

Ligand-induced decarbonylation in bisphosphine-ligated palladium acetates $[\text{CH}_3\text{CO}_2\text{Pd}((\text{PR}_2)_2\text{CH}_2)]^+$ (R = Me and Ph).

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Supporting Information

Reagents

Bis(diphenylphosphino)methane (dppm), bis(dimethylphosphino)methane (dmpm), and $\text{Pd}(\text{O}_2\text{CCH}_3)_2$ were purchased from Sigma Aldrich and used without further purification. Acetic acid-1- ^{13}C and acetic acid- d_4 were obtained from Isotech and Cambridge Isotopes respectively.

The desired precursor complexes, $[\text{CH}_3\text{CO}_2\text{Pd}((\text{PR}_2)_2\text{CH}_2)]^+$, were typically generated by combining stock solutions of 5 mM palladium acetate in methanol with 5 mM ligand (dppm or dmpm) in methanol at 1:1 ratio followed by 10-fold dilution with methanol resulting in a theoretical complex concentration of 0.5 mM. For experiments utilizing a labeled acetate ligand, the requisite acid was added to this solution in 10-fold molar excess. The solutions were vortexed and allowed to sit for 5 min prior to analysis.

Mass spectrometry experiments

All experiments with the dppm ligand were carried out using a commercially available Finnigan LTQ linear ion trap fitted with the standard factory electrospray ionization source described in detail elsewhere.¹ Solutions prepared as above were introduced into the mass spectrometer at 3.0 $\mu\text{L}/\text{min}$ via ESI. Typical ESI conditions used were: positive ion mode; spray voltage, 4.5 kV; capillary temperature, 300 °C; nitrogen sheath pressure, 10-20 (arbitrary units). The capillary voltage and the tube lens offset were tuned to maximise the desired peak. The injection time was set using the automatic gain control function. For the multistage mass spectrometry (MS^n) experiments, the desired ions produced via ESI were trapped in the LTQ and subjected to CID at a He bath gas pressure of ca. 5×10^{-3} Torr. Low-energy CID was carried out by mass selecting the desired ions with a 0.8-1.0 m/z units window and subjecting them to multiple collisions with the He bath gas using the following typical conditions: normalised collision energy between 16% and 40%, which determines the translational kinetic

energy of the ions; activation (Q), 0.25, which assigns the radio-frequency (RF) used to fragment ions, and activation time of 30 ms that is the time set to excite the ions via CID.

All experiments with the dmpm ligand were carried out using a commercially available Bruker Esquire 3000 ion trap mass spectrometer. Samples prepared as described above were introduced via ESI to the mass spectrometer at a flowrate of 3.0 $\mu\text{L}/\text{min}$. Source parameters were set to 12 PSI, 4.0kV respectively for the nebulizer pressure and the needle voltage and the source temperature was maintained at 250 $^{\circ}\text{C}$. All other tunable instrument parameters were optimized to give the maximum yield of the desired complex ion. Tandem mass spectrometry experiments utilized CID, with the helium bath gas pressure unmodified from normal usage. Isolation of the desired precursor ion was achieved with isolation windows of 0.8-1.3 m/z units. Fragmentation amplitudes ranged from 0.4 to 0.8 V and were optimised for generation of the product ion while ensuring that 15-25 % of the precursor ion remained.

Gas-phase Infrared Spectroscopy Experiments

IRMPD spectroscopy was performed employing a commercial Bruker Esquire 3000+ quadrupole ion trap mass spectrometer into which pulsed IR light is coupled. The detailed layout of this experimental apparatus is described elsewhere.² IR spectroscopy in the 1000–2000 cm^{-1} spectral range was carried out using the free electron laser (FEL) at CLIO.³

Desired mass-selected ions are trapped in a 3D ion trap where ions normally are collisionally thermalised by high-purity helium buffer gas. The ions are then irradiated by the FEL. Upon resonant vibrational excitation, dissociation of the selected decarbonylated $[\text{CH}_3\text{CO}_2^{106}\text{Pd}((\text{PPh}_2)_2\text{CH}_2)]^+$, **1a-CO**, was monitored via the formation of fragment peaks at m/z 305 and 397, which are the same ions formed upon CID (see Figures S1 below). The abundances of these photofragments and their corresponding precursors were recorded as a

function of the IR wavelength in order to derive the IR action spectra, where the IRMPD efficiency is plotted against the photon energy.

Computational Methods

Standard DFT calculations were carried out with Gaussian 09.⁴ Starting geometries for the complexes $[\text{CH}_3\text{CO}_2\text{Pd}((\text{PR}_2)_2\text{CH}_2)]^+$, **1a** and **1b**, were assumed to be the most stable square planar four coordinate complexes, which were allowed to fully optimize. The geometries of species associated with the decarboxylation pathway were chosen based on the previously calculated decarboxylation of the related $[\text{CH}_3\text{CO}_2\text{Pd}(\text{phen})]^+$ system.⁵ For the decarbonylation pathways, several geometries were considered that allowed one of the P atoms of the bisphosphine ligand to interact with one of the O atoms of the acetate ligand. For example, a higher energy pathway that connects **1b** and the key intermediate **7b** via **TS1b-7b** was found but since this is higher in energy (63.5 kcal/mol) than the highest energy decarboxylation **TS12b-13b** (36.7 kcal/mol), this is unlikely to operate under the low energy CID conditions of the ion trap mass spectrometer. The related pathways for **1a** are shown in Figure S5.

Geometries for all structures were optimized with the M06 procedure⁶ with the 6-31G(d) basis set for all C, H, P and O atoms and the SDD basis set for the Pd atom.⁷ Following each geometry optimization, harmonic frequency analysis was carried out to confirm the nature of the stationary point as an equilibrium structure (no imaginary frequencies) or a transition structure (one imaginary frequency) and to determine the zero-point vibrational energies (E_{zpv}), which were used to calculate the reaction energies: $E_{\text{reported}} = E_{\text{electronic}} + E_{\text{zpv}}$. IRC calculations and potential energy surface scans were performed on transition states to confirm that they

connect the stated reactants and products. The calculated vibrational frequencies were scaled using 0.98 scale factor.

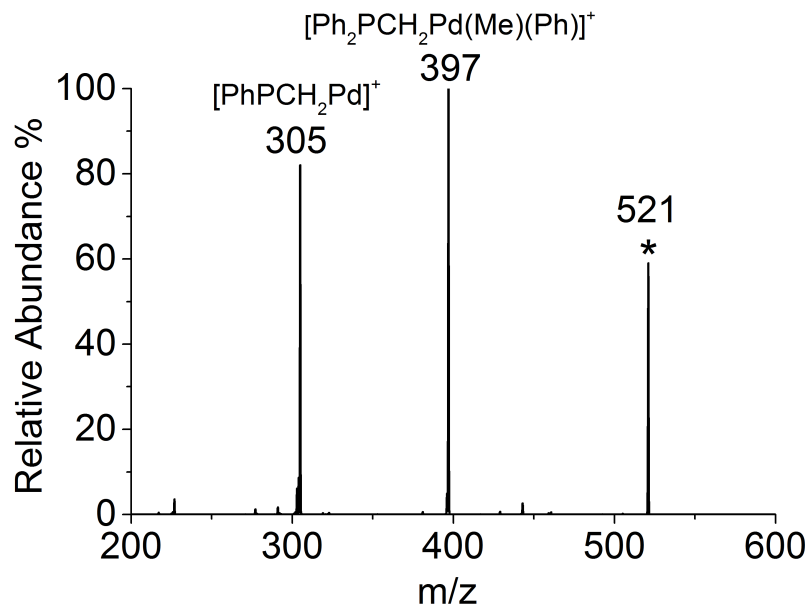


Figure S1: LTQ MS³ CID spectrum of $[\text{CH}_3\text{CO}_2^{106}\text{Pd}((\text{PPh}_2)_2\text{CH}_2) - \text{CO}]^+$, **1b-CO**. The mass-selected precursor is marked with an asterisk.

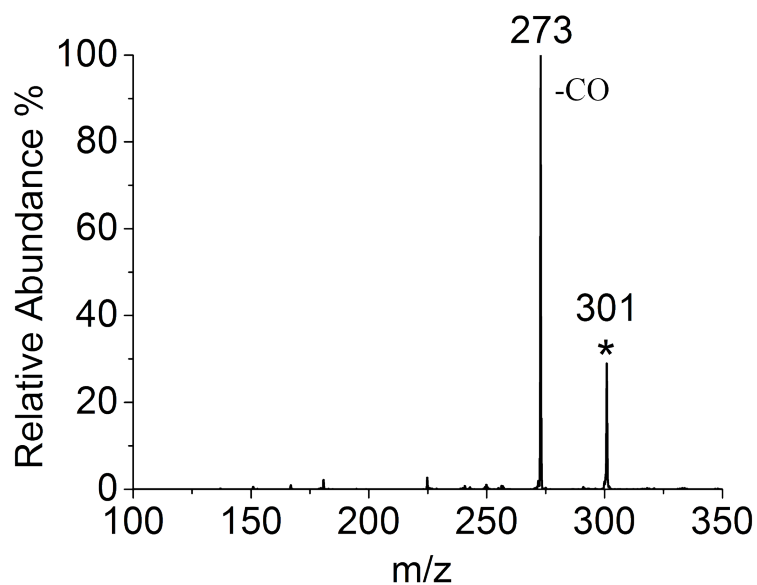


Figure S2: Esquire 3000 MS² CID spectrum of $[\text{CH}_3\text{CO}_2^{106}\text{Pd}((\text{PMe}_2)_2\text{CH}_2)]^+$, **1b**. Product ion is labelled according to the neutral fragment that was lost from the mass-selected precursor, which is marked with an asterisk.

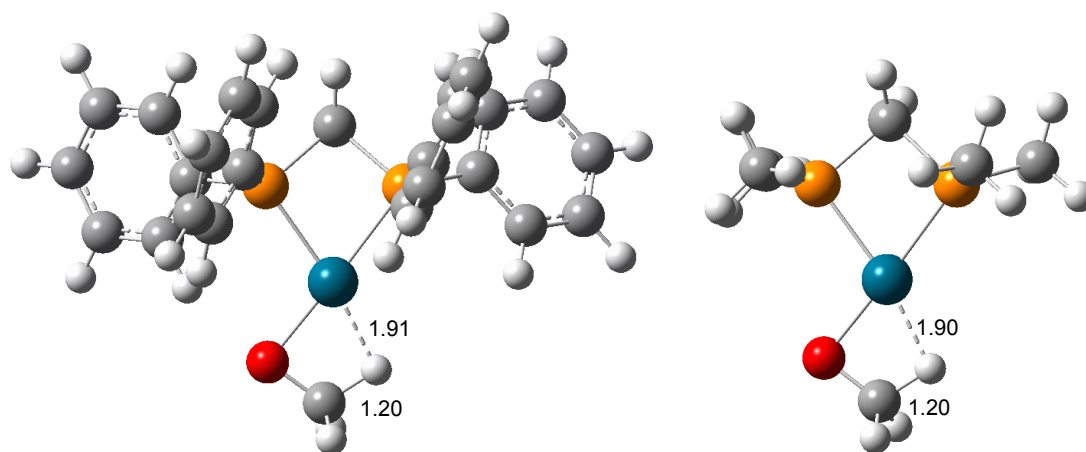


Figure S3: DFT calculated structures of isomers $[\text{CH}_3\text{OPd}((\text{PMe}_2)_2\text{CH}_2)]^+$, **4a** (left) and **4b** (right) at the M06/SDD6-31G(d) level of theory showing agostic interactions.

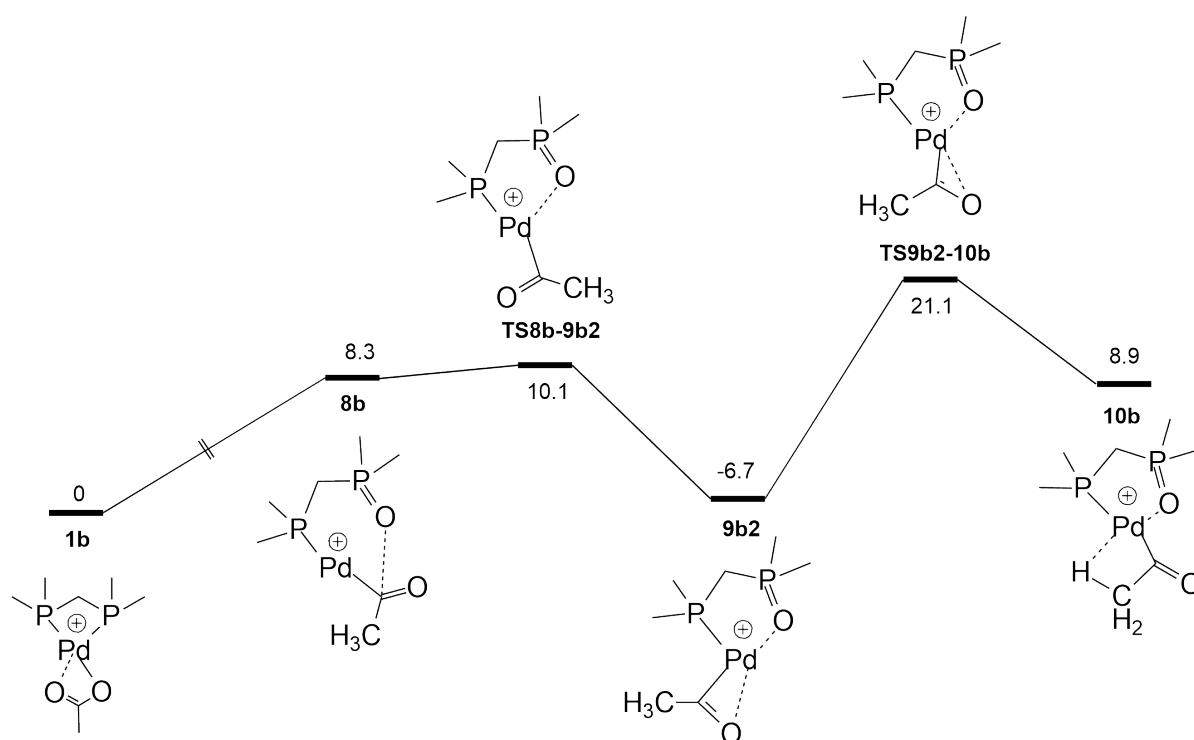


Figure S4: Alternative higher energy pathway to isomerize **8b** to **10b** at the M06/def2-TZVP//M06/SDD6-31G(d) level of theory. Energies are in kcal/mol and are given as ΔE .

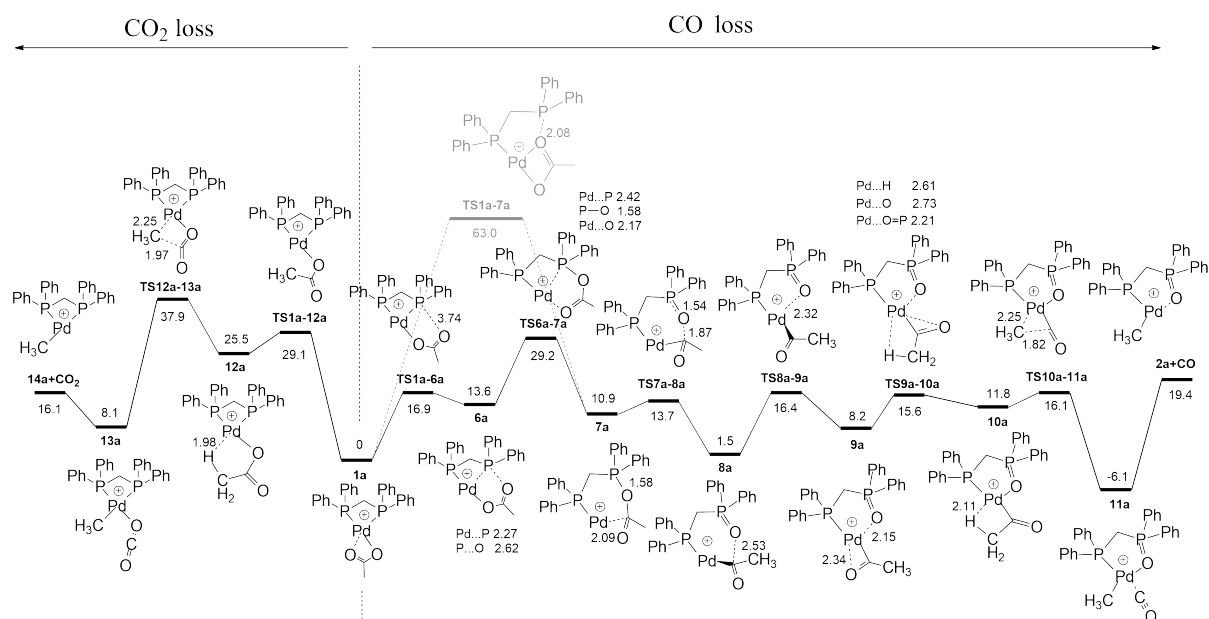


Figure S5: Results of DFT calculations on the competition between decarboxylation and decarbonylation of $[\text{CH}_3\text{CO}_2\text{Pd}((\text{PPh}_2)_2\text{CH}_2)]^+$, **1b** at the M06/def2-TZVP//M06/SDD6-31G(d) level of theory. Energies are in kcal mol⁻¹ and are given as ΔE .

Table S1: IRMPD experimental and theoretical vibrational frequency of three $[\text{CH}_3\text{CO}_2^{106}\text{Pd}(\text{PPh}_2)_2\text{CH}_2 - \text{CO}]^+$ isomers, **2**, **3** and **4**.

Experimental	Theoretical vibrational frequencies			Vibrational Modes
	2	3	4	
1000 (0.09)	980 (0.05)	980 (0.10)	980 (0.10)	In-plane ring deformation
-	1034 (0.05)	-	-	ρCH_2
-	-	1042 (0.60)	-	$\rho\text{CH}_2, \delta\text{CH}$
1060-1080 (0.50)	1075 (0.35)	-	-	δCH
1080-1170 (1.0)	1110-1180 [1134] (1.0)	1170-1250 [1125] (1.0)	1155-1145 [1110] (1.0)	$\nu\text{Pd-C}, \gamma\text{CH}_2, \nu\text{Pd=O},$
1180-1200 (0.4)	1195 (0.05)	-	-	νCH_3
1220 (0.10)	-	-	1210 (0.20)	$\nu\text{O-CH}_3$
1300 (0.10)	1295 (0.05)	1295 (0.05)	1300 (0.10)	δCPC
-	1365 (0.07)	1370 (0.10)	1365 (0.10)	ρCH_2
1400-1440 (0.20)	1442 (0.23)	1445 (0.20)	1420-1500 [1445] (0.40)	Ring deformation, δCH
-	-	1480 (0.05)	-	δCPC
-	-	-	1580 (0.40)	νCH_3
-	1620 (0.10)	1625 (0.10)	1620 (0.10)	In-plane ring deformation

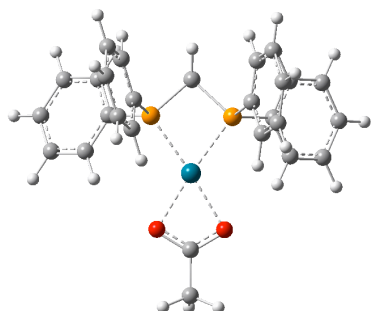
Relative intensities, scaled by a factor of 0.98, are in parenthesis. Frequencies in cm^{-1} . When a frequencies range is reported the most intense frequency is in brackets.

References:

- (1) Feketeová, L.; Khairallah, G. N.; O'Hair, R. A. J. *Eur. J. Mass Spectrom.* **2008**, *14*, 107.
- (2) Bakker, J. M.; Besson, T.; Lemaire, J.; Scuderi, D.; Maitre, P. *J. Phys. Chem. A* **2007**, *111*, 13415.
- (3) Prazeres, R.; Glotin, F.; Insa, C.; Jaroszynski, D. A.; Ortega, J. M., *Eur. Phys. J. D*, **1998**, *3*, 87.
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- (7) (a) Petersson, G. A.; Allaham, M. A. *J. Chem. Phys.* **1991**, *94*, 6081. (b) Clark, T.; Chandrasekhar, J.; Spitznagel, G. W.; Schleyer, P. V. *J. Comput. Chem.* **1983**, *4*, 294.

Structures, Cartesian coordinates and energies (in Hartrees) of all species.

1a



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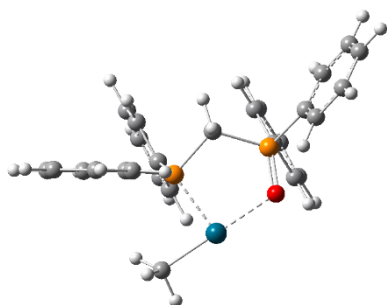
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2a

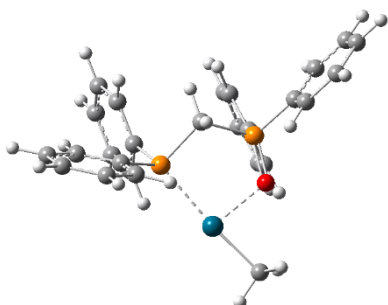


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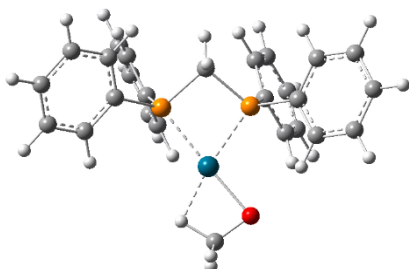
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4a

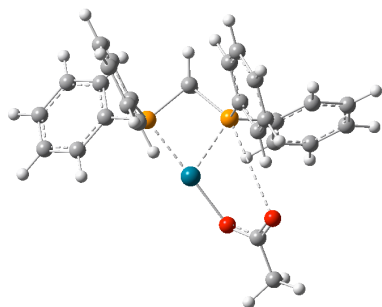


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SPE= -1891.057994

Pd	-0.12136900	-0.90573200	1.45052500
P	1.45026900	-0.25014600	-0.12882800
P	-1.23932100	-0.20420400	-0.40794100
C	0.22154800	-0.37765000	-1.52270600
H	0.21426200	-1.41126700	-1.89687200
H	0.32925200	0.32119900	-2.36169000
O	-1.52933600	-1.48598600	2.75982800
C	-0.51396900	-1.79578500	3.60163400
H	-0.47572200	-1.18666700	4.52067200
H	-0.40904200	-2.87122500	3.82411000
H	0.55131300	-1.55218100	3.11242200
C	-2.64005900	-1.17685600	-0.98041200
C	-3.10786500	-1.00734000	-2.28933500
C	-3.27710400	-2.04899800	-0.09335500
C	-4.21665200	-1.72593800	-2.71239100
H	-2.61429100	-0.30993000	-2.96883500
C	-4.39214100	-2.75836500	-0.53000100
H	-2.90346500	-2.16403600	0.92583700
C	-4.85589000	-2.59874900	-1.83167500
H	-4.58884700	-1.60402700	-3.72732900
H	-4.89830400	-3.43906800	0.15088000
H	-5.72715700	-3.15816900	-2.16642500
C	-1.68881700	1.54086300	-0.29783900
C	-2.42300500	1.93300400	0.82818400
C	-1.31748500	2.48105400	-1.26151400
C	-2.78256800	3.26516500	0.98373100
H	-2.70165700	1.19389600	1.58249600
C	-1.67681200	3.81391700	-1.09444800
H	-0.73671800	2.18988700	-2.13643400
C	-2.40554800	4.20401900	0.02547300
H	-3.35424400	3.57279300	1.85669100
H	-1.38182000	4.54976800	-1.83958000
H	-2.68171700	5.24868400	0.15376800
C	1.89448300	1.50637400	-0.06397400
C	1.45876400	2.28906900	1.00847400
C	2.58559700	2.09683700	-1.12784900
C	1.69591300	3.65947300	1.00819800

H	0.91715200	1.82587900	1.83492500
C	2.82303800	3.46491300	-1.12096300
H	2.94322600	1.48725100	-1.95958500
C	2.37376100	4.24501300	-0.05591200
H	1.35336900	4.26853800	1.84206300
H	3.36221100	3.92647600	-1.94568000
H	2.56143300	5.31687500	-0.05523200
C	2.90684100	-1.23060200	-0.55083700
C	3.22730200	-1.55456700	-1.87268300
C	3.73680500	-1.64732300	0.49558200
C	4.37754800	-2.28731800	-2.14268500
H	2.58429800	-1.23753800	-2.69451800
C	4.88647500	-2.37540100	0.21778500
H	3.48136200	-1.40224400	1.52790900
C	5.20436300	-2.69550200	-1.09970900
H	4.62808100	-2.54155700	-3.17038700
H	5.53191900	-2.70042000	1.03080900
H	6.10140500	-3.27195000	-1.31590600

TS1a-6a



E = -2003.430037

H = -2003.398926

G = -2003.494771

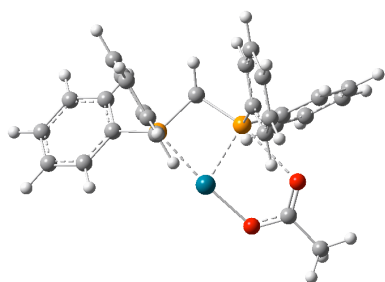
SPE = -2004.420086

Imaginary frequency = -21.35

Pd	0.24597800	-0.94878500	1.12846000
P	0.90812400	0.11549500	-0.75821200
P	-1.63659700	-0.37309300	-0.07863100
C	-0.65674100	-0.24753300	-1.65698000
H	-0.55394200	-1.25460200	-2.08614500
H	-0.98884700	0.45327400	-2.43252500
O	3.19281300	0.05399600	2.20586000
O	1.84372400	-1.73833200	2.03195900
C	2.91493400	-1.10932100	2.45723600
C	3.79819600	-1.98856000	3.30600700
H	4.10920300	-2.86994300	2.73358200
H	4.67746300	-1.43057100	3.63716600
H	3.24063800	-2.35326800	4.17627800
C	-2.34384500	1.26667300	0.21127000
C	-3.30478400	1.77676900	-0.66955700
C	-1.87551900	2.04590900	1.27229500
C	-3.78292200	3.06780300	-0.49129900
H	-3.68599200	1.16318600	-1.48784400

C	-2.35637500	3.33977100	1.44225800
H	-1.12281500	1.64573600	1.95305600
C	-3.30608700	3.84810700	0.56157100
H	-4.53241300	3.46792300	-1.17090500
H	-1.98704500	3.95010600	2.26363900
H	-3.68353000	4.85962700	0.69745900
C	-2.95448500	-1.58184200	-0.32308400
C	-3.51590800	-2.17909500	0.81140700
C	-3.42758100	-1.90853200	-1.59799000
C	-4.55083900	-3.09430400	0.66774700
H	-3.14367000	-1.92690600	1.80552800
C	-4.46361200	-2.82517100	-1.73265400
H	-2.99756900	-1.44742200	-2.48773200
C	-5.02171800	-3.41698300	-0.60257400
H	-4.98624800	-3.56164200	1.54816000
H	-4.83607000	-3.07970800	-2.72261200
H	-5.82883500	-4.13788900	-0.71392200
C	2.36230100	-0.62327400	-1.50598500
C	2.52331600	-2.01380800	-1.45946200
C	3.32228400	0.18902100	-2.11980500
C	3.63475900	-2.59112100	-2.05532800
H	1.79682500	-2.63374700	-0.93161500
C	4.43325800	-0.40238600	-2.70882400
H	3.20508200	1.27161700	-2.13596300
C	4.58734000	-1.78523700	-2.67774200
H	3.76914400	-3.66987400	-2.02002000
H	5.18489000	0.22091000	-3.18783200
H	5.46407000	-2.24042300	-3.13382600
C	1.08331600	1.89123800	-0.56046400
C	1.91893900	2.35892600	0.46452900
C	0.38428500	2.78578800	-1.38089300
C	2.04492300	3.72942000	0.65654900
H	2.44564700	1.64924200	1.10961600
C	0.52432200	4.15194500	-1.17636600
H	-0.27669400	2.43032600	-2.16979700
C	1.34958900	4.62123000	-0.15663600
H	2.68862000	4.10059500	1.45099900
H	-0.01662900	4.85096400	-1.81052400
H	1.45045000	5.69266300	0.00534200

6a



E = -2003.435406

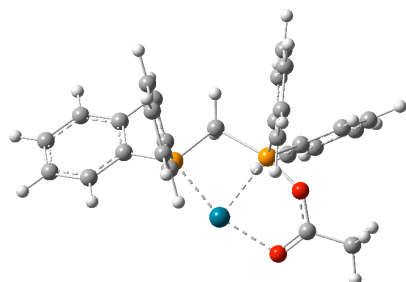
H = -2003.403809

G = -2003.500053
SPE= -2004.425451

Pd	-0.17248000	-0.87153200	-1.43775100
P	-1.07132900	-0.00051000	0.45833100
P	1.59555300	-0.41532700	-0.02344200
C	0.45302100	-0.44553500	1.43059500
H	0.32592000	-1.48699900	1.75748500
H	0.72061200	0.17521000	2.29452500
O	-3.03249100	0.14175600	-1.27752800
O	-1.85185000	-1.33958200	-2.46475600
C	-2.94224800	-0.70964500	-2.17149400
C	-4.12967600	-1.09672000	-3.01055700
H	-4.33916300	-2.16372000	-2.87313100
H	-5.00594800	-0.50772500	-2.73158600
H	-3.90003400	-0.95016400	-4.07167400
C	2.30912700	1.24978300	-0.05088100
C	3.17117400	1.64175400	0.97982700
C	1.94281500	2.15753700	-1.04604200
C	3.65443000	2.94265400	1.01399500
H	3.47146100	0.92880700	1.74987700
C	2.42880700	3.46032800	-1.00434200
H	1.26474300	1.84765300	-1.84228500
C	3.28039800	3.85021700	0.02404900
H	4.32734000	3.25065800	1.81152400
H	2.14133000	4.17016100	-1.77727900
H	3.66192600	4.86889100	0.05395100
C	2.92436400	-1.61045300	0.23825200
C	3.71863600	-1.95062000	-0.86324000
C	3.17984700	-2.17716700	1.49012000
C	4.76438000	-2.85091200	-0.70890800
H	3.52134500	-1.50673200	-1.84055700
C	4.22863800	-3.07868300	1.63627000
H	2.57185800	-1.91294600	2.35585300
C	5.01620800	-3.41579400	0.53925400
H	5.38100100	-3.11716800	-1.56455300
H	4.43020200	-3.51948700	2.61026500
H	5.83136600	-4.12656200	0.65721300
C	-2.43622100	-0.82949800	1.28564900
C	-2.40459700	-2.21953700	1.43280200
C	-3.50478100	-0.08161700	1.78485800
C	-3.43651000	-2.85857900	2.10714700
H	-1.59094900	-2.80616600	1.00227000
C	-4.52407900	-0.73056900	2.47076000
H	-3.54293400	0.99570200	1.63075700
C	-4.49069500	-2.11300700	2.63077900
H	-3.42139100	-3.94037200	2.21991800
H	-5.35471000	-0.15384000	2.87154200
H	-5.29770400	-2.61621300	3.15936000
C	-1.15306400	1.80603900	0.48442600
C	-1.54801900	2.53654100	-0.64185600
C	-0.71716000	2.47792100	1.63484100
C	-1.49257600	3.92441000	-0.61618800
H	-1.90805800	2.01136000	-1.52237900

C	-0.67135600	3.86529700	1.65223300
H	-0.42379000	1.92790300	2.52817200
C	-1.04979100	4.58825000	0.52394500
H	-1.79901300	4.48997200	-1.49369400
H	-0.34165000	4.38265400	2.55063700
H	-1.00471800	5.67539300	0.53750300

TS6a-7a



E = -2003.405141

H = -2003.3748

G = -2003.467282

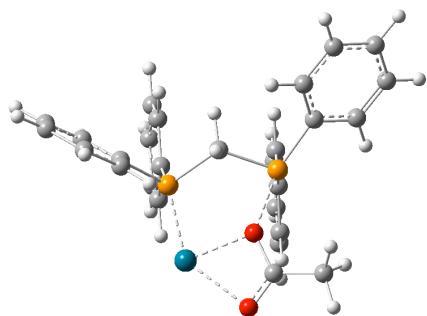
SPE = -2004.400616

imaginary frequency = -58.35

Pd	0.05321000	-0.99388900	1.69051300
P	1.32651300	0.04145400	-0.08271200
P	-1.54832900	-0.53507200	0.14743300
C	-0.21537800	-0.59027300	-1.11710900
H	-0.03359000	-1.64752700	-1.34493700
H	-0.38186300	-0.03877100	-2.05565900
O	2.31465500	0.43130800	1.09081400
O	1.97387900	-1.09116200	2.68916500
C	2.71613800	-0.27901100	2.15216100
C	4.10172500	0.01858300	2.58570200
H	4.79447100	-0.31828800	1.80255300
H	4.24118300	1.09998600	2.69286100
H	4.32573700	-0.49330100	3.52335800
C	-2.19825300	1.16090000	0.17360200
C	-2.71385200	1.71827100	-1.00146300
C	-2.19933700	1.90123500	1.35710200
C	-3.21089100	3.01443700	-0.99255500
H	-2.73500600	1.13292800	-1.92280600
C	-2.70173300	3.19892400	1.36281800
H	-1.80246900	1.45917700	2.27247000
C	-3.20233900	3.75392200	0.18969300
H	-3.61109000	3.44921400	-1.90619000
H	-2.70665200	3.77516000	2.28604700
H	-3.59855700	4.76758300	0.19565200
C	-2.92439500	-1.58021000	-0.39568400
C	-3.99231000	-1.76934800	0.48878400
C	-2.94580800	-2.18317600	-1.65492700
C	-5.07243100	-2.55630800	0.11357600
H	-3.97780300	-1.29493400	1.47186500

C	-4.03281700	-2.96844000	-2.02642900
H	-2.12232000	-2.03928200	-2.35502800
C	-5.09123700	-3.15717000	-1.14355700
H	-5.90068000	-2.70389700	0.80334700
H	-4.05169000	-3.43571100	-3.00892300
H	-5.93616900	-3.77793800	-1.43453800
C	2.59188800	-0.91911300	-0.97770800
C	2.47239200	-2.30334400	-1.14059200
C	3.75358700	-0.26987500	-1.41572500
C	3.49323200	-3.02455300	-1.75030700
H	1.59568400	-2.83431300	-0.76840200
C	4.75827000	-0.99206500	-2.04809600
H	3.86235500	0.80647500	-1.27725800
C	4.62959700	-2.36913900	-2.21334800
H	3.39836600	-4.10246700	-1.86339100
H	5.64732000	-0.47890400	-2.40895100
H	5.42221800	-2.93393100	-2.69965900
C	1.19524700	1.77235900	-0.63508600
C	1.03505600	2.79794600	0.29952500
C	1.18986000	2.07673300	-2.00043900
C	0.85835300	4.11015600	-0.12544100
H	1.03368500	2.57227600	1.36536600
C	1.04423100	3.39314200	-2.41951400
H	1.32935100	1.29036400	-2.74337700
C	0.86950600	4.40924600	-1.48326500
H	0.71640800	4.90098000	0.60838700
H	1.06774700	3.62622600	-3.48203300
H	0.74487000	5.43793600	-1.81530500

TS1a-7a



E = -2003.36226

H = -2003.331048

G = -2003.425495

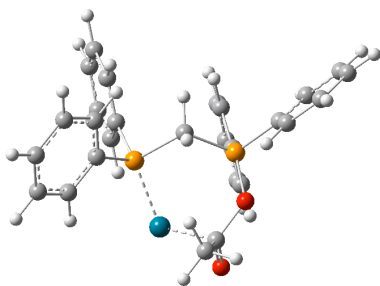
SPE = -2004.346682

Imaginary frequency = -148.86

Pd	-1.45928100	-1.29551000	-1.73462500
P	-1.47103800	0.03741500	0.12281300
P	1.62408300	-0.74620400	0.30979700
C	-0.00569100	-0.53892100	1.16416400
H	-0.29864800	-1.52626300	1.54595600
H	0.11537100	0.12923700	2.03126500
O	0.50368500	-1.88318400	-1.02431700

O	-0.08522300	-2.90631400	-2.85754300
C	0.78567400	-2.75341400	-2.00863600
C	2.10693000	-3.43839400	-2.00238600
H	2.90767500	-2.70277000	-2.15844200
H	2.28798300	-3.91397500	-1.03214500
H	2.14144400	-4.18332200	-2.80101000
C	-1.24998300	1.83774100	0.00311800
C	-1.28647900	2.44462500	-1.25319700
C	-1.03724500	2.62057300	1.14610800
C	-1.12332600	3.82228300	-1.36745600
H	-1.44428300	1.83201100	-2.14201800
C	-0.87462000	3.99446900	1.02859400
H	-1.02209100	2.15953300	2.13524100
C	-0.92082700	4.59523200	-0.22914800
H	-1.15833600	4.29125500	-2.34895100
H	-0.72006000	4.60074000	1.91897200
H	-0.80083600	5.67323300	-0.31901900
C	-2.85912000	-0.24431200	1.26724000
C	-3.70452000	0.78363600	1.69536200
C	-3.14307400	-1.56807700	1.63454000
C	-4.80031500	0.49214700	2.50199400
H	-3.51261700	1.81326000	1.39801200
C	-4.23326600	-1.85195200	2.44410900
H	-2.51962600	-2.38655000	1.26790500
C	-5.06267900	-0.81990600	2.88004600
H	-5.45364600	1.29698600	2.83252700
H	-4.44602600	-2.88110700	2.72588800
H	-5.92249400	-1.04409200	3.50797900
C	2.86318600	-0.64084800	1.62114800
C	4.18495500	-0.29704500	1.28666100
C	2.56731900	-1.05478200	2.92973100
C	5.17007200	-0.29983900	2.26141000
H	4.43131900	-0.00645600	0.26532800
C	3.56082200	-1.05322000	3.89959900
H	1.55995700	-1.37046400	3.19932900
C	4.85971400	-0.67477400	3.56868100
H	6.18700900	-0.01194700	2.00344500
H	3.32217200	-1.35289800	4.91785200
H	5.63726300	-0.68308500	4.32950500
C	1.89783000	0.68378500	-0.77077900
C	2.18821400	1.92474600	-0.18261700
C	1.79244200	0.59240900	-2.16303000
C	2.35297000	3.05037000	-0.97764600
H	2.27141400	2.01359600	0.90073500
C	1.97378500	1.72190300	-2.95478700
H	1.56405700	-0.35661300	-2.64249800
C	2.24879900	2.94970300	-2.36360300
H	2.55991400	4.01192900	-0.51188900
H	1.89941500	1.63723500	-4.03687400
H	2.38782400	3.83298600	-2.98393800

7a

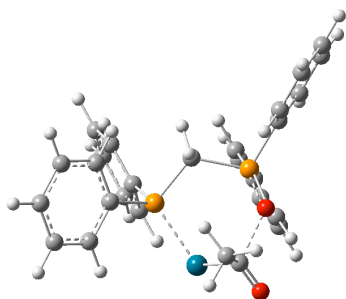


E = -2003.433054
H = -2003.402117
G = -2003.495476
SPE= -2004.429742

Pd	-0.89984800	0.02785700	-2.08420500
P	-1.44493200	-0.00542400	0.12659800
P	1.58545600	-0.58298500	-0.01212900
C	0.05088600	-0.80808000	0.93789000
H	-0.12259200	-1.89335000	1.00010600
H	0.22942100	-0.44733300	1.96217600
O	1.54368000	-1.44254900	-1.34211100
O	0.65902100	-0.88329400	-3.41495600
C	0.47590000	-1.52487900	-2.37372300
C	-0.15635000	-2.88208900	-2.27390600
H	0.60682200	-3.64613100	-2.47888600
H	-0.57108400	-3.06438900	-1.27560900
H	-0.95275700	-2.96772500	-3.01894300
C	-2.80461400	-1.04926000	0.74134200
C	-2.84188900	-1.59494300	2.03041900
C	-3.86061900	-1.29863100	-0.14068900
C	-3.92558400	-2.36713600	2.42954700
H	-2.02411600	-1.42630100	2.73209700
C	-4.94649100	-2.06814500	0.26389300
H	-3.82401500	-0.88863300	-1.15116400
C	-4.97871500	-2.60109500	1.54819000
H	-3.94970300	-2.78904300	3.43230700
H	-5.76437800	-2.25630200	-0.42836200
H	-5.82573800	-3.20668800	1.86401200
C	-1.54888200	1.60701900	0.97483300
C	-1.53198000	2.76039300	0.18720600
C	-1.62997000	1.72573800	2.36688400
C	-1.58893100	4.01824600	0.78030300
H	-1.46172000	2.66979600	-0.89894900
C	-1.67745200	2.98127500	2.95839100
H	-1.67114700	0.83726100	2.99806700
C	-1.65708700	4.12757100	2.16490400
H	-1.58244500	4.91190500	0.15918300
H	-1.74327300	3.06884700	4.04108000
H	-1.70486300	5.10964500	2.63153700
C	1.85605200	1.15101300	-0.33725500
C	1.82728500	2.05281800	0.73523900
C	2.07631400	1.60135500	-1.64426600
C	2.01480000	3.40691700	0.49685200
H	1.65839700	1.70685100	1.75640800
C	2.25356300	2.96253800	-1.86955700

H	2.09907500	0.89607400	-2.47469400
C	2.22074200	3.85948500	-0.80518300
H	1.98995200	4.11003900	1.32653300
H	2.42179300	3.32176700	-2.88232600
H	2.36302900	4.92233400	-0.99060600
C	2.92652600	-1.30400900	0.92483900
C	2.87139300	-2.67674600	1.20446000
C	4.00677000	-0.53501400	1.36657700
C	3.89321200	-3.27079200	1.92930300
H	2.04375700	-3.28562900	0.83807100
C	5.02427600	-1.13996500	2.09604800
H	4.06067700	0.52725700	1.13313500
C	4.96626100	-2.50094000	2.37670600
H	3.85861600	-4.33668300	2.14261400
H	5.86967000	-0.54675700	2.43693500
H	5.76766900	-2.97123000	2.94271600

TS7a-8a



E = -2003.428289

H = -2003.397402

G = -2003.491238

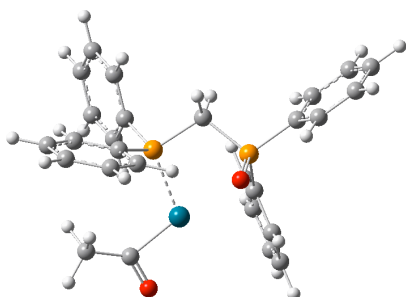
SPE = -2004.425279

Imaginary frequency = -221.00

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P	-1.64739800	-0.62040800	0.12596300
C	-0.17212800	-0.83740900	-0.93708600
H	-0.00875400	-1.92290900	-1.01368500
H	-0.38738900	-0.46727200	-1.94970400
O	-1.47568000	-1.36737600	1.45855400
O	-0.27728500	-0.85562700	3.65311700
C	-0.00750600	-1.41588500	2.62075100
C	0.44401800	-2.80525000	2.33734900
H	-0.35483600	-3.49888300	2.62592100
H	0.68621300	-2.94530900	1.28145400
H	1.33419200	-3.00194700	2.94649200
C	-3.01377800	-1.34094300	-0.78797200
C	-3.00462300	-2.72898700	-0.97703000
C	-4.05828500	-0.56925400	-1.30275600
C	-4.03021300	-3.33577700	-1.68750500
H	-2.20689700	-3.33705700	-0.54806200
C	-5.08177300	-1.18504500	-2.01542500
H	-4.08283500	0.50719100	-1.13881900
C	-5.06579400	-2.56225300	-2.20902500

H	-4.02835100	-4.41414400	-1.83019600
H	-5.89851000	-0.58672700	-2.41309400
H	-5.87077000	-3.04078900	-2.76310700
C	-1.88537700	1.14432200	0.35885300
C	-1.87380200	2.03206900	-0.72363000
C	-2.04558900	1.62590800	1.66358500
C	-2.02052900	3.39495300	-0.49967700
H	-1.74573000	1.66847300	-1.74486200
C	-2.18289000	2.99391400	1.87922700
H	-2.07124900	0.92784100	2.50037300
C	-2.16869100	3.87409200	0.80049300
H	-2.01058100	4.08501800	-1.34091300
H	-2.31057100	3.37174500	2.89144000
H	-2.28134100	4.94274400	0.97284500
C	1.49423600	1.53410400	-1.11623400
C	1.50137300	2.72131100	-0.38156500
C	1.56585800	1.58475200	-2.51252900
C	1.56742100	3.94954300	-1.03247500
H	1.43587800	2.68628300	0.70900000
C	1.62177900	2.81105600	-3.16153300
H	1.58950000	0.66494300	-3.09848800
C	1.62077600	3.99257500	-2.42126300
H	1.57507200	4.87092800	-0.45354200
H	1.67688200	2.84833600	-4.24755000
H	1.67163600	4.95162000	-2.93311700
C	2.70598600	-1.12407100	-0.78266800
C	2.66795600	-1.81496000	-1.99964700
C	3.83235400	-1.23595800	0.03889200
C	3.74634000	-2.60089000	-2.38763000
H	1.79647300	-1.74911400	-2.65195900
C	4.91169800	-2.01866000	-0.35613500
H	3.85882200	-0.70659900	0.99289000
C	4.86765800	-2.70106000	-1.56792900
H	3.71172800	-3.13828900	-3.33313400
H	5.78575900	-2.09954400	0.28652700
H	5.70993500	-3.31799900	-1.87423500

8a



E = -2003.447988

H = -2003.416015

G = -2003.513287

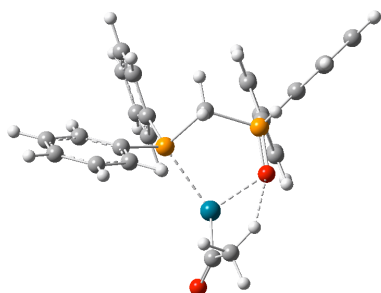
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P 1.05431900 -0.55652000 -0.25477000

P	-1.87161100	-0.57361800	0.55600700
C	-0.59604400	-1.36494100	-0.50242300
H	-0.55626900	-2.42774600	-0.22395500
H	-0.85956300	-1.30822200	-1.56794300
O	-1.59651600	-0.76204300	2.01361100
O	1.75208900	3.21701400	1.68843800
C	2.16440200	2.12180100	1.41287200
C	3.44447700	1.45158600	1.73980100
H	3.23183200	0.52757900	2.29447300
H	3.94310900	1.15471600	0.80788200
H	4.08779100	2.11508200	2.32758100
C	-3.45463300	-1.23575500	0.01740600
C	-4.19181600	-1.96480400	0.95365300
C	-3.94576200	-1.05353400	-1.27967800
C	-5.41466500	-2.51695200	0.58653100
H	-3.79891100	-2.08711200	1.96206800
C	-5.16671200	-1.60710500	-1.63935400
H	-3.38361500	-0.47075700	-2.01181200
C	-5.89821300	-2.34005600	-0.70566000
H	-5.99226800	-3.08485100	1.31275900
H	-5.55395500	-1.46581800	-2.64626200
H	-6.85560400	-2.77212900	-0.99013300
C	-1.81624000	1.20196700	0.10805100
C	-1.49481500	1.71398700	-1.16774000
C	-2.20559000	2.10207400	1.12329600
C	-1.57909200	3.08713500	-1.41791600
H	-1.20895000	1.04477100	-1.98138400
C	-2.28764600	3.46499500	0.86211200
H	-2.43319000	1.70637900	2.11286800
C	-1.98183700	3.95600800	-0.40887800
H	-1.33515200	3.46936400	-2.40686400
H	-2.58927700	4.14844500	1.65267000
H	-2.05062300	5.02309000	-0.60872200
C	2.00330600	-1.60429500	0.87921400
C	1.42979800	-1.95399600	2.10946600
C	3.33034100	-1.94482400	0.59581400
C	2.18971600	-2.65098000	3.04172000
H	0.39864100	-1.67214900	2.33822000
C	4.08077500	-2.63804500	1.53969200
H	3.77984200	-1.67098100	-0.35857100
C	3.51232800	-2.98873800	2.76074400
H	1.74588000	-2.92978700	3.99522300
H	5.11151700	-2.90718600	1.31792900
H	4.10192300	-3.53032500	3.49773300
C	1.86564000	-0.61728200	-1.87549500
C	2.34423200	0.55856800	-2.45947700
C	2.00969100	-1.83802200	-2.54871300
C	2.96418600	0.51650100	-3.70538700
H	2.22198800	1.51037200	-1.93780000
C	2.62885000	-1.87435000	-3.79103300
H	1.64877700	-2.76220200	-2.09469300
C	3.10608300	-0.69805900	-4.36777700
H	3.33615400	1.43374000	-4.15712900
H	2.74267100	-2.82317700	-4.31114800
H	3.59130000	-0.73175700	-5.34108200

TS8a-9a



E = -2003.424961

H = -2003.393464

G = -2003.489498

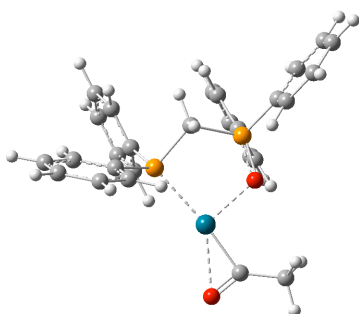
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Imaginary frequency = -85.42

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P	-1.75662700	-0.34419100	-0.16386100
C	-0.20597500	-0.30751400	-1.14310800
H	-0.03630700	-1.33104200	-1.50804400
H	-0.29419100	0.34289500	-2.02390900
O	-1.60017800	-1.31894200	1.00387600
O	1.28476400	-1.99912600	3.92604800
C	0.67530500	-2.27703800	2.94604900
C	0.18073000	-3.53060700	2.31908800
H	-0.73520200	-3.33808500	1.75236800
H	0.96016400	-3.89021500	1.63493100
H	0.02364400	-4.27787000	3.10559200
C	1.45328800	1.95302200	-0.37542500
C	1.46920800	2.83473400	0.70710700
C	1.56540300	2.45450300	-1.67861800
C	1.58665200	4.20484100	0.49258900
H	1.37911500	2.44521000	1.72285000
C	1.68317300	3.82188900	-1.89003800
H	1.57561100	1.77317400	-2.53113200
C	1.69188300	4.69665600	-0.80367500
H	1.59708100	4.88683600	1.34046400
H	1.77577100	4.20919300	-2.90282000
H	1.78641500	5.76772500	-0.97225800
C	2.64095100	-0.69784600	-0.79499100
C	3.80632700	-0.03147900	-1.17780200
C	2.58027400	-2.09320200	-0.89670200
C	4.88758900	-0.75270700	-1.67682700
H	3.87447200	1.05193800	-1.08913800
C	3.65829900	-2.80754000	-1.40221300
H	1.68047600	-2.62776100	-0.57931500
C	4.81454800	-2.13595700	-1.79422100
H	5.79128400	-0.22588400	-1.97650800
H	3.59997600	-3.89079600	-1.48870100
H	5.66101900	-2.69499300	-2.18727400
C	-3.07786600	-0.81163200	-1.28517700
C	-3.01587600	-2.07454400	-1.88779300
C	-4.16098200	0.03294600	-1.54118600
C	-4.02704000	-2.48205900	-2.74608100

H	-2.18550800	-2.74753300	-1.67093500
C	-5.17041900	-0.38144700	-2.40342300
H	-4.22282900	1.00978100	-1.06308500
C	-5.10176500	-1.63369200	-3.00508500
H	-3.98087600	-3.46384700	-3.21232300
H	-6.01511000	0.27454200	-2.60197800
H	-5.89424100	-1.95547800	-3.67771700
C	-1.99425700	1.34299200	0.42529100
C	-1.89959300	2.44220300	-0.43568900
C	-2.19562500	1.54481400	1.79520500
C	-1.99120500	3.73100900	0.07281700
H	-1.74696100	2.29649900	-1.50619000
C	-2.28683700	2.83968800	2.29974900
H	-2.29952300	0.68383700	2.45735100
C	-2.18070200	3.92842900	1.43986700
H	-1.91117700	4.58479900	-0.59707600
H	-2.44997200	2.99648100	3.36406100
H	-2.25209900	4.93954000	1.83603000

9a

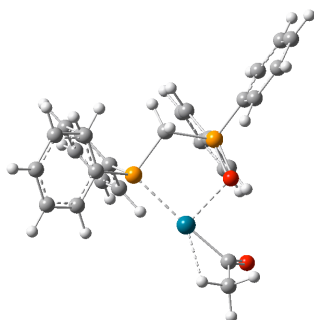


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H = -2003.406523
G = -2003.504132
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P	1.42748000	0.00048800	-0.29313500
P	-1.55013700	-0.38334700	-0.33551500
C	-0.06050600	-0.30598500	-1.38711300
H	0.05176800	-1.29798600	-1.85001400
H	-0.16141400	0.43020700	-2.19581900
O	-1.29885000	-1.38975100	0.80275900
O	1.33689000	-2.02130400	3.78557800
C	0.23861900	-2.15761600	3.32193400
C	-0.99717400	-2.83365800	3.77005900
H	-1.31707400	-3.53614300	2.99184900
H	-0.84162300	-3.34586700	4.72538400
H	-1.79276400	-2.08375500	3.85728800
C	1.59546000	1.81032300	-0.32150900
C	1.58605700	2.49951900	0.89301800
C	1.66808800	2.52820700	-1.52243800
C	1.64170400	3.89018700	0.90964600
H	1.52937000	1.94190100	1.82931800
C	1.72966300	3.91532900	-1.50309000
H	1.68884900	2.00030000	-2.47767000
C	1.71483500	4.59620900	-0.28625500

H	1.63396900	4.42148000	1.85933100
H	1.79467500	4.46874900	-2.43795300
H	1.76486100	5.68325500	-0.27305700
C	2.80374400	-0.70875000	-1.25317100
C	3.88503100	0.04726700	-1.70917400
C	2.79700100	-2.09518500	-1.45151300
C	4.93489400	-0.57685500	-2.37739200
H	3.91477800	1.12267800	-1.53969100
C	3.84190800	-2.71125000	-2.12639800
H	1.97398100	-2.70101000	-1.06392100
C	4.91246500	-1.95021000	-2.59147900
H	5.77617900	0.01695900	-2.72902400
H	3.82828500	-3.78832100	-2.28036400
H	5.73564600	-2.43357600	-3.11358800
C	-2.92233600	-0.90612000	-1.36481400
C	-2.89234100	-2.20312100	-1.89403400
C	-3.99454500	-0.05663300	-1.64950000
C	-3.92717600	-2.63940400	-2.70884200
H	-2.06759100	-2.87491900	-1.65395100
C	-5.02713500	-0.50101700	-2.46811700
H	-4.02850600	0.94739900	-1.22848500
C	-4.99145600	-1.78690800	-2.99729600
H	-3.90761700	-3.64688800	-3.11866900
H	-5.86350000	0.15814000	-2.69001100
H	-5.80125500	-2.13115400	-3.63741600
C	-1.83805700	1.27453900	0.29878700
C	-1.76565600	2.39774300	-0.53292800
C	-2.09242300	1.43028300	1.66422500
C	-1.93546900	3.66722600	0.00291300
H	-1.57022100	2.28634800	-1.60066600
C	-2.26727600	2.70419700	2.19464200
H	-2.14690900	0.54893800	2.30338800
C	-2.18660900	3.81878200	1.36538000
H	-1.87291200	4.54069000	-0.64271200
H	-2.46872100	2.82758400	3.25676700
H	-2.32116200	4.81458800	1.78338000

TS9a-10a



E = -2003.425996

H = -2003.394739

G = -2003.48936

SPE = -2004.422279

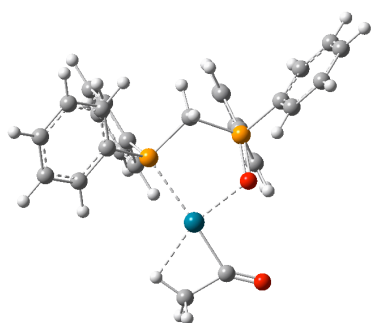
Imaginary frequency = -47.90

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P	-1.55455600	-0.50963800	-0.25681000
C	-0.01097100	-0.73000000	-1.21913100
H	0.08351600	-1.81290100	-1.39253600
H	-0.07846400	-0.23357900	-2.19776700
O	-1.39310600	-1.15531500	1.12615800
O	-1.06365300	-0.04483700	4.15286600
C	-0.28196600	-0.83925500	3.76039900
C	0.36302300	-2.05039000	4.37686500
H	-0.37943800	-2.85736800	4.35177200
H	1.25618600	-2.38804400	3.83459100
H	0.62732900	-1.82100200	5.41582900
C	1.66338900	1.57811000	-0.65899500
C	1.41003100	2.53687700	0.32446400
C	2.03321000	1.98735600	-1.94450400
C	1.50614500	3.89188700	0.02524400
H	1.12052600	2.22079100	1.32925500
C	2.13156500	3.34100100	-2.24091700
H	2.26319800	1.24611300	-2.71155800
C	1.86615200	4.29250900	-1.25695100
H	1.30490200	4.63393600	0.79555200
H	2.42616000	3.65684400	-3.23983900
H	1.94986800	5.35191400	-1.49192100
C	2.86947100	-1.05721500	-0.98332300
C	4.00257800	-1.25055200	-0.18610400
C	2.87411300	-1.50837400	-2.30716900
C	5.12918700	-1.87491600	-0.70809900
H	4.00025300	-0.90806700	0.85020600
C	4.00000400	-2.14034100	-2.82372000
H	1.99964400	-1.37207800	-2.94375800
C	5.12646300	-2.32117900	-2.02642600
H	6.00783500	-2.02030300	-0.08322500
H	3.99799200	-2.49190000	-3.85345900
H	6.00564000	-2.81584600	-2.43417400
C	-2.86068700	-1.31417000	-1.18847500
C	-2.84432200	-2.71311500	-1.26382500
C	-3.87354000	-0.58913100	-1.82081400
C	-3.83308800	-3.37720800	-1.97566200
H	-2.07005700	-3.28048800	-0.74627700
C	-4.85995800	-1.26205700	-2.53363000
H	-3.90114700	0.49745400	-1.74904600
C	-4.83809200	-2.65073500	-2.61170700
H	-3.82578500	-4.46360300	-2.03091500
H	-5.65190200	-0.70016800	-3.02402000
H	-5.61436300	-3.17386000	-3.16657200
C	-1.86228800	1.25707700	-0.13245800
C	-1.70935500	2.11894500	-1.22498800
C	-2.23299900	1.76393900	1.11692700
C	-1.91969000	3.48172100	-1.06270100
H	-1.41131300	1.73187900	-2.20067600
C	-2.44350300	3.13057800	1.27124400
H	-2.34514800	1.08610800	1.96275400
C	-2.28724500	3.98504000	0.18445200
H	-1.79438400	4.15459900	-1.90845800
H	-2.73476200	3.52690400	2.24169300
H	-2.45254300	5.05377500	0.30742500

10a



E = -2003.429563

H = -2003.397875

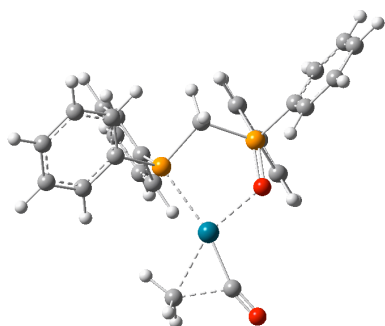
G = -2003.494147

SPE= -2004.428261

Pd	0.63294100	-0.57679000	2.04893800
P	1.40056200	-0.22686600	-0.29491000
P	-1.59606300	-0.49089400	-0.16471800
C	-0.12298800	-0.79026000	-1.20616400
H	-0.06380600	-1.88271500	-1.32803900
H	-0.22887000	-0.33853600	-2.20253600
O	-1.31827000	-1.02656500	1.24714400
O	-0.91875800	-0.70543300	4.47405000
C	0.10015500	-0.65878000	3.89189900
C	1.57059200	-0.54836300	4.25498400
H	1.85465600	-1.44853500	4.80934800
H	2.26945100	-0.47640200	3.38128500
H	1.72257100	0.35427100	4.85469000
C	1.59500300	1.50682200	-0.82651600
C	1.37305700	2.52910500	0.09867000
C	1.91356500	1.82869800	-2.14970300
C	1.44502300	3.86065800	-0.29903400
H	1.12064600	2.27960300	1.13179100
C	1.99021400	3.15848200	-2.54360000
H	2.11717400	1.03728900	-2.87270000
C	1.75226900	4.17395300	-1.61895800
H	1.26491200	4.65292300	0.42530200
H	2.24366400	3.40561300	-3.57271600
H	1.81504900	5.21524500	-1.92920100
C	2.76048700	-1.14782400	-1.07761800
C	3.94509300	-1.27613400	-0.34480100
C	2.68479200	-1.69208400	-2.36363100
C	5.04251900	-1.92820700	-0.89405000
H	4.00794200	-0.85930800	0.66221200
C	3.78167000	-2.35239200	-2.90675000
H	1.77055000	-1.60622900	-2.95112100
C	4.95926300	-2.46837800	-2.17419500
H	5.96210400	-2.02129900	-0.32007100
H	3.71578900	-2.77699600	-3.90645400
H	5.81563000	-2.98507500	-2.60257700
C	-2.96297800	-1.37160500	-0.91933600
C	-2.98735200	-2.76528300	-0.78278200
C	-3.96418700	-0.71609400	-1.64036700
C	-4.00585600	-3.49673100	-1.37682600
H	-2.22118600	-3.26902000	-0.19297700

C	-4.97988400	-1.45715700	-2.23409100
H	-3.96028800	0.36994800	-1.72698300
C	-4.99831700	-2.84231500	-2.10438400
H	-4.03234500	-4.57872400	-1.26759100
H	-5.76424400	-0.94992600	-2.79165900
H	-5.79659000	-3.41771700	-2.56889100
C	-1.90537600	1.27909600	-0.14801900
C	-1.82820300	2.06222400	-1.30488100
C	-2.19913700	1.87142000	1.08434700
C	-2.03841900	3.43268600	-1.22570400
H	-1.59460100	1.60965400	-2.26987300
C	-2.41195500	3.24451900	1.15530500
H	-2.25340700	1.25006800	1.97905100
C	-2.33150600	4.02118700	0.00338700
H	-1.97215200	4.04420400	-2.12320100
H	-2.64564200	3.70791200	2.11170000
H	-2.49882500	5.09497600	0.06184500

TS10a-11a



E = -2003.423433

H = -2003.391864

G = -2003.488499

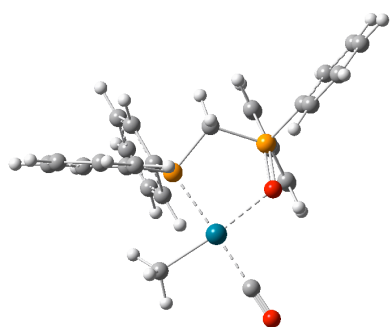
SPE = -2004.421511

Imaginary frequency = -315.41

Pd	0.79137900	-0.96645500	1.83485100
P	1.28629200	-0.11470900	-0.43293500
P	-1.65615100	-0.46725700	-0.13178200
C	-0.28192200	-0.54010400	-1.33274500
H	-0.22849700	-1.59526100	-1.64131700
H	-0.45381600	0.07463000	-2.22672900
O	-1.21465300	-1.23590300	1.12151900
O	0.47119800	-2.01468400	4.61488300
C	0.81636300	-1.57365200	3.60304800
C	2.53002500	-1.06699100	3.26484400
H	3.01174400	-2.03334500	3.42994200
H	3.00974400	-0.56949900	2.41286000
H	2.61645100	-0.41044400	4.13351700
C	1.42728600	1.69083100	-0.61419100
C	1.25948800	2.50497800	0.50858100
C	1.64752600	2.27056500	-1.86813800
C	1.28805400	3.88990400	0.37630500
H	1.09078500	2.05143900	1.48759900
C	1.67644300	3.65310700	-1.99664800
H	1.80874300	1.63794900	-2.74272300

C	1.49267900	4.46125300	-0.87530900
H	1.15257900	4.52170600	1.25191500
H	1.85021700	4.10439500	-2.97159900
H	1.52007500	5.54424200	-0.97943300
C	2.61721300	-0.81412700	-1.45617600
C	3.91024900	-0.78323000	-0.92045300
C	2.41303800	-1.35526800	-2.72780100
C	4.98202700	-1.28646900	-1.64595600
H	4.08090600	-0.35102700	0.06755400
C	3.48847200	-1.86600400	-3.44852100
H	1.41793000	-1.37981100	-3.17101900
C	4.76994300	-1.83347400	-2.90929300
H	5.98441400	-1.25600300	-1.22408600
H	3.32299300	-2.28885000	-4.43738400
H	5.60805500	-2.23469000	-3.47509700
C	-3.08074700	-1.25033200	-0.88602600
C	-3.09184100	-2.64898900	-0.95731800
C	-4.13745300	-0.50769300	-1.41944500
C	-4.15536200	-3.29723100	-1.56938800
H	-2.27936000	-3.22364600	-0.51243900
C	-5.19779200	-1.16573500	-2.03235700
H	-4.14141400	0.57942900	-1.34703900
C	-5.20441700	-2.55501300	-2.10861300
H	-4.17203800	-4.38365100	-1.62055100
H	-6.02456200	-0.59199800	-2.44519300
H	-6.03732300	-3.06599000	-2.58752000
C	-1.99583400	1.26053600	0.21932900
C	-1.96687800	2.24287300	-0.77732600
C	-2.29088100	1.60987500	1.54108500
C	-2.22632600	3.56709700	-0.44963100
H	-1.73053500	1.98398700	-1.81051700
C	-2.55257800	2.93799400	1.86149400
H	-2.31080700	0.83971200	2.31170500
C	-2.51952200	3.91253200	0.86840200
H	-2.19461800	4.33258800	-1.22216100
H	-2.78700900	3.21110700	2.88826300
H	-2.72609300	4.95075200	1.12133500

11a

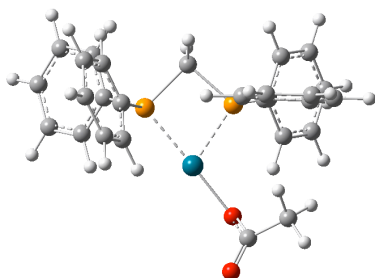


E = -2003.45823
H = -2003.426098
G = -2003.522763
SPE = -2004.456843

Pd 0.86454400 -0.77897100 1.78844100

P	1.22655900	-0.11274500	-0.41373800
P	-1.70685200	-0.47243400	-0.06024100
C	-0.34168900	-0.60600900	-1.27576800
H	-0.26844600	-1.66767700	-1.55400200
H	-0.51154500	-0.02675300	-2.19284400
O	-1.23784900	-1.15605100	1.22483100
O	0.49593300	-1.74098000	4.74362600
C	0.63556500	-1.38746800	3.67345800
C	2.87950200	-0.48366000	2.11340500
H	3.33821500	-1.47049500	1.97257900
H	3.31329900	0.23005600	1.40452000
H	3.03828800	-0.12556700	3.13531900
C	1.39827000	1.66734400	-0.70058900
C	1.41958000	2.54554500	0.38552200
C	1.46926900	2.17104700	-2.00640800
C	1.51473100	3.91672000	0.16816700
H	1.35540300	2.15346900	1.40143600
C	1.56485800	3.53990500	-2.21739600
H	1.46377900	1.49176300	-2.86049600
C	1.58824400	4.41149300	-1.12950700
H	1.53294000	4.59822100	1.01611100
H	1.62731400	3.92957000	-3.23137700
H	1.66786900	5.48380800	-1.29717900
C	2.56989500	-0.97076200	-1.27800600
C	2.51779200	-2.36818500	-1.36002500
C	3.69159000	-0.28894600	-1.75596000
C	3.56031800	-3.06929700	-1.95002500
H	1.66750700	-2.91516000	-0.94736200
C	4.73610800	-0.99910000	-2.34054500
H	3.75397600	0.79551900	-1.67570200
C	4.66888100	-2.38385300	-2.44381500
H	3.51270300	-4.15399000	-2.01836000
H	5.60647900	-0.46440100	-2.71492900
H	5.48636200	-2.93456100	-2.90434800
C	-3.14118200	-1.28584700	-0.76398700
C	-3.12681900	-2.68534700	-0.82140200
C	-4.23958800	-0.57269000	-1.25106600
C	-4.20363900	-3.36284800	-1.37536500
H	-2.28349300	-3.24010200	-0.40925600
C	-5.31410900	-1.25943000	-1.80523800
H	-4.26523200	0.51441900	-1.18658300
C	-5.29390500	-2.64898500	-1.86968400
H	-4.19861400	-4.44982100	-1.41597800
H	-6.17311600	-0.70736700	-2.18019800
H	-6.13755700	-3.18237000	-2.30303800
C	-2.01623300	1.28255500	0.17534200
C	-2.11182800	2.16995800	-0.90307300
C	-2.13080800	1.75638000	1.48536000
C	-2.31788300	3.52287000	-0.66904500
H	-2.02761700	1.80798300	-1.92933000
C	-2.33169200	3.11373100	1.71343200
H	-2.05767400	1.05749100	2.31809900
C	-2.42320100	3.99314900	0.63901100
H	-2.39542200	4.21361100	-1.50602900
H	-2.42315800	3.48504500	2.73204300
H	-2.58371600	5.05428400	0.81988900

TS1a-12a



E = -2003.410544

H = -2003.379263

G = -2003.476004

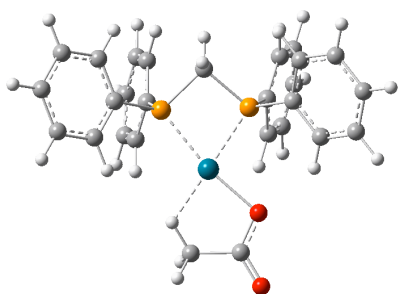
SPE= -2004.400721

Imaginary frequency = -60.05

P	-0.98628400	-0.33067200	-0.70667600
P	1.64696800	-0.10862100	-0.14460400
C	0.59420000	-0.44675600	-1.64957700
H	0.69588300	0.26971100	-2.47409700
H	0.73719600	-1.47143200	-2.01717300
Pd	-0.09916200	-0.19739800	1.34704600
O	-1.56542300	-0.33075900	2.67245100
C	-2.16277500	0.78348200	3.11483100
O	-1.84042900	1.31834900	4.15017700
C	-3.26959500	1.30648100	2.22856200
H	-3.90457100	1.99580100	2.79197300
H	-2.83436200	1.85897400	1.38153200
H	-3.87446600	0.48821300	1.81801600
C	2.95480000	-1.35095900	-0.08260100
C	3.51226800	-1.88798400	-1.24790200
C	3.42894400	-1.74583500	1.17295200
C	4.54566600	-2.81124000	-1.15278600
H	3.14521100	-1.58996100	-2.23093300
C	4.46287300	-2.67046000	1.25900100
H	2.98797000	-1.33429500	2.08170400
C	5.01831900	-3.20121400	0.09844600
H	4.98178300	-3.23027700	-2.05704800
H	4.83001900	-2.98268000	2.23403300
H	5.82368600	-3.92923200	0.16895000
C	2.35414700	1.54413700	-0.36216300
C	2.11231900	2.52532500	0.60507400
C	3.13979900	1.84013300	-1.48246200
C	2.65126000	3.79848300	0.44809800
H	1.50126900	2.29571300	1.47931000
C	3.67390200	3.11264500	-1.63210700
H	3.34302900	1.07544000	-2.23363900
C	3.42878500	4.08990400	-0.66768800
H	2.46608700	4.56040400	1.20208100
H	4.28592300	3.34507500	-2.50098200
H	3.85231900	5.08492100	-0.78826900
C	-1.91118600	1.12344700	-1.21450100
C	-1.25392200	2.35693700	-1.32725500
C	-3.29275600	1.03402900	-1.41704100

C	-1.98126000	3.49178900	-1.65369500
H	-0.17921400	2.43651000	-1.15167900
C	-4.00965600	2.17862400	-1.74625600
H	-3.80458200	0.07749400	-1.31630300
C	-3.35750500	3.40277600	-1.86042600
H	-1.47631200	4.45087200	-1.74459300
H	-5.08272900	2.11282300	-1.91063100
H	-3.92513900	4.29620000	-2.11181300
C	-1.97575500	-1.81762200	-0.89087100
C	-2.62682800	-2.35788100	0.22424400
C	-2.12555100	-2.38940100	-2.16166600
C	-3.42633000	-3.48403100	0.05749900
H	-2.50252600	-1.90013600	1.20881400
C	-2.92583000	-3.51377000	-2.31020100
H	-1.63182200	-1.95424300	-3.03196000
C	-3.57032400	-4.06036700	-1.20102100
H	-3.93140400	-3.91670700	0.91815800
H	-3.04785000	-3.96585100	-3.29209800
H	-4.19100700	-4.94576400	-1.32156600

12a

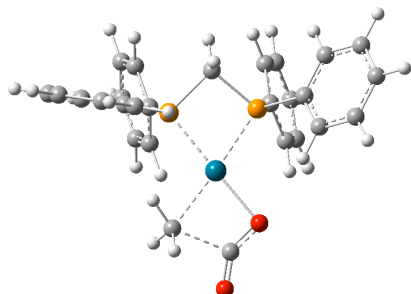


E = -2003.416742
H = -2003.384894
G = -2003.483055
SPE = -2004.406529

Pd	0.15513200	-0.83035100	1.13146400
C	-0.09361000	-1.63894400	3.61165000
H	-0.35548900	-2.55609400	4.15144500
H	-0.73743100	-1.69015200	2.67869600
H	-0.44289600	-0.78021400	4.19754400
P	1.16837300	0.02194500	-0.70409700
P	-1.49007100	-0.22129600	-0.38020900
C	-0.30354100	-0.09796400	-1.80652200
H	-0.29033900	-1.07364000	-2.31242400
H	-0.44676200	0.70310000	-2.54115100
O	1.82350100	-1.13686000	2.24451300
C	1.42204500	-1.55696400	3.42511900
O	2.15484200	-1.83525300	4.34111800
C	-2.08256800	1.45396200	-0.03463200
C	-2.25849300	2.41200400	-1.03675500
C	-2.34961800	1.78235800	1.29959700
C	-2.68247300	3.69210800	-0.70106600
H	-2.06265200	2.17182100	-2.08186600
C	-2.78590100	3.05984000	1.62812700

H	-2.20831300	1.03481800	2.08313600
C	-2.94382700	4.01515000	0.62821800
H	-2.81297800	4.44042000	-1.47991800
H	-2.99470800	3.31222000	2.66544900
H	-3.27366200	5.01947900	0.88560800
C	-2.84799600	-1.31237500	-0.85275900
C	-3.29349300	-2.27113500	0.06054700
C	-3.46725300	-1.18300100	-2.10113600
C	-4.36025300	-3.09841200	-0.27283600
H	-2.80354700	-2.37445800	1.02942600
C	-4.52838900	-2.01609200	-2.42865600
H	-3.12440200	-0.43337400	-2.81597600
C	-4.97308100	-2.97081400	-1.51510500
H	-4.70962700	-3.84604800	0.43574800
H	-5.01166000	-1.92131800	-3.39868500
H	-5.80506200	-3.62092900	-1.77736500
C	1.54989600	1.76885200	-0.47072600
C	1.63773200	2.30448400	0.81645900
C	1.76177200	2.57594900	-1.59550700
C	1.91796000	3.65735600	0.97534500
H	1.49171600	1.66306100	1.68621200
C	2.04442900	3.92416800	-1.42536100
H	1.71294100	2.15347800	-2.60084200
C	2.11719100	4.46262600	-0.14136700
H	1.98976200	4.08082600	1.97467400
H	2.21292700	4.55675000	-2.29413600
H	2.33818300	5.52023800	-0.01243900
C	2.55855800	-0.89650600	-1.36983800
C	2.68493500	-1.09559900	-2.74985700
C	3.53481200	-1.36104300	-0.47929000
C	3.80232400	-1.75862500	-3.24005900
H	1.92376600	-0.73053200	-3.44059300
C	4.64475600	-2.02552000	-0.98683500
H	3.41111200	-1.22265800	0.59589300
C	4.77691700	-2.22281100	-2.35902300
H	3.91243600	-1.91611700	-4.31074800
H	5.40494700	-2.39838400	-0.30417200
H	5.64742000	-2.74726000	-2.74770400

TS12a-13a



E = -2003.396306

H = -2003.364907

G = -2003.461404

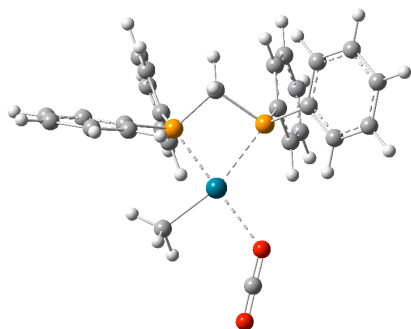
SPE = -2004.386632

Imaginary frequency = -427.88

P	-1.34413800	-0.07731100	-0.53206300
P	1.35673500	-0.09886700	-0.49662600
C	0.02476700	-0.11873400	-1.78384000
H	0.06508600	0.65409900	-2.56095600
H	0.00555900	-1.10835500	-2.26181500
Pd	-0.00022300	-0.86015600	1.18696500
O	-1.26765300	-1.43604400	2.73416000
C	-0.37135100	-1.43726800	3.59401500
O	-0.17717300	-1.40542100	4.75701300
C	1.40290800	-1.62886700	2.76492700
H	1.94493800	-0.90191300	3.37485700
H	1.40555800	-2.61361100	3.24597700
H	1.97806700	-1.80649100	1.83518700
C	2.75163500	-1.11738800	-1.02485100
C	2.51838400	-2.47723500	-1.27116700
C	4.04246900	-0.59344200	-1.13254700
C	3.56921800	-3.29929700	-1.65182800
H	1.51686800	-2.89693000	-1.15363000
C	5.09053100	-1.42736500	-1.50953900
H	4.23103300	0.45883600	-0.92419100
C	4.85444300	-2.77283800	-1.77149000
H	3.38921800	-4.35420200	-1.84713900
H	6.09582800	-1.02121700	-1.59768200
H	5.67891400	-3.41972700	-2.06373000
C	1.86186600	1.62271400	-0.30160600
C	1.84118600	2.21429100	0.96480300
C	2.23186100	2.37547400	-1.42367800
C	2.18548900	3.55460700	1.10645900
H	1.54538600	1.62834600	1.83648500
C	2.57934800	3.71128900	-1.27377500
H	2.26075200	1.91545600	-2.41301900
C	2.55235500	4.29925500	-0.00978600
H	2.16697600	4.01671400	2.09092300
H	2.87050800	4.29698500	-2.14313800
H	2.82041300	5.34766800	0.10360000
C	-1.83425200	1.64631600	-0.29861700
C	-1.75267900	2.60132300	-1.31609000
C	-2.30507100	2.00987300	0.96908400
C	-2.13511100	3.91346100	-1.06236200
H	-1.38752000	2.33427700	-2.30819200
C	-2.68612100	3.32304200	1.21433000
H	-2.36813400	1.26338700	1.76290300
C	-2.59681900	4.27363400	0.20072000
H	-2.06934300	4.65815900	-1.85284300
H	-3.04978500	3.60602900	2.19973400
H	-2.88929000	5.30322900	0.39645300
C	-2.73620300	-1.06480500	-1.11344200
C	-3.11869200	-2.19959400	-0.39350000
C	-3.42074800	-0.69175400	-2.27624400
C	-4.18727300	-2.96751200	-0.84672300
H	-2.58947100	-2.47161800	0.52036200
C	-4.48241800	-1.46632700	-2.72115500
H	-3.12998300	0.20538600	-2.82522100
C	-4.86280600	-2.60211900	-2.00636200
H	-4.49366000	-3.84966600	-0.28888400
H	-5.02034200	-1.18391100	-3.62360900

H -5.69915700 -3.20378400 -2.35628800

13a

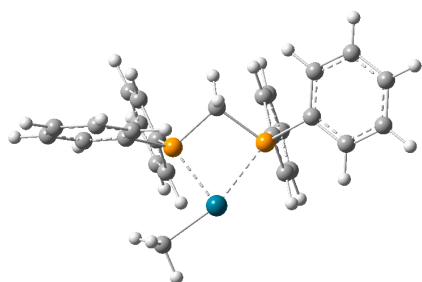


E = -2003.441064
H = -2003.408074
G = -2003.50986
SPE= -2004.434261

Pd	-0.14505900	-1.13800300	1.08567400
C	-1.86351700	-1.74063500	2.04278300
H	-1.96916400	-2.81075900	1.81121300
H	-2.78933600	-1.22367400	1.76685400
H	-1.66915100	-1.58322300	3.11443900
P	1.45111100	-0.02843800	-0.40537200
P	-1.34419800	-0.02912100	-0.45395500
C	0.05819800	0.13092500	-1.64599900
H	0.08296000	-0.76347900	-2.28448200
H	0.02706600	1.02415700	-2.28416900
O	0.50065000	-4.02418800	4.13784300
C	0.80452200	-3.20236800	3.38484500
O	1.12574500	-2.36807400	2.62298600
C	1.76204600	1.67948200	0.14791300
C	2.01567700	1.87773000	1.50902900
C	1.72768500	2.78095900	-0.71212400
C	2.23168400	3.15946800	2.00344500
H	2.03524200	1.01948700	2.18357900
C	1.93639900	4.06161800	-0.21552300
H	1.53303100	2.64803300	-1.77668000
C	2.18882900	4.25081100	1.14136200
H	2.43133300	3.30680300	3.06301300
H	1.90560500	4.91581800	-0.88891400
H	2.35186800	5.25478000	1.52824900
C	2.89474900	-0.61819200	-1.33387600
C	3.26352400	-0.07586200	-2.56999900
C	3.65563900	-1.64540500	-0.76937700
C	4.38540300	-0.55913100	-3.22993000
H	2.67804000	0.72618600	-3.02109700
C	4.78217100	-2.12253800	-1.43182600
H	3.36022600	-2.07053000	0.19128500
C	5.14468800	-1.57981400	-2.65987900
H	4.67230300	-0.13863300	-4.19162800
H	5.37430500	-2.92130200	-0.99021400
H	6.02401200	-1.95427100	-3.18006100
C	-1.80055900	1.65269600	0.02021200
C	-2.18577000	2.56843800	-0.96833400

C	-1.69039800	2.06352800	1.35047700
C	-2.45500800	3.88508100	-0.62083300
H	-2.27843600	2.25118700	-2.00840900
C	-1.95934400	3.38505700	1.69100900
H	-1.38538100	1.34732200	2.11460800
C	-2.33808000	4.29222200	0.70727700
H	-2.75733700	4.59681500	-1.38616500
H	-1.86875300	3.70617200	2.72638800
H	-2.54720700	5.32609500	0.97482600
C	-2.74941600	-0.84277000	-1.24656100
C	-4.03035100	-0.28548700	-1.21035100
C	-2.54589600	-2.09470100	-1.84068900
C	-5.09383800	-0.96612000	-1.79527300
H	-4.19853200	0.67900500	-0.73257700
C	-3.61086200	-2.76411900	-2.42617200
H	-1.55605500	-2.55520500	-1.83606400
C	-4.88461400	-2.19793800	-2.40563600
H	-6.09009700	-0.52983900	-1.77081800
H	-3.45117100	-3.73369000	-2.89315500
H	-5.71886400	-2.72526800	-2.86355900

14a

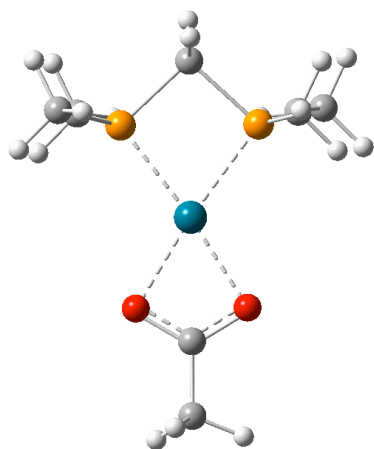


E = -1814.937328
H = -1814.908684
G = -1814.996611
SPE= -1815.837157

Pd	-0.26688100	-0.77020300	1.83885600
C	-2.07616800	-0.81133700	2.78451000
H	-2.50455400	-1.81111700	2.63826100
H	-2.80319500	-0.04699900	2.48613700
H	-1.77373800	-0.65106400	3.83171700
P	1.50578200	-0.48234700	0.14841800
P	-1.30024100	-0.28553200	-0.09648900
C	0.15758400	-0.76011100	-1.12291100
H	0.11843600	-1.84138100	-1.31618600
H	0.22719900	-0.22876100	-2.08176900
C	1.91327200	1.28982200	-0.00198700
C	2.22263800	1.97802300	1.17550800
C	1.88891600	1.98216300	-1.21585800
C	2.50184000	3.33989500	1.14129100
H	2.23708300	1.44287800	2.12684600
C	2.15157300	3.34608100	-1.24621000
H	1.66089900	1.46425200	-2.14788900
C	2.45813300	4.02484100	-0.06892400

H	2.74851800	3.86736300	2.06062500
H	2.12087500	3.88192800	-2.19299800
H	2.66690500	5.09248300	-0.09715400
C	2.93770300	-1.43018500	-0.44240900
C	3.19384700	-1.62164300	-1.80393300
C	3.81793700	-1.94746700	0.51180700
C	4.32275700	-2.32616700	-2.20270500
H	2.51344000	-1.22181600	-2.55674700
C	4.95122100	-2.64419600	0.10745100
H	3.61362100	-1.80575800	1.57404700
C	5.20074900	-2.83465600	-1.24805200
H	4.52027000	-2.47904400	-3.26181900
H	5.63636900	-3.04540300	0.85125100
H	6.08349800	-3.38683600	-1.56398000
C	-1.57122500	1.47919600	-0.37262000
C	-1.91947400	1.92311200	-1.65593800
C	-1.34082700	2.40136000	0.65029400
C	-2.03321100	3.28398200	-1.90554600
H	-2.10841100	1.20524400	-2.45585300
C	-1.45212700	3.76325500	0.39121400
H	-1.05933500	2.05060800	1.64406500
C	-1.79454900	4.20185900	-0.88361600
H	-2.30834800	3.63086300	-2.89934900
H	-1.26576800	4.48228400	1.18609200
H	-1.88148600	5.26782800	-1.08440200
C	-2.76876700	-1.20412500	-0.59585100
C	-4.00822700	-0.56126300	-0.68086800
C	-2.68050200	-2.58678300	-0.80057400
C	-5.14423600	-1.29560100	-1.00288600
H	-4.08716200	0.51098200	-0.50507800
C	-3.81906700	-3.31096600	-1.12459500
H	-1.72501900	-3.10338700	-0.69762100
C	-5.04991600	-2.66474800	-1.22888500
H	-6.10680800	-0.79431800	-1.07727200
H	-3.74843600	-4.38351900	-1.29156600
H	-5.94071300	-3.23584800	-1.48190100

1b



E = -1237.331990

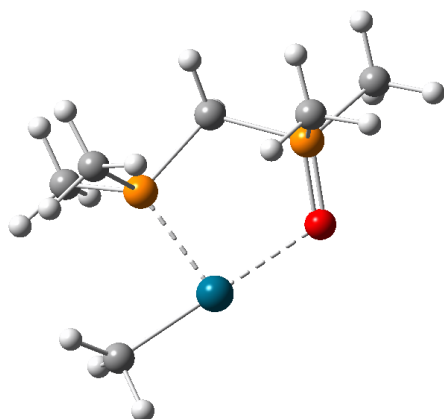
H = -1237.312875

G = -1237.378312

SPE= -1237.83551737

Pd	-0.51475100	0.00110200	-0.00431700
P	1.32488200	-1.35640900	-0.04331700
P	1.32818000	1.35395400	-0.04313500
C	1.46359100	-2.60395400	-1.35595000
H	0.69475200	-3.37052700	-1.20575500
H	1.29643900	-2.13947700	-2.33388300
H	2.45490200	-3.07438000	-1.33485000
C	1.76068800	2.16286000	1.52577800
H	1.77491500	1.42800800	2.33865600
H	2.74432800	2.64428100	1.45008800
H	1.00487500	2.91953200	1.76463900
C	2.55817200	-0.00266000	-0.34043900
H	2.88846200	-0.00306100	-1.38855600
H	3.44455100	-0.00374700	0.30732500
C	1.75631300	-2.16800200	1.52449100
H	0.99876500	-2.92304400	1.76300200
H	2.73871100	-2.65177700	1.44764300
H	1.77294700	-1.43405200	2.33813100
C	1.47012300	2.60262000	-1.35432400
H	2.46231200	3.07113500	-1.33227700
H	1.30237600	2.13964600	-2.33286200
H	0.70269100	3.37049700	-1.20348400
O	-2.32751600	-1.08928100	0.03395800
O	-2.32474900	1.09828900	0.03115300
C	-2.98366000	0.00601700	0.04334000
C	-4.46783300	0.00102000	0.05177300
H	-4.83310500	-0.35136000	-0.92063500
H	-4.83446500	-0.70003300	0.80923200
H	-4.85708800	1.00504300	0.24006200

2b



E = -1124.043284

H = -1124.026137

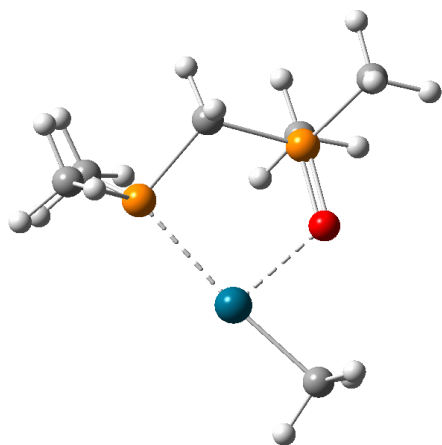
G = -1124.086366

SPE= -1124.505198

Pd	0.95974200	-1.04610300	-0.00340600
C	2.95481500	-0.75919000	0.14736400

H	3.25375000	-1.72248100	0.59123600
H	3.30256300	0.05592400	0.79243800
H	3.36880000	-0.64739900	-0.86299000
P	0.69183600	1.15730800	-0.07622700
P	-2.05701000	-0.12961900	-0.04854700
C	1.63337600	2.09919200	-1.31291800
H	2.69661000	2.08973800	-1.04359700
H	1.52332200	1.64121700	-2.30233900
H	1.28375400	3.13966300	-1.34862200
C	-2.55903200	0.11469500	1.66814400
H	-1.68165900	0.09181400	2.32621200
H	-3.09203900	1.06488700	1.79983800
H	-3.22045300	-0.70729800	1.96760700
C	-1.09052900	1.35520200	-0.54470000
H	-1.13022500	1.41230400	-1.64331900
H	-1.51188700	2.29038700	-0.14578500
C	0.91735700	2.07755700	1.47806800
H	1.97364800	2.04448500	1.77033900
H	0.62157000	3.12660000	1.34151400
H	0.32796800	1.63586300	2.28862900
C	-3.55162300	-0.12507700	-1.04981600
H	-4.11578100	0.80531200	-0.90796900
H	-3.29121600	-0.23555100	-2.10869600
H	-4.18455800	-0.97248200	-0.76067500
O	-1.20261000	-1.37273400	-0.25530200

3b

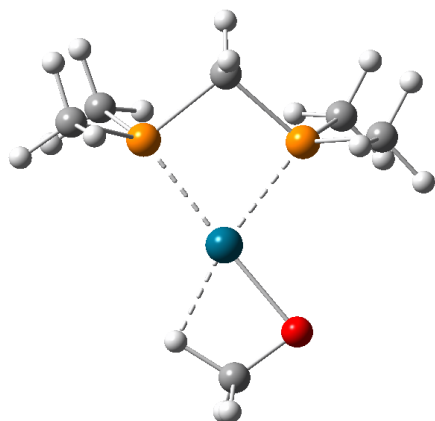


E = -1124.010804
H = -1123.993155
G = -1124.055314
SPE= -1124.467551

Pd	1.44256700	-0.32128000	0.02685200
C	2.45463700	-2.05219700	0.03798200
H	2.29795900	-2.54498400	-0.92639400
H	3.48238000	-1.67890400	0.17796200
H	2.09711600	-2.66103000	0.87397700
P	-0.01037700	1.67582400	-0.04608900
P	-1.61092400	-0.89003700	-0.08102000
C	0.15101200	3.04293000	-1.25394700
H	0.99662100	3.67997600	-0.96926400
H	0.34938600	2.64321700	-2.25475500

H	-0.75853300	3.65672700	-1.28094500
C	-2.06111300	-0.94420100	1.66445600
H	-1.27546900	-0.47704400	2.27125100
H	-3.01302300	-0.42917900	1.84463100
H	-2.15664500	-1.98906100	1.98237000
C	-1.59776600	0.85666900	-0.59485200
H	-1.60924500	0.86398400	-1.69525700
H	-2.49082200	1.39392900	-0.24329000
C	-0.51097100	2.55966500	1.48108200
H	0.33052900	3.16309700	1.84121500
H	-1.36235000	3.22583000	1.28962700
H	-0.77745100	1.85348600	2.27563900
C	-2.89539800	-1.74019100	-1.00866100
H	-3.87256300	-1.27281900	-0.83544400
H	-2.66101400	-1.70524400	-2.07846400
H	-2.94008000	-2.79002100	-0.69694800
O	-0.23972300	-1.53449300	-0.35760700

4b

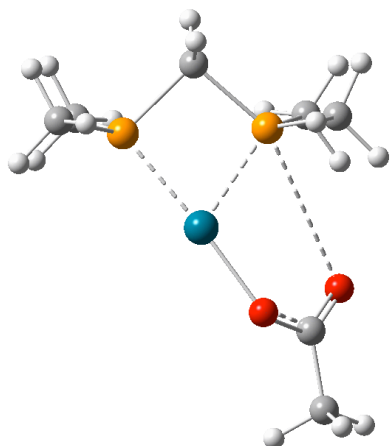


E = -1123.995784
H = -1123.978496
G = -1124.039528
SPE = -1124.446436

Pd	-0.72473200	-0.58070800	0.01908200
P	1.59974800	-0.68672800	-0.05562700
P	0.01798400	1.56923400	-0.07508800
C	2.55811600	-1.62600800	-1.28831900
H	2.53105500	-2.69308800	-1.03948200
H	2.12246900	-1.49490900	-2.28492300
H	3.60236800	-1.28871800	-1.29831100
C	0.03093000	2.48136400	1.49633300
H	0.52603400	1.88756400	2.27320100
H	0.55682900	3.43773300	1.37716100
H	-0.99991500	2.67193800	1.81548000
C	1.76276800	1.11892700	-0.48836300
H	1.92165900	1.22509100	-1.57106700
H	2.54761700	1.67638400	0.04068300
C	2.49943500	-0.88735400	1.51795100
H	2.44930600	-1.93193200	1.84546300
H	3.55233800	-0.60122600	1.39718400
H	2.04233700	-0.26676400	2.29778800

C	-0.68024600	2.67112400	-1.33675800
H	-0.16002700	3.63741900	-1.33866500
H	-0.60009100	2.20585900	-2.32517600
H	-1.74313600	2.82798400	-1.11801700
O	-2.70524500	-0.40192400	0.07862800
C	-2.76718700	-1.75427200	0.10653900
H	-3.16826900	-2.17898200	1.04174200
H	-3.22348000	-2.21480100	-0.78528100
H	-1.66633800	-2.23183400	0.08184800

TS1b-6b



E = -1237.301122

H = -1237.282559

G = -1237.34659

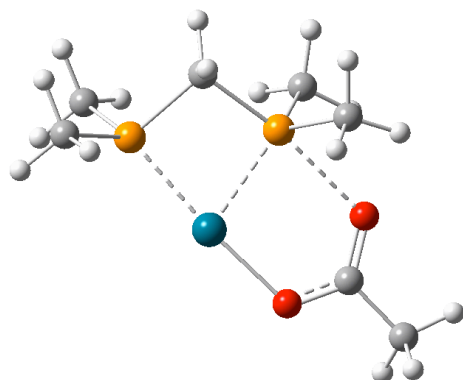
SPE = -1237.807122

Imaginary frequency = -40.67

P	0.68468373	2.30052336	0.03592242
P	2.37085173	0.20366236	-0.23802058
C	0.19354973	3.16413236	-1.47443558
H	-0.89725227	3.08120736	-1.56318858
H	0.65432773	2.69788336	-2.35212558
H	0.50470073	4.21625936	-1.41062658
C	3.49407073	-0.66622264	0.89783242
H	3.24557373	-0.41845564	1.93595042
H	4.53844373	-0.39881064	0.69345442
H	3.36922473	-1.74754664	0.76617142
C	2.51476773	2.03568836	0.05008442
H	3.08790873	2.59947136	-0.69792358
H	2.93197173	2.23876436	1.04668542
C	0.16574673	3.30197736	1.45276942
H	-0.92774627	3.38718236	1.43651842
H	0.61391573	4.30283136	1.37638642
H	0.47189973	2.83358236	2.39416842
C	2.96058773	-0.11988664	-1.92884358
H	4.02127773	0.14596936	-2.02529358
H	2.37099373	0.45779736	-2.65038958
H	2.83317573	-1.18289564	-2.16419658
Pd	0.10371473	0.13166436	0.11539342
O	-1.82810927	-0.05722664	0.46170142

C	-2.77473127	0.46710036	-0.29903158
O	-2.61669027	1.46134936	-0.98961058
C	-4.05438627	-0.32314964	-0.20044258
H	-4.84319427	0.12344836	-0.81189158
H	-4.37578927	-0.38047964	0.84713242
H	-3.87195027	-1.35536764	-0.52777458

6b

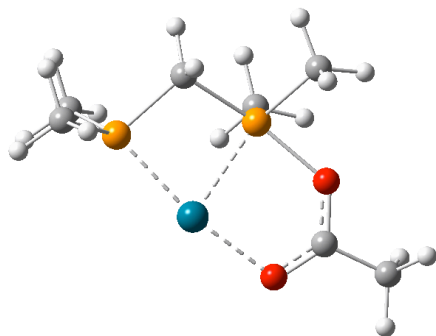


E = -1237.313002
H = -1237.29394
G = -1237.358839
SPE=-1237.819776

P	0.13266200	1.30525100	0.12591700
P	-2.17084200	-0.26975600	-0.02929100
C	0.34923300	2.23089800	-1.41946000
H	1.41256400	2.32263400	-1.65057800
H	-0.15488300	1.71665400	-2.24590400
H	-0.10582000	3.22216900	-1.28763000
C	-3.44871200	-0.86276300	1.12407000
H	-3.05149100	-0.89273600	2.14456900
H	-4.32147500	-0.19747500	1.09240800
H	-3.76267800	-1.87522100	0.84571500
C	-1.70388200	1.45007300	0.45411500
H	-2.22957900	2.26162500	-0.06933200
H	-1.86467600	1.56704800	1.53601600
C	0.88068000	2.18282500	1.52759300
H	1.91526900	2.44001500	1.28969800
H	0.28627200	3.08413200	1.72752700
H	0.86927100	1.54243000	2.41700900
C	-2.98464500	-0.15684700	-1.65476900
H	-3.87450400	0.48281800	-1.58615000
H	-2.29630900	0.26062900	-2.39817600
H	-3.28715100	-1.15401700	-1.99380900
Pd	0.01691400	-0.96773700	0.04411300
O	1.99757600	-1.39006300	0.10831700
C	2.80480200	-0.41594700	-0.10975300
O	2.43656000	0.76575400	-0.25199900
C	4.25915400	-0.78257600	-0.18269200

H	4.86859900	0.09278500	-0.41530800
H	4.57391800	-1.21328900	0.77457400
H	4.40445900	-1.55622000	-0.94440300

TS6b-7b



E = -1237.303447

H = -1237.285527

G = -1237.347734

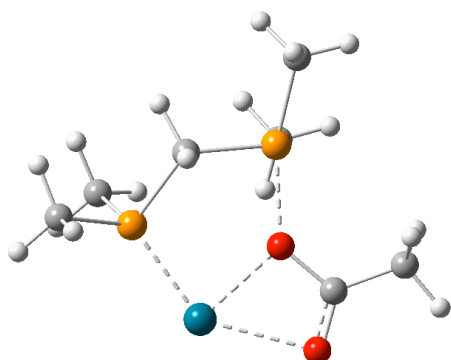
SPE=-1237.813213

Imaginary frequency = -37.21

P	-0.40253900	1.21829600	-0.07995900
P	2.17012400	-0.16151400	-0.00980200
C	-0.58497700	1.70470300	1.66361000
H	-1.63990200	1.92280900	1.86208400
H	-0.26349400	0.90249700	2.33774500
H	0.01485400	2.60394400	1.85426400
C	3.53972100	-0.46696300	-1.17265400
H	3.14936700	-0.59616400	-2.18808700
H	4.23203100	0.38596700	-1.15682400
H	4.08782500	-1.37372200	-0.89292400
C	1.43395400	1.46032900	-0.47001700
H	1.88668900	2.36474200	-0.02997200
H	1.49200900	1.54742800	-1.56613300
C	-0.97826100	2.61765900	-1.10292000
H	-1.96108300	2.96055200	-0.76861400
H	-0.24304300	3.42835500	-1.02415100
H	-1.05980900	2.31812700	-2.15468000
C	2.99549700	0.12467900	1.59226300
H	3.70707000	0.95550000	1.48536900
H	2.26433700	0.37850000	2.36763200
H	3.54104100	-0.76929700	1.91360900
Pd	0.07497300	-1.09137500	-0.06617500
O	-1.96472289	-1.55067585	-0.11268196
C	-2.66614087	-0.52458251	-0.04772727
O	-2.20781290	0.66801162	-0.24024193
C	-4.12194434	-0.57541826	0.27306715
H	-4.27914543	-0.10827385	1.25265566
H	-4.67915641	0.01512969	-0.46190466

H -4.48595970 -1.60358701 0.29067718

TS1b-7b



E = -1237.232202

H = -1237.213357

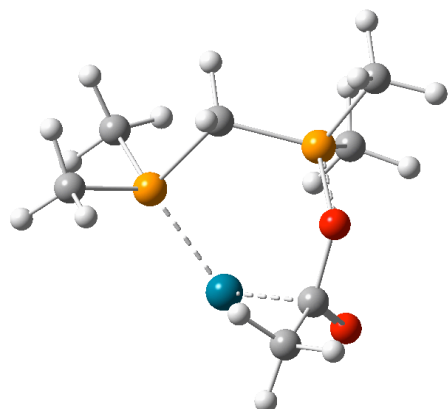
G = -1237.277799

SPE= -1237.73232

Imaginary frequency = -209.26

Pd	0.88295300	-1.44735000	0.05613300
P	1.67561600	0.69201000	-0.06200300
P	-1.46803600	1.45924500	-0.13578800
C	2.99641400	1.17682100	-1.22893000
H	3.94692200	0.74240600	-0.89779000
H	2.77800700	0.79534400	-2.23261900
H	3.10104200	2.27016700	-1.26828100
C	-1.49963400	1.60083600	1.67850700
H	-0.98529800	0.75512600	2.14859900
H	-1.02775500	2.54239000	1.99524200
H	-2.53983400	1.60946400	2.02639500
C	0.26411000	1.75743700	-0.70231200
H	0.25532500	1.59494000	-1.79125600
H	0.51136200	2.82233500	-0.54574100
C	2.18249800	1.53960800	1.47815100
H	3.13542100	1.11804500	1.81967400
H	2.31680000	2.61645400	1.30178300
H	1.44683400	1.38781600	2.27464600
C	-2.33215300	2.98687300	-0.71123200
H	-1.82422900	3.86906500	-0.28855700
H	-2.31207700	3.04745400	-1.80432900
H	-3.37567400	2.97597000	-0.37807500
O	-1.02500900	-0.49443400	-0.26537000
O	-1.16826000	-2.64924900	0.02302000
C	-1.78983500	-1.61351900	-0.15008000
C	-3.26880600	-1.49779000	-0.24014400
H	-3.65004500	-0.85821900	0.56633700
H	-3.56052600	-1.04017100	-1.19236100
H	-3.71522900	-2.49146100	-0.15388700

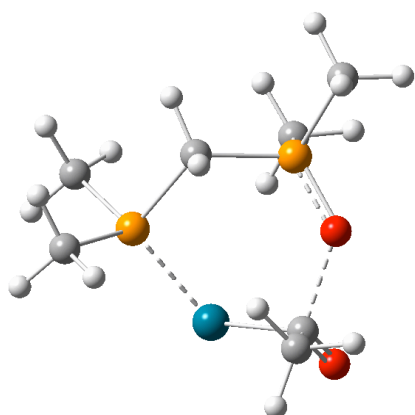
7b



E = -1237.306442
 H = -1237.288056
 G = -1237.350534
 SPE= -1237.820236

Pd	0.60114700	-1.26598800	0.49316800
P	1.65783900	0.62467500	-0.23019900
P	-1.35663500	1.31594200	0.02979800
C	2.62980300	0.76867700	-1.77529800
H	3.56797500	0.21450800	-1.65543500
H	2.08000000	0.31662200	-2.60917800
H	2.86472000	1.81474800	-2.01229800
C	-1.37232000	1.18259700	1.82093300
H	-0.59360500	0.49293900	2.16963300
H	-1.21009500	2.17990500	2.25145100
H	-2.34623500	0.79938300	2.14779900
C	0.26067300	1.84220000	-0.59055600
H	0.14472800	1.94161000	-1.68093600
H	0.48351500	2.84470400	-0.19244600
C	2.65497400	1.58868300	0.96969200
H	3.55744200	1.02080600	1.22388000
H	2.95489900	2.56242100	0.55970200
H	2.08910300	1.74119800	1.89707100
C	-2.58323200	2.52997800	-0.45984100
H	-2.33891100	3.51084300	-0.03438600
H	-2.61642400	2.60833000	-1.55224000
H	-3.57046700	2.21806900	-0.09972600
O	-1.81178000	-0.00212000	-0.72681000
O	-1.63439700	-1.86880500	0.65436200
C	-1.36390600	-1.38040400	-0.43553900
C	-1.23004800	-2.09097000	-1.74566500
H	-2.22896200	-2.19735300	-2.19224900
H	-0.59982100	-1.53053200	-2.44340800
H	-0.81494800	-3.08920300	-1.57970200

TS7b-8b



E = -1237.301439

H = -1237.283157

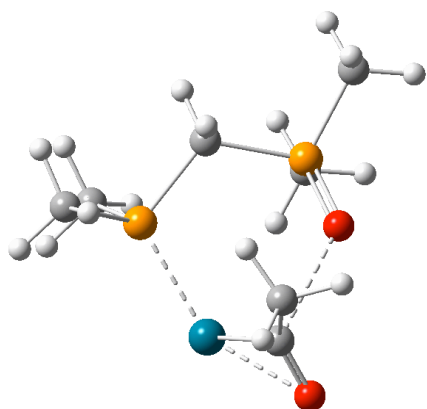
G = -1237.345508

SPE= -1237.816172

Imaginary frequency = -221.33

Pd	-1.33542400	-0.50318000	-0.57197300
P	-0.69264400	1.52689500	0.27886800
P	1.98686700	-0.00131000	-0.04986800
C	-1.45327600	2.20702200	1.79588900
H	-2.50026900	2.45887000	1.59114100
H	-1.43651200	1.45957300	2.59752300
H	-0.92731300	3.11167400	2.12826100
C	1.99101800	0.30574000	-1.82711100
H	0.97665200	0.21633700	-2.23686100
H	2.39507300	1.30137100	-2.05124900
H	2.61811700	-0.44962400	-2.31532200
C	1.10104100	1.37401400	0.76430100
H	1.14893100	1.17097300	1.84535200
H	1.63622600	2.32019200	0.58852900
C	-0.68640400	2.95920700	-0.86199200
H	-1.71711300	3.20221900	-1.14550300
H	-0.23689400	3.83828900	-0.38090200
H	-0.13198700	2.72330800	-1.77771600
C	3.69409400	0.10662900	0.50987700
H	4.13665500	1.06942300	0.22597000
H	3.73926100	-0.00604400	1.59873800
H	4.27635800	-0.70243700	0.05409000
O	1.40835900	-1.37099500	0.33350200
O	-0.62615400	-2.68361300	-0.46857900
C	-0.35101600	-1.94329700	0.43858500
C	-0.43536000	-2.10072000	1.91549300
H	0.27605100	-2.87530900	2.22642900
H	-0.20173000	-1.16890100	2.43467700
H	-1.45357000	-2.42210400	2.16297300

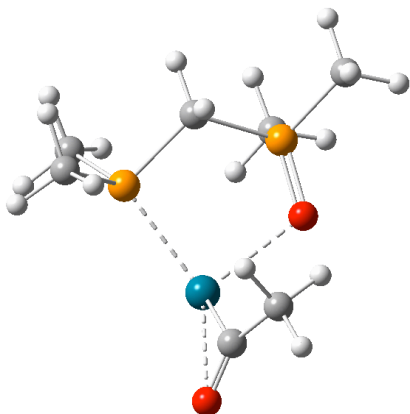
8b



E = -1237.305274
H = -1237.285877
G = -1237.351548
SPE= -1237.822327

Pd	-1.45215700	0.03942600	-0.61629100
P	-0.02424500	1.58447000	0.35072600
P	1.99380300	-0.73864500	-0.07962400
C	-0.54761400	2.47343500	1.85856500
H	-1.43761700	3.07315500	1.63584600
H	-0.80397800	1.76454200	2.65405600
H	0.25229400	3.13774000	2.21134100
C	2.33162700	-0.22700800	-1.78217500
H	1.40878700	0.11146600	-2.27011000
H	3.08203900	0.57325000	-1.82098200
H	2.70581600	-1.08886400	-2.34722500
C	1.58110200	0.80535800	0.83725200
H	1.50839600	0.52162500	1.89868700
H	2.39281300	1.54520800	0.75670600
C	0.46636300	2.93507200	-0.78341000
H	-0.41548300	3.52714700	-1.05493100
H	1.19615200	3.59543400	-0.29593100
H	0.90543600	2.53504600	-1.70460700
C	3.58415000	-1.23944000	0.61384400
H	4.33761100	-0.45048700	0.49762000
H	3.47048500	-1.47556300	1.67803100
H	3.93400000	-2.14229700	0.09978100
O	0.90738400	-1.77128100	0.05687700
O	-2.10499800	-2.17789900	-0.40546200
C	-1.53457000	-1.58876000	0.45705600
C	-1.24074600	-1.86963300	1.87777800
H	-0.70504700	-2.82442600	1.92776600
H	-0.63497500	-1.08504800	2.33123400
H	-2.20184700	-1.95959400	2.40080700

TS8b-9b



E = -1237.300014

H = -1237.280985

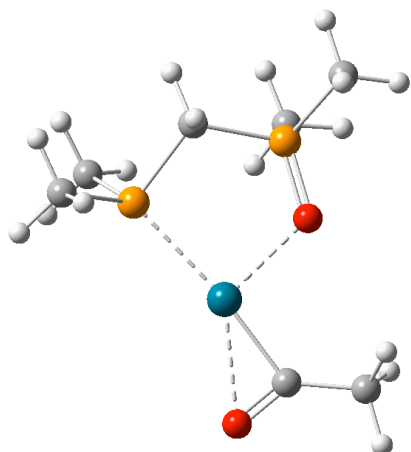
G = -1237.346663

SPE = -1237.813308

Imaginary frequency = -82.77

Pd	-1.12708400	0.00659900	-0.69030000
P	0.44186600	1.65261500	0.25292800
P	1.78766100	-1.10225700	0.05018100
C	-0.01965400	2.64961700	1.71939900
H	-0.67930300	3.46852700	1.41005900
H	-0.56427800	2.03006000	2.44200800
H	0.86987300	3.07337400	2.20422800
C	2.63625700	-0.78147600	-1.51315600
H	2.01512400	-0.15342500	-2.16501700
H	3.60452200	-0.29017400	-1.35201100
H	2.80478000	-1.73344900	-2.03077100
C	1.71622500	0.48750700	0.96053800
H	1.39588500	0.23591700	1.98446400
H	2.70946700	0.95741600	1.03073000
C	1.45638300	2.82809500	-0.72475800
H	0.80978700	3.61488500	-1.12971700
H	2.22841200	3.29230700	-0.09556700
H	1.93765800	2.32196300	-1.56987600
C	2.86648700	-2.17579800	1.01571600
H	3.85725200	-1.72087100	1.14092700
H	2.42727500	-2.35536800	2.00383100
H	2.97911400	-3.13991400	0.50689800
O	0.39104200	-1.68207100	-0.13976000
O	-3.52663100	-0.39582400	-0.18826300
C	-2.53951500	-0.75467200	0.35508700
C	-2.20753600	-1.60909200	1.52378800
H	-1.37975000	-2.27772100	1.26397600
H	-1.87823600	-0.96062000	2.34657500
H	-3.10178800	-2.16376300	1.82091500

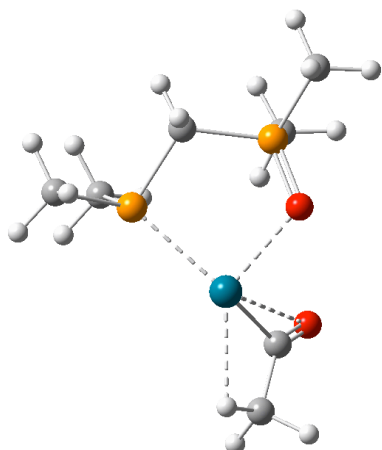
9b



E = -1237.315536
 H = -1237.29589
 G = -1237.362775
 SPE= -1237.827719

Pd	-1.07685200	-0.42324500	0.00303700
P	1.13986600	-1.48923300	-0.06137000
P	1.39046700	1.52692900	-0.06336600
C	1.63615000	-2.76867700	-1.27301200
H	1.17570600	-3.72443000	-0.99708200
H	1.28273800	-2.49929900	-2.27456300
H	2.72650000	-2.89320200	-1.29238100
C	1.77631600	1.74971500	1.68678200
H	1.26410500	0.98619800	2.28522100
H	2.85696000	1.68432700	1.86529400
H	1.42079400	2.73208400	2.01906700
C	2.17600200	-0.02848900	-0.59505300
H	2.18558500	-0.01849800	-1.69553800
H	3.21763100	-0.09941600	-0.24835000
C	1.98040600	-2.05012500	1.46867700
H	1.51204000	-2.97825600	1.81647000
H	3.04568800	-2.24135000	1.28443800
H	1.87942500	-1.30709000	2.26810500
C	2.18145200	2.87327000	-0.95815500
H	3.26323300	2.87407700	-0.77608200
H	1.99638300	2.76495000	-2.03265800
H	1.76466100	3.83151500	-0.62732500
O	-0.11876800	1.48214800	-0.33495600
O	-3.34434600	-0.88937700	0.19682200
C	-2.89366700	0.20905200	0.03617300
C	-3.45573300	1.56741200	-0.09927800
H	-3.21249000	2.12569800	0.81379500
H	-2.95847700	2.08285100	-0.92788900
H	-4.54093400	1.52854500	-0.24091900

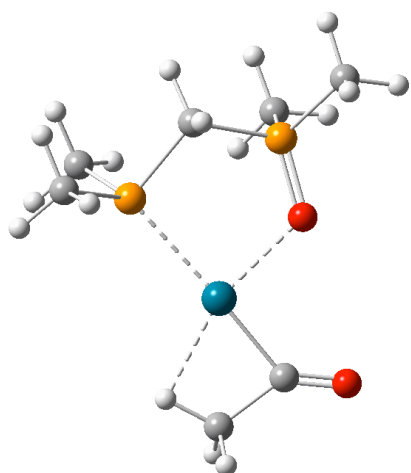
TS9b-10b



E = -1237.301281
 H = -1237.282589
 G = -1237.346447
 SPE = -1237.815854
 Imaginary frequency = -53.59

Pd	1.14867900	0.18753500	-0.47425500
P	-0.76361600	1.65925800	0.11628100
P	-1.62091500	-1.27833100	-0.13341300
C	-1.39421200	3.20641700	-0.63750100
H	-0.71840900	4.03293300	-0.38957700
H	-1.43110500	3.11145300	-1.72817800
H	-2.39741700	3.44285900	-0.25926100
C	-1.55994700	-1.71719400	1.61733100
H	-0.71780900	-1.20615600	2.10023200
H	-2.49276100	-1.45689800	2.13312600
H	-1.38912600	-2.79611000	1.71265100
C	-2.15699000	0.47107500	-0.23496300
H	-2.46875800	0.64116900	-1.27690600
H	-3.02881600	0.66142000	0.40937000
C	-0.94778400	1.99204800	1.91069900
H	-0.26430700	2.79876700	2.20056000
H	-1.97470300	2.29895800	2.15049700
H	-0.68869300	1.10558600	2.50132600
C	-2.93447000	-2.25420600	-0.88471000
H	-3.89193700	-2.07268200	-0.38062900
H	-3.02857500	-1.99450800	-1.94514800
H	-2.68774000	-3.31950200	-0.81045400
O	-0.27925500	-1.47720000	-0.83541300
O	2.25328400	-1.55495700	1.36105800
C	2.44938800	-0.78599000	0.49501600
C	3.63042000	-0.13983000	-0.18286900
H	3.35513300	0.61319600	-0.94702100
H	4.24427300	0.35914800	0.57500800
H	4.19882100	-0.93680000	-0.67608100

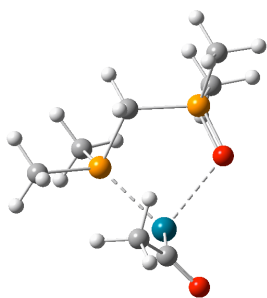
10b



E = -1237.306472
 H = -1237.287069
 G = -1237.353454
 SPE=-1237.821341

Pd	1.15594000	0.22742500	-0.04817700
P	-0.94355300	1.58954700	-0.05368600
P	-1.60574200	-1.36971100	-0.05948200
C	-1.35907900	2.95914800	-1.19806800
H	-0.78233000	3.85024200	-0.92408100
H	-1.09852800	2.68827600	-2.22729200
H	-2.42844500	3.20183000	-1.14697600
C	-2.00992400	-1.58763900	1.68685600
H	-1.40237700	-0.90986900	2.29929600
H	-3.07307400	-1.39860100	1.88064800
H	-1.77054800	-2.61464100	1.98693800
C	-2.18352800	0.28917100	-0.55334400
H	-2.23162600	0.29063800	-1.65292400
H	-3.19154900	0.50763600	-0.17077300
C	-1.62026900	2.20033800	1.53918200
H	-1.04615400	3.07571100	1.86492400
H	-2.67349400	2.49209800	1.43343300
H	-1.53434000	1.43664600	2.32065600
C	-2.56812700	-2.57450000	-0.98747200
H	-3.64021700	-2.44658700	-0.79334700
H	-2.37651200	-2.45383400	-2.05954600
H	-2.26919500	-3.58746800	-0.69453800
O	-0.10764400	-1.50324500	-0.33760200
O	3.10008700	-1.89583100	-0.00190700
C	2.80612500	-0.76166900	0.02562700
C	3.52155100	0.56974400	0.14933900
H	4.20407500	0.67447200	-0.70011100
H	2.85788200	1.47232100	0.13993200
H	4.06261600	0.58711500	1.10076400

TS8b-9b2



E = -1237.536085

H = -1237.284898

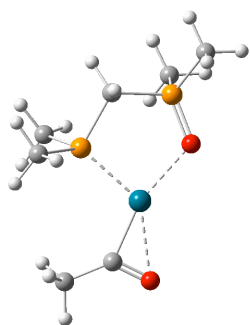
G = -1237.348967

SPE= -1237.819499

Imaginary frequency = -76.88

Pd	-1.17886500	-0.10775100	-0.81774100
P	0.08925800	1.53902200	0.23359800
P	1.99886700	-0.87746100	0.10926500
C	-0.53882200	2.58608800	1.59411800
H	-1.37312100	3.19853800	1.23334600
H	-0.89558600	1.96663600	2.42509800
H	0.25568100	3.24728400	1.96438700
C	2.92808400	-0.36174500	-1.35542800
H	2.25746000	0.11586600	-2.08059200
H	3.74162200	0.32900800	-1.10013200
H	3.35613400	-1.24837000	-1.83809600
C	1.53933400	0.67701000	0.99265100
H	1.23956800	0.37555000	2.00852700
H	2.39576600	1.36168000	1.09210700
C	0.83274700	2.75628900	-0.91352000
H	0.04699500	3.40187800	-1.32258200
H	1.56505900	3.38157800	-0.38501900
H	1.33144300	2.25589800	-1.75150800
C	3.19281200	-1.67192000	1.20540800
H	4.03280800	-1.00188200	1.42794800
H	2.70409100	-1.96140000	2.14277400
H	3.57878700	-2.57964900	0.72736100
O	0.77659300	-1.70375900	-0.20038900
O	-2.80302300	-1.74698200	-0.22423800
C	-2.21822300	-1.03059600	0.52357600
C	-2.17783600	-0.89280300	1.99659200
H	-1.16558500	-1.14679900	2.33612700
H	-2.39718600	0.14279100	2.27715400
H	-2.90516000	-1.57349300	2.45289900

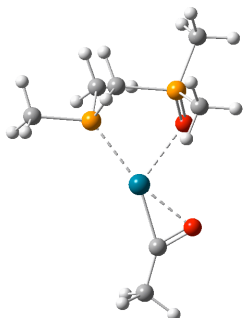
9b2



E = -1237.564785
H = -1237.312414
G = -1237.3778
SPE= -1237.846117

Pd	0.83889300	-0.73395300	-0.07700300
P	0.04497500	1.40910500	-0.08091900
P	-2.33569400	-0.45236800	-0.01676600
C	0.64843200	2.61711700	-1.30866100
H	1.68480800	2.88934000	-1.07479400
H	0.62350500	2.18128600	-2.31355800
H	0.03471600	3.52746100	-1.29084100
C	-2.81601300	-0.37839100	1.72166700
H	-1.93639500	-0.19714100	2.35100000
H	-3.56069000	0.40780600	1.89770100
H	-3.24258900	-1.34363600	2.01936500
C	-1.75900500	1.22502600	-0.48359000
H	-1.85431000	1.30359500	-1.57721100
H	-2.36293300	2.02626700	-0.03329100
C	0.08894200	2.34255200	1.48934200
H	1.13175800	2.56164200	1.74966800
H	-0.45493100	3.29141300	1.39040600
H	-0.34532500	1.75776000	2.30763800
C	-3.83009700	-0.77379700	-0.96614600
H	-4.58742700	-0.00277300	-0.77865800
H	-3.59220000	-0.79831900	-2.03549600
H	-4.23844300	-1.75058000	-0.68172600
O	-1.22461700	-1.45439300	-0.29593400
O	2.86034000	-1.88325300	0.06328000
C	2.75408500	-0.68376500	0.08354500
C	3.79222700	0.37130600	0.18586200
H	3.79979500	0.94548600	-0.74949100
H	3.53464600	1.06107600	0.99842400
H	4.78051400	-0.06904500	0.35741200

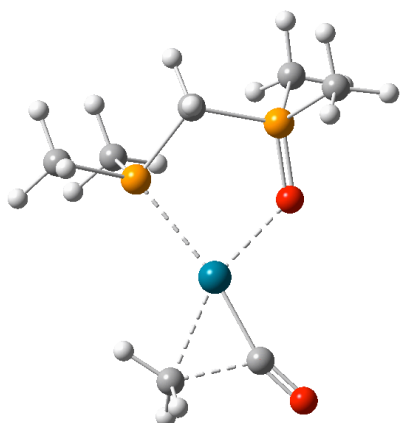
TS9b2-10b



E = -1237.519904
H = -1237.269175
G = -1237.334455
SPE= -1237.801873
Imaginary frequency = -75.61

Pd	1.16501100	0.04988300	0.01689500
P	-0.73238000	1.55847100	-0.10935700
P	-1.95603200	-1.12064800	-0.05761200
C	-0.95597600	3.12970800	-1.02021800
H	-0.25981000	3.88076900	-0.62977200
H	-0.73794500	2.98425200	-2.08397300
H	-1.98153500	3.50634600	-0.90917900
C	-3.43914500	-1.43720800	0.91652800
H	-3.54289000	-0.67169100	1.69459300
H	-4.33410400	-1.43177400	0.28214100
H	-3.35463100	-2.41481600	1.40501500
C	-2.11583900	0.53742000	-0.80971600
H	-1.98920400	0.48350100	-1.90012300
H	-3.08597600	1.01254700	-0.60107300
C	-1.31006300	1.97217200	1.57603000
H	-0.66377700	2.75442600	1.99105400
H	-2.34174100	2.34977000	1.54622100
H	-1.25000900	1.09426900	2.22776200
C	-1.92336500	-2.32146100	-1.40291700
H	-2.83036900	-2.25136000	-2.01617500
H	-1.04566000	-2.13574900	-2.03463000
H	-1.84611000	-3.33527800	-0.99348900
O	-0.68667400	-1.09555800	0.78256300
O	2.48421500	-1.49831600	0.49391700
C	3.08898000	-0.55188400	0.04064700
C	4.50211300	-0.24685200	-0.22914400
H	4.60130500	0.10142400	-1.26307600
H	4.79826600	0.58971500	0.41619300
H	5.13927000	-1.11867900	-0.04323300

TS10b-11b

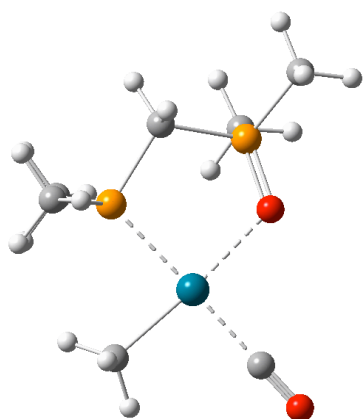


E = -1237.298803
H = -1237.279531
G = -1237.345438
SPE= -1237.813298

Imaginary frequency = -317.26

Pd	1.18307600	-0.05931900	0.00624600
P	-0.63688800	1.60716800	-0.07956700
P	-1.92898700	-1.11268900	-0.06929800
C	-0.79136000	3.14733400	-1.05445900
H	-0.05695900	3.87974800	-0.69910200
H	-0.59284900	2.95092000	-2.11401700
H	-1.79503100	3.57887200	-0.94884500
C	-2.99402700	-1.26664600	1.37761100
H	-2.69052100	-0.55680200	2.15558500
H	-4.04246800	-1.08273900	1.11221600
H	-2.90296400	-2.28017500	1.78542300
C	-2.07682800	0.60176100	-0.68945900
H	-2.01670800	0.57529800	-1.78766500
H	-3.04078700	1.05491400	-0.41449000
C	-1.17787500	2.11673000	1.59597500
H	-0.47982500	2.86327200	1.99282700
H	-2.18552000	2.55278000	1.57677800
H	-1.16155300	1.25750400	2.27757700
C	-2.60049100	-2.20384800	-1.33512000
H	-3.63530100	-1.93046500	-1.57632100
H	-1.98855500	-2.14189800	-2.24226900
H	-2.58015800	-3.23909700	-0.97522900
O	-0.46586500	-1.42092000	0.25106100
O	3.48177900	-1.95379500	0.19378800
C	2.75971400	-1.05935200	0.09015800
C	3.30114200	0.66585900	-0.16908300
H	3.88030800	0.46831100	-1.07409900
H	2.77242400	1.61822300	-0.29420100
H	3.93415500	0.72952400	0.71893500

11b

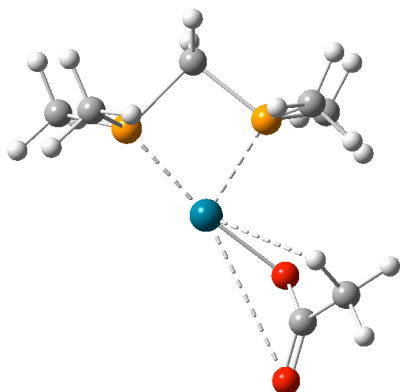


E = -1237.331572
H = -1237.311718
G = -1237.378460
SPE = -1237.847416

Pd	1.12652600	-0.21237000	-0.01357400
C	2.66619400	1.15166100	0.14714000
H	3.52032000	0.67929200	0.63983800

H	2.36966800	2.03503700	0.72368200
H	2.92665600	1.43382400	-0.88089000
P	-0.34280700	1.58523200	-0.06924800
P	-2.01126400	-0.92281900	-0.05088500
C	-0.04585700	2.88905200	-1.30507000
H	0.87155000	3.43198700	-1.04613200
H	0.08721100	2.44413200	-2.29787300
H	-0.88186100	3.60003600	-1.33156700
C	-2.52434300	-1.00195100	1.67769900
H	-1.74807700	-0.57207400	2.32272000
H	-3.47257400	-0.47468700	1.84190700
H	-2.65021100	-2.05286800	1.96509500
C	-1.97928100	0.84513800	-0.53255800
H	-2.05542400	0.88126100	-1.63001700
H	-2.82216400	1.41775100	-0.11849500
C	-0.64150100	2.49509200	1.48330200
H	0.27752500	3.01049400	1.78771800
H	-1.43205100	3.24386300	1.34206200
H	-0.92803200	1.81407200	2.29243000
C	-3.29632000	-1.71642500	-1.02871500
H	-4.26825600	-1.23428200	-0.86466300
H	-3.03927200	-1.66464400	-2.09284200
H	-3.37023100	-2.77219700	-0.74217800
O	-0.63185400	-1.52544500	-0.29241700
O	3.17820700	-2.59593500	0.01710700
C	2.44365600	-1.73208700	0.01121500

TS1b-12b



E = -1237.275690

H = -1237.257017

G = -1237.321964

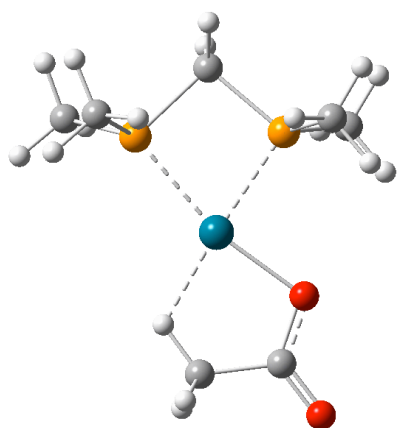
SPE= -1237.78292

Imaginary frequency = -94.00

P	0.35751200	1.49655800	0.12546500
P	2.06184000	-0.63430200	-0.16879000
C	-0.15510100	2.35576600	-1.38342000
H	-1.24841000	2.43893100	-1.39302200
H	0.15948400	1.79681400	-2.27200200
H	0.28727600	3.36091400	-1.40693800
C	3.30009200	-1.41174700	0.91573700

H	3.06284200	-1.20998900	1.96613500
H	4.30200600	-1.02765800	0.68489000
H	3.28944600	-2.49723700	0.76479600
C	2.17741900	1.21292900	0.10198900
H	2.73271900	1.77451500	-0.66128200
H	2.60921700	1.43088700	1.08900900
C	-0.18736000	2.45983400	1.55435900
H	-1.28388600	2.44528300	1.57409400
H	0.17595100	3.49317400	1.48018400
H	0.17559400	2.00157800	2.48068400
C	2.62793800	-0.90937700	-1.87808600
H	3.65471400	-0.54185200	-2.00360100
H	1.96689800	-0.39275800	-2.58358100
H	2.60015500	-1.97977100	-2.11140600
Pd	-0.21594800	-0.64523300	0.25792100
O	-2.09593500	-0.30431700	0.77756400
C	-3.08296900	-0.67459700	-0.05862800
O	-3.69997000	-1.69864600	0.10329500
C	-3.37330200	0.30487500	-1.17054700
H	-4.27535700	0.00935700	-1.71232500
H	-2.53371900	0.32625500	-1.88158700
H	-3.50468300	1.31605800	-0.76381900

12b

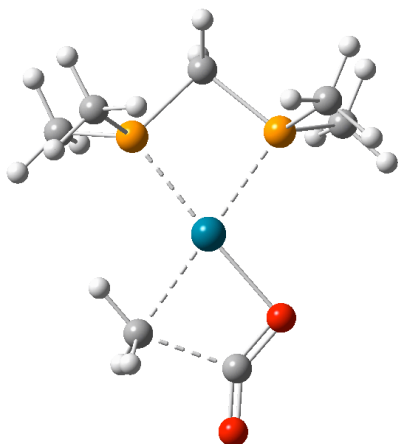


E = -1237.288987
 H = -1237.269863
 G = -1237.335365
 SPE = -1237.795075

Pd	0.40700800	-0.39005200	-0.03246500
C	2.65704800	-1.83288800	0.05448100
H	2.95025500	-2.30948400	0.99657400
H	3.11729200	-2.38473200	-0.77290600
H	1.54426900	-2.03009000	-0.05347500
P	-0.67611300	1.57339400	-0.04592900
P	-1.86986200	-0.90367000	-0.02452900
C	-0.17064800	2.68872000	-1.37603000
H	0.89641100	2.90905900	-1.24231800
H	-0.30543100	2.20816800	-2.35112000
H	-0.74968900	3.62077200	-1.33722600

C	-2.63091800	-1.38988700	1.55747600
H	-2.24747500	-0.75921100	2.36863300
H	-3.72281400	-1.28768800	1.50315800
H	-2.38076200	-2.43117300	1.79064200
C	-2.36744900	0.88078500	-0.28271300
H	-2.71348400	1.04515100	-1.31311100
H	-3.13299700	1.26081200	0.40748200
C	-0.54699900	2.45797500	1.52745600
H	0.51038600	2.69261500	1.70483400
H	-1.12891500	3.38870600	1.49366000
H	-0.90627400	1.83013900	2.35086300
C	-2.70572600	-1.87848300	-1.31531900
H	-3.79243400	-1.73518000	-1.25358600
H	-2.35333100	-1.57433300	-2.30722700
H	-2.47841800	-2.94226500	-1.18065900
O	2.19821200	0.53899300	-0.00572200
C	3.13642000	-0.38723800	0.03793900
O	4.31807500	-0.14382200	0.07150900

TS12b-13b



E = -1237.267632

H = -1237.248332

G = -1237.314780

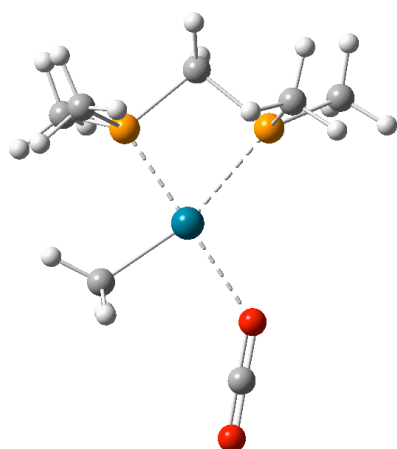
SPE = -1237.773299

Imaginary frequency = -447.71

P	-1.22720700	1.41085700	-0.05028400
P	-1.33148900	-1.32093800	-0.05763900
C	-1.31036500	2.66846700	-1.35979100
H	-0.53294900	3.42137600	-1.18531800
H	-1.12610000	2.20799300	-2.33663900
H	-2.29325900	3.15671300	-1.36187900
C	-1.85788800	-2.08976800	1.50457000
H	-1.84422200	-1.35147300	2.31454300
H	-2.86947000	-2.50469100	1.40593300
H	-1.16424600	-2.89665800	1.76928600
C	-2.48364100	0.08790200	-0.39875400
H	-2.76674000	0.10072700	-1.46082000
H	-3.39792300	0.11671600	0.20888500
C	-1.71811200	2.23226300	1.49678800
H	-0.96957800	2.98737000	1.76222500
H	-2.69481900	2.71884200	1.37589200

H	-1.77253900	1.50509600	2.31486900
C	-1.52952700	-2.58525500	-1.34943600
H	-2.55351000	-2.98008000	-1.34747100
H	-1.30383800	-2.15767300	-2.33263800
H	-0.82937800	-3.40902100	-1.16419300
Pd	0.57313300	-0.04514900	0.02045900
O	2.21659400	1.18165300	0.06522000
C	3.09697300	0.30272000	0.03619600
O	4.26382400	0.14718100	0.00164900
C	2.32175300	-1.47932000	0.06240900
H	2.85878000	-1.77659300	-0.84256200
H	2.88715900	-1.72530300	0.96606300
H	1.43045500	-2.13800700	0.10471800

13b

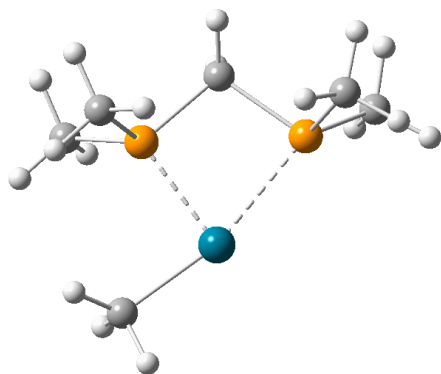


E = -1237.318386
 H = -1237.297801
 G = -1237.368708
 SPE = -1237.827204

Pd	0.54851200	-0.22661800	0.03334100
C	1.44047600	-2.07670900	0.17823100
H	1.97913200	-2.21522500	-0.76969000
H	0.79981100	-2.94572800	0.36195700
H	2.13727600	-1.96540500	1.02088800
P	-1.08153300	1.62554900	-0.05708500
P	-1.46832600	-1.18595200	-0.09949000
C	-1.37417200	3.00993900	-1.21899300
H	-0.73280700	3.85778200	-0.95106600
H	-1.12838600	2.70764600	-2.24307100
H	-2.42273000	3.33351100	-1.17811400
C	-2.15076700	-1.85948200	1.44460100
H	-2.06799900	-1.11847400	2.24802400
H	-3.20589100	-2.13149800	1.30790100
H	-1.58571700	-2.75118500	1.74174200
C	-2.38753800	0.35730200	-0.51014800
H	-2.55236700	0.38869100	-1.59742400
H	-3.35964800	0.47325700	-0.00882300
C	-1.68921500	2.28246300	1.54204500
H	-1.00941900	3.06027700	1.90868600
H	-2.69447300	2.71146100	1.43388400

H	-1.71719800	1.48406800	2.29392500
C	-1.79252600	-2.43269300	-1.38067500
H	-2.86737800	-2.64976200	-1.43594100
H	-1.44346700	-2.06908700	-2.35367800
H	-1.25340300	-3.35763100	-1.14365700
O	4.94718100	0.28392400	-0.09524200
C	3.81704800	0.50862400	-0.00756600
O	2.67296200	0.75121600	0.08204400

14b



E = -1048.814927
H = -1048.798326
G = -1048.857397
SPE = -1049.229404

Pd	-0.47363800	-1.09852700	0.04545800
C	-2.49509700	-1.41579900	0.09092900
H	-2.85847300	-1.45278000	-0.94386800
H	-3.10001200	-0.71977000	0.68274400
H	-2.52414300	-2.41302000	0.55789600
P	1.77360300	-0.08906900	-0.04452500
P	-0.83226800	1.10436200	-0.08104500
C	3.11346500	-0.21415200	-1.28519400
H	3.74246600	-1.08297100	-1.05810900
H	2.69260500	-0.35315100	-2.28744700
H	3.73934600	0.68793300	-1.27539300
C	-1.30163000	1.93702700	1.46404100
H	-0.63845200	1.63280000	2.28150200
H	-1.24247700	3.02618900	1.33455300
H	-2.32873500	1.66493100	1.73458600
C	0.91594000	1.53213500	-0.46728200
H	1.00605000	1.71218800	-1.54875600
H	1.29792100	2.41628300	0.06411600
C	2.66962800	0.30077900	1.50490400
H	3.26118400	-0.56838700	1.81579000
H	3.34400600	1.15586000	1.36448100
H	1.96179000	0.52674500	2.31133700
C	-1.93376900	1.75969200	-1.36634000
H	-1.85527200	2.85395400	-1.41224100
H	-1.67185000	1.33356200	-2.34119300
H	-2.96983500	1.48441300	-1.13388400

CO

E = -113.243564
H = -113.240259
G = -113.262702
SPE= -113.3009614

C	0.00000000	0.00000000	-0.64993800
O	0.00000000	0.00000000	0.48745400

CO₂

E = -188.490100
H = -188.486537
G = -188.510798
SPE= -188.5842447

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16412500
O	0.00000000	0.00000000	-1.16412500