

Supporting information

Generation and Direct EPR Spectroscopic Observation of Triplet Arylphosphinidenes: Stabilisation Versus Internal Rearrangements

Eugenii Ya. Misochko,^a Alexander V. Akimov,^a Denis V. Korchagin,^a Yulia S. Ganushevich,^b Egor A. Melnikov,^b and Vasili A. Miluykov^b

^a Institute of Problems of Chemical Physics, Russian Academy of Sciences, 142432 Chernogolovka, Moscow Region, Russian Federation

^b Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russian Academy of Sciences, 420088 Kazan, Russian Federation

The content:

1. Experimental and computational details.
2. Experimental and calculated fine and hyperfine parameters of the studied triplet phosphinidenes
3. Calculated equilibrium structures and potential energy profiles for internal rearrangements of the studied phosphinidenes.
4. Cartesian coordinates of molecules under consideration.

1. Experimental and computational details

A. Synthesis of 1-arylphosphiranes

All manipulations were performed under a nitrogen atmosphere using high-vacuum and standard Schlenk techniques. NMR spectra were recorded on Bruker 500 and 400 MHz NMR spectrometers. ¹H and ¹³C NMR data are reported with reference to solvent resonances, and ³¹P NMR spectra were reported with respect to external 85% H₃PO₄ (0 ppm). GC-MS data were recorded on an Agilent Technologies 5977A MSD (He) using an HP-5MS column (150 °C).

PhPC₂H₄ (**1**), AnthPC₂H₄ (**2**), TippPC₂H₄ (**3**) and Mes*PC₂H₄ (**4**) were prepared according to the literature through reactions of corresponding arylphosphine and ethylene glycol ditosylate [1].

1-Phenylphosphirane (1).

¹H NMR (400 MHz, C₆D₆): δ = 7.24 – 7.18 (m, 2H, CHAr), 7.04 – 6.95 (m, 3H, CHAr), 1.09 – 1.01 (m, 2H, CH₂), 0.95 – 0.85 (m, 2H, CH₂). ¹³C{¹H} NMR (100 MHz, C₆D₆): δ = 139.6 (d, ¹J_{C-P} = 40.6 Hz, CAr), 131.5 (d, ²J_{C-P} = 19.4 Hz, CAr), 127.9 (bs, CAr), 127.6 (bs, CAr), 127.4 (bs, CAr) 9.7 (d, ¹J_{C-P} = 40.6 Hz, CH₂). ³¹P{¹H} NMR (162 MHz, C₆D₆): δ = -236.9. MS (EI): 136.0 [M]⁺

1-(9-Anthracene)phosphirane (2).

^1H NMR (400 MHz, CDCl_3): $\delta = 8.93\text{-}8.87$ (m, 2H, CHAr), 8.38 (s, 1H, CHAr), 8.00-7.96 (m, 2H, CHAr), 7.60-7.42 (m, 4H, CHAr), 1.74-1.38 (m, 4H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 135.1$ (d, $J_{\text{C-P}} = 7.7$ Hz, CAr), 131.3-125.1 (CAr), 13.9 (d, $^1J_{\text{C-P}} = 39.6$ Hz, CH_2). $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, CDCl_3): $\delta = -247.1$. MS (EI): 236.0 [M]⁺.

1-(2,4,6-Triisopropylphenyl)phosphirane (3).

^1H NMR (500 MHz, CDCl_3): $\delta = 7.14$ (d, $^4J_{\text{P-H}} = 1.8$ Hz, 2H, CHAr), 4.23 (m, 2H, ^iPr), 3.05 (m, 1H, ^iPr), 1.49 (m, 18H, ^iPr), 1.45 (m, 4H, CH_2). $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, CDCl_3): $\delta = 153.3$ (d, $J_{\text{C-P}} = 8.6$ Hz, CAr), 134.6 (d, $^1J_{\text{C-P}} = 41.4$ Hz, CAr), 122.2 (bs, CAr), 121.3 (bs, CAr), 34.38 (bs), 32.37 (d, $J_{\text{C-P}} = 8.9$ Hz), 24.7, 24.3, 24.0 (^iPr), 12.7 (d, $^1J_{\text{C-P}} = 39.7$ Hz, CH_2). $^{31}\text{P}\{^1\text{H}\}$ NMR (202 MHz, C_6D_6): $\delta = -242.1$. MS (EI): 262.0 [M]⁺

*1-(2,4,6-Tri-*t*-butylphenyl)phosphirane (4).*

^1H NMR (400 MHz, CDCl_3): $\delta = 7.16$ (d, $^4J_{\text{P-H}} = 1.9$ Hz, 2H, CHAr), 1.61 (bs, 18H, ^tBu), 1.26 (bs, 9H, ^tBu), 1.11-1.01 (m, 2H, CH_2), 0.91 – 0.85 (m, 2H, CH_2). $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, C_6D_6): $\delta = 156.2$, 148.6 (d, $^1J_{\text{C-P}} = 41.4$ Hz, CAr), 139.7, 122.2 (bs, CAr), 121.3 (bs, CAr), 122.4 (bs, CAr), 38.5, 34.3, 31.0, 14.5 (d, $^1J_{\text{C-P}} = 39.9$ Hz, CH_2). $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, C_6D_6): $\delta = -216.2$. MS (EI): 304.3 [M]⁺

B. Sample preparation and EPR measurements.

The X-band cw EPR spectra of triplet phosphinidenes were recorded after UV-irradiation of the corresponding 1-arylphosphirane (see Scheme 2) in glassy methylcyclohexane (MCH) at 5 K. In a typical procedure, the 1-arylphosphirane was dissolved in freshly distilled MCH in the ratio of 1:500 (1:1000 in the case of AnthPC₂H₄ due to its low solubility in MCH), placed in a 3 mm o.d. quartz EPR tube, and sealed under vacuum. The sample tube was placed in the cavity of an EPR spectrometer equipped with a helium gas-flow thermostat. Then, the sample was cooled to 5 K to form glass and photolyzed at 60 K using a low-pressure mercury lamp (at $\lambda = 254$ nm). EPR spectra were recorded at 5 K using a standard 9 GHz spectrometer (*Bruker Elexsys 500*, the modulation frequency 100 KHz) at a sufficiently low microwave power to avoid the saturation effects.

C. Computational details.

The geometries of all systems under consideration were optimized within the density functional theory (DFT) method at the B3LYP/def2-TZVP level of theory. The equilibrium (no imaginary frequency) and transition state (one imaginary frequency) geometry configurations were confirmed by vibrational frequency calculations. The Cartesian coordinates of the optimized species

are given in the Section 4. The based on DFT formalism ZFS parameters including the spin-spin (SS) and spin-orbit coupling (SOC) contributions to the total \mathbf{D} tensor were obtained at the PBE/Ahlich-DZ level of theory by using modified McWeeny-Mizuno equation [2] and coupled perturbed (CP) approach [3], respectively. Hyperfine constants were calculated at the B3LYP/def2-TZVPP level of theory.

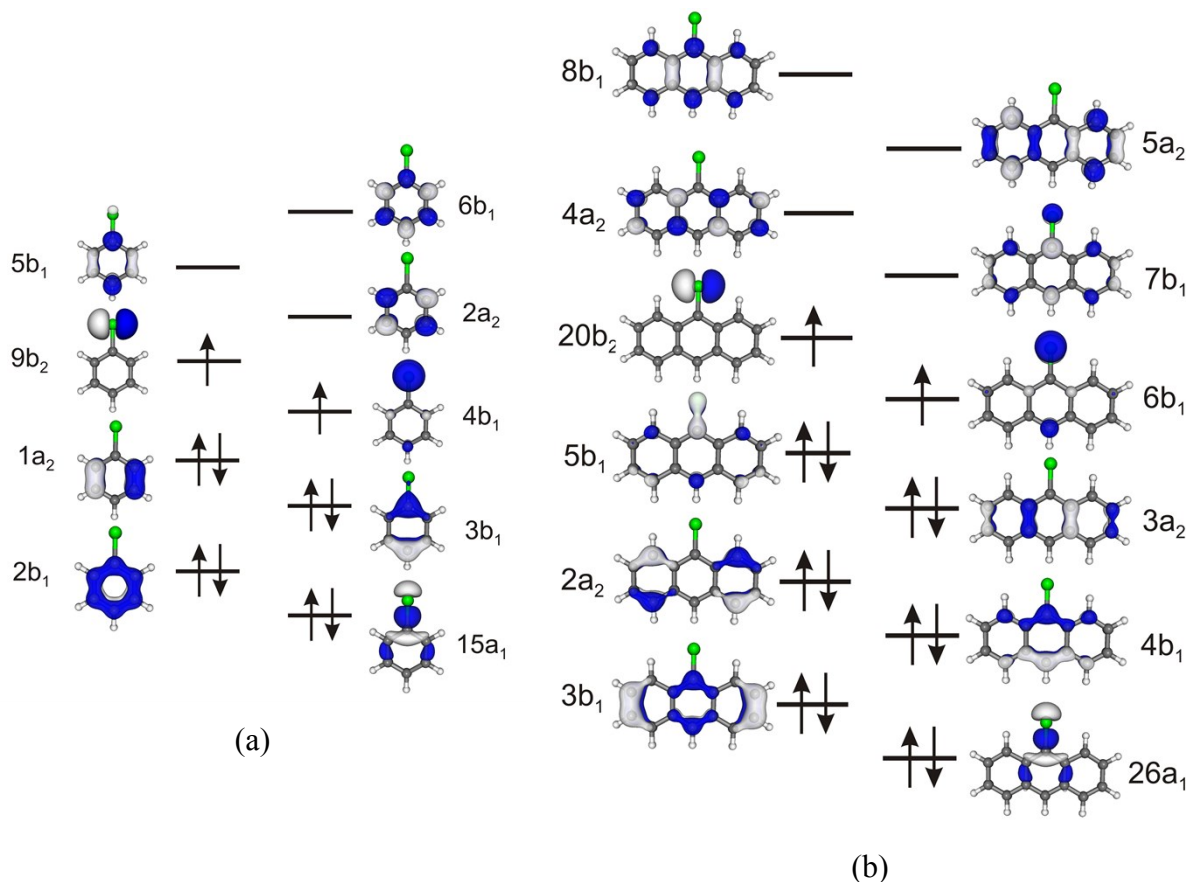


Fig. S1. The CASSCF active space of the phosphinidenes PhP (MesP, TippP, Mes*P) (a) and AnthP (b).

In *ab initio* post Hartree-Fock calculations, the values of the \hat{D} tensor for phosphinidenes PhP, MesP, TippP, Mes*P and AnthP were obtained employing the multiconfigurational formalism with ground triplet and three excited singlet states on the top of the state-average CASSCF wave function. The CASSCF active space consists of 9 orbitals and 10 electrons and 12 orbitals and 14 electrons for phosphinidenes PhP, MesP, TippP, Mes*P and AnthP, respectively. The CASSCF active space of these phosphinidenes is shown in Fig. S1. Scalar relativistic effects were taken into account by a standard second-order Douglas-Kroll-Hess (DKH) procedure [4]. An all-electron relativistically contracted version of Ahlich polarized triple- ζ basis set DKH-def2-TZVP [5] was used for all atoms. The spin-orbit effects were included using the quasi degenerate perturbation

theory (QDPT) [6]. Dynamic electron correlations were taken into account including the N-electron valence second-order perturbation theory (NEVPT2) [7]. All calculations were performed with the ORCA program package (version 4.0.1.2) [8].

2. Experimental and calculated fine and hyperfine parameters of the studied triplet phosphinidenes

Table S1. Calculated and experimental ZFS parameters D (cm^{-1}) in triplet phosphinidenes R -P^{**} and calculated spin densities on phosphorus atom $\rho(\text{P}\cdot)$.

R-P	PBE/Ahlfriech-DZ / CASSCF/NEVPT2 calculations					Expt.	
	D_{SS}	D_{SO}	$D_{\text{SS+SO}}$	E/D	$\rho(\text{P}\cdot)$	D	E/D
Anth	0.298 / 0.286	3.748 / 2.967	4.046 / 3.253	0.0284/0.000	1.63	3.741	0.0013
Mes	0.319 / 0.303	3.890 / 3.296	4.209 / 3.599	0.0200/0.0005	1.80	4.116 ^{a)}	0.0010
Tipp	0.315 / 0.304	4.005 / 3.329	4.320 / 3.633	0.0165/0.0009	1.78	4.252	0.0014
Ph	0.336 / 0.308	4.029 / 3.439	4.365 / 3.747	0.0153/0.0002	1.86	4.322	0.0010
H	0.414 / 0.367	3.951 / 3.043	4.365 / 3.410	0.000 / 0.001	2.0	4.4 ^{b)}	-
Dmp	0.326 / - ^{c)}	4.016 / - ^{c)}	4.342 / - ^{c)}	0.0167 / - ^{c)}	1.82	-	-
Mes*	0.310 / 0.315	4.120 / 3.563	4.430 / 3.877	0.0176 / 0.000	1.75	-	-

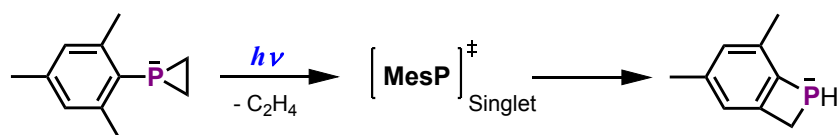
^{a)} data from Ref. [9]. ^{b)} data from Ref. [10], ^{c)} unable to calculate by *ab initio* approach

Table S2. The DFT calculated contributions of different excitations to the spin-orbit term of the ZFS parameter D .

Contribution	<i>PhP</i>	<i>AnthP</i>	<i>MesP</i>	<i>TippP</i>	<i>Mes*P</i>	<i>DmpP</i>
SPIN-ORBIT	4.029	3.748	3.885	4.005	4.120	4.016
SOMO->VMO (alpha->alpha)	-0.005	-0.044	-0.023	-0.017	-0.019	-0.019
DOMO->SOMO (beta ->beta)	0.309	0.198	0.288	0.279	0.274	0.301
SOMO->SOMO (alpha->beta)	3.845	3.707	3.738	3.860	3.980	3.852
DOMO->VMO (beta ->alpha)	-0.119	-0.114	-0.118	-0.117	-0.116	-0.118

4. Calculated equilibrium structures and potential energy profiles for internal rearrangements of the studied phosphinidenes.

A. Internal rearrangement of *MesP*:



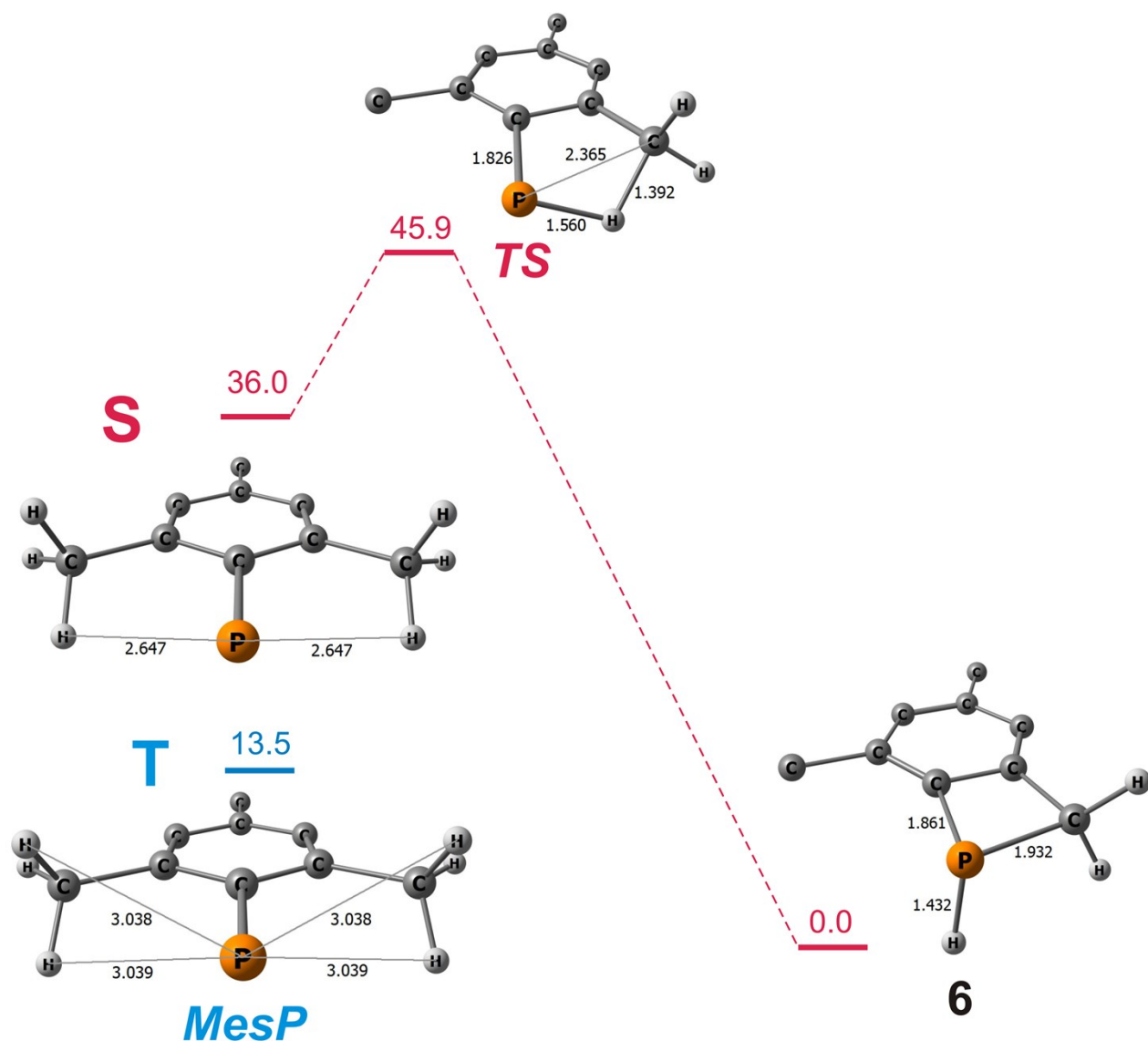
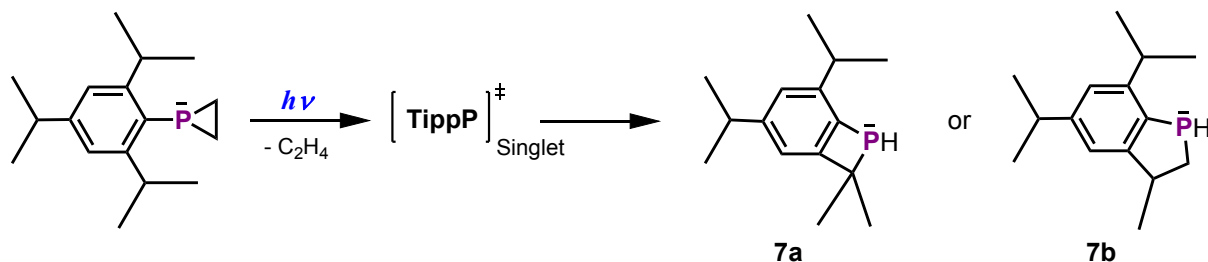


Fig. S2. Calculated potential energy profile for internal rearrangement of singlet MesP.

B. Internal rearrangements of TippP.

We examined two possible rearrangements of the excited intermediates TippP* producing the products with four-membered (**7a**) or five-membered (**7b**) cycles. Figure S3 demonstrates the rearrangements in TippP, producing both products, **7a** and **7b**.



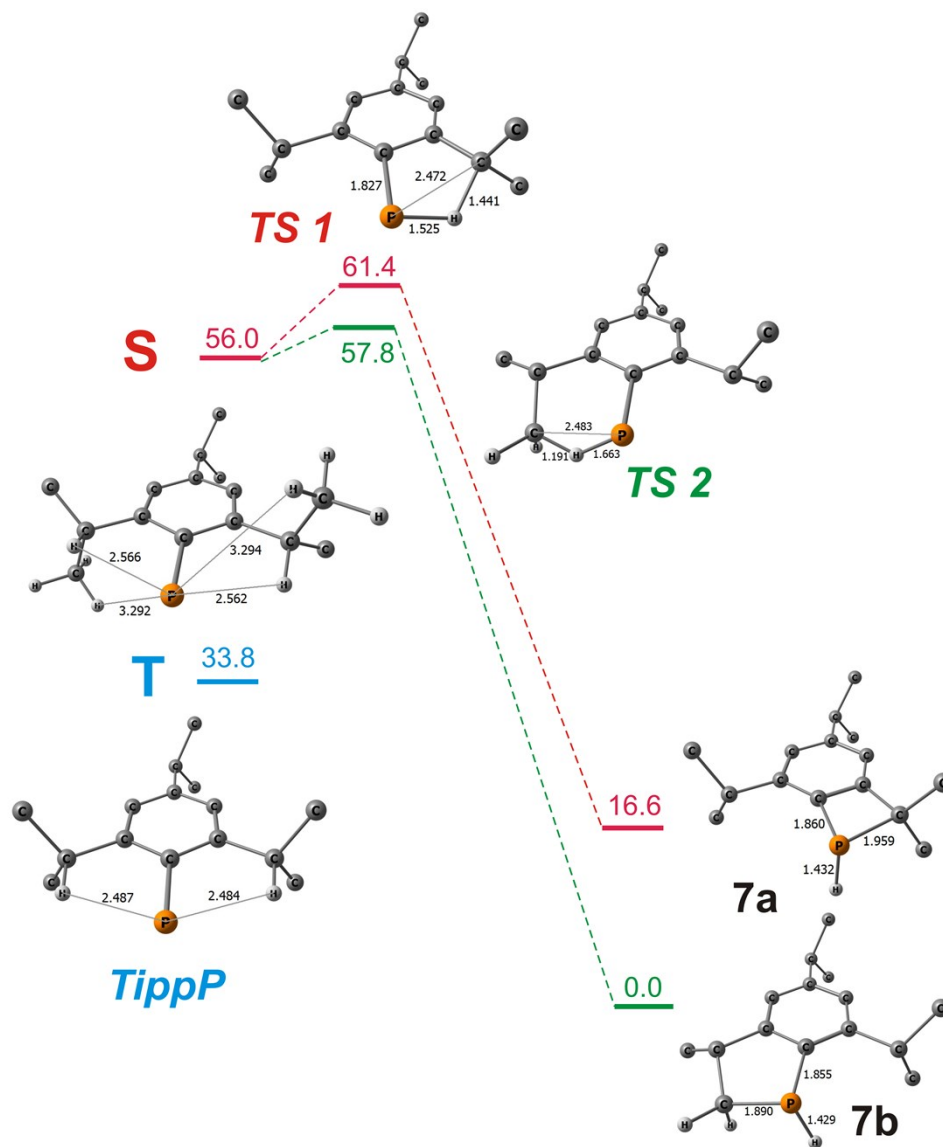
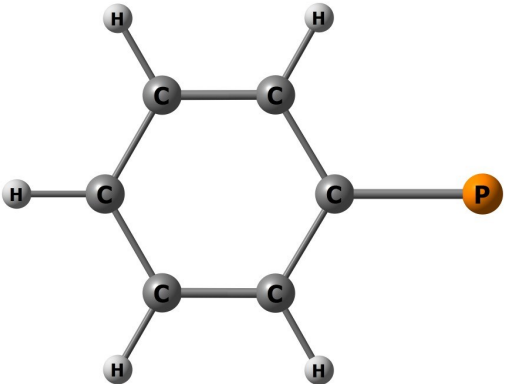


Fig. S3. Calculated potential energy profile for internal rearrangement of singlet TippP.

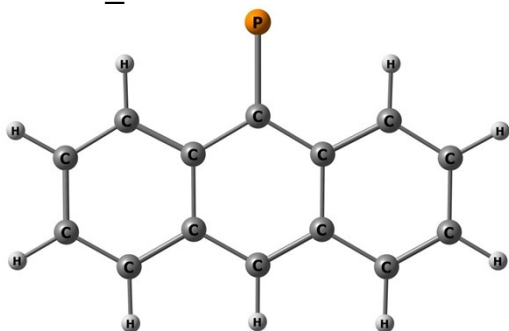
References

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4. Cartesian coordinates of molecules under consideration.

PhP_T		Method : UB3LYP/def2-TZVP Charge : 0 Multiplicity : 3 Total energy: -572.8298164 a.u.	
			
6	0.000000000	0.000000000	0.512087000
6	0.000000000	1.210089000	-0.211981000
6	0.000000000	-1.210089000	-0.211981000
1	0.000000000	2.152828000	0.321763000
1	0.000000000	-2.152828000	0.321763000
6	0.000000000	1.206640000	-1.599085000
6	0.000000000	-1.206640000	-1.599085000
1	0.000000000	2.144369000	-2.142031000
1	0.000000000	-2.144369000	-2.142031000
6	0.000000000	0.000000000	-2.296861000
1	0.000000000	0.000000000	-3.378535000
15	0.000000000	0.000000000	2.321017000

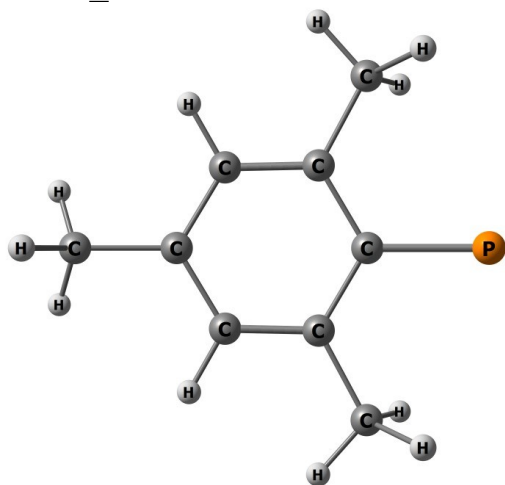
AnthP_T



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Charge : 0
Multiplicity : 3
Total energy: -880.00765085 a.u.

6	-1.273261000	0.024059000	-2.105973000
6	-1.273261000	-0.043781000	-0.686090000
6	-1.273261000	-1.288117000	0.028378000
6	-1.273261000	1.199398000	0.034926000
6	-1.273261000	1.187443000	1.432418000
6	-1.273261000	-0.006599000	2.159942000
6	-1.273261000	-1.263775000	1.462951000
6	-1.273261000	1.222399000	-2.768294000
6	-1.273261000	2.428963000	-0.687060000
1	-1.273261000	2.133162000	1.963030000
6	-1.273261000	0.004067000	3.584553000
6	-1.273261000	-2.449539000	2.247930000
6	-1.273261000	-2.403686000	3.616431000
6	-1.273261000	-1.161534000	4.296748000
1	-1.273261000	0.963047000	4.089896000
1	-1.273261000	-3.409464000	1.745676000
1	-1.273261000	-3.323489000	4.188287000
1	-1.273261000	-1.142624000	5.378242000
6	-1.273261000	2.444606000	-2.052729000
1	-1.273261000	-0.899201000	-2.672733000
1	-1.273261000	1.238012000	-3.850085000
1	-1.273261000	3.355493000	-0.124110000
1	-1.273261000	3.382606000	-2.594364000
15	-1.273261000	-2.845710000	-0.857917000

MesP_T



Method : UB3LYP/def2-TZVP

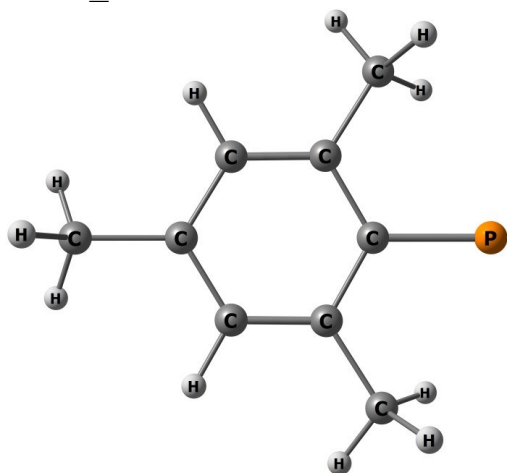
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Multiplicity : 3

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6	1.256161000	1.197066000	-0.011123000
6	1.256161000	-1.197066000	-0.011123000
6	-0.132729000	-1.224927000	-0.003441000
6	1.973889000	0.000000000	-0.011720000
15	-2.659767000	0.000000000	0.009740000
1	1.798467000	-2.136981000	-0.018559000
1	1.798467000	2.136981000	-0.018559000
6	-0.847766000	-2.552719000	-0.004084000
1	-1.485924000	-2.664846000	0.876392000
1	-1.492190000	-2.661026000	-0.880461000
1	-0.134413000	-3.377484000	-0.008309000
6	-0.847766000	2.552719000	-0.004084000
1	-1.492190000	2.661026000	-0.880461000
1	-1.485924000	2.664846000	0.876392000
1	-0.134413000	3.377484000	-0.008309000
6	3.479277000	0.000000000	0.017118000
1	3.887799000	-0.884269000	-0.474819000
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MesP_S



Method : UB3LYP/def2-TZVP

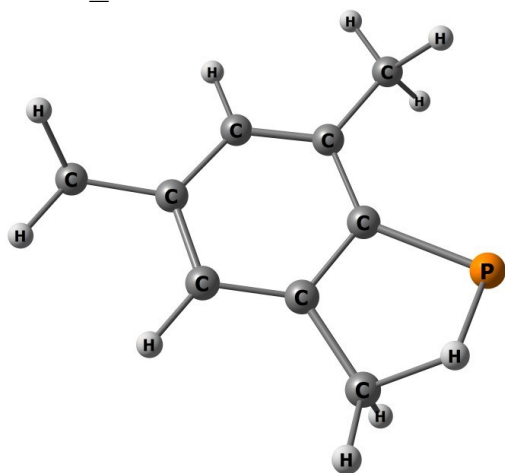
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Multiplicity : 1

Total energy: -690.9784672 a.u.

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6	-1.270973000	-1.195983000	-0.011522000
6	-1.270978000	1.195979000	-0.011521000
6	0.118542000	1.218545000	0.003706000
6	-1.991824000	-0.000003000	-0.013619000
15	2.618789000	0.000001000	-0.021068000
1	-1.806683000	2.140527000	-0.035248000
1	-1.806673000	-2.140533000	-0.035251000
6	0.918377000	2.491689000	0.029689000
1	1.325808000	2.688376000	1.027159000
1	1.771175000	2.422400000	-0.668261000
1	0.335893000	3.363933000	-0.270385000
6	0.918389000	-2.491682000	0.029690000
1	1.771190000	-2.422387000	-0.668256000
1	1.325816000	-2.688371000	1.027161000
1	0.335912000	-3.363928000	-0.270393000
6	-3.499770000	-0.000006000	0.001820000
1	-3.903367000	0.882537000	-0.498141000
1	-3.903364000	-0.882550000	-0.498142000
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MesP_TS



Method : UB3LYP/def2-TZVP

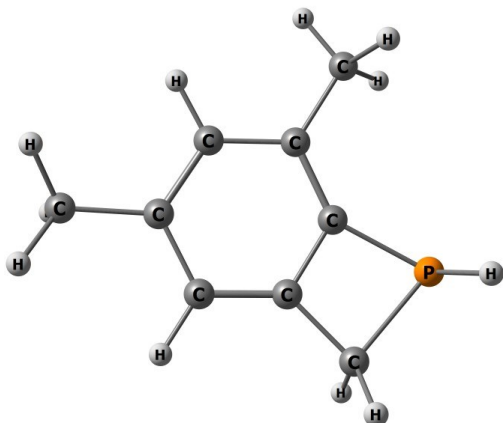
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6	1.440594000	1.034109000	0.015360000
6	1.109923000	-1.351727000	-0.020263000
6	-0.257700000	-1.112953000	0.047044000
6	1.980543000	-0.263589000	-0.023618000
15	-2.593081000	-0.023346000	-0.073158000
1	1.497622000	-2.365027000	-0.038090000
1	2.125738000	1.876959000	0.014962000
6	-1.396944000	-2.052887000	0.129976000
1	-1.808251000	-2.231042000	1.118098000
1	-2.301586000	-1.414898000	-0.714443000
1	-1.385849000	-2.964570000	-0.470558000
6	-0.474249000	2.695520000	0.042893000
1	-1.091889000	2.883860000	-0.841314000
1	-1.106177000	2.867866000	0.919754000
1	0.324858000	3.437493000	0.055778000
6	3.476268000	-0.460461000	-0.042226000
1	3.735448000	-1.507802000	-0.203593000
1	3.946250000	0.125833000	-0.835944000
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6



Method : UB3LYP/def2-TZVP

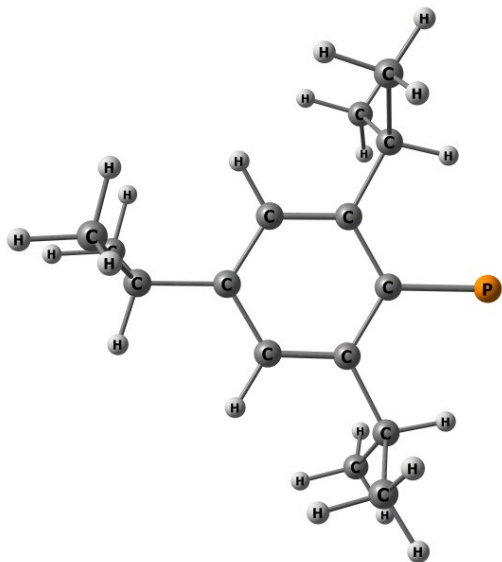
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Total energy: -691.0485691 a.u.

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6	-1.521563000	0.967573000	0.009001000
6	-1.020412000	-1.401758000	0.017297000
6	0.322786000	-1.060004000	0.025266000
6	-1.960640000	-0.364038000	0.012316000
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1	-1.345746000	-2.436728000	0.020039000
1	-2.268190000	1.755819000	0.006498000
6	1.634036000	-1.815528000	0.027834000
1	1.800282000	-2.478821000	-0.821685000
1	2.931337000	0.032994000	1.242502000
1	1.854772000	-2.351535000	0.951307000
6	0.271932000	2.766751000	0.009738000
1	0.663027000	3.054915000	0.990053000
1	1.070042000	2.935699000	-0.717246000
1	-0.553932000	3.438180000	-0.228423000
6	-3.437432000	-0.672749000	-0.024730000
1	-3.664812000	-1.595806000	0.511502000
1	-4.024684000	0.131235000	0.421719000
1	-3.786231000	-0.799818000	-1.054307000

TippP_T



Method : UB3LYP/def2-TZVP

Charge : 0

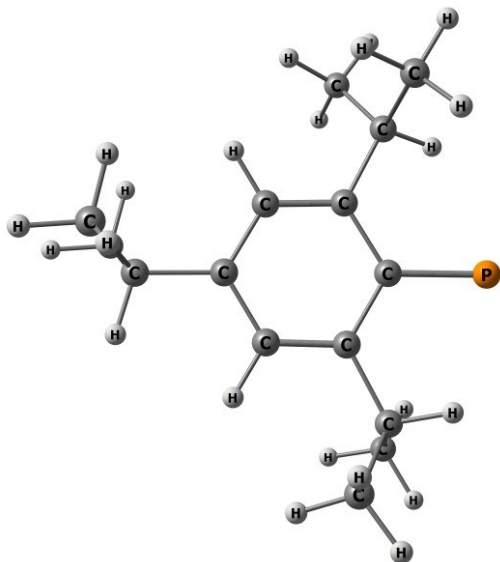
Multiplicity : 3

Total energy: -926.9819478 a.u.

6	-0.510175000	1.143485000	0.000105000
6	0.888673000	0.878788000	0.000037000
6	-1.403043000	0.079786000	0.000010000
6	0.394075000	-1.495438000	-0.000191000
6	1.334569000	-0.470530000	-0.000064000
6	-0.977739000	-1.250380000	-0.000175000
15	2.085148000	2.244564000	-0.000063000
1	0.735930000	-2.524922000	-0.000299000
1	-2.466331000	0.290623000	0.000059000
6	-1.969638000	-2.400968000	-0.000291000
1	-1.382414000	-3.324669000	-0.000867000
6	-2.840413000	-2.408883000	-1.267330000
6	-2.839449000	-2.409842000	1.267401000
1	-2.224520000	-2.437164000	2.168927000
1	-3.471729000	-1.520469000	1.321084000
1	-3.495136000	-3.283978000	1.275745000
1	-3.473001000	-1.519652000	-1.319692000
1	-3.495859000	-3.283194000	-1.275964000
1	-2.226167000	-2.435192000	-2.169348000
6	2.816678000	-0.823339000	0.000001000
1	3.375393000	0.118026000	0.000040000
6	3.225856000	-1.587150000	-1.269314000
6	3.225661000	-1.587154000	1.269386000
1	2.965029000	-1.025761000	2.168622000
1	2.731755000	-2.560138000	1.327173000
1	4.304386000	-1.761373000	1.278645000
1	2.731949000	-2.560128000	-1.327209000
1	4.304578000	-1.761389000	-1.278381000
1	2.965394000	-1.025743000	-2.168591000
6	-1.051236000	2.568286000	0.000233000

1	-0.189515000	3.243598000	0.000493000
6	-1.860574000	2.876949000	1.269521000
6	-1.860082000	2.877241000	-1.269321000
1	-1.268835000	2.692601000	-2.168218000
1	-2.761194000	2.262393000	-1.329478000
1	-2.171993000	3.924505000	-1.277185000
1	-2.761756000	2.262158000	1.329215000
1	-2.172451000	3.924223000	1.277497000
1	-1.269697000	2.692096000	2.168620000

TippP_S



Method : UB3LYP/def2-TZVP

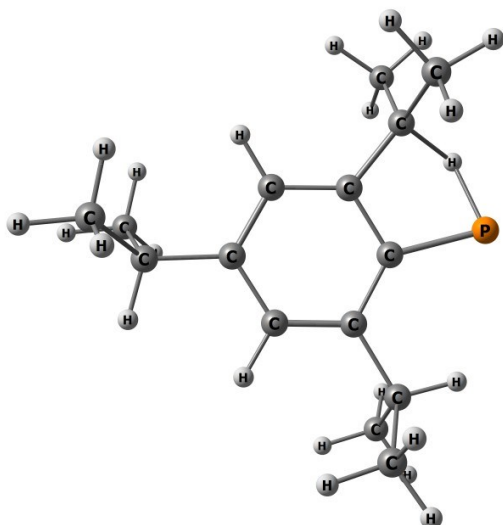
Charge : 0

Multiplicity : 1

Total energy: -926.9465104 a.u.

6	-0.501643000	1.152721000	-0.073665000
6	0.915563000	0.858320000	-0.008903000
6	-1.416047000	0.114290000	-0.041826000
6	0.342762000	-1.518597000	0.046391000
6	1.314720000	-0.529197000	0.075979000
6	-1.020574000	-1.226695000	0.001622000
15	2.129770000	2.153580000	-0.064338000
1	0.642775000	-2.559228000	0.077590000
1	-2.473720000	0.343781000	-0.068416000
6	-2.043627000	-2.346556000	0.003460000
1	-1.485692000	-3.287062000	0.039797000
6	-2.882419000	-2.355656000	-1.285725000
6	-2.943521000	-2.294692000	1.249748000
1	-2.352179000	-2.314207000	2.166995000
1	-3.553323000	-1.388695000	1.262752000
1	-3.620657000	-3.151848000	1.263301000
1	-3.485275000	-1.449337000	-1.375008000
1	-3.563300000	-3.209956000	-1.287955000
1	-2.247876000	-2.424618000	-2.171155000
6	2.777473000	-0.928028000	0.135537000
1	3.306226000	-0.050554000	0.520515000
6	3.341025000	-1.202902000	-1.271131000
6	3.055229000	-2.111851000	1.071834000
1	2.631304000	-1.945108000	2.063998000
1	2.657362000	-3.054554000	0.687454000
1	4.133624000	-2.242147000	1.186404000
1	2.835090000	-2.048846000	-1.744574000
1	4.406942000	-1.436699000	-1.212827000
1	3.222670000	-0.334475000	-1.922023000
6	-0.998009000	2.585479000	-0.112372000

1	-0.174158000	3.168925000	-0.536807000
6	-1.240819000	3.129570000	1.308075000
6	-2.239963000	2.789838000	-0.989320000
1	-2.098264000	2.372867000	-1.988256000
1	-3.137702000	2.339585000	-0.557653000
1	-2.439512000	3.858167000	-1.097963000
1	-2.031633000	2.571528000	1.816855000
1	-1.541894000	4.179191000	1.265263000
1	-0.338265000	3.063329000	1.918568000

TippP_TS1

Method : UB3LYP/def2-TZVP

Charge : 0

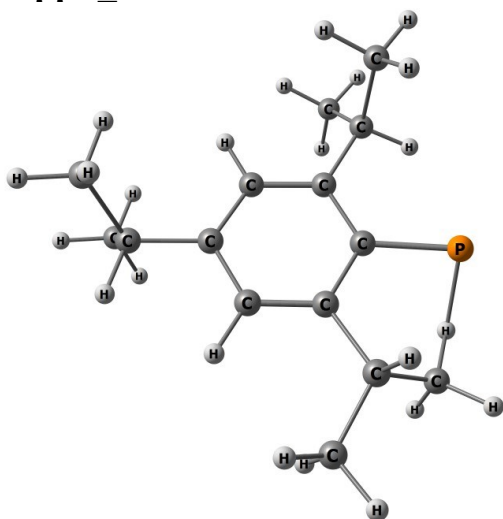
Multiplicity : 1

Total energy: -926.9379159 a.u.

6	-0.394806000	-1.103107000	-0.032551000
6	-1.111655000	0.098392000	-0.057867000
6	0.990572000	-1.125567000	-0.059187000
6	0.957362000	1.277807000	0.023896000
6	-0.439062000	1.322193000	-0.001736000
6	1.690855000	0.086271000	-0.013296000
15	-2.883835000	-0.330358000	-0.179165000
1	1.510043000	2.211434000	0.065368000
1	1.528972000	-2.066982000	-0.075384000
6	3.211190000	0.119072000	0.020133000
1	3.502598000	1.174282000	0.023279000
6	3.835426000	-0.523496000	-1.228888000
6	3.774680000	-0.513723000	1.303406000
1	3.361794000	-0.034650000	2.193263000
1	3.535095000	-1.578839000	1.357366000
1	4.862952000	-0.416595000	1.337852000
1	3.603350000	-1.590082000	-1.285843000
1	4.923794000	-0.423585000	-1.211860000
1	3.464644000	-0.052975000	-2.141479000
6	-1.204744000	2.635425000	0.007175000
1	-2.271778000	2.381911000	0.010765000
6	-0.941388000	3.462618000	-1.261224000
6	-0.932986000	3.458007000	1.276141000
1	-1.156117000	2.880359000	2.175054000
1	0.113140000	3.768883000	1.329556000
1	-1.548474000	4.361022000	1.289898000
1	0.105945000	3.769034000	-1.319434000
1	-1.554497000	4.367420000	-1.267835000
1	-1.171793000	2.888336000	-2.160385000
6	-1.346023000	-2.257617000	0.000637000
1	-2.421905000	-1.665360000	-0.753838000

6	-1.727469000	-2.798751000	1.365426000
6	-1.122550000	-3.347925000	-1.034396000
1	-0.996150000	-2.938541000	-2.036580000
1	-0.205237000	-3.886497000	-0.772205000
1	-1.938930000	-4.071837000	-1.041214000
1	-0.952011000	-3.508211000	1.683486000
1	-2.673112000	-3.343059000	1.334155000
1	-1.801198000	-2.007692000	2.107472000

TippP_TS2



Method : UB3LYP/def2-TZVP

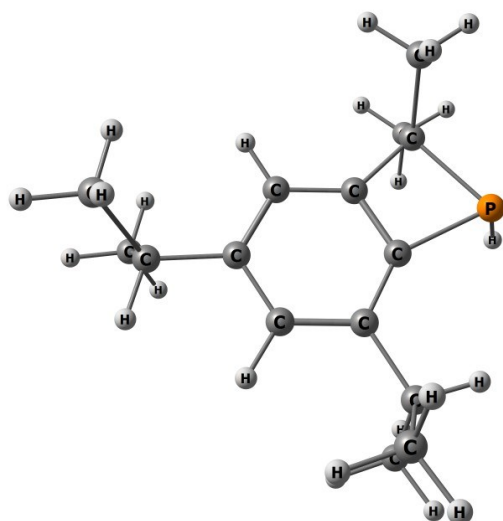
Charge : 0

Multiplicity : 1

Total energy: -926.9437653 a.u.

6	-0.155560000	1.163571000	-0.057000000
6	1.035387000	0.417389000	0.010515000
6	-1.374567000	0.485924000	-0.046450000
6	-0.260341000	-1.624982000	0.103089000
6	0.972671000	-0.987180000	0.121652000
6	-1.454861000	-0.904215000	0.021658000
15	2.684516000	1.209772000	-0.008402000
1	-0.309131000	-2.706098000	0.162694000
1	-2.290586000	1.062330000	-0.105546000
6	-2.792421000	-1.627667000	0.010471000
1	-2.571932000	-2.697898000	0.081390000
6	-3.558957000	-1.405121000	-1.303347000
6	-3.661728000	-1.259523000	1.223740000
1	-3.131768000	-1.446251000	2.159751000
1	-3.942356000	-0.203567000	1.205157000
1	-4.583658000	-1.846843000	1.230972000
1	-3.825062000	-0.353288000	-1.432793000
1	-4.485105000	-1.985671000	-1.314299000
1	-2.959161000	-1.704348000	-2.165088000
6	2.297758000	-1.704385000	0.330530000
1	2.597122000	-1.479824000	1.362869000
6	3.375665000	-1.107815000	-0.570407000
6	2.259361000	-3.226538000	0.164730000
1	1.582973000	-3.684738000	0.887809000
1	1.928594000	-3.511321000	-0.837135000
1	3.250452000	-3.654995000	0.329138000
1	3.365132000	-1.558653000	-1.571458000
1	4.378559000	-1.144979000	-0.155262000
1	3.198627000	-0.014581000	-1.009111000
6	-0.091948000	2.682569000	-0.093209000
1	0.924295000	2.939024000	-0.430865000
6	-0.277070000	3.286176000	1.310679000

6	-1.061131000	3.320473000	-1.096490000
1	-0.937897000	2.893762000	-2.093385000
1	-2.102439000	3.183050000	-0.795758000
1	-0.883087000	4.396329000	-1.162651000
1	-1.284804000	3.087911000	1.684527000
1	-0.132040000	4.369398000	1.289490000
1	0.431977000	2.862612000	2.024626000

7a

Method : UB3LYP/def2-TZVP

Charge : 0

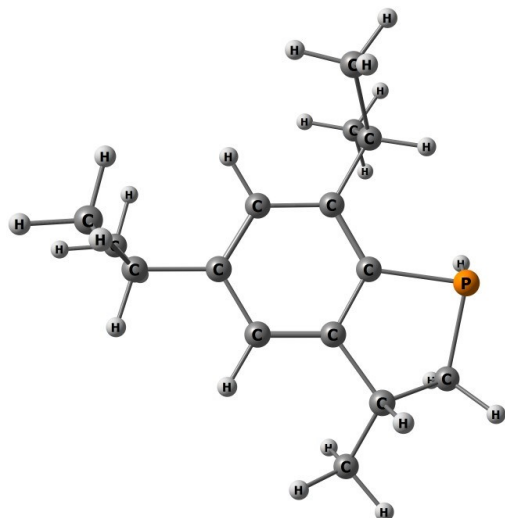
Multiplicity : 1

Total energy: -927.0094392 a.u.

6	0.655737000	-0.944046000	0.005633000
6	0.994786000	0.406958000	0.004194000
6	-0.664954000	-1.357522000	-0.000678000
6	-1.294417000	0.979571000	-0.000748000
6	0.039973000	1.414306000	-0.009539000
6	-1.663356000	-0.370429000	0.003694000
15	2.828758000	0.125682000	-0.130301000
1	-2.088237000	1.719769000	0.000559000
1	-0.929438000	-2.409131000	-0.004429000
6	-3.136797000	-0.751270000	0.011138000
1	-3.705732000	0.183774000	0.007389000
6	-3.526139000	-1.519630000	1.284500000
6	-3.535867000	-1.535789000	-1.249161000
1	-3.288443000	-0.979755000	-2.155457000
1	-3.020789000	-2.498329000	-1.297101000
1	-4.610534000	-1.734612000	-1.254321000
1	-3.009049000	-2.480611000	1.341336000
1	-4.600472000	-1.719782000	1.299858000
1	-3.273159000	-0.951375000	2.181666000
6	0.414534000	2.885527000	-0.020602000
1	1.506930000	2.929635000	-0.075260000
6	-0.011178000	3.593206000	1.276250000
6	-0.136268000	3.614664000	-1.256098000
1	0.191595000	3.131376000	-2.178283000
1	-1.228754000	3.628985000	-1.255819000
1	0.208768000	4.651368000	-1.274271000
1	-1.098535000	3.597930000	1.384697000
1	0.328563000	4.631911000	1.276609000
1	0.409163000	3.097597000	2.153424000
6	2.007888000	-1.648139000	-0.004485000
1	3.182416000	0.287556000	1.247840000

6	2.263665000	-2.502395000	-1.246798000
6	2.325697000	-2.417995000	1.276075000
1	2.120556000	-1.821607000	2.166229000
1	1.717603000	-3.327070000	1.332803000
1	3.375416000	-2.722473000	1.301797000
1	1.613253000	-3.383065000	-1.244401000
1	3.298453000	-2.852542000	-1.274677000
1	2.069228000	-1.946878000	-2.165944000

7b



Method : UB3LYP/def2-TZVP

Charge : 0

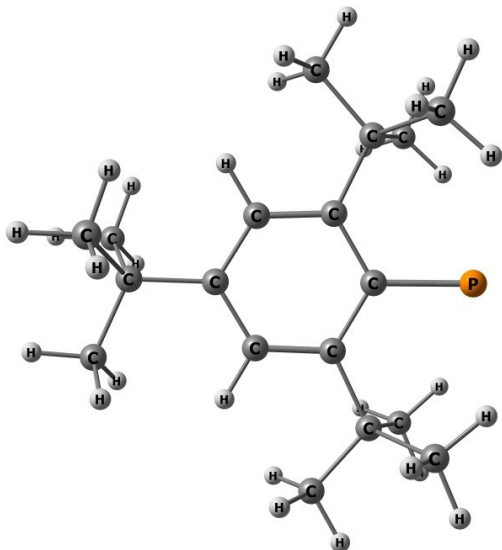
Multiplicity : 1

Total energy: -927.0358344 a.u.

6	0.129796000	1.143835000	-0.070421000
6	-1.016768000	0.344233000	-0.130814000
6	1.370424000	0.504917000	-0.017798000
6	0.334345000	-1.654799000	-0.137720000
6	-0.918346000	-1.052077000	-0.177380000
6	1.495635000	-0.885401000	-0.048653000
15	-2.776382000	0.910691000	-0.289606000
1	0.419819000	-2.735344000	-0.171835000
1	2.267183000	1.109989000	0.049835000
6	2.858871000	-1.557623000	0.010154000
1	2.678984000	-2.636866000	-0.026238000
6	3.593001000	-1.260989000	1.327654000
6	3.733272000	-1.198323000	-1.201873000
1	3.229063000	-1.442821000	-2.138779000
1	3.969445000	-0.131622000	-1.219231000
1	4.678296000	-1.746598000	-1.170779000
1	3.827488000	-0.197895000	1.421108000
1	4.534669000	-1.813582000	1.375969000
1	2.986831000	-1.545490000	2.189879000
6	-2.239754000	-1.790232000	-0.331828000
1	-2.396999000	-1.949681000	-1.407431000
6	-3.343627000	-0.832972000	0.166890000
6	-2.305774000	-3.157033000	0.353681000
1	-1.576873000	-3.855407000	-0.062313000
1	-2.111769000	-3.064668000	1.425082000
1	-3.294924000	-3.602482000	0.225244000
1	-3.442559000	-0.913293000	1.250999000
1	-4.309827000	-1.063926000	-0.281685000
1	-2.929567000	1.527442000	0.989993000
6	0.026327000	2.661355000	-0.015500000
1	-1.000184000	2.922517000	-0.292135000

6	0.949258000	3.363657000	-1.021782000
6	0.264141000	3.184302000	1.411567000
1	-0.418528000	2.716857000	2.123854000
1	1.284639000	2.970914000	1.739459000
1	0.115376000	4.266170000	1.457495000
1	2.003462000	3.207965000	-0.781631000
1	0.768348000	4.441127000	-1.013447000
1	0.778548000	2.999243000	-2.036402000

Mes*P_T

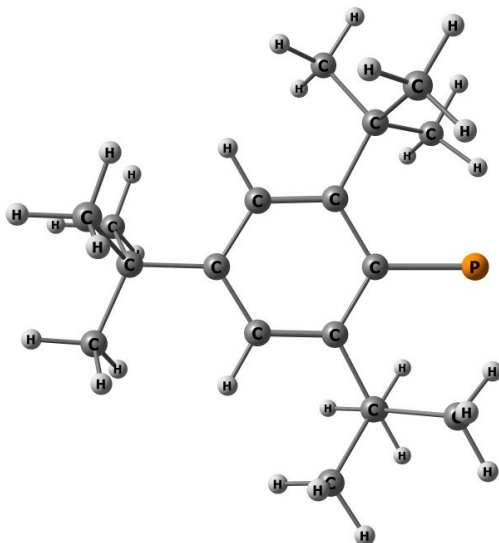


Method : UB3LYP/def2-TZVP
Charge : 0
Multiplicity : 3
Total energy: -1044.9346599 a.u.

6	0.559102000	-1.207475000	-0.000095000
6	1.180550000	0.085095000	0.000032000
6	-0.834322000	-1.276949000	-0.000235000
6	-1.030022000	1.091671000	-0.000090000
6	0.349111000	1.259549000	-0.000036000
6	-1.654321000	-0.155331000	-0.000201000
15	2.993660000	0.237161000	0.000288000
1	-1.657748000	1.967144000	0.000002000
1	-1.301081000	-2.245439000	-0.000396000
6	-3.188740000	-0.244186000	0.000027000
6	-3.745277000	0.454575000	1.260367000
6	-3.695039000	-1.696038000	-0.000926000
1	-3.364075000	-2.243045000	-0.886229000
1	-3.364457000	-2.244196000	0.883807000
1	-4.787011000	-1.700824000	-0.001114000
1	-3.366230000	-0.019070000	2.168527000
1	-4.836595000	0.393492000	1.275541000
1	-3.471419000	1.509901000	1.294458000
6	0.905439000	2.711647000	-0.000074000
6	1.741749000	2.979894000	1.272078000
6	-0.214028000	3.774193000	-0.000278000
1	-0.847562000	3.711190000	-0.887197000
1	-0.847669000	3.711424000	0.886584000
1	0.245921000	4.764077000	-0.000378000
1	1.137572000	2.823344000	2.168616000
1	2.093374000	4.014851000	1.275395000
1	2.618024000	2.335514000	1.343680000
6	1.349711000	-2.547358000	-0.000072000
6	0.419228000	-3.779908000	-0.000212000
6	2.218181000	-2.674298000	1.272160000
1	2.975803000	-1.893591000	1.344028000

1	1.596268000	-2.619817000	2.168564000
1	2.735850000	-3.636986000	1.275500000
1	-0.216348000	-3.820021000	0.886416000
1	1.034479000	-4.681452000	-0.000218000
1	-0.216214000	-3.819944000	-0.886939000
6	2.218432000	-2.674156000	-1.272144000
1	2.975969000	-1.893352000	-1.343830000
1	2.736212000	-3.636788000	-1.275444000
1	1.596667000	-2.619710000	-2.168654000
6	1.741977000	2.979678000	-1.272128000
1	2.093714000	4.014599000	-1.275513000
1	2.618197000	2.335204000	-1.343529000
1	1.137908000	2.823100000	-2.168733000
6	-3.746174000	0.456379000	-1.258873000
1	-4.837473000	0.394886000	-1.273528000
1	-3.472833000	1.511878000	-1.291521000
1	-3.367490000	-0.015687000	-2.168014000

Mes*P_S

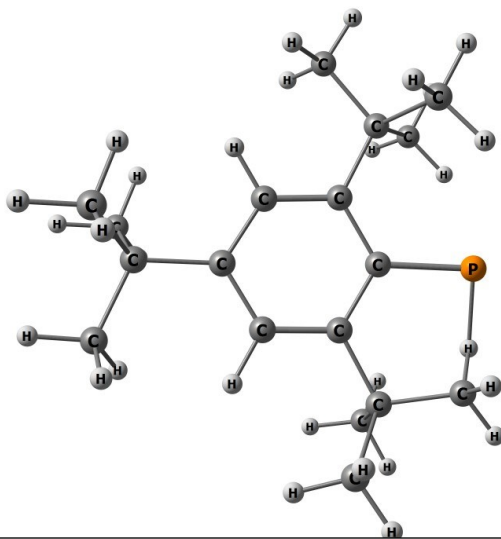


Method : UB3LYP/def2-TZVP
Charge : 0
Multiplicity : 1
Total energy: -1044.9128014 a.u.

6	-0.485790000	-1.211272000	-0.029676000
6	-1.154722000	0.041554000	0.002612000
6	0.908498000	-1.244944000	-0.039261000
6	1.021598000	1.119201000	0.041069000
6	-0.363766000	1.226973000	0.031175000
6	1.696854000	-0.100775000	0.001468000
15	-2.984426000	0.134831000	0.005052000
1	1.604542000	2.028194000	0.071175000
1	1.392966000	-2.207537000	-0.071096000
6	3.233735000	-0.135523000	0.000661000
6	3.769930000	0.616019000	-1.237628000
6	3.787023000	-1.569603000	-0.038834000
1	3.472252000	-2.151175000	0.830386000
1	3.473496000	-2.102272000	-0.939204000
1	4.878784000	-1.540429000	-0.037254000
1	3.410644000	0.153351000	-2.159442000
1	4.863197000	0.598645000	-1.251618000
1	3.454709000	1.660618000	-1.244513000
6	-1.010990000	2.625323000	-0.006793000
6	-1.373838000	2.974665000	-1.467891000
6	-0.087882000	3.730197000	0.544403000
1	0.257314000	3.501906000	1.554894000
1	0.785199000	3.886699000	-0.089796000
1	-0.630530000	4.677753000	0.577154000
1	-0.471024000	3.021463000	-2.079313000
1	-1.871207000	3.947559000	-1.520843000
1	-2.040244000	2.226163000	-1.898776000
6	-1.267872000	-2.538854000	0.004285000
6	-0.467709000	-3.724131000	-0.571419000
6	-2.535063000	-2.421721000	-0.845104000
1	-3.262778000	-1.694730000	-0.397327000

1	-2.332376000	-2.126096000	-1.873110000
1	-3.116378000	-3.347854000	-0.839406000
1	-0.113084000	-3.518255000	-1.583508000
1	-1.104123000	-4.611300000	-0.608666000
1	0.393209000	-3.976938000	0.048349000
6	-1.647124000	-2.863980000	1.466532000
1	-2.235543000	-2.058453000	1.908343000
1	-2.232773000	-3.786422000	1.519769000
1	-0.746675000	-2.999114000	2.068250000
6	-2.272639000	2.645671000	0.858984000
1	-2.753367000	3.627540000	0.849425000
1	-3.076277000	1.990957000	0.434248000
1	-2.086449000	2.341889000	1.887945000
6	3.770215000	0.545839000	1.278656000
1	4.863467000	0.527961000	1.290505000
1	3.454557000	1.588056000	1.345005000
1	3.412130000	0.031533000	2.173196000

Mes*P_TS

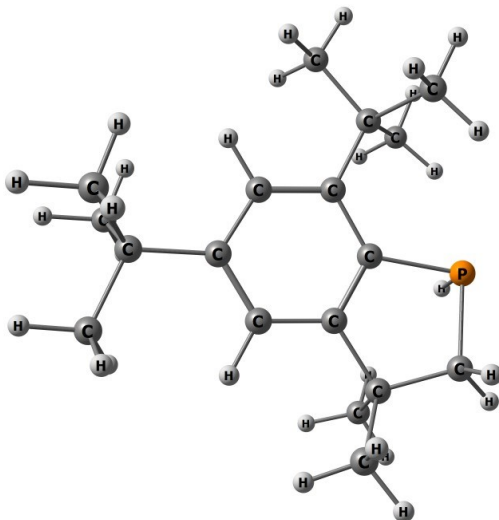


Method : UB3LYP/def2-TZVP
Charge : 0
Multiplicity : 1
Total energy: -1044.9111453 a.u.

6	-0.488905000	-1.209214000	-0.045427000
6	-1.148870000	0.038842000	-0.005846000
6	0.902100000	-1.276912000	-0.036605000
6	1.029106000	1.089138000	0.010323000
6	-0.357405000	1.225298000	0.008010000
6	1.696188000	-0.138178000	-0.007327000
15	-2.994222000	0.088628000	-0.014777000
1	1.628412000	1.985874000	0.024532000
1	1.368108000	-2.251449000	-0.053862000
6	3.232976000	-0.182514000	0.001150000
6	3.783701000	0.557158000	-1.237626000
6	3.775405000	-1.621077000	-0.026149000
1	3.451311000	-2.194857000	0.844892000
1	3.462816000	-2.156726000	-0.925183000
1	4.867299000	-1.600681000	-0.018366000
1	3.426405000	0.092633000	-2.159303000
1	4.876808000	0.529257000	-1.244027000
1	3.478659000	1.604516000	-1.252412000
6	-0.978072000	2.644841000	-0.001326000
6	-1.734622000	2.878125000	-1.328916000
6	0.080216000	3.759947000	0.105845000
1	0.662921000	3.687374000	1.026513000
1	0.768615000	3.760146000	-0.741208000
1	-0.424997000	4.728037000	0.112595000
1	-1.046129000	2.813864000	-2.174284000
1	-2.189234000	3.872331000	-1.334298000
1	-2.529209000	2.149152000	-1.495833000
6	-1.302248000	-2.511167000	-0.004757000
6	-0.739972000	-3.601483000	-0.938095000
6	-2.720332000	-2.196017000	-0.469524000
1	-3.133585000	-1.430099000	0.416638000

1	-2.796914000	-1.943717000	-1.520054000
1	-3.456657000	-2.967966000	-0.230970000
1	-0.632899000	-3.230620000	-1.958922000
1	-1.407694000	-4.466935000	-0.954364000
1	0.235462000	-3.953467000	-0.600249000
6	-1.342266000	-3.043368000	1.445007000
1	-1.780377000	-2.306700000	2.122076000
1	-1.928765000	-3.964606000	1.508531000
1	-0.333029000	-3.258716000	1.797823000
6	-1.927528000	2.833000000	1.199390000
1	-2.375411000	3.829484000	1.174029000
1	-2.749637000	2.111547000	1.221538000
1	-1.385385000	2.722431000	2.141102000
6	3.764879000	0.502177000	1.279248000
1	4.857853000	0.476277000	1.299365000
1	3.456157000	1.546900000	1.337072000
1	3.396322000	-0.004279000	2.174035000

8

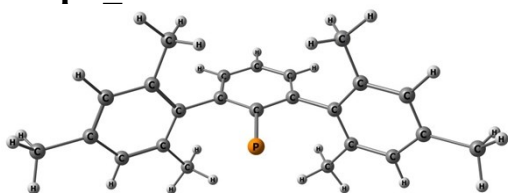


Method : UB3LYP/def2-TZVP
 Charge : 0
 Multiplicity : 1
 Total energy: -1045.0055624 a.u.

6	-0.488905000	-1.209214000	-0.045427000
6	-1.148870000	0.038842000	-0.005846000
6	0.902100000	-1.276912000	-0.036605000
6	1.029106000	1.089138000	0.010323000
6	-0.357405000	1.225298000	0.008010000
6	1.696188000	-0.138178000	-0.007327000
15	-2.994222000	0.088628000	-0.014777000
1	1.628412000	1.985874000	0.024532000
1	1.368108000	-2.251449000	-0.053862000
6	3.232976000	-0.182514000	0.001150000
6	3.783701000	0.557158000	-1.237626000
6	3.775405000	-1.621077000	-0.026149000
1	3.451311000	-2.194857000	0.844892000
1	3.462816000	-2.156726000	-0.925183000
1	4.867299000	-1.600681000	-0.018366000
1	3.426405000	0.092633000	-2.159303000
1	4.876808000	0.529257000	-1.244027000
1	3.478659000	1.604516000	-1.252412000
6	-0.978072000	2.644841000	-0.001326000
6	-1.734622000	2.878125000	-1.328916000
6	0.080216000	3.759947000	0.105845000
1	0.662921000	3.687374000	1.026513000
1	0.768615000	3.760146000	-0.741208000
1	-0.424997000	4.728037000	0.112595000
1	-1.046129000	2.813864000	-2.174284000
1	-2.189234000	3.872331000	-1.334298000
1	-2.529209000	2.149152000	-1.495833000
6	-1.302248000	-2.511167000	-0.004757000
6	-0.739972000	-3.601483000	-0.938095000
6	-2.720332000	-2.196017000	-0.469524000
1	-3.133585000	-1.430099000	0.416638000

1	-2.796914000	-1.943717000	-1.520054000
1	-3.456657000	-2.967966000	-0.230970000
1	-0.632899000	-3.230620000	-1.958922000
1	-1.407694000	-4.466935000	-0.954364000
1	0.235462000	-3.953467000	-0.600249000
6	-1.342266000	-3.043368000	1.445007000
1	-1.780377000	-2.306700000	2.122076000
1	-1.928765000	-3.964606000	1.508531000
1	-0.333029000	-3.258716000	1.797823000
6	-1.927528000	2.833000000	1.199390000
1	-2.375411000	3.829484000	1.174029000
1	-2.749637000	2.111547000	1.221538000
1	-1.385385000	2.722431000	2.141102000
6	3.764879000	0.502177000	1.279248000
1	4.857853000	0.476277000	1.299365000
1	3.456157000	1.546900000	1.337072000
1	3.396322000	-0.004279000	2.174035000

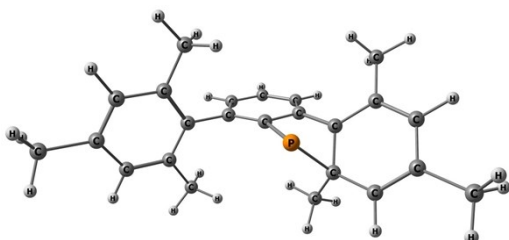
DmpP_T



Method : UB3LYP/def2-TZVP
Charge : 0
Multiplicity : 3
Total energy: -1271.2594820 a.u.

6	-1.225298000	0.000100000	1.007018000
6	0.000001000	0.000021000	0.293062000
6	-1.204405000	0.000245000	2.399330000
6	1.204397000	0.000239000	2.399335000
6	1.225298000	0.000100000	1.007021000
6	-0.000005000	0.000310000	3.095418000
15	0.000004000	-0.000194000	-1.522058000
1	2.143540000	0.000300000	2.940562000
1	-2.143549000	0.000309000	2.940554000
6	-2.540873000	0.000027000	0.289470000
6	-3.169699000	-1.217286000	-0.029906000
6	-3.169711000	1.217285000	-0.030114000
6	-4.406010000	-1.193633000	-0.673919000
6	-4.406019000	1.193521000	-0.674120000
6	-5.042810000	-0.000089000	-1.004381000
1	-4.882558000	-2.135733000	-0.924421000
1	-4.882574000	2.135574000	-0.924779000
6	2.540878000	0.000025000	0.289482000
6	3.169726000	1.217284000	-0.030107000
6	3.169694000	-1.217286000	-0.029894000
6	4.406038000	1.193513000	-0.674091000
6	4.406009000	-1.193639000	-0.673914000
6	5.042819000	-0.000106000	-1.004367000
1	4.882613000	2.135567000	-0.924717000
1	4.882555000	-2.135741000	-0.924409000
1	-0.000006000	0.000413000	4.178860000
6	-2.528450000	-2.542668000	0.301399000
1	-1.575106000	-2.666251000	-0.218298000
1	-2.321465000	-2.635827000	1.369732000
1	-3.177784000	-3.368449000	0.009638000
6	-6.394368000	-0.000155000	-1.672726000
1	-6.528450000	-0.883627000	-2.299206000
1	-7.199510000	-0.000181000	-0.931370000
1	-6.528526000	0.883286000	-2.299232000
6	-2.528477000	2.542726000	0.301001000
1	-2.321729000	2.636134000	1.369361000
1	-1.575018000	2.666142000	-0.218515000
1	-3.177718000	3.368461000	0.008905000
6	2.528444000	-2.542670000	0.301408000
1	2.321321000	-2.635770000	1.369718000
1	1.575173000	-2.666315000	-0.218411000

1	3.177840000	-3.368448000	0.009778000
6	2.528452000	2.542730000	0.300906000
1	1.575406000	2.666412000	-0.219321000
1	2.320898000	2.635893000	1.369123000
1	3.178021000	3.368450000	0.009494000
6	6.394377000	-0.000143000	-1.672710000
1	7.199524000	0.001764000	-0.931363000
1	6.529192000	-0.884537000	-2.297722000
1	6.527792000	0.882372000	-2.300688000

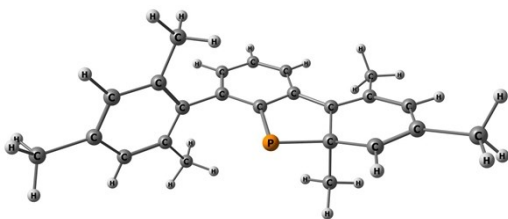
9a

Method : UB3LYP/def2-TZVP
 Charge : 0
 Multiplicity : 1
 Total energy: -1271.2400280 a.u.

6	-1.200938000	1.347036000	0.367252000
6	-0.049982000	0.593799000	0.124454000
6	-1.132522000	2.629062000	0.872579000
6	1.290180000	2.414989000	0.840008000
6	1.223529000	1.097166000	0.342100000
6	0.147100000	3.159978000	1.101213000
15	-0.866800000	-0.958066000	-0.526518000
1	2.264443000	2.856508000	1.017603000
1	-2.017165000	3.220725000	1.074895000
6	-2.309028000	0.387369000	0.021661000
6	-3.468336000	0.692291000	-0.800450000
6	-2.268682000	-0.849291000	0.867543000
6	-4.434116000	-0.247623000	-0.946498000
6	-3.343400000	-1.802535000	0.559232000
6	-4.357589000	-1.536045000	-0.296415000
1	-5.286918000	-0.043732000	-1.584765000
1	-3.324259000	-2.747371000	1.092487000
6	2.463664000	0.316242000	0.044562000
6	3.003034000	0.319511000	-1.254116000
6	3.094518000	-0.423490000	1.060038000
6	4.162584000	-0.411778000	-1.510659000
6	4.252316000	-1.141025000	0.760204000
6	4.805381000	-1.146711000	-0.517761000
1	4.572299000	-0.406541000	-2.515527000
1	4.731765000	-1.713085000	1.547959000
1	0.246695000	4.170732000	1.478362000
6	-3.536733000	2.012347000	-1.514493000
1	-3.579474000	2.851892000	-0.816668000
1	-2.649136000	2.163650000	-2.135010000
1	-4.417323000	2.059644000	-2.155453000
6	-5.447843000	-2.536203000	-0.570992000
1	-6.430264000	-2.118992000	-0.331534000
1	-5.466653000	-2.810375000	-1.629837000
1	-5.312128000	-3.447550000	0.011556000
6	2.534285000	-0.466189000	2.461052000
1	2.450374000	0.532740000	2.894503000
1	1.532664000	-0.902639000	2.475453000
1	3.170813000	-1.065172000	3.113064000
6	2.347920000	1.093679000	-2.372297000

1	1.355116000	0.700079000	-2.604488000
1	2.216919000	2.145968000	-2.110980000
1	2.948782000	1.041613000	-3.280736000
6	6.076937000	-1.902459000	-0.810956000
1	6.955712000	-1.268257000	-0.657963000
1	6.183728000	-2.770175000	-0.157708000
1	6.103474000	-2.251284000	-1.844810000
6	-1.849774000	-0.824944000	2.325698000
1	-2.681381000	-0.481101000	2.949519000
1	-1.579157000	-1.831439000	2.650469000
1	-1.001968000	-0.165902000	2.499602000

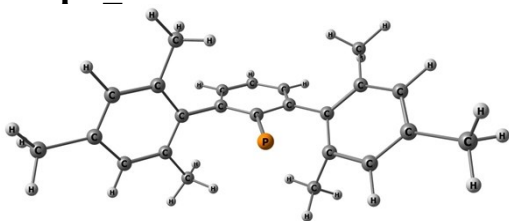
9b



Method : UB3LYP/def2-TZVP
Charge : 0
Multiplicity : 1
Total energy: -1271.2446414 a.u.

6	-1.297312000	1.247944000	-0.003719000
6	-0.049089000	0.488203000	0.022473000
6	-1.214821000	2.669619000	-0.166527000
6	1.207905000	2.525023000	-0.291447000
6	1.209645000	1.168265000	-0.124110000
6	-0.004061000	3.276446000	-0.306239000
15	-0.229518000	-1.230644000	0.226297000
1	2.150508000	3.046506000	-0.412808000
1	-2.109089000	3.271122000	-0.173791000
6	-2.434118000	0.445187000	0.117939000
6	-3.825455000	0.767658000	-0.050430000
6	-2.093161000	-0.979517000	0.454525000
6	-4.702999000	-0.261811000	-0.256880000
6	-3.045920000	-1.993637000	-0.079999000
6	-4.312857000	-1.651842000	-0.374958000
1	-5.750748000	-0.022552000	-0.408174000
1	-2.721234000	-3.027309000	-0.131340000
6	2.494297000	0.399976000	-0.110484000
6	3.028975000	-0.098441000	-1.311489000
6	3.176251000	0.186745000	1.100942000
6	4.231021000	-0.805426000	-1.277430000
6	4.375310000	-0.524157000	1.088480000
6	4.921567000	-1.028298000	-0.089415000
1	4.635003000	-1.193829000	-2.206648000
1	4.893383000	-0.691320000	2.027304000
1	0.048320000	4.351643000	-0.428903000
6	-4.348107000	2.182173000	-0.075316000
1	-4.028404000	2.750298000	0.800955000
1	-4.006525000	2.723157000	-0.961718000
1	-5.438300000	2.178992000	-0.094341000
6	-5.344856000	-2.650742000	-0.826349000
1	-6.196309000	-2.674802000	-0.139598000
1	-5.737424000	-2.394576000	-1.814761000
1	-4.926096000	-3.656115000	-0.879603000
6	2.632261000	0.707488000	2.408565000
1	2.558246000	1.797427000	2.408526000
1	1.630366000	0.318783000	2.603772000
1	3.275996000	0.413751000	3.238208000
6	2.333821000	0.122581000	-2.633311000
1	1.298314000	-0.222291000	-2.606492000

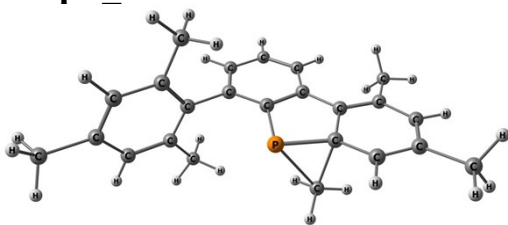
1	2.310040000	1.181905000	-2.900851000
1	2.847766000	-0.412663000	-3.432296000
6	6.234772000	-1.769509000	-0.080046000
1	7.078252000	-1.076898000	-0.162064000
1	6.366649000	-2.334053000	0.844820000
1	6.303440000	-2.467770000	-0.915839000
6	-2.215886000	-1.095970000	2.049537000
1	-3.259686000	-0.914618000	2.311036000
1	-1.936717000	-2.093437000	2.387002000
1	-1.586077000	-0.359405000	2.547276000

DmpP_TS1

Method : UB3LYP/def2-TZVP
Charge : 0
Multiplicity : 1
Total energy: -1271.223557 a.u.

6	-1.277733000	1.295315000	0.415530000
6	-0.098115000	0.517662000	0.219110000
6	-1.198193000	2.676648000	0.613153000
6	1.202280000	2.541097000	0.409286000
6	1.161176000	1.168869000	0.217466000
6	0.039944000	3.298029000	0.625646000
15	-0.342413000	-1.241874000	-0.053938000
1	2.164930000	3.041110000	0.397097000
1	-2.095132000	3.258376000	0.783704000
6	-2.471832000	0.465033000	0.291318000
6	-3.558668000	0.759849000	-0.560192000
6	-2.356951000	-0.859345000	0.859731000
6	-4.425542000	-0.269672000	-0.899740000
6	-3.294521000	-1.859785000	0.455451000
6	-4.306055000	-1.595766000	-0.430113000
1	-5.224823000	-0.048238000	-1.600779000
1	-3.201783000	-2.846961000	0.895866000
6	2.411503000	0.380694000	-0.019252000
6	2.908499000	0.224916000	-1.325838000
6	3.097036000	-0.203943000	1.062624000
6	4.079270000	-0.507740000	-1.525955000
6	4.262981000	-0.925856000	0.817765000
6	4.773801000	-1.087955000	-0.468722000
1	4.454256000	-0.628476000	-2.537098000
1	4.783890000	-1.377546000	1.655981000
1	0.114308000	4.364014000	0.798863000
6	-3.755075000	2.120154000	-1.180065000
1	-4.098243000	2.851964000	-0.445028000
1	-2.824553000	2.500768000	-1.603456000
1	-4.503397000	2.075213000	-1.971488000
6	-5.268634000	-2.654852000	-0.898547000
1	-6.306018000	-2.342953000	-0.755276000
1	-5.134911000	-2.860787000	-1.964268000
1	-5.119323000	-3.589908000	-0.358370000
6	2.576230000	-0.079516000	2.472008000
1	2.437258000	0.963878000	2.762296000
1	1.606555000	-0.575223000	2.566519000
1	3.263966000	-0.541810000	3.181064000
6	2.206238000	0.845475000	-2.509936000
1	1.144964000	0.590719000	-2.526508000

1	2.272736000	1.936490000	-2.486409000
1	2.652976000	0.503958000	-3.444404000
6	6.054391000	-1.849302000	-0.702094000
1	6.927770000	-1.214055000	-0.524365000
1	6.135918000	-2.707305000	-0.031759000
1	6.118826000	-2.214330000	-1.728366000
6	-1.919925000	-0.980168000	2.334707000
1	-2.790644000	-0.781906000	2.967622000
1	-1.555137000	-1.981978000	2.553660000
1	-1.140816000	-0.265954000	2.583919000

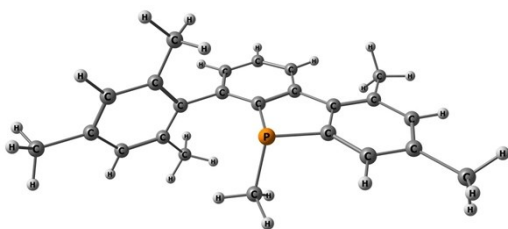
DmpP_TS2

Method : UB3LYP/def2-TZVP
Charge : 0
Multiplicity : 1
Total energy: -1271.2299937 a.u.

6	-1.291283000	1.267693000	-0.042204000
6	-0.059471000	0.524303000	-0.045719000
6	-1.205363000	2.683486000	-0.067654000
6	1.219420000	2.560740000	-0.114912000
6	1.199517000	1.182586000	-0.073374000
6	0.020551000	3.302290000	-0.109552000
15	-0.282945000	-1.233107000	-0.005805000
1	2.169884000	3.079976000	-0.152703000
1	-2.095898000	3.290540000	-0.061695000
6	-2.454921000	0.434642000	-0.011546000
6	-3.837995000	0.774538000	-0.034158000
6	-2.103145000	-0.972870000	0.066380000
6	-4.767364000	-0.240216000	-0.141773000
6	-3.097984000	-1.964294000	-0.242086000
6	-4.413040000	-1.610603000	-0.309560000
1	-5.819757000	0.021859000	-0.161202000
1	-2.796909000	-2.999174000	-0.360414000
6	2.478365000	0.403449000	-0.078321000
6	3.049119000	-0.008259000	-1.295814000
6	3.123309000	0.098799000	1.133889000
6	4.247329000	-0.722486000	-1.276749000
6	4.319901000	-0.616333000	1.106363000
6	4.900386000	-1.036125000	-0.087984000
1	4.680131000	-1.041445000	-2.219307000
1	4.809582000	-0.852413000	2.045636000
1	0.069832000	4.384552000	-0.138652000
6	-4.336830000	2.196294000	0.026579000
1	-3.966201000	2.722342000	0.909440000
1	-4.027167000	2.769647000	-0.851130000
1	-5.426379000	2.211757000	0.061348000
6	-5.496367000	-2.623033000	-0.575911000
1	-6.226943000	-2.638654000	0.237760000
1	-6.042584000	-2.384922000	-1.492857000
1	-5.085269000	-3.627729000	-0.679599000
6	2.543361000	0.525689000	2.460411000
1	2.428002000	1.609952000	2.520385000
1	1.552914000	0.093112000	2.620953000
1	3.185243000	0.207417000	3.282348000
6	2.396042000	0.311862000	-2.618645000
1	1.385351000	-0.097651000	-2.678986000

1	2.309307000	1.389903000	-2.772300000
1	2.976443000	-0.100993000	-3.444163000
6	6.211122000	-1.781691000	-0.093466000
1	7.057956000	-1.088412000	-0.102050000
1	6.315025000	-2.410748000	0.792504000
1	6.302444000	-2.419269000	-0.974354000
6	-1.696660000	-1.293689000	1.923000000
1	-2.740955000	-1.144770000	2.175882000
1	-1.387401000	-2.309865000	2.145973000
1	-1.070479000	-0.549052000	2.401097000

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Method : UB3LYP/def2-TZVP
 Charge : 0
 Multiplicity : 1
 Total energy: -1271.3256086 a.u.

6	1.352309000	1.289787000	0.047243000
6	0.135661000	0.563683000	0.056434000
6	1.291190000	2.687920000	0.028142000
6	-1.124711000	2.606362000	0.018958000
6	-1.104432000	1.208648000	0.051919000
6	0.059751000	3.332194000	0.010013000
15	0.414785000	-1.249657000	0.217496000
1	-2.077533000	3.122437000	0.009266000
1	2.186944000	3.286438000	0.027273000
6	2.552533000	0.423369000	0.059903000
6	3.917331000	0.786000000	0.040783000
6	2.222594000	-0.948365000	0.093843000
6	4.870510000	-0.233377000	0.041064000
6	3.197768000	-1.936152000	0.109986000
6	4.546042000	-1.590855000	0.067618000
1	5.918446000	0.048283000	0.026006000
1	2.912986000	-2.981993000	0.162297000
6	-2.395302000	0.448798000	0.077805000
6	-2.909103000	-0.034022000	1.295889000
6	-3.114836000	0.244038000	-1.113384000
6	-4.118395000	-0.728619000	1.293938000
6	-4.317951000	-0.461130000	-1.069014000
6	-4.838091000	-0.956426000	0.123632000
1	-4.507418000	-1.100684000	2.236177000
1	-4.862063000	-0.625506000	-1.993518000
1	0.025751000	4.415141000	-0.004972000
6	4.411681000	2.211000000	0.020523000
1	4.063629000	2.750988000	-0.863448000
1	4.080780000	2.769807000	0.899299000
1	5.501661000	2.230874000	0.009632000
6	5.623443000	-2.644316000	0.036810000
1	5.926596000	-2.867292000	-0.990949000
1	6.515612000	-2.318713000	0.574950000
1	5.279077000	-3.577539000	0.485337000
6	-2.623589000	0.782773000	-2.436010000
1	-2.741157000	1.868366000	-2.491319000
1	-1.564687000	0.575305000	-2.595503000
1	-3.186359000	0.346927000	-3.262337000
6	-2.182513000	0.185826000	2.599792000
1	-1.262700000	-0.402627000	2.644135000

1	-1.901114000	1.232270000	2.732202000
1	-2.808698000	-0.108004000	3.442777000
6	-6.156894000	-1.687083000	0.153333000
1	-6.983038000	-0.999041000	0.357874000
1	-6.364952000	-2.171739000	-0.802023000
1	-6.170834000	-2.452020000	0.931775000
6	0.030482000	-1.905484000	-1.496789000
1	0.465159000	-1.288937000	-2.283032000
1	0.430330000	-2.917844000	-1.569518000
1	-1.051064000	-1.957461000	-1.619426000