	3.136381	0.924201
42	1	0	0.121178	1.344940	2.325698
43	17	0	1.982466	-0.565542	2.728246
44	17	0	3.553973	-2.792172	0.047573
45	17	0	1.446619	-0.728711	-2.238350
46	7	0	3.761827	0.572677	0.291936
47	6	0	4.958713	0.434700	-0.557941
48	6	0	4.717306	0.978794	-1.947496
49	1	0	5.612021	0.848369	-2.558353

50	1	0	3.891150	0.457802	-2.434036
51	1	0	4.488158	2.048511	-1.918849
52	1	0	5.798495	0.957444	-0.088891
53	1	0	5.208836	-0.626639	-0.598286
54	1	0	3.362251	1.505368	0.200076
55	1	0	4.005124	0.458445	1.272752
56	7	0	0.347317	-2.439930	0.631363
57	6	0	-0.160130	-3.243985	-0.485901
58	6	0	-1.214900	-4.247035	-0.063375
59	1	0	-2.049683	-3.753129	0.442420
60	1	0	-1.601501	-4.785499	-0.931978
61	1	0	-0.800035	-4.982922	0.629444
62	1	0	-0.545878	-2.550985	-1.237505
63	1	0	0.692531	-3.740257	-0.953163
64	1	0	-0.425307	-1.973826	1.118874
65	1	0	0.793124	-3.042256	1.319196

	1	2	3
	A	A	A
Frequencies --	25.1215	36.5398	38.7554
Red. masses --	4.4488	4.1513	2.7885
Frc consts --	0.0017	0.0033	0.0025
IR Inten --	0.7576	0.5610	0.3485

Sum of electronic and zero-point Energies=	-5419.405216
Sum of electronic and thermal Energies=	-5419.321707
Sum of electronic and thermal Enthalpies=	-5419.320272
Sum of electronic and thermal Free Energies=	-5419.555884

Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{L}_{Zn_C}$, a minimum energy conformer of a zinc-activated indium-phosphine complex.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	-2.108319	-0.404347	-0.123419
2	17	0	-0.695568	-1.749326	-1.704463
3	17	0	-4.051250	-1.902300	-0.200314
4	17	0	-3.151079	1.270926	1.468149
5	7	0	-3.223975	0.760643	-1.800484
6	6	0	-2.641041	1.605865	-2.859153
7	6	0	-2.064230	0.774097	-3.981494
8	1	0	-1.606297	1.424339	-4.729085
9	1	0	-1.311507	0.077896	-3.610051
10	1	0	-2.844482	0.190615	-4.477606
11	1	0	-3.408612	2.281694	-3.249890
12	1	0	-1.866797	2.226826	-2.403819
13	1	0	-3.801416	0.028227	-2.207482
14	1	0	-3.847794	1.309126	-1.213185
15	7	0	-1.232627	-1.710615	1.509800
16	6	0	-1.867382	-1.699581	2.837062
17	6	0	-1.296052	-2.752987	3.762995
18	1	0	-0.222340	-2.608693	3.904861
19	1	0	-1.782058	-2.702529	4.739675
20	1	0	-1.454550	-3.756548	3.359518
21	1	0	-1.738565	-0.701553	3.258593
22	1	0	-2.940015	-1.840427	2.689896
23	1	0	-1.339675	-2.631779	1.090385
24	1	0	-0.221187	-1.569317	1.599480
25	15	0	-0.132015	1.430048	0.251992
26	7	0	1.388314	1.237463	-0.550222
27	6	0	1.275280	1.332955	-2.030459
28	6	0	2.606740	1.656794	-2.669478
29	1	0	2.956184	2.648284	-2.371649
30	1	0	3.386964	0.949210	-2.385336
31	1	0	2.500289	1.648314	-3.755477
32	1	0	0.875338	0.383256	-2.388307
33	1	0	0.549651	2.108685	-2.289622
34	1	0	2.053952	1.944338	-0.238655
35	30	0	2.651606	-0.479066	0.071733
36	17	0	4.501628	0.781222	0.292176
37	17	0	2.063193	-1.799536	1.790269
38	7	0	2.599950	-1.704859	-1.588886
39	1	0	3.012012	-1.270844	-2.409150
40	1	0	1.606224	-1.836399	-1.796385

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    41          6           0        3.227269   -3.021959   -1.365446
    42          6           0        3.063599   -3.958597   -2.542511
    43          1           0        3.534693   -4.920606   -2.330498
    44          1           0        2.006452   -4.139377   -2.753109
    45          1           0        3.528039   -3.548619   -3.443596
    46          1           0        4.282535   -2.851051   -1.141894
    47          1           0        2.775585   -3.438681   -0.464080
    48          7           0        0.323559    1.319880    1.839080
    49          6           0        1.464707    1.928416    2.522557
    50          6           0        1.636219    1.307131    3.891769
    51          1           0        2.491152    1.753249    4.402893
    52          1           0        0.749260    1.475433    4.509429
    53          1           0        1.803666    0.233221    3.798410
    54          1           0        2.369945    1.749923    1.935646
    55          1           0        1.342403    3.014018    2.614420
    56          1           0       -0.494386    1.225834    2.429756
    57          7           0       -0.676006    2.951568   -0.193573
    58          6           0       -0.159408    4.232247    0.303002
    59          6           0        1.263836    4.528066   -0.123692
    60          1           0        1.511904    5.561808    0.123163
    61          1           0        1.996211    3.903823    0.393536
    62          1           0        1.386751    4.398282   -1.200986
    63          1           0       -0.817491    5.003906   -0.102787
    64          1           0       -0.243860    4.288998    1.394879
    65          1           0       -1.687958    2.931394   -0.126082
 ---------------------------------------------------------------------

                     1                      2                      3
                     A                      A                      A
 Frequencies --     25.4730                35.1288                39.1360
 Red. masses --      4.4356                 3.7564                 3.3116
 Frc consts  --      0.0017                 0.0027                 0.0030
 IR Inten    --      0.1700                 1.2633                 0.6626

 Sum of electronic and zero-point Energies=          -5419.404725
 Sum of electronic and thermal Energies=             -5419.320938
 Sum of electronic and thermal Enthalpies=           -5419.319503
 Sum of electronic and thermal Free Energies=        -5419.556248
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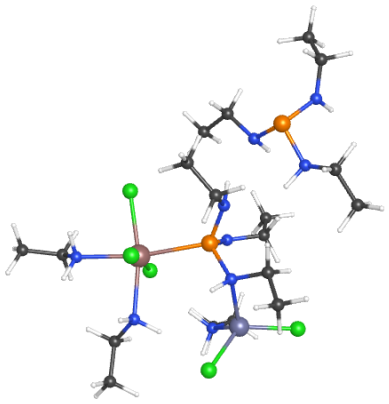
Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{D}_{ZnI}$, the starting geometry of the zinc-activated disproportionation reaction where a second aminophosphine, P_{Am}(III), hydrogen bonds with $\mathbf{L}_{Zn}$.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	-1.887879	-1.619619	-0.323666
2	17	0	-0.328590	-3.444990	0.272557
3	17	0	-1.619662	-1.671429	-2.824398
4	17	0	-2.461238	-1.084028	2.081981
5	7	0	-3.686859	-0.242314	-0.934607
6	6	0	-4.956841	-0.300508	-0.195044
7	6	0	-6.056479	0.525382	-0.831412
8	1	0	-6.970825	0.461613	-0.237339
9	1	0	-5.761352	1.574248	-0.903078
10	1	0	-6.283147	0.169477	-1.839847
11	1	0	-5.261428	-1.347298	-0.121328
12	1	0	-4.758891	0.027532	0.826336
13	1	0	-3.411272	0.740126	-1.038418
14	1	0	-3.823395	-0.557811	-1.893098
15	7	0	-3.382302	-3.366106	-0.530805
16	6	0	-3.911340	-3.957171	0.709522
17	6	0	-4.715009	-5.217302	0.470424
18	1	0	-4.103977	-5.987804	-0.006752
19	1	0	-5.082248	-5.618185	1.417430
20	1	0	-5.579582	-5.021071	-0.169813
21	1	0	-3.053901	-4.154253	1.355013
22	1	0	-4.510951	-3.195916	1.211591
23	1	0	-2.779590	-4.040679	-0.997073
24	1	0	-4.135307	-3.165312	-1.182787
25	15	0	0.143989	0.086027	-0.225219
26	7	0	0.466129	0.474097	1.329770
27	6	0	1.450258	1.425065	1.837743
28	6	0	1.884029	1.051792	3.238268

29	1	0	2.620631	1.767354	3.607753
30	1	0	1.036040	1.058006	3.928786
31	1	0	2.321953	0.051905	3.259523
32	1	0	2.313104	1.422060	1.168698
33	1	0	1.037908	2.440666	1.822129
34	1	0	-0.215432	0.119169	1.989457
35	7	0	-0.238690	1.539699	-1.113347
36	30	0	-1.560104	2.886562	0.009925
37	17	0	-3.229304	3.006430	-1.521395
38	17	0	-0.314545	4.624950	0.648871
39	7	0	-2.553526	2.185698	1.684083
40	6	0	-2.037748	2.647401	2.986085
41	6	0	-2.903390	2.214813	4.149651
42	1	0	-2.979459	1.125903	4.196853
43	1	0	-3.912606	2.626130	4.060933
44	1	0	-2.479214	2.569935	5.091183
45	1	0	-1.025061	2.254515	3.090118
46	1	0	-1.940428	3.732461	2.938151
47	1	0	-2.619929	1.163417	1.706174
48	1	0	-3.505105	2.524795	1.562119
49	6	0	0.863789	2.382752	-1.651444
50	6	0	0.347863	3.340076	-2.701042
51	1	0	1.177184	3.937436	-3.084055
52	1	0	-0.096748	2.798918	-3.540481
53	1	0	-0.400117	4.021897	-2.293711
54	1	0	1.290394	2.933285	-0.812223
55	1	0	1.643005	1.749647	-2.076247
56	1	0	-0.853466	1.267599	-1.881744
57	7	0	1.613780	-0.365424	-0.828719
58	6	0	1.835452	-0.762573	-2.217069
59	6	0	2.097440	-2.245644	-2.375658
60	1	0	1.252546	-2.830104	-2.011382
61	1	0	2.991907	-2.537152	-1.819380
62	1	0	2.264372	-2.483188	-3.428676
63	1	0	0.959088	-0.481419	-2.806435
64	1	0	2.685617	-0.193640	-2.614118
65	1	0	2.246817	-0.806347	-0.155837
66	7	0	4.578270	0.961496	-0.482629
67	6	0	5.179875	1.877054	-1.444404
68	6	0	4.710338	3.298373	-1.208327
69	1	0	4.963445	3.625950	-0.197653
70	1	0	5.174419	3.982392	-1.922667
71	1	0	3.626673	3.381987	-1.325018
72	1	0	6.264595	1.821573	-1.321853
73	1	0	4.966573	1.583740	-2.483879

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    74         15           0        5.206967   -0.645017   -0.434763
    75          7           0        6.685094   -0.294346    0.268281
    76          1           0        6.722658    0.361865    1.037694
    77          6           0        7.892035   -1.053455    0.020410
    78          6           0        8.267065   -2.002567    1.145503
    79          1           0        8.400864   -1.459419    2.085152
    80          1           0        9.202741   -2.521684    0.921037
    81          1           0        7.486285   -2.751994    1.296951
    82          1           0        7.737226   -1.617336   -0.904291
    83          1           0        8.722417   -0.363957   -0.172196
    84          7           0        4.090743   -1.146513    0.771286
    85          1           0        4.060453   -0.504584    1.559086
    86          6           0        4.158286   -2.535691    1.213814
    87          6           0        3.005956   -2.878182    2.134623
    88          1           0        3.035161   -2.266358    3.041156
    89          1           0        2.043411   -2.721794    1.643247
    90          1           0        3.061735   -3.924745    2.442132
    91          1           0        5.110338   -2.752855    1.718678
    92          1           0        4.126133   -3.170094    0.322861
    93          1           0        3.571417    0.921185   -0.609787
 -------------------------------------------------------------------

                     1                      2                      3
                     A                      A                      A
 Frequencies --     16.6761                19.0352                23.9066
 Red. masses --      4.4139                 4.5151                 4.4035
 Frc consts  --      0.0007                 0.0010                 0.0015
 IR Inten    --      0.6277                 0.0694                 0.9116

 Sum of electronic and zero-point Energies=          -6163.857465
 Sum of electronic and thermal Energies=             -6163.741404
 Sum of electronic and thermal Enthalpies=           -6163.739969
 Sum of electronic and thermal Free Energies=        -6164.053895
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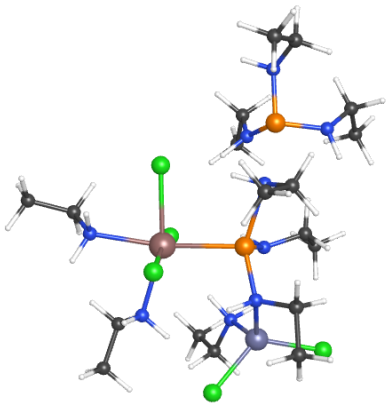
Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{D}^{\ddagger}_{Zn}$, the transition state of the zinc-activated disproportionation reaction.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	0.826399	1.756287	-0.349488
2	17	0	-1.508398	2.781700	-0.434368
3	17	0	1.293217	1.889130	-2.837851
4	17	0	0.813836	1.445388	2.163704
5	7	0	3.167127	1.489808	-0.304922
6	6	0	3.953391	2.008202	0.823055
7	6	0	5.448835	1.914645	0.597692
8	1	0	5.990433	2.281325	1.472412
9	1	0	5.749623	0.881145	0.411077
10	1	0	5.754180	2.511495	-0.265692
11	1	0	3.656272	3.043961	1.004335
12	1	0	3.654389	1.456155	1.715038
13	1	0	3.463494	0.526149	-0.495836
14	1	0	3.410916	1.982160	-1.162189
15	7	0	1.355987	4.006195	-0.268083
16	6	0	1.105808	4.729537	0.989106
17	6	0	1.291093	6.226342	0.858025
18	1	0	0.605058	6.643013	0.116020
19	1	0	1.093480	6.718352	1.812693
20	1	0	2.312448	6.475331	0.556618
21	1	0	0.087698	4.484305	1.295485
22	1	0	1.769320	4.314380	1.749496
23	1	0	0.725345	4.349128	-0.989321
24	1	0	2.295305	4.195209	-0.606047
25	15	0	-0.177662	-0.607252	-0.780937
26	7	0	-0.204236	-1.408142	0.696487
27	6	0	-1.106550	-2.523682	0.962652
28	6	0	-0.728950	-3.210852	2.257330

29	1	0	-1.447495	-3.997572	2.496752
30	1	0	0.259495	-3.667699	2.175750
31	1	0	-0.729328	-2.498149	3.087960
32	1	0	-2.141439	-2.172997	1.013183
33	1	0	-1.028034	-3.233611	0.134759
34	1	0	-0.179847	-0.744166	1.465743
35	7	0	1.138823	-1.470663	-1.632138
36	30	0	2.529877	-2.222577	-0.210475
37	17	0	4.464381	-1.439431	-1.140462
38	17	0	2.110063	-4.413250	0.041137
39	7	0	2.615783	-1.484717	1.730038
40	6	0	3.948763	-1.482926	2.351297
41	6	0	3.937874	-0.981490	3.780080
42	1	0	3.312119	-1.614343	4.414946
43	1	0	3.548799	0.039008	3.835708
44	1	0	4.948473	-0.982960	4.193990
45	1	0	4.337901	-2.501626	2.295305
46	1	0	4.600803	-0.874265	1.723045
47	1	0	1.998991	-2.111228	2.240184
48	1	0	2.184504	-0.563426	1.820654
49	6	0	0.719835	-2.534707	-2.576761
50	6	0	1.885034	-3.015389	-3.411517
51	1	0	1.543734	-3.778394	-4.113990
52	1	0	2.320645	-2.193380	-3.985110
53	1	0	2.666627	-3.450956	-2.787198
54	1	0	0.315469	-3.357426	-1.983945
55	1	0	-0.073527	-2.153641	-3.226447
56	1	0	1.625569	-0.752637	-2.175117
57	7	0	-2.257814	-0.377738	-1.058081
58	6	0	-2.613938	-0.993072	-2.368375
59	6	0	-2.234521	-0.155344	-3.570601
60	1	0	-1.162814	0.056040	-3.593582
61	1	0	-2.755041	0.805747	-3.543376
62	1	0	-2.510239	-0.666429	-4.496550
63	1	0	-2.137802	-1.975922	-2.406853
64	1	0	-3.694412	-1.162655	-2.377261
65	1	0	-2.152241	0.631902	-1.209005
66	7	0	-4.554412	-1.680989	0.062131
67	6	0	-5.445321	-2.305347	1.027633
68	6	0	-4.722057	-2.972324	2.184853
69	1	0	-4.114232	-2.251303	2.735135
70	1	0	-5.439354	-3.418922	2.878178
71	1	0	-4.060664	-3.766982	1.829798
72	1	0	-6.120767	-1.531945	1.397819
73	1	0	-6.067261	-3.041070	0.506496

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    74         15           0       -4.102978   -0.077923   -0.009305
    75          7           0       -5.632726    0.623696    0.257092
    76          1           0       -5.536526    1.590959    0.541331
    77          6           0       -6.702507    0.435509   -0.711961
    78          6           0       -6.519692    1.205085   -2.009941
    79          1           0       -6.450747    2.279469   -1.820155
    80          1           0       -7.361252    1.032908   -2.685499
    81          1           0       -5.602222    0.895444   -2.517301
    82          1           0       -6.777543   -0.634770   -0.918645
    83          1           0       -7.642912    0.726775   -0.233195
    84          7           0       -3.294683    0.456953    1.338707
    85          1           0       -2.443733    0.963174    1.127339
    86          6           0       -3.837715    0.728317    2.656702
    87          6           0       -2.815068    0.419271    3.733185
    88          1           0       -2.542736   -0.639026    3.715195
    89          1           0       -1.902949    1.001983    3.578920
    90          1           0       -3.210485    0.658851    4.723164
    91          1           0       -4.732377    0.117571    2.793973
    92          1           0       -4.159581    1.774643    2.746351
    93          1           0       -3.899259   -2.313835   -0.369808
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                     1                    2                    3
                     A                    A                    A
 Frequencies --   -512.8951             10.6012              26.2238
 Red. masses --      9.2227              5.0642               3.6113
 Frc consts  --      1.4294              0.0003               0.0015
 IR Inten    --   2000.9766              1.0029               0.2360

 Sum of electronic and zero-point Energies=          -6163.773703
 Sum of electronic and thermal Energies=             -6163.658609
 Sum of electronic and thermal Enthalpies=           -6163.657173
 Sum of electronic and thermal Free Energies=        -6163.966039
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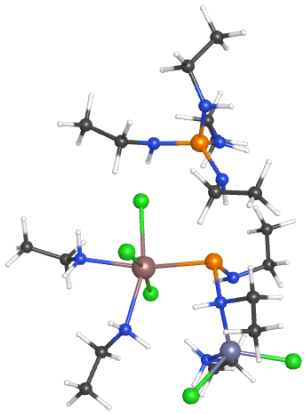
Cartesian coordinates, three lower frequencies, and thermochemistry of $\mathbf{D}_{Zn_{II}}$, the terminal geometry of the zinc-activated disproportionation reaction where the oxidized quaternary aminophosphine is separated from the reduced indium-phosphorus compound.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	17	0	-0.797255	1.116207	-2.331359
4	17	0	1.947852	2.069840	1.880695
5	7	0	2.236992	1.793754	-1.510876
6	6	0	3.185549	2.892451	-1.279916
7	6	0	4.139091	3.110908	-2.437628
8	1	0	4.832857	3.924296	-2.212444
9	1	0	4.717335	2.206177	-2.636131
10	1	0	3.595136	3.373673	-3.349296
11	1	0	2.619780	3.804533	-1.076396
12	1	0	3.728593	2.666317	-0.360967
13	1	0	2.785389	0.940937	-1.664792
14	1	0	1.737150	1.936549	-2.386240
15	7	0	-0.053793	3.685244	-0.544405
16	6	0	0.242994	4.730862	0.445520
17	6	0	-0.325829	6.081978	0.066452
18	1	0	-1.414290	6.036104	-0.025410
19	1	0	-0.084523	6.823827	0.830680
20	1	0	0.082104	6.434514	-0.885124
21	1	0	-0.162914	4.387340	1.398054
22	1	0	1.326116	4.778016	0.567742
23	1	0	-1.060523	3.607619	-0.667405
24	1	0	0.319874	3.930946	-1.456585
25	15	0	0.254266	-1.050473	0.328110
26	7	0	1.234138	-1.278696	1.694476
27	6	0	0.984945	-2.391307	2.600223
28	6	0	-0.100867	-2.113456	3.621891

29	1	0	-0.246939	-2.970462	4.284930
30	1	0	0.155119	-1.245778	4.235792
31	1	0	-1.046105	-1.894476	3.120124
32	1	0	0.723993	-3.262115	1.993002
33	1	0	1.924550	-2.648563	3.100338
34	1	0	1.518574	-0.427299	2.165506
35	7	0	1.348731	-1.624459	-0.979897
36	30	0	3.340602	-1.616788	-0.294195
37	17	0	4.330461	-0.700461	-2.193377
38	17	0	3.879215	-3.699326	0.343842
39	7	0	4.180353	-0.248326	1.020544
40	6	0	4.646926	-0.785425	2.307370
41	6	0	5.322075	0.256670	3.174401
42	1	0	4.639565	1.082226	3.391663
43	1	0	6.207120	0.665785	2.679123
44	1	0	5.641048	-0.181840	4.122614
45	1	0	3.776930	-1.205270	2.814744
46	1	0	5.313274	-1.623021	2.095244
47	1	0	3.539541	0.529796	1.198154
48	1	0	4.964840	0.139850	0.502718
49	6	0	0.983524	-2.965273	-1.490984
50	6	0	1.742906	-3.314443	-2.750601
51	1	0	1.437635	-4.301222	-3.105113
52	1	0	1.542615	-2.589324	-3.544071
53	1	0	2.818569	-3.331327	-2.569273
54	1	0	1.211121	-3.684291	-0.701285
55	1	0	-0.094329	-3.002078	-1.675884
56	1	0	1.288020	-0.971251	-1.760334
57	7	0	-4.124655	0.598654	-0.241001
58	6	0	-4.438825	1.288713	-1.491446
59	6	0	-4.997727	2.666964	-1.206473
60	1	0	-4.281193	3.260703	-0.633259
61	1	0	-5.924028	2.606878	-0.630266
62	1	0	-5.203470	3.193086	-2.141034
63	1	0	-3.534999	1.365777	-2.103620
64	1	0	-5.161373	0.690389	-2.049503
65	1	0	-3.400895	1.077096	0.309391
66	15	0	-4.072224	-1.009947	-0.057049
67	7	0	-2.919621	-1.940990	-0.731054
68	6	0	-2.802813	-2.140117	-2.178718
69	6	0	-2.827843	-3.607709	-2.554195
70	1	0	-3.783450	-4.066149	-2.287491
71	1	0	-2.681026	-3.727617	-3.630075
72	1	0	-2.038742	-4.159818	-2.039104
73	1	0	-3.617791	-1.613600	-2.680072

74	1	0	-1.881282	-1.658387	-2.516118
75	1	0	-2.012296	-1.857790	-0.257911
76	7	0	-5.446941	-1.552921	-0.758409
77	1	0	-5.434830	-2.531919	-1.005158
78	6	0	-6.776538	-0.987561	-0.561614
79	6	0	-7.604087	-1.756310	0.450215
80	1	0	-7.734105	-2.796733	0.141311
81	1	0	-8.595782	-1.309437	0.547872
82	1	0	-7.127024	-1.750333	1.432742
83	1	0	-6.655329	0.048626	-0.241375
84	1	0	-7.287884	-0.962188	-1.528444
85	7	0	-3.800767	-1.211864	1.537321
86	1	0	-3.437225	-2.118048	1.793983
87	6	0	-4.424178	-0.461599	2.623787
88	6	0	-3.496369	-0.350733	3.813682
89	1	0	-3.243414	-1.337101	4.211786
90	1	0	-2.576168	0.161251	3.528814
91	1	0	-3.980737	0.215857	4.611622
92	1	0	-5.367994	-0.935490	2.919699
93	1	0	-4.666672	0.532018	2.246713

	1	2	3
	A	A	A
Frequencies --	16.3438	20.8156	25.7007
Red. masses --	3.4327	4.2232	4.5555
Frc consts --	0.0005	0.0011	0.0018
IR Inten --	0.8789	1.4845	1.1042

Sum of electronic and zero-point Energies= -6163.870906
Sum of electronic and thermal Energies= -6163.754896
Sum of electronic and thermal Enthalpies= -6163.753461
Sum of electronic and thermal Free Energies= -6164.068293