ELECTRONIC SUPPLEMENTARY INFORMATION

Why do silanes reduce electron-rich phosphine oxides faster than electron-poor phosphine oxides?

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Computational methods

Density functional theory calculations were performed in Gaussian 16.[1] The M06-2X functional[2] and 6-311+G(d,p) basis set were used in conjunction with the "ultrafine" pruned (99,590) integration grid. The toluene solvent was simulated with the SMD implicit solvent model.[3] Vibrational frequency calculations were performed to identify the nature of each stationary point (local minimum or first-order saddle point) and to obtain thermochemical quantities. Selected transition states were further characterized by means of intrinsic reaction coordinate (IRC) calculations[4] to identify the nearest local minima on the reactant and product sides of the TS. Errors in computed entropies associated with the harmonic treatment of low frequency modes were minimized by use of Truhlar's approximation[5] in which all harmonic frequencies below 100 cm^{-1} were raised to 100 cm^{-1} before evaluation of the vibrational component of the thermal contribution to entropy. Gibbs free energies are reported at a standard state of 1 mol/L and 298.15 K. Natural bond orbital (NBO) analyses[6] were performed at the same level of theory as used for geometry optimizations. Molecular structures were drawn with CYLview.[7]

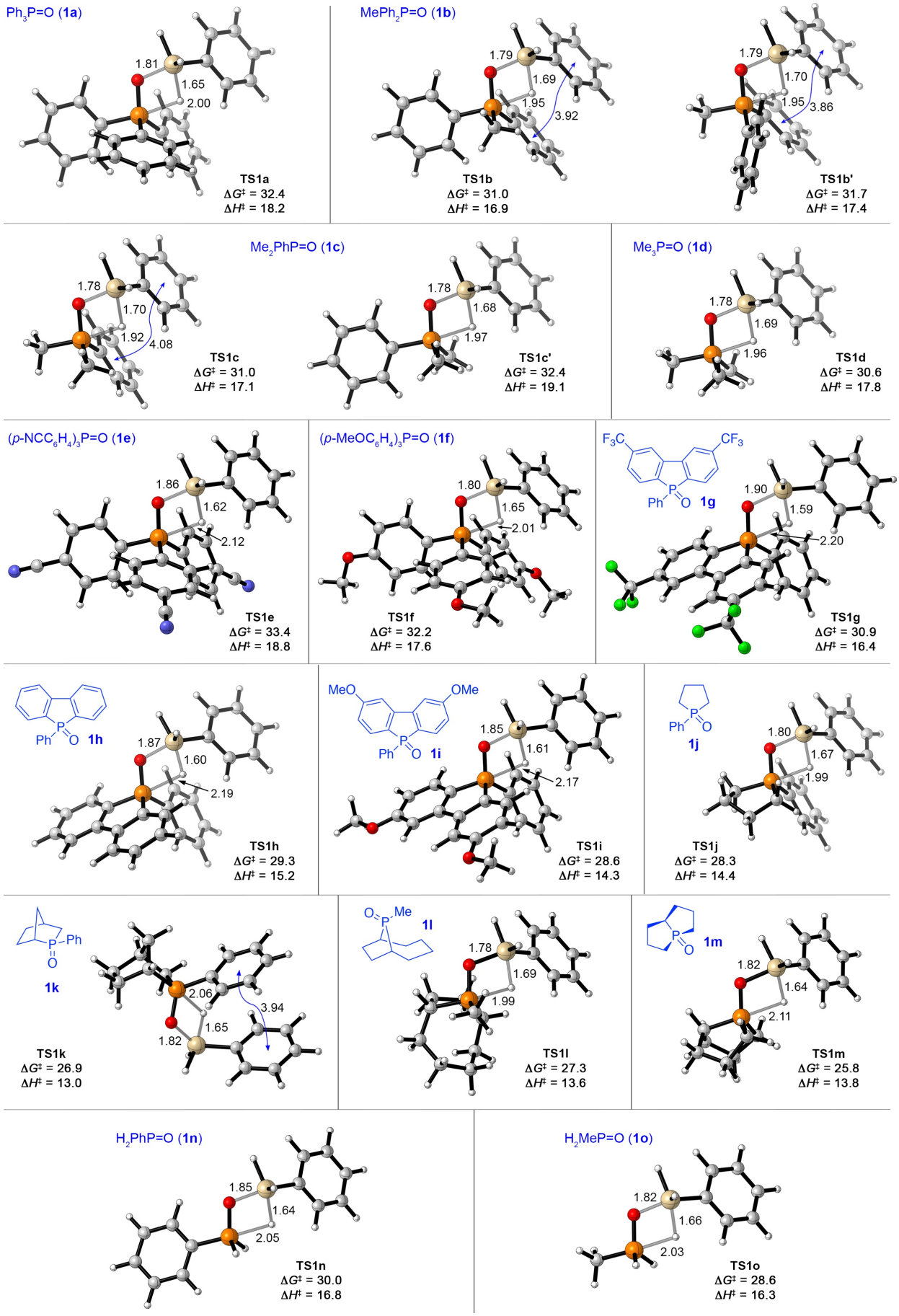

Figure S1. Transition states for hydride transfer from $PhSiH_3$ to phosphine oxides **1a**–**1o**. Distances in Å; $\Delta G^{\ddagger}$ and $\Delta H^{\ddagger}$ in kcal/mol.

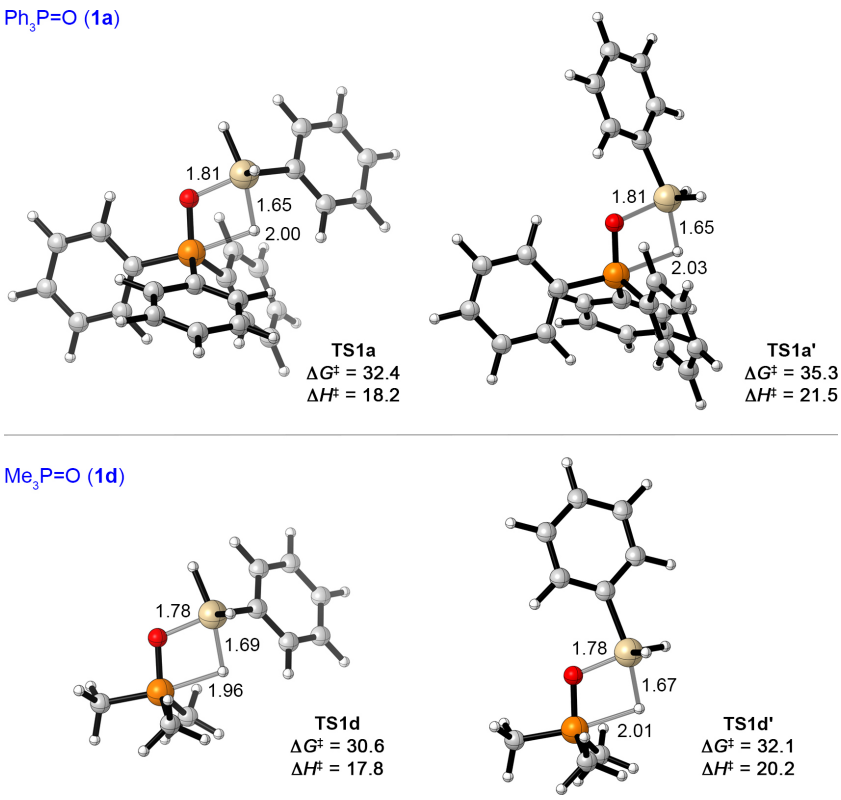

Figure S2. Transition states for hydride transfer from $PhSiH_3$ to $Ph_3P{=}O$ (**1a**) and $Me_3P{=}O$ (**1d**) in which the Si–Ph group occupies an equatorial or apical position on the Si trigonal bipyramid. The preferred TSs have the Si–Ph group occupying the equatorial position.

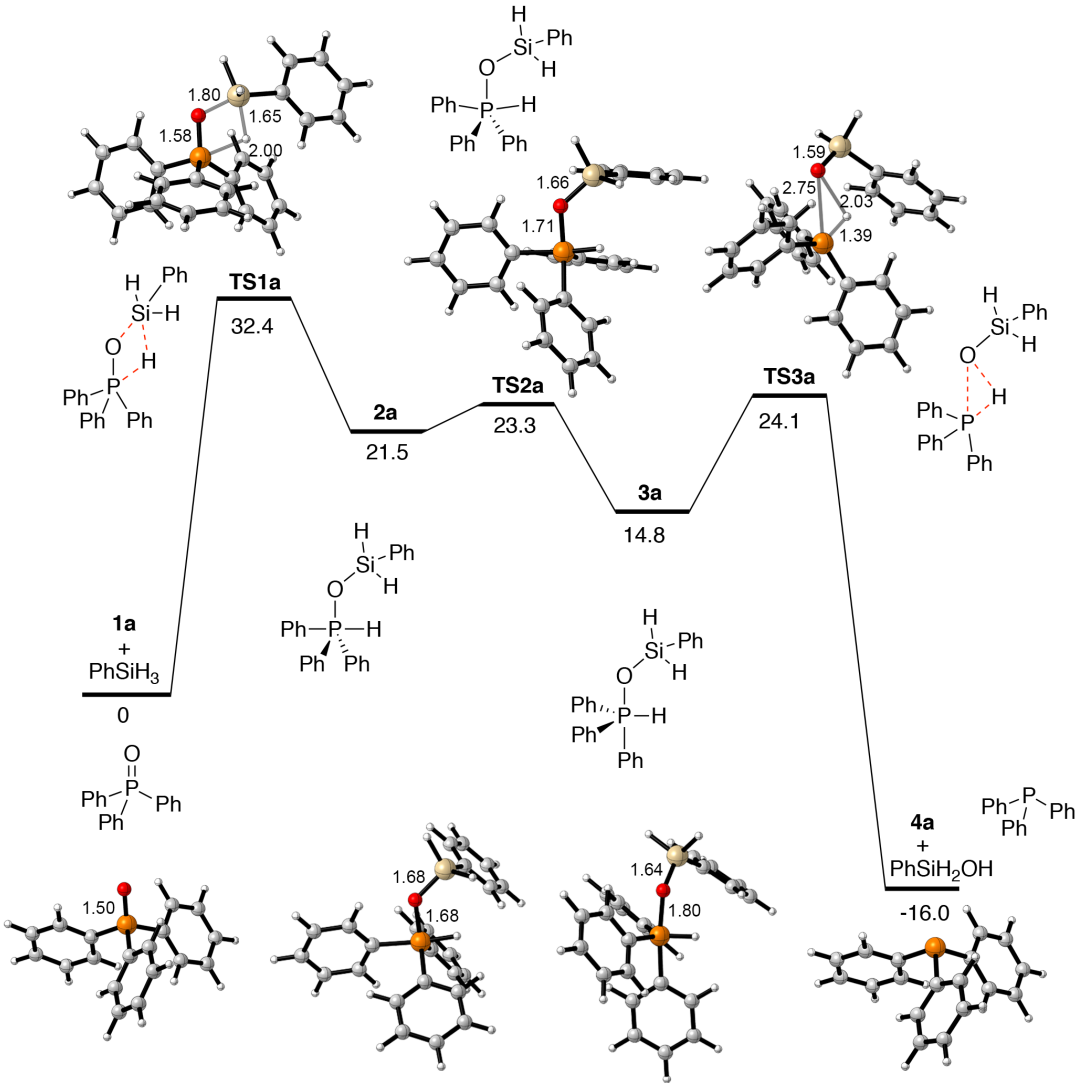

Figure S3. Free energy profile for the reduction of triphenylphosphine oxide (**1a**) by $PhSiH_3$, calculated with M06-2X/6-311+G(d,p) in SMD toluene. Distances in Å, ΔG in kcal/mol.

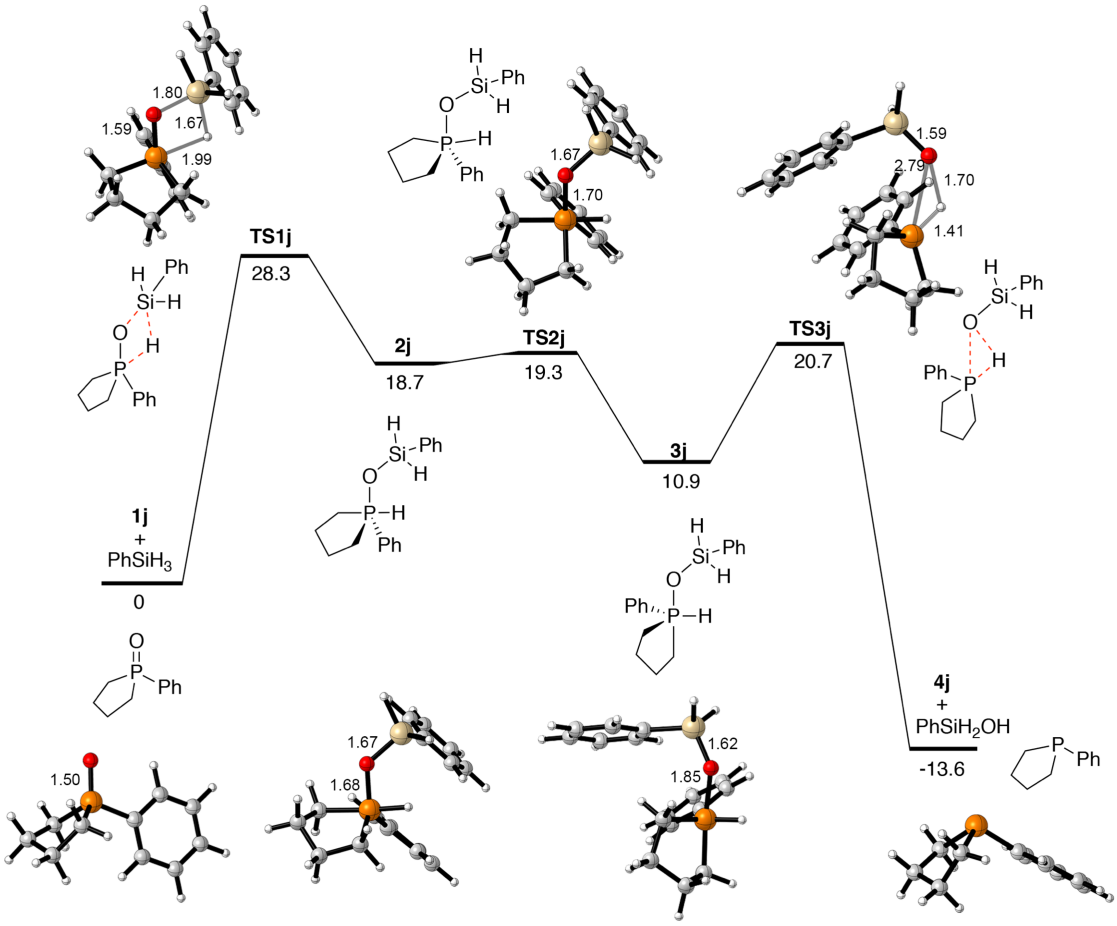

Figure S4. Free energy profile for the reduction of 1-phenylphospholane oxide (**1j**) by $PhSiH_3$, calculated with M06-2X/6-311+G(d,p) in SMD toluene. Distances in Å, ΔG in kcal/mol.

Comments about the mechanism of the extrusion step

We describe the final step in the reductions of phosphine oxides by phenylsilane as an "extrusion"; that is, a concerted elimination of phenylsilanol from the phosphorane intermediate **3**. This mechanism was deduced from an IRC calculation performed on **TS3d**, which showed that the TS led to the conversion of phosphorane **3d** into PMe_3 + $PhSiH_2(OH)$. Similar observations were made in the IRC calculations performed on the corresponding TSs in the reductions of $Ph_3P{=}O$ (**1a**) and 1-phenylphospholane oxide (**1j**). In contrast, for other oxide/silane combinations, Fianchini recently described[8] this process differently: the phosphorane intermediates were described as close ion-pairs $[R_3PH]^+[OSiR_3]^-$ (drawn as **A**) and the process leading from **A** to the phosphine and silanol was described as a proton transfer. Although the P–O distances in phosphoranes of type **A** are long, (1.8–1.9 Å), suggestive of a weakened P–O interaction, we find that a P–O σ bonding orbital is still present, as shown in Figure S5 for the three phosphoranes **3a**, **3d**, and **3j**. Therefore, these intermediates are best described as covalently-bonded phosphoranes rather than as ion pairs. Their conversion into the phosphine and silanol is best described as a concerted extrusion process, albeit a highly asynchronous one in which the early stages of the reaction are dominated by the breaking of the P–O bond and the latter stages are dominated by the proton transfer from P to O.

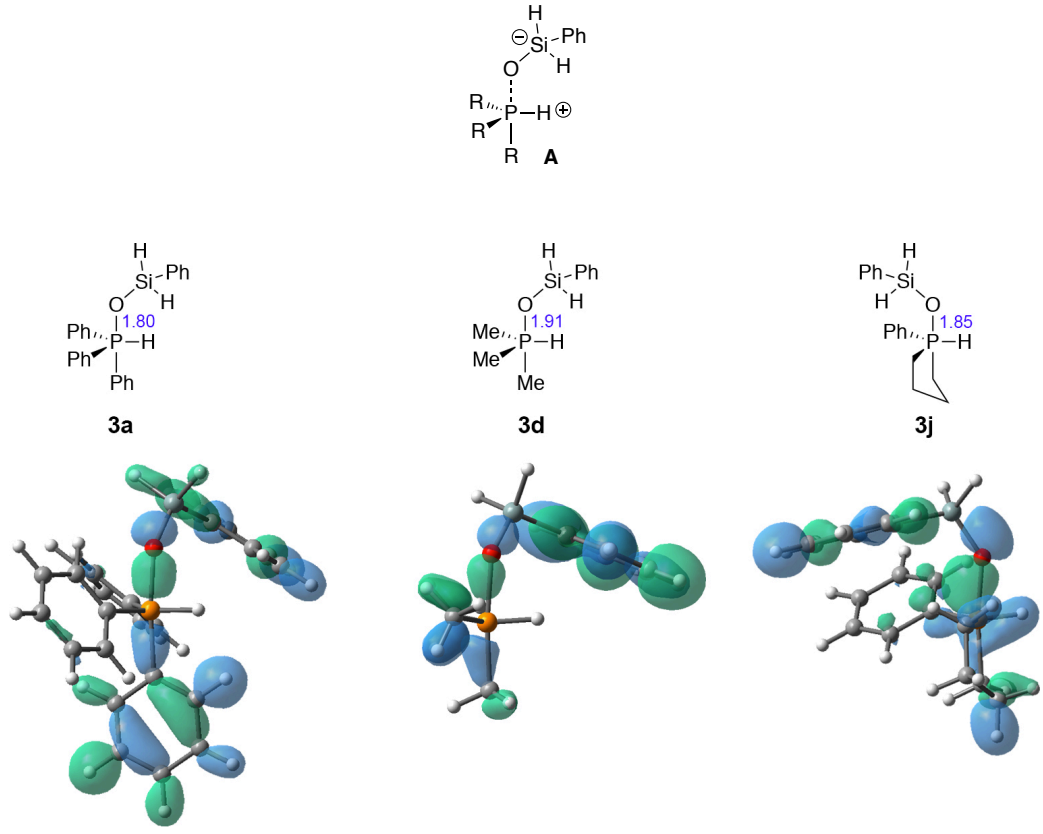

Figure S5. P–O σ bonding orbitals in **3a**, **3d**, and **3j** indicative of a covalent P–O interaction. Molecular orbitals (not NBOs) were calculated with HF/6-31G(d) on the M06-2X geometries and are plotted using an isovalue of 0.04. The P–O bond lengths (Å) are shown in blue.

Comments about the identity of the reducing agent

Fianchini's recent computational study[8] showed that in silane-mediated reductions of phosphine oxides, the silanes themselves are not the only active reducing agents. Silanols, which are formally the byproducts of the reduction, were shown to be more active reducing agents than the starting silanes. For example, in the reduction of 1-phenylphospholane oxide **1j**, on going from $PhSiH_3$ to $Ph(HO)SiH_2$ to $Ph(HO)_2SiH$, each successive OH group on silicon lowered the hydride transfer barrier by 2–3 kcal/mol. Silanols were shown to play a significant or even dominant role in the reduction. It is likely that silanols are also important in the phenylsilane-mediated reductions of phosphine oxides **1a**–**1o** studied here. For example, we calculate that the barrier for hydride transfer to $Me_3P{=}O$ (**1d**) from $Ph(HO)SiH_2$ is 24.3 kcal/mol, which is 6 kcal/mol lower than the corresponding barrier for hydride transfer from $PhSiH_3$ (30.6 kcal/mol). In our analysis of substituent effects, we have focused on $PhSiH_3$ as the hydride donor. $PhSiH_3$ is expected to be the dominant reducing agent during the early stages of the reduction.

Analysis of orbital interactions in the hydride transfer TSs

The key bond-forming orbital interactions in the hydride transfer TSs were quantified by means of a second order perturbation theory analysis of the Fock matrix in the NBO basis (Tables S1 and S2).

The oxygen lone pair displayed significant interactions with the antibonding orbitals of two Si–H bonds. The stronger of the two interactions involved the bond between Si and the transferring hydride, which is denoted "Si–H_{tr}" in Tables S1 and S2. The smaller interaction involved the Si–H bond to the non-transferring apical hydride, which is denoted "Si–H_{ap}" in the tables.

Table S1 compares the TSs for reductions of $Ph_3P{=}O$ (**TS1a**) and $Me_3P{=}O$ (**TS1d**). All four of the listed orbital interactions are stronger in **TS1d** than in **TS1a**. **TS1d** is 0.6 kcal/mol lower in energy ($\Delta E^{\ddagger}$) than **TS1a**. The strongest interaction is that between the oxygen lone pair and the σ* orbital of the breaking Si–H bond.

Table S1. NBO analysis of key orbital interactions in the hydride transfer TSs for triphenyl- and trimethylphosphine oxides.[a]

	TS1a	**TS1d**
Phosphine oxide	$Ph_3P{=}O$	$Me_3P{=}O$
$\Delta E^{\ddagger}$ [b]	17.7	17.1
Charge on P	1.94	1.87
Charge on O	–1.10	–1.12
O lone pair → Si–H_{tr} σ*	59.5	69.0
O lone pair → Si–H_{ap} σ*	37.2	39.0
Si–H σ → P–C σ*	19.5	21.8
Si–H σ → P–O σ*	15.8	17.0

[a] Interaction energies in kcal/mol. [b] $\Delta E^{\ddagger}$ calculated with M06-2X/6-311+G(d,p) in SMD toluene.

Table S2 compares the TSs for the reductions of three triarylphosphine oxides bearing different *para* substituents. The $\Delta E^{\ddagger}$ values for these oxides decrease as the electron density of the aryl substituent increases. The *p*-methoxy substituted oxide has the smallest $\Delta E^{\ddagger}$ overall (**TS1f**). In **TS1f**, the interactions of Si–H with the oxide P–C and P–O σ* orbitals are weaker than those for $Ph_3P{=}O$ in **TS1a**, but the interactions of the O lone pair with Si–H σ* orbitals are stronger, consistent with the greater nucleophilicity of the oxygen in this oxide. In contrast, the electron-deficient *p*-cyano substituted phosphine oxide has the highest $\Delta E^{\ddagger}$ (**TS1e**). All four bond-forming interactions are weakest in this TS.

Table S2. NBO analysis of key orbital interactions in the hydride transfer TSs for triarylphosphine oxides.[a]

	TS1e	**TS1a**	**TS1f**
Phosphine oxide	$(p\text{-}NCC_6H_4)_3P{=}O$	$Ph_3P{=}O$	$(p\text{-}MeOC_6H_4)_3P{=}O$
$\Delta E^{\ddagger}$ [b]	18.3	17.7	17.2
Charge on P	1.93	1.94	1.95
Charge on O	–1.09	–1.10	–1.11
O lone pair → $Si–H_{tr}$ σ*	50.1	59.5	60.2
O lone pair → $Si–H_{ap}$ σ*	33.7	37.2	38.6
Si–H σ → P–C σ*	13.7	19.5	18.9
Si–H σ → P–O σ*	11.5	15.8	15.6

[a] Interaction energies in kcal/mol. [b] $\Delta E^{\ddagger}$ calculated with M06-2X/6-311+G(d,p) in SMD toluene.

Computed geometries and energies

The Cartesian coordinates of species optimized with M06-2X/6-311+G(d,p) in SMD toluene are listed below. Underneath each set of coordinates are listed the following energies (all in Hartree):

E: electronic potential energy

H: enthalpy at 298.15 K

G: Gibbs free energy at 298.15 K and 1 mol/L

$PhSiH_3$

Si	2.341632	0.000066	0.005585
H	-2.185811	2.144040	0.003577
C	-1.646123	1.203972	0.003021
C	-0.254479	1.201802	-0.009764
H	0.273975	2.150248	-0.021762
C	0.464646	0.000189	-0.012164
C	-0.254373	-1.201750	-0.009766
H	0.274091	-2.150313	-0.021785
C	-1.645717	-1.204293	0.003097
H	-2.185245	-2.144449	0.003772
C	-2.343194	-0.000119	0.010330
H	-3.427143	-0.000301	0.017858
H	2.838801	1.241465	-0.629611
H	2.843788	-1.181899	-0.731077
H	2.860140	-0.058527	1.392310

0 imaginary frequencies

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G = -522.790010

1a

C	1.876888	3.832264	-0.763477
C	2.077887	2.629198	-1.432731
C	1.532990	1.451683	-0.928525
C	1.134205	3.861718	0.414220
H	2.305021	4.747447	-1.156010
H	2.664474	2.604688	-2.343638
C	0.587123	2.688520	0.920403
C	0.780583	1.480142	0.246486
H	1.701502	0.513870	-1.447358
H	0.985409	4.797422	0.940271
H	0.017623	2.701097	1.843695
H	2.347795	-1.338840	1.830577
C	2.046327	-1.837278	0.915324
C	0.892003	-1.417396	0.249385
C	2.792981	-2.895801	0.411738
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C	0.484515	-2.069989	-0.914730
H	-0.419973	-1.760179	-1.427344
C	2.389166	-3.539670	-0.755278
C	1.235829	-3.129257	-1.416183
H	2.970850	-4.366787	-1.145768
H	0.915712	-3.637173	-2.318419
H	-1.294678	1.199594	-1.459331
H	-3.587559	0.987026	-2.353732
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C   -3.316994    0.474281   -1.438117
C   -1.675170   -0.064023    0.246400
C   -4.260901   -0.292017   -0.761563
H   -5.267798   -0.379369   -1.153322
C   -2.627418   -0.826021    0.927714
C   -3.917279   -0.939681    0.422350
H   -2.355194   -1.317116    1.855969
H   -4.655136   -1.529150    0.953863
P   -0.002107   -0.000195    0.957254
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TS1a

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H    0.810697    1.255915   -0.327179
C   -1.660191    1.561811    0.070260
C    3.067755    0.552373   -1.118463
C    4.048650   -0.032752   -1.928462
H    3.818344   -0.252984   -2.966696
C    5.313090   -0.340146   -1.430183
H    6.056494   -0.792596   -2.077430
C    5.619865   -0.067977   -0.100664
H    6.601792   -0.308030    0.292077
C    4.658004    0.509468    0.725196
H    4.888807    0.717402    1.764425
C    3.397609    0.809002    0.218477
H    2.646719    1.236622    0.877699
H    1.611532    0.413843   -3.238669
H    1.101693    2.402315   -2.191832
C   -2.966844    1.719501   -0.400590
C   -3.671109    2.888179   -0.127553
C   -3.086976    3.891680    0.635215
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C   -1.069104    2.585724    0.817637
H   -3.439898    0.937165   -0.982086
H   -4.677638    3.007605   -0.510109
H   -3.639030    4.798587    0.853237
H   -1.325123    4.520512    1.699476
H   -0.043740    2.485813    1.153007
C    0.174584   -0.658507    1.046656
C   -0.028914   -0.260676    2.368925
H   -0.764357    0.498106    2.611527
C    0.725310   -0.841053    3.383479
H    0.571198   -0.529449    4.409911
C    1.673378   -1.814904    3.083438
H    2.261967   -2.259797    3.877143
C    1.864291   -2.218364    1.765677
H    2.603613   -2.973473    1.526869
C    1.115796   -1.644846    0.744804
H    1.275703   -1.953540   -0.283194
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C   -2.359921   -1.825773   -1.745621
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C   -3.398802   -2.747512   -1.861286
H   -3.576654   -3.237897   -2.811248
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H   -5.007545   -3.756722   -0.857210
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TS1a'

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H    0.215606    0.357666   -1.915365
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C    3.493059    0.149870   -0.546184
C    4.539205    0.982750   -0.955806
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C    5.809354    0.904403   -0.384793
H    6.598961    1.567473   -0.722103
C    6.061446   -0.022053    0.620684
H    7.046183   -0.087479    1.069992
C    5.037216   -0.864934    1.048365
H    5.225642   -1.589816    1.833435
C    3.774145   -0.774566    0.471182
H    2.987134   -1.435483    0.823511
H    2.040193    1.556921   -2.135854
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H    0.348927   -2.594868   -0.666449
C   -1.400045    1.631923   -0.425157
C   -1.747855    2.028696   -1.720800
H   -1.526982    1.380518   -2.560393
C   -2.357594    3.257600   -1.930124
H   -2.632475    3.554460   -2.935173
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H   -3.948141   -1.006339    3.419819
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H = -1633.858200
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2a

Si	1.406668	-0.191451	-2.641828
O	0.093787	-0.679903	-1.722501
P	-0.648885	0.168702	-0.480047
H	-0.005359	1.354247	-1.032280
C	-2.208449	1.222244	-0.379357
C	2.894401	0.042039	-1.535256
C	3.778724	-1.017215	-1.297315
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C	4.827035	-0.885276	-0.390424
H	5.502946	-1.715269	-0.218018
C	5.002659	0.311455	0.296722
H	5.813289	0.413892	1.009573
C	4.136045	1.378052	0.070232
H	4.267834	2.309685	0.608810
C	3.094903	1.243408	-0.841063
H	2.420566	2.080178	-1.001133
H	1.645891	-1.291934	-3.595582
H	1.094128	1.071017	-3.347141
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C	-4.586098	1.597377	-0.081006
C	-4.409814	2.964952	-0.261752
C	-3.137799	3.464750	-0.519391
C	-2.054866	2.595753	-0.595239
H	-3.667997	-0.326118	0.006920
H	-5.576468	1.196687	0.102269
H	-5.260337	3.635495	-0.215465
H	-2.989814	4.526780	-0.678005
H	-1.074186	2.994849	-0.834224
C	0.397896	0.297253	1.029998
C	0.463877	1.477956	1.767443
H	-0.187244	2.311020	1.521328
C	1.361717	1.591096	2.825104
H	1.396527	2.505174	3.406879
C	2.218116	0.536578	3.128410
H	2.927548	0.630929	3.942686
C	2.165496	-0.637670	2.382502
H	2.838753	-1.457004	2.607100
C	1.249925	-0.761632	1.342710
H	1.203591	-1.680493	0.766286
C	-1.529333	-1.450793	-0.007655
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H	-3.602101	-4.580275	1.037322
C	-2.629928	-2.779123	1.704033
H	-2.894445	-2.923071	2.745665
C	-1.893516	-1.660312	1.325641
H	-1.609013	-0.938211	2.084956

0 imaginary frequencies
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H = -1633.879524
G = -1633.951089

TS2a

Si	1.513858	-0.751057	-2.498801
O	0.156936	-0.995419	-1.569851
P	-0.661602	0.102081	-0.539446
H	-0.029309	1.129935	-1.331003
C	-2.090237	1.349181	-0.373705
C	2.981331	-0.365814	-1.403064
C	3.266069	-1.178421	-0.296266
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C	5.123371	0.232621	0.307763
H	5.949326	0.465171	0.970717
C	4.855658	1.051021	-0.784192
H	5.472435	1.922064	-0.975289
C	3.789639	0.752835	-1.630832
H	3.583944	1.406603	-2.473615
H	1.705122	-2.006360	-3.253866
H	1.333025	0.383940	-3.435510
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C	-2.902574	3.549243	0.235897
C	-4.103608	3.302281	-0.423736
C	-4.296360	2.082844	-1.063344
C	-3.300097	1.109799	-1.027310
H	-0.964134	2.804969	0.753896
H	-2.747129	4.493894	0.745181
H	-4.883008	4.055391	-0.437567
H	-5.226397	1.881618	-1.583086
H	-3.477979	0.151341	-1.505621
C	0.411585	0.320444	0.930893
C	1.291329	1.408389	0.948874
H	1.299527	2.112208	0.123507
C	2.179735	1.584345	2.002647
H	2.856579	2.430871	1.998870
C	2.215906	0.661019	3.043229
H	2.915678	0.790647	3.861029
C	1.366433	-0.439236	3.018811
H	1.401539	-1.171816	3.816974
C	0.468571	-0.611476	1.968602
H	-0.175249	-1.482081	1.959304
C	-1.792535	-1.333291	-0.042403
C	-1.879233	-2.551200	-0.716833
H	-1.264218	-2.720711	-1.588834
C	-2.750402	-3.548525	-0.276863
H	-2.812015	-4.483035	-0.823196
C	-3.528919	-3.351711	0.855928
H	-4.199401	-4.130400	1.201358
C	-3.443586	-2.143719	1.545293
H	-4.044226	-1.977479	2.432239
C	-2.596684	-1.142093	1.088352
H	-2.557118	-0.200423	1.627109

0 imaginary frequencies
E = -1634.302039
H = -1633.878075
G = -1633.948259

3a

Si	1.591849	-2.409580	-0.943777
O	0.079235	-1.789372	-0.851002
P	-0.699714	-0.200259	-0.501040
H	-0.268874	0.161231	-1.790333
C	2.890721	-1.051311	-0.976090

```
C    3.839751   -0.921941    0.043333
H    3.861114   -1.643836    0.854695
C    4.750510    0.132370    0.048032
H    5.475724    0.218010    0.849838
C    4.720399    1.081627   -0.968009
H    5.424259    1.906363   -0.963093
C    3.785438    0.968975   -1.994978
H    3.763803    1.703578   -2.792332
C    2.884194   -0.090562   -1.997675
H    2.165634   -0.168970   -2.809958
H    1.892171   -3.273522    0.228445
H    1.693205   -3.225463   -2.177818
C    0.428368    0.038933    0.938085
C    0.583234   -0.959200    1.900528
C    1.168945    1.217521    1.045834
C    1.453362   -0.771610    2.970486
H    0.028014   -1.885799    1.818828
C    2.069048    1.383855    2.092228
H    1.054442    2.004089    0.308433
C    2.204948    0.395286    3.062379
H    1.550576   -1.544438    3.724316
H    2.661933    2.289308    2.148902
H    2.896553    0.532895    3.885668
C   -1.450544    1.544954   -0.313089
C   -1.409511    2.426137   -1.389326
C   -2.033125    1.982933    0.882096
C   -1.939396    3.715127   -1.289048
H   -0.959560    2.110877   -2.328353
C   -2.563706    3.260904    0.991778
H   -2.071153    1.313396    1.737933
C   -2.517827    4.132486   -0.098225
H   -1.897564    4.387034   -2.139109
H   -3.012154    3.584119    1.924625
H   -2.929630    5.131612   -0.012806
C   -2.305516   -1.091578   -0.282536
C   -3.508722   -0.476638   -0.641246
C   -2.343664   -2.392687    0.230572
C   -4.719304   -1.146436   -0.490440
H   -3.514813    0.525630   -1.048855
C   -3.557658   -3.042544    0.419324
H   -1.420791   -2.905320    0.459870
C   -4.749265   -2.424189    0.054386
H   -5.638746   -0.659615   -0.793757
H   -3.568340   -4.043464    0.834899
H   -5.693940   -2.939191    0.186055
0 imaginary frequencies
E = -1634.314831
H = -1633.890081
G = -1633.961785
```

TS3a

```
Si   1.302978   -2.781296   -1.367125
O   -0.204929   -2.266325   -1.391724
P   -0.700415    0.169083   -0.214281
H    0.051791   -0.257130   -1.306351
C    2.537426   -1.339580   -1.107512
C    2.994296   -0.982253    0.169335
H    2.687472   -1.571250    1.031195
C    3.836739    0.111277    0.365997
H    4.175594    0.361487    1.366009
C    4.248817    0.876813   -0.722047
H    4.912687    1.721808   -0.574715
```

```
C    3.809675    0.545038   -2.002056
H    4.131371    1.132531   -2.855462
C    2.963486   -0.547222   -2.184941
H    2.636943   -0.794971   -3.192097
H    1.628741   -3.722883   -0.242475
H    1.771140   -3.448018   -2.623896
C   -0.112156   -0.517435    1.352593
C   -0.287563   -1.883545    1.594984
C    0.508351    0.300750    2.297672
C    0.181237   -2.426328    2.784755
H   -0.748454   -2.501941    0.831953
C    0.976399   -0.256620    3.483435
H    0.641567    1.360241    2.112799
C    0.817113   -1.617308    3.723899
H    0.060145   -3.486671    2.971380
H    1.466836    0.373988    4.215380
H    1.189270   -2.049644    4.645626
C   -0.500083    1.966665   -0.137848
C    0.782388    2.445913   -0.424329
C   -1.525081    2.851842    0.193483
C    1.039183    3.809832   -0.361475
H    1.578277    1.754784   -0.692156
C   -1.260835    4.216799    0.248524
H   -2.526065    2.487134    0.392855
C    0.017690    4.693826   -0.023877
H    2.033422    4.179570   -0.582833
H   -2.056788    4.907588    0.499561
H    0.216878    5.758274    0.019322
C   -2.420683   -0.277287   -0.470041
C   -2.809977   -0.832855   -1.688690
C   -3.349802   -0.060240    0.550386
C   -4.151033   -1.136888   -1.894100
H   -2.057485   -1.073298   -2.429891
C   -4.686469   -0.371765    0.334511
H   -3.029978    0.330260    1.511554
C   -5.085348   -0.901568   -0.889984
H   -4.462048   -1.577104   -2.833800
H   -5.412107   -0.211225    1.122746
H   -6.127860   -1.148188   -1.055004
1 imaginary frequency
E = -1634.297742
H = -1633.874954
G = -1633.946979
```

PPh_3 (4a)

```
C   -1.523218    3.907358   -0.710111
C   -0.396425    3.286375   -1.237929
C    0.093912    2.114971   -0.665556
C   -2.157270    3.358978    0.401840
H   -1.902764    4.817820   -1.158834
H    0.103324    3.711124   -2.100927
C   -1.660836    2.197412    0.981969
C   -0.538084    1.556452    0.447273
H    0.968590    1.637151   -1.092119
H   -3.031646    3.841165    0.823227
H   -2.151361    1.779874    1.855947
H    2.619755    0.976220    1.852290
C    2.735606    0.340675    0.979730
C    1.618505   -0.311664    0.446556
C    3.990149    0.186507    0.400633
H    4.845370    0.702726    0.821041
```

```
C     1.785721   -1.140613   -0.664594
H     0.934107   -1.659393   -1.090260
C     4.147625   -0.639911   -0.708765
C     3.045572   -1.305058   -1.235804
H     5.126012   -0.767937   -1.156774
H     3.163171   -1.952384   -2.097203
H    -0.482003   -2.750073    1.864463
H    -1.832857   -4.539383    0.832924
C    -1.082133   -2.534539    0.985691
C    -1.843825   -3.542974    0.406719
C    -1.077441   -1.244178    0.445062
C    -2.627958   -3.268410   -0.710815
H    -3.229297   -4.050534   -1.159145
C    -1.869075   -0.976610   -0.673504
C    -2.641916   -1.984436   -1.245213
H    -1.884397    0.018205   -1.104362
H    -3.253663   -1.764073   -2.112402
P     0.000947   -0.000168    1.277536
0 imaginary frequencies
E = -1036.183724
H = -1035.891828
G = -1035.946818
```

$PhSiH_2(OH)$

```
Si   -1.909334   -0.547386    0.115329
C    -0.077131   -0.209521    0.036442
C     0.839750   -1.263645   -0.057063
C     0.412880    1.100040    0.091721
C     2.208630   -1.018704   -0.085042
C     1.782141    1.348829    0.059914
C     2.680483    0.289801   -0.026179
H     0.486786   -2.289773   -0.113922
H    -0.284101    1.929523    0.151429
H     2.906336   -1.845130   -0.158081
H     2.147738    2.368617    0.099921
H     3.746899    0.483153   -0.051375
H    -2.261557   -1.627669   -0.834929
H    -2.332914   -0.973058    1.470804
O    -2.648124    0.889292   -0.278665
H    -3.574042    1.022601   -0.067887
0 imaginary frequencies
E = -598.157105
H = -598.025275
G = -598.063995
```

1b

```
P     0.036939    1.267119    0.117443
H    -3.688782   -1.605973    1.759184
C    -3.210357   -1.145303    0.902807
C    -2.078686   -0.355757    1.083811
H    -1.691142   -0.206497    2.085581
C    -1.461028    0.243813   -0.015624
C    -1.991505    0.057353   -1.293993
H    -1.520696    0.543699   -2.141598
C    -3.121146   -0.732790   -1.471475
H    -3.530300   -0.873525   -2.465042
C    -3.729241   -1.336038   -0.373887
H    -4.611988   -1.949376   -0.513033
H     2.476370    1.396292   -1.346745
C     2.519134    0.466949   -0.789238
C     3.628593   -0.369840   -0.875313
H     4.467755   -0.090946   -1.501883
```

```
C     3.657088   -1.564042   -0.163108
H     4.520136   -2.216044   -0.232714
C     2.574925   -1.928609    0.635281
H     2.593296   -2.864205    1.181816
C     1.465943   -1.095735    0.722990
H     0.617645   -1.392294    1.332505
C     1.438760    0.107891    0.015658
O     0.116725    2.325912   -0.939008
C     0.073905    1.902804    1.812478
H     0.131637    1.100500    2.549956
H    -0.814033    2.511679    1.993431
H     0.963895    2.528437    1.906635
0 imaginary frequencies
E = -919.727134
H = -919.486636
G = -919.536961
```

TS1b

```
Si   -1.017851    2.310809   -0.626941
O     0.620108    1.841443   -0.078316
P     1.054190    0.500016   -0.809159
H    -0.632751    1.017198   -1.640082
C     2.636187    0.201931    0.077706
C     0.087863   -0.970534   -0.401062
C     1.634028    0.551426   -2.526190
H     2.039055    1.556654   -2.676552
H     0.827931    0.385425   -3.236383
H     2.443611   -0.168206   -2.662737
H    -1.037047    3.388694    0.431539
C    -0.261434   -1.915036   -1.365144
C    -1.046343   -3.004739   -1.005517
C    -1.496506   -3.139397    0.305567
C    -1.150673   -2.192349    1.264171
C    -0.349386   -1.110647    0.916237
H     0.061077   -1.796187   -2.394322
H    -1.316905   -3.742151   -1.752108
H    -2.122437   -3.981212    0.577838
H    -1.510032   -2.288658    2.281727
H    -0.082642   -0.368548    1.662265
C     3.284412    1.231410    0.761322
C     4.513661    0.997933    1.373193
C     5.099406   -0.261150    1.309362
C     4.454566   -1.293951    0.633133
C     3.228793   -1.063140    0.020880
H     2.726273   -1.878651   -0.491310
H     6.054137   -0.441094    1.789981
H     4.902631   -2.279718    0.589257
H     2.819922    2.207757    0.821706
H     5.009558    1.801840    1.904671
C    -2.516719    1.307023   -0.030878
C    -3.090637    1.587276    1.214269
C    -3.047718    0.240929   -0.768959
C    -4.149670    0.828495    1.710974
H    -2.698616    2.407055    1.809115
C    -4.112194   -0.512682   -0.288606
H    -2.604921   -0.012659   -1.727849
C    -4.661777   -0.223635    0.959360
H    -4.573359    1.058692    2.682479
H    -4.505556   -1.334090   -0.877901
H    -5.484172   -0.817410    1.343005
H    -1.174712    3.147195   -1.852145
```

```
1 imaginary frequency
E = -1442.578745
H = -1442.213631
G = -1442.277639
```

TS1b'

```
Si    0.487891   -2.251603    0.112436
O    -0.456008   -1.531331    1.450714
P    -1.066407   -0.139494    0.985976
H    -0.317874   -0.946924   -0.625732
C     0.105780    1.160591    0.521852
C    -2.593960   -0.133050    0.008315
C    -1.663566    0.440320    2.608843
H    -2.423728   -0.248058    2.982067
H    -0.830004    0.460465    3.312566
H    -2.086128    1.443200    2.532375
C     2.137386   -1.457816   -0.388737
C     3.297827   -1.755270    0.334698
H     3.247559   -2.466855    1.153670
C     4.516390   -1.150862    0.029112
H     5.401535   -1.390849    0.608125
C     4.595816   -0.242253   -1.020769
H     5.541691    0.230367   -1.261772
C     3.454337    0.058950   -1.761908
H     3.510196    0.768321   -2.580711
C     2.240657   -0.537759   -1.440386
H     1.349812   -0.274719   -2.003370
H     1.019214   -3.287762    1.073552
H    -0.181061   -3.141506   -0.881135
C    -3.377754    1.022739   -0.034413
C    -4.577206    1.020779   -0.738317
C    -5.010719   -0.139506   -1.371901
C    -4.238736   -1.296033   -1.313563
C    -3.025965   -1.292410   -0.634705
H    -3.050925    1.929984    0.462970
H    -5.173991    1.923935   -0.784880
H    -5.949950   -0.142045   -1.912523
H    -4.574388   -2.200691   -1.806234
H    -2.414786   -2.187216   -0.613074
C    -0.062037    1.928900   -0.629893
C     0.886568    2.888651   -0.959979
C     2.013913    3.062920   -0.160253
C     2.188270    2.284608    0.978414
C     1.228402    1.340514    1.330054
H     1.376503    0.724006    2.211059
H     2.762217    3.797877   -0.433097
H     3.074336    2.402601    1.590663
H    -0.914510    1.759279   -1.279418
H     0.755547    3.488024   -1.853341
1 imaginary frequency
E = -1442.578207
H = -1442.212929
G = -1442.276501
```

1c

```
O    -1.851911   -1.679453    0.000000
P    -0.375985   -1.421077    0.000000
C     0.488986   -2.100987    1.439944
H     1.558197   -1.881997    1.408804
C     0.488986   -2.100987   -1.439944
H     1.558197   -1.881997   -1.408804
```

```
H     0.057882   -1.667736   -2.344277
H     0.341671   -3.183107   -1.459647
H     0.057882   -1.667736    2.344277
H     0.341671   -3.183107    1.459647
C     0.007668    0.358491    0.000000
C     1.319341    0.840036    0.000000
H     2.158460    0.150968    0.000000
C     1.558699    2.209066    0.000000
H     2.576753    2.580647    0.000000
C     0.488986    3.101935    0.000000
H     0.677020    4.169428    0.000000
C    -0.817683    2.625826    0.000000
H    -1.649314    3.320833    0.000000
C    -1.060086    1.254853    0.000000
H    -2.072734    0.866194    0.000000
0 imaginary frequencies
E = -728.018899
H = -727.835453
G = -727.879105
```

TS1c

```
Si   -0.122823    2.283927    0.343516
O    -1.485027    1.757930   -0.677351
P    -2.120255    0.433382   -0.059894
H    -0.779809    0.974383    1.207691
C    -1.076073   -1.039395   -0.138258
C    -3.170372    0.519227    1.414753
H    -3.466170    1.566237    1.526692
H    -2.632397    0.218626    2.310714
H    -4.068577   -0.085318    1.270961
H     0.215840    3.352846   -0.667923
C    -1.128825   -2.032009    0.839938
C    -0.287267   -3.134936    0.746762
C     0.609773   -3.243595   -0.312746
C     0.660598   -2.252593   -1.287510
C    -0.185587   -1.152068   -1.206667
H    -1.810599   -1.944590    1.679154
H    -0.327066   -3.906413    1.506849
H     1.273044   -4.098410   -0.374081
H     1.366810   -2.326862   -2.105881
H    -0.129311   -0.369913   -1.957347
C     1.522585    1.333486    0.299063
C     2.484734    1.667012   -0.661290
C     1.808315    0.270066    1.165660
C     3.684723    0.964272   -0.759994
H     2.290632    2.485887   -1.347725
C     3.008122   -0.427441    1.084694
H     1.068080   -0.026606    1.903322
C     3.948091   -0.084800    0.114242
H     4.412118    1.236294   -1.517074
H     3.206346   -1.247029    1.766978
H     4.879927   -0.634623    0.040462
H    -0.409075    3.128933    1.538470
C    -3.356432    0.111320   -1.362719
H    -4.092332    0.918407   -1.381332
H    -3.862509   -0.837467   -1.171795
H    -2.865719    0.065185   -2.335715
1 imaginary frequency
E = -1250.870344
H = -1250.562149
G = -1250.619713
```

TS1c'

Si	1.377650	0.363854	1.530029
O	-0.285606	0.680075	0.965101
P	-0.916538	-0.650506	0.368995
H	0.887279	-1.149784	0.977334
C	-1.363795	-1.975936	1.526583
H	-2.398285	-2.286579	1.376813
C	-2.559249	0.011137	-0.118992
C	-0.249353	-1.267425	-1.202418
H	0.250175	-2.223007	-1.047860
H	0.488186	-0.542402	-1.555170
H	-1.039819	-1.359342	-1.948088
H	-0.682550	-2.818367	1.419574
H	-1.261733	-1.572424	2.537029
C	2.869600	0.254116	0.352424
C	3.584545	1.415156	0.033535
H	3.265924	2.366247	0.449284
C	4.695925	1.375108	-0.805934
H	5.230286	2.288594	-1.042784
C	5.120527	0.162365	-1.338459
H	5.986374	0.126717	-1.990247
C	4.427048	-1.006353	-1.032045
H	4.756065	-1.954960	-1.442168
C	3.310766	-0.953719	-0.203377
H	2.769286	-1.868437	0.021027
H	1.509739	1.829554	1.874846
H	1.538735	-0.240052	2.884900
C	-2.907897	1.342396	0.105517
C	-4.164805	1.809415	-0.273970
C	-5.077824	0.953715	-0.877746
C	-4.735946	-0.377682	-1.105495
C	-3.483708	-0.844171	-0.727834
H	-2.194208	2.007135	0.575232
H	-4.426948	2.845824	-0.095820
H	-6.054482	1.320101	-1.172065
H	-5.443812	-1.049680	-1.576361
H	-3.229400	-1.884840	-0.912352

1 imaginary frequency
E = -1250.867647
H = -1250.559030
G = -1250.617431

1d

O	0.586249	1.569685	0.000000
P	0.061504	0.165307	0.000000
C	-1.748858	0.067353	0.000000
H	-2.093410	-0.968936	0.000000
C	0.586249	-0.805590	1.438699
C	0.586249	-0.805590	-1.438699
H	1.677150	-0.849077	1.459470
H	1.677150	-0.849077	-1.459470
H	0.241103	-0.309501	2.348107
H	0.241103	-0.309501	-2.348107
H	0.184145	-1.820398	1.404691
H	0.184145	-1.820398	-1.404691
H	-2.132886	0.576386	0.886390
H	-2.132886	0.576386	-0.886390

0 imaginary frequencies
E = -536.309213
H = -536.182792
G = -536.218467

TS1d

Si	0.041212	-1.303539	0.639803
O	1.477514	-1.167751	-0.399745
P	2.210880	0.221482	-0.134096
H	0.675601	0.201443	1.079390
C	3.574687	0.030315	-1.326374
H	4.219289	0.911973	-1.311839
C	3.098909	0.433695	1.433174
C	1.393709	1.734763	-0.710541
H	2.584125	1.147569	2.073585
H	1.100993	2.355336	0.135103
H	3.120028	-0.533328	1.941390
H	0.493526	1.449364	-1.260003
H	4.124480	0.756540	1.242718
H	2.058333	2.288347	-1.377083
H	4.166102	-0.851438	-1.072794
H	3.168768	-0.101483	-2.330982
C	-1.610199	-0.434764	0.258550
C	-2.579529	-1.099851	-0.502650
H	-2.366018	-2.094227	-0.882895
C	-3.812730	-0.513633	-0.780172
H	-4.545807	-1.047636	-1.374775
C	-4.103573	0.756019	-0.292209
H	-5.062911	1.214973	-0.503939
C	-3.155740	1.435883	0.469291
H	-3.378511	2.424932	0.854683
C	-1.922879	0.846387	0.730880
H	-1.186318	1.388051	1.317511
H	-0.284710	-2.629978	-0.006883
H	0.256807	-1.743987	2.049280

1 imaginary frequency
E = -1059.160032
H = -1058.908384
G = -1058.959777

TS1d'

Si	0.020245	-1.182208	0.320430
O	-0.821252	0.338263	-0.085643
P	-2.398033	0.139238	-0.064864
H	-1.586957	-1.649427	0.341279
C	-2.894573	1.844790	-0.452909
H	-3.982422	1.929541	-0.491558
C	-3.191895	-0.157915	1.536241
C	-3.146575	-0.811389	-1.413089
H	-3.501255	-1.197133	1.628094
H	-3.435423	-1.804583	-1.075937
H	-2.462892	0.059244	2.320504
H	-2.403496	-0.912606	-2.207779
H	-4.047422	0.510587	1.652923
H	-4.011161	-0.271458	-1.805536
H	-2.508541	2.521578	0.311481
H	-2.476114	2.136270	-1.418074
C	1.740510	-0.332929	0.078072
C	1.990233	1.038179	0.229874
H	1.160508	1.710268	0.422174
C	3.277547	1.561390	0.131401
H	3.440445	2.627343	0.251994
C	4.356546	0.719691	-0.125818
H	5.359415	1.124473	-0.205174
C	4.136056	-0.644817	-0.285463
H	4.968759	-1.308829	-0.491916
C	2.843295	-1.154883	-0.184622

```
H    2.691178   -2.223803   -0.319944
H    0.275885   -2.339759   -0.590848
H    0.109717   -1.528162    1.768273
1 imaginary frequency
E = -1059.155469
H = -1058.904523
G = -1058.957264
```

2d

```
Si    0.049048  -1.878854    0.391657
O    -1.298029  -1.178487   -0.302141
P    -1.944743   0.345102    0.084600
H    -1.165873   0.221653    1.327807
C    -2.897778   0.201771   -1.533810
H    -3.495539   1.102114   -1.699317
C    -3.433168   0.710124    1.110068
C    -1.055538   1.891007   -0.349008
H    -3.139456   1.316735    1.969172
H    -0.785464   2.431025    0.560207
H    -3.808467  -0.246418    1.487315
H    -0.130397   1.609984   -0.862776
H    -4.228930   1.196779    0.544972
H    -1.643201   2.525567   -1.013897
H    -3.563936  -0.663992   -1.507839
H    -2.208671   0.072111   -2.371081
C     1.519538  -0.734194    0.199829
C     2.180927  -0.629552   -1.031218
H     1.886001  -1.266347   -1.860605
C     3.215606   0.283083   -1.214283
H     3.716536   0.350685   -2.173333
C     3.606983   1.108013   -0.163526
H     4.412116   1.820334   -0.303991
C     2.966485   1.014612    1.068809
H     3.272282   1.653911    1.889253
C     1.931400   0.101338    1.245882
H     1.433669   0.043455    2.209472
H     0.269113  -3.131713   -0.357420
H    -0.157808  -2.157769    1.830533
0 imaginary frequencies
E = -1059.172904
H = -1058.919256
G = -1058.972235
```

TS2d

```
Si  -0.153129    1.822117    0.343830
O    1.208967    0.946571    0.704990
P    2.000014   -0.243180   -0.269560
H    1.089222    0.210107   -1.311911
C    2.753483   -0.833832    1.345385
H    3.533100   -1.572726    1.145804
C    3.508870    0.398255   -1.067750
C    1.746370   -1.968932   -0.920269
H    3.382950    0.419069   -2.151121
H    1.687089   -1.926764   -2.010708
H    3.677680    1.418099   -0.714236
H    0.780351   -2.330719   -0.552367
H    4.374201   -0.211436   -0.803275
H    2.521969   -2.668286   -0.603142
H    3.175683    0.004739    1.900081
H    1.984557   -1.298498    1.968096
C   -1.596246    0.641446    0.140286
C   -1.631546   -0.548341    0.878754
```

```
H   -0.821613   -0.779661    1.565586
C   -2.689447   -1.443042    0.747681
H   -2.700244   -2.359737    1.326565
C   -3.734974   -1.157906   -0.125997
H   -4.560098   -1.853224   -0.230634
C   -3.717488    0.019793   -0.867394
H   -4.528094    0.241821   -1.552213
C   -2.654321    0.908627   -0.735872
H   -2.648510    1.817418   -1.330867
H   -0.360838    2.744999    1.478901
H   -0.023739    2.613875   -0.903633
1 imaginary frequency
E = -1059.171786
H = -1058.919045
G = -1058.970799
```

3d

```
Si  -0.192556    1.930504   -0.058680
O    1.239518    1.242968   -0.389334
P    2.008599   -0.470366   -0.056841
H    0.949281   -0.895991   -0.869009
C    3.510354    0.242891   -0.800933
H    4.364426   -0.422036   -0.678926
C    2.654675   -2.227434    0.113937
C    1.701366   -0.198502    1.721362
H    1.883891   -2.865569    0.557985
H    0.635695   -0.362489    1.906947
H    2.896360   -2.631475   -0.874464
H    1.941195    0.830929    1.982387
H    3.551683   -2.283530    0.737360
H    2.274199   -0.896011    2.332024
H    3.315165    0.405379   -1.862105
H    3.699182    1.215361   -0.350256
C   -1.591470    0.661052   -0.085091
C   -2.358852    0.392166    1.054467
H   -2.165137    0.938413    1.973587
C   -3.375052   -0.561504    1.034736
H   -3.959169   -0.751296    1.928382
C   -3.639595   -1.268994   -0.132908
H   -4.430199   -2.010646   -0.152492
C   -2.888149   -1.019231   -1.279288
H   -3.094518   -1.566238   -2.192554
C   -1.876300   -0.065269   -1.251148
H   -1.302331    0.121027   -2.155374
H   -0.239898    2.533578    1.304734
H   -0.491030    2.994225   -1.050223
0 imaginary frequencies
E = -1059.184518
H = -1058.930623
G = -1058.984372
```

TS3d

```
Si  -0.624367    2.373095   -0.255714
O    0.935895    2.074587   -0.383859
P    1.999410   -0.490933   -0.017365
H    1.347695    0.418664   -0.884000
C    3.480366    0.356917    0.557606
H    3.976706   -0.218616    1.340643
C    2.465476   -2.082902   -0.739228
C    0.935446   -0.821078    1.398131
H    1.565895   -2.601987   -1.075546
H    0.034143   -1.344272    1.071587
```

```
H    3.125254   -1.922169   -1.593153
H    0.655284    0.131049    1.849997
H    2.978357   -2.695448    0.004843
H    1.476971   -1.433133    2.122898
H    4.163193    0.507481   -0.279954
H    3.161823    1.331209    0.931310
C   -1.593325    0.726455   -0.184342
C   -2.351695    0.349525    0.930140
H   -2.492228    1.057028    1.743062
C   -2.922500   -0.918936    1.032418
H   -3.504275   -1.184383    1.908710
C   -2.742054   -1.847507    0.011522
H   -3.182667   -2.835396    0.087518
C   -2.002770   -1.494065   -1.116677
H   -1.874609   -2.206484   -1.925181
C   -1.439996   -0.223319   -1.207082
H   -0.870015    0.036192   -2.096885
H   -1.055754    3.077146    0.997267
H   -1.216640    3.156560   -1.386697
1 imaginary frequency
E = -1059.172465
H = -1058.921220
G = -1058.975474
```

PMe_3 (4d)

```
P    0.607230    0.000227    0.000000
C   -0.280627   -0.811411    1.404676
H   -1.366970   -0.745671    1.293111
C   -0.280627   -0.811411   -1.404676
C   -0.280627    1.622524    0.000000
H    0.008191   -0.336437   -2.345100
H    0.007207    2.198779   -0.882313
H    0.006465   -1.863919   -1.461494
H    0.007207    2.198779    0.882313
H   -1.366970   -0.745671   -1.293111
H   -1.366950    1.492877    0.000000
H    0.006465   -1.863919    1.461494
H    0.008191   -0.336437    2.345100
0 imaginary frequencies
E = -461.049447
H = -460.928543
G = -460.962203
```

1e

```
C    2.024785    0.406201   -0.704260
C    1.486446    0.787624    0.525753
C    2.083766    1.805781    1.271433
C    3.207563    2.456413    0.783225
C    3.733150    2.078129   -0.454549
C    3.148344    1.052435   -1.200417
P    0.001987    0.012444    1.241450
C   -0.065271   -1.665121    0.533827
C    0.630915   -2.662993    1.220412
C    0.643111   -3.961417    0.733990
C   -0.049502   -4.257914   -0.442856
C   -0.756749   -3.268665   -1.128566
C   -0.763879   -1.970991   -0.634846
O    0.009067    0.016440    2.734935
C   -1.421793    0.901228    0.533460
C   -1.353656    1.629212   -0.654786
C   -2.486196    2.264784   -1.145878
C   -3.686289    2.168660   -0.438593
```

```
C   -3.759563    1.449726    0.757299
C   -2.623244    0.819299    1.241567
H   -0.419503    1.712644   -1.198951
H   -2.445111    2.835359   -2.065354
C   -4.861104    2.824064   -0.945864
H   -4.696276    1.394133    1.297707
H   -2.662945    0.271151    2.176395
H    1.152514   -2.422690    2.140362
H    1.178227   -4.743898    1.257197
C   -0.040202   -5.602346   -0.951785
H   -1.297296   -3.519667   -2.032719
H   -1.323587   -1.204934   -1.160345
H    1.673121    2.077366    2.237551
H    3.680721    3.246616    1.352671
C    4.897815    2.747331   -0.966761
H    3.577527    0.764547   -2.151942
H    1.579009   -0.399699   -1.276749
N   -0.032254   -6.676786   -1.360866
N   -5.800062    3.346987   -1.354200
N    5.828113    3.281548   -1.380344
0 imaginary frequencies
E = -1388.149853
H = -1387.850814
G = -1387.919290
```

TS1e

```
C   -2.090420   -1.998600   -1.675812
C   -1.811166   -1.276713   -0.516570
C   -2.479979   -1.571136    0.675317
C   -3.428227   -2.579496    0.711095
C   -3.705269   -3.298589   -0.456278
C   -3.040599   -3.012809   -1.648260
P   -0.545681    0.039965   -0.540327
C   -1.467798    1.527878   -0.034458
C   -0.860310    2.577276    0.661439
C   -1.600843    3.689199    1.026608
C   -2.949442    3.766953    0.667118
C   -3.558267    2.736330   -0.047444
C   -2.816767    1.612878   -0.387330
O   -0.014054   -0.053513   -2.007733
Si   1.402573    1.118203   -2.307893
C    3.203441    0.824736   -1.750041
C    3.672666    1.240189   -0.497234
C    4.984738    1.007004   -0.099445
C    5.857970    0.332515   -0.950599
C    5.412983   -0.096084   -2.197190
C    4.098170    0.150087   -2.588715
C    0.647088   -0.498927    0.709678
C    0.562615   -0.120416    2.051260
C    1.506763   -0.582273    2.955977
C    2.527512   -1.428953    2.516151
C    2.600858   -1.827011    1.180109
C    1.656330   -1.362582    0.278016
H    1.012413    1.459330   -0.778125
H    1.043905    2.501860   -2.739129
H    1.511400    0.434074   -3.649877
H    2.991242    1.742980    0.184659
H    5.326560    1.340175    0.874557
H    6.879136    0.140160   -0.640902
H    6.088463   -0.622156   -2.862817
H    3.760087   -0.191205   -3.562880
H    0.194902    2.533994    0.901084
```

```
H   -1.138821    4.502137    1.572292
C   -3.716900    4.925632    1.035767
H   -4.600706    2.812648   -0.329511
H   -3.299169    0.809435   -0.931154
H   -0.226522    0.537176    2.397254
H    1.458933   -0.289491    3.997356
C    3.512136   -1.895702    3.453140
H    3.397894   -2.481653    0.850626
H    1.721098   -1.660218   -0.762765
H   -2.265288   -1.011963    1.580716
H   -3.952154   -2.816409    1.628597
C   -4.689273   -4.346094   -0.424714
H   -3.266853   -3.579885   -2.542647
H   -1.565081   -1.765737   -2.593306
N   -4.331371    5.849997    1.334680
N    4.297870   -2.266549    4.206242
N   -5.477622   -5.182477   -0.398389
1 imaginary frequency
E = -1910.998735
H = -1910.574799
G = -1910.656140
```

1f

```
C   -0.661693    2.032432   -0.417505
C   -1.016237    1.325048    0.726334
C   -2.228396    1.627368    1.363081
C   -3.063981    2.603755    0.857170
C   -2.701852    3.306097   -0.299624
C   -1.495076    3.021405   -0.938536
P    0.000623   -0.000222    1.432840
C    1.656049    0.217580    0.724310
C    2.527480    1.109445    1.365691
C    3.791105    1.343581    0.860029
C    4.214619    0.685154   -0.301668
C    3.361077   -0.210811   -0.945512
C    2.088002   -0.437734   -0.424062
O    0.001928   -0.000948    2.931877
C   -0.637716   -1.542867    0.723812
C   -1.449483   -1.588195   -0.404682
C   -1.888997   -2.804737   -0.925564
C   -1.509479   -3.993420   -0.302548
C   -0.698114   -3.957350    0.838992
C   -0.271101   -2.745445    1.345102
H   -1.757714   -0.668841   -0.891532
H   -2.525120   -2.809073   -1.800310
O   -1.878892   -5.223734   -0.723485
H   -0.425627   -4.893783    1.310858
H    0.346482   -2.720847    2.236916
H    2.207446    1.611268    2.272855
H    4.476704    2.026503    1.347189
O    5.466368    0.977124   -0.720176
H    3.671740   -0.739806   -1.836274
H    1.435014   -1.143981   -0.926186
H   -2.505451    1.094797    2.266825
H   -4.001213    2.850878    1.341258
O   -3.580921    4.243922   -0.718022
H   -1.189719    3.559296   -1.825733
H    0.279128    1.824866   -0.916496
C   -2.711179   -5.312800   -1.867056
H   -2.885606   -6.374477   -2.029136
H   -3.668096   -4.809919   -1.699197
H   -2.219782   -4.888065   -2.747591
```

```
C    5.946144    0.328922   -1.885449
H    6.957043    0.700298   -2.040199
H    5.975864   -0.756178   -1.750033
H    5.331951    0.576557   -2.756424
C   -3.253577    4.993120   -1.875541
H   -4.082151    5.680603   -2.032185
H   -2.332348    5.564552   -1.728795
H   -3.151314    4.344476   -2.750622
0 imaginary frequencies
E = -1454.980271
H = -1454.576031
G = -1454.648051
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TS1f

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C   -2.221035   -1.935269   -1.678081
C   -1.617809   -1.376025   -0.544679
C   -1.942082   -1.889809    0.708458
C   -2.853153   -2.932542    0.849275
C   -3.452513   -3.475381   -0.289295
C   -3.129335   -2.971422   -1.553375
P   -0.478682    0.042278   -0.691482
C   -1.520035    1.462501   -0.223494
C   -0.998062    2.730934    0.044392
C   -1.816425    3.788735    0.419811
C   -3.196926    3.596626    0.508945
C   -3.737328    2.338154    0.228729
C   -2.911386    1.288084   -0.123672
O   -0.037816   -0.154309   -2.204449
Si   1.289625    0.983523   -2.618532
C    3.048764    0.659069   -1.961953
C    3.526851    1.253362   -0.786539
C    4.787621    0.954841   -0.282888
C    5.598384    0.031716   -0.941455
C    5.145414   -0.571944   -2.109619
C    3.885170   -0.253266   -2.614264
C    0.798815   -0.355767    0.520841
C    1.002241    0.373862    1.685396
C    2.047179    0.053970    2.550038
C    2.902463   -1.003099    2.234333
C    2.690070   -1.751024    1.070924
C    1.646019   -1.432098    0.225184
H    0.872254    1.476513   -1.102116
H    0.976850    2.358703   -3.116858
H    1.429450    0.264958   -3.943521
H    2.886604    1.943779   -0.244000
H    5.134474    1.426150    0.630961
H    6.575599   -0.217217   -0.542603
H    5.771199   -1.291507   -2.626477
H    3.540512   -0.731414   -3.526703
H    0.066000    2.903881   -0.052567
H   -1.370302    4.753280    0.620541
O   -4.076892    4.558641    0.848627
H   -4.810427    2.205823    0.293482
H   -3.361453    0.324926   -0.327104
H    0.354360    1.208328    1.930651
H    2.185976    0.637856    3.449929
O    3.958429   -1.377724    2.990910
H    3.368789   -2.563629    0.842442
H    1.498844   -2.008546   -0.682746
H   -1.478759   -1.479839    1.600553
H   -3.077861   -3.312565    1.836649
O   -4.346616   -4.488428   -0.266634
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H   -3.598276   -3.414782   -2.423580
H   -1.967080   -1.555924   -2.660234
C   -3.574862    5.856991    1.125443
H   -4.442519    6.466760    1.367700
H   -2.892323    5.841566    1.979990
H   -3.068153    6.277110    0.252226
C   -4.695014   -5.039911    0.991683
H   -5.413512   -5.830081    0.783952
H   -3.820688   -5.467813    1.490790
H   -5.159267   -4.288838    1.637588
C    4.244104   -0.621010    4.153620
H    5.132975   -1.069321    4.592741
H    4.451419    0.423789    3.902951
H    3.421169   -0.672561    4.872859
1 imaginary frequency
E = -1977.830951
H = -1977.301893
G = -1977.386698
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1g

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C   -0.741799   -0.544988   -0.381210
C   -1.302625    0.663579   -0.821157
P   -0.000088    1.868420   -1.243504
C    1.302565    0.663700   -0.821167
C    0.741861   -0.544920   -0.381209
C   -0.000157    3.119931    0.066996
C   -0.000207    4.461176   -0.310261
H   -0.000189    4.717120   -1.364078
C   -0.000285    5.450862    0.669325
H   -0.000328    6.495189    0.380493
C   -0.000311    5.098021    2.014094
H   -0.000370    5.869775    2.775156
C   -0.000262    3.755288    2.389774
H   -0.000286    3.484253    3.438798
C   -0.000189    2.764043    1.417945
H   -0.000165    1.717244    1.708235
O   -0.000128    2.463238   -2.611818
C    1.572904   -1.587893    0.001438
C    2.952812   -1.401483   -0.069095
C    3.511028   -0.208360   -0.512760
C    2.673807    0.840076   -0.891323
C   -1.572743   -1.588052    0.001389
C   -2.952672   -1.401798   -0.069165
C   -3.511004   -0.208724   -0.512813
C   -2.673883    0.839804   -0.891346
H   -1.168407   -2.532767    0.349655
H   -4.586493   -0.095945   -0.559757
H   -3.094579    1.777853   -1.235391
H    1.168664   -2.532634    0.349748
H    4.586508   -0.095476   -0.559681
H    3.094410    1.778166   -1.235368
C    3.832086   -2.548932    0.342260
C   -3.831812   -2.549337    0.342236
F   -3.684119   -3.605093   -0.476054
F   -5.130747   -2.231301    0.342322
F   -3.530377   -2.983539    1.577955
F    3.530254   -2.983667    1.577686
F    3.685045   -3.604419   -0.476504
F    5.130932   -2.230529    0.342992
0 imaginary frequencies
E = -1784.344793
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H = -1784.053168
G = -1784.122757

TS1g

Si	2.943834	0.199155	-2.021099
O	1.358610	-0.816413	-1.738899
P	0.612267	-0.408790	-0.438576
H	2.336835	0.928572	-0.749124
C	1.555167	-0.760983	1.054712
C	-0.903305	-1.404355	-0.377786
C	-0.325763	1.142627	-0.307700
C	4.649286	0.132547	-1.153623
C	4.882223	0.756897	0.077436
H	4.065869	1.279723	0.570063
C	6.129856	0.706807	0.692548
H	6.285790	1.196891	1.647608
C	7.176458	0.018662	0.083605
H	8.149466	-0.025656	0.560273
C	6.965819	-0.619319	-1.135610
H	7.776065	-1.161026	-1.611463
C	5.711513	-0.566523	-1.739334
H	5.553432	-1.079901	-2.683876
H	3.239265	-0.878202	-3.036314
H	2.741369	1.379011	-2.913559
C	1.260905	-0.130943	2.264811
C	2.007278	-0.443363	3.394265
C	3.036278	-1.378963	3.316042
C	3.321855	-2.008225	2.109075
C	2.582182	-1.702372	0.972123
H	0.466842	0.605987	2.324335
H	1.789210	0.048523	4.334675
H	3.620052	-1.613470	4.198368
H	4.129983	-2.726770	2.044353
H	2.820331	-2.176536	0.025555
C	-2.026358	-0.584310	-0.242432
C	-1.697613	0.859387	-0.198141
C	-1.013870	-2.785599	-0.449359
C	-2.278383	-3.356905	-0.378352
C	-3.398435	-2.537821	-0.239126
C	-3.293555	-1.154332	-0.171086
H	-4.183570	-0.545548	-0.069916
H	-0.134622	-3.409298	-0.561571
H	-2.399404	-4.432726	-0.433808
C	-2.606593	1.901559	-0.055432
C	-2.126845	3.205752	-0.029145
C	-0.768220	3.489440	-0.138361
C	0.143718	2.449023	-0.279109
H	-0.424229	4.516763	-0.119391
H	-3.668972	1.710114	0.032143
H	1.202722	2.652771	-0.372300
C	-3.079649	4.353940	0.166630
C	-4.745065	-3.200886	-0.153997
F	-4.355423	3.999855	-0.026405
F	-2.815749	5.367803	-0.669052
F	-2.995242	4.851216	1.412832
F	-4.836998	-3.990504	0.929204
F	-5.749052	-2.319193	-0.084009
F	-4.979347	-3.985253	-1.217767

1 imaginary frequency
E = -2307.197657
H = -2306.780949
G = -2306.863599

1h

C	-1.827617	-0.742573	-0.204156
C	-0.732205	-1.302559	0.468553
P	0.354072	0.000018	1.126007
C	-0.732259	1.302547	0.468544
C	-1.827652	0.742510	-0.204154
C	1.858052	0.000039	0.107561
C	3.089632	0.000021	0.758822
H	3.114917	0.000004	1.843031
C	4.265321	0.000026	0.012099
H	5.224540	0.000011	0.516334
C	4.206505	0.000049	-1.376932
H	5.122110	0.000053	-1.957130
C	2.973439	0.000068	-2.028007
H	2.930810	0.000086	-3.110826
C	1.798484	0.000063	-1.288071
H	0.836613	0.000076	-1.792946
O	0.668772	0.000028	2.587209
C	-2.775939	1.578694	-0.785324
C	-2.620484	2.959035	-0.680972
C	-1.531631	3.508613	-0.007269
C	-0.575453	2.676557	0.572016
C	-2.775856	-1.578801	-0.785339
C	-2.620341	-2.959135	-0.680983
C	-1.531473	-3.508663	-0.007262
C	-0.575339	-2.676562	0.572030
H	-3.629377	-1.166574	-1.311709
H	-3.358194	-3.614447	-1.129189
H	-1.428821	-4.584647	0.066719
H	0.276010	-3.095657	1.097572
H	-3.629451	1.166427	-1.311676
H	-3.358373	3.614313	-1.129168
H	-1.429026	4.584603	0.066708
H	0.275881	3.095692	1.097549

0 imaginary frequencies
E = -1110.244854
H = -1109.970117
G = -1110.024642

TS1h

Si	1.554519	1.020677	-1.812467
O	0.045768	-0.078855	-1.810665
P	-0.715572	-0.058619	-0.446539
H	0.957467	1.348734	-0.366287
C	0.245787	-0.792699	0.890461
C	-2.191834	-1.082323	-0.673825
C	-1.696327	1.364915	0.097524
C	3.261719	0.676562	-1.016820
C	3.517358	0.929540	0.336384
H	2.716469	1.313756	0.963428
C	4.765803	0.680850	0.898858
H	4.938951	0.883981	1.950275
C	5.790646	0.160145	0.112049
H	6.763821	-0.039522	0.547003
C	5.557639	-0.109347	-1.233395
H	6.350561	-0.519047	-1.849810
C	4.303354	0.143091	-1.785275
H	4.128132	-0.080651	-2.833886
H	1.859600	0.349338	-3.133992
H	1.341514	2.423399	-2.285549
C	-0.043527	-0.512520	2.226640
C	0.711832	-1.109781	3.228345

```
C    1.745537   -1.983404    2.898773
C    2.025607   -2.265351    1.566012
C    1.276370   -1.671842    0.555927
H   -0.842206    0.175551    2.482738
H    0.496790   -0.888791    4.267103
H    2.336561   -2.440669    3.683657
H    2.837113   -2.934884    1.307312
H    1.511337   -1.873865   -0.483888
C   -3.342277   -0.369268   -0.318615
C   -3.060094    1.017991    0.120134
C   -2.260952   -2.392516   -1.122776
C   -3.509992   -3.002346   -1.214324
C   -4.660326   -2.300839   -0.858063
C   -4.586656   -0.984624   -0.409678
H   -5.626850   -2.785105   -0.933689
H   -5.490912   -0.450989   -0.140958
H   -1.361738   -2.931049   -1.400806
H   -3.587571   -4.023927   -1.566271
C   -3.997170    1.956747    0.536678
C   -3.570286    3.224157    0.924640
C   -2.219638    3.560370    0.902001
C   -1.271135    2.628482    0.485934
H   -4.300529    3.957482    1.246555
H   -1.902474    4.551344    1.203054
H   -5.051849    1.708440    0.560117
H   -0.218640    2.881173    0.456287
1 imaginary frequency
E = -1633.099716
H = -1632.699903
G = -1632.767932
```

1i

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C   -0.750646   -1.165843   -0.180345
C   -1.294437    0.020789   -0.702618
P    0.014142    1.170146   -1.205303
C    1.300713    0.001054   -0.690286
C    0.734460   -1.177988   -0.174982
C    0.015400    2.539046   -0.007691
C    0.082440    3.841538   -0.497848
H    0.125675    4.000645   -1.569733
C    0.090756    4.915263    0.389550
H    0.142550    5.928907    0.009547
C    0.031577    4.685485    1.759446
H    0.037651    5.521615    2.449344
C   -0.036881    3.382006    2.249915
H   -0.084414    3.204967    3.318011
C   -0.045435    2.308771    1.368636
H   -0.101455    1.292949    1.748895
O    0.029319    1.678425   -2.612182
C    1.547073   -2.202648    0.273700
C    2.938458   -2.054164    0.201994
C    3.505464   -0.885223   -0.314376
C    2.675184    0.143378   -0.759051
C   -1.583037   -2.174772    0.267447
C   -2.971322   -2.003212    0.187717
C   -3.515938   -0.826532   -0.335119
C   -2.665960    0.186460   -0.778401
H   -1.198164   -3.101119    0.678005
H   -4.586657   -0.690928   -0.401840
H   -3.088343    1.100100   -1.182909
H    1.144237   -3.124479    0.677351
H    4.578605   -0.767627   -0.375818
```

```
H     3.115114    1.050389   -1.159796
O    -3.709706   -3.038244    0.644744
O     3.656979   -3.103161    0.659064
C     5.071481   -3.016524    0.611750
H     5.436850   -2.188329    1.225961
H     5.441798   -3.956012    1.016577
H     5.425790   -2.900559   -0.416556
C    -5.122266   -2.927098    0.591789
H    -5.510382   -3.858327    0.999013
H    -5.475480   -2.090221    1.201372
H    -5.470719   -2.809037   -0.438266
0 imaginary frequencies
E = -1339.274533
H = -1338.928671
G = -1338.993631
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TS1i

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Si    2.242169    0.454134   -2.001916
O     0.751636   -0.604792   -1.726816
P    -0.004875   -0.245223   -0.402232
H     1.669210    1.112010   -0.652745
C     0.964832   -0.668874    1.059475
C    -1.492042   -1.268758   -0.378937
C    -0.959165    1.273094   -0.216292
C     3.954109    0.266410   -1.166248
C     4.231238    0.797592    0.099463
H     3.442611    1.315088    0.640135
C     5.485234    0.658953    0.686895
H     5.674380    1.077520    1.669653
C     6.494776   -0.027332    0.015810
H     7.472198   -0.141493    0.471647
C     6.240615   -0.572289   -1.239472
H     7.021340   -1.111551   -1.765061
C     4.980759   -0.428540   -1.816806
H     4.789006   -0.866941   -2.792141
H     2.531008   -0.477892   -3.160791
H     2.032461    1.726544   -2.761584
C     0.706731   -0.073138    2.294683
C     1.466167   -0.435353    3.400547
C     2.473361   -1.389741    3.275942
C     2.722025   -1.987112    2.044950
C     1.969102   -1.628987    0.931612
H    -0.071810    0.676568    2.388974
H     1.275016    0.031415    4.359646
H     3.067563   -1.663661    4.139911
H     3.512655   -2.720926    1.943008
H     2.180514   -2.076582   -0.033837
C    -2.638319   -0.477957   -0.209122
C    -2.334363    0.970031   -0.116425
C    -1.598774   -2.643082   -0.499046
C    -2.853717   -3.247126   -0.446894
C    -3.994583   -2.457028   -0.273185
C    -3.888395   -1.065225   -0.153693
H    -4.795567   -0.486166   -0.026713
H    -0.715203   -3.256635   -0.636839
H    -2.930711   -4.320956   -0.546066
C    -3.256722    1.982880    0.053134
C    -2.817215    3.312368    0.121407
C    -1.456155    3.616309    0.024419
C    -0.530500    2.589330   -0.145521
H    -1.107621    4.638615    0.070417
H    -4.318968    1.784575    0.132232
```

```
H    0.524032    2.821202   -0.230203
O   -3.786371    4.233725    0.280709
O   -5.249859   -2.949474   -0.210661
C   -3.409966    5.601314    0.346093
H   -4.335947    6.159005    0.466788
H   -2.758324    5.788825    1.204022
H   -2.913219    5.916406   -0.575548
C   -5.426399   -4.351238   -0.339418
H   -4.919507   -4.888178    0.467474
H   -6.498188   -4.524440   -0.270270
H   -5.063237   -4.706559   -1.307888
1 imaginary frequency
E = -1862.130640
H = -1861.659871
G = -1861.738075
```

1j

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H    1.920705   -2.173683   -0.367844
C    2.542216   -1.300406   -0.591419
H    3.388942   -1.646367   -1.186812
C    1.716201   -0.249425   -1.350260
H    2.368745    0.458337   -1.869828
H    1.021306   -0.670195   -2.077649
P    0.848308    0.732394   -0.060100
C    1.741822   -0.024138    1.355935
H    1.954055    0.743616    2.100815
H    1.113114   -0.790797    1.817128
C    2.993541   -0.651230    0.725346
H    3.728095    0.131531    0.511820
H    3.463880   -1.372719    1.395465
C   -0.880423    0.166736   -0.002087
C   -1.890461    1.126447   -0.002487
H   -1.619149    2.176102   -0.033056
C   -3.224833    0.729779    0.032191
H   -4.009934    1.476942    0.033274
C   -3.549220   -0.622248    0.062289
H   -4.588256   -0.929749    0.087846
C   -2.540843   -1.584277    0.057849
H   -2.794253   -2.637814    0.078241
C   -1.208638   -1.190724    0.026178
H   -0.424635   -1.942931    0.020478
O    0.944575    2.223592   -0.186199
0 imaginary frequencies
E = -805.424192
H = -805.201866
G = -805.246580
```

TS1j

```
Si  -0.274484   -2.226136    0.267195
O    1.072328   -1.634363   -0.769994
P    1.705225   -0.330245   -0.125305
H    0.339363   -0.966138    1.179622
C    0.610569    1.103595   -0.189307
C    3.086860    0.045218   -1.284991
C    2.782113   -0.482091    1.344888
H   -0.595930   -3.244010   -0.805272
C    0.680905    2.130149    0.752274
C   -0.190078    3.209578    0.658202
C   -1.128432    3.264002   -0.369623
C   -1.192452    2.241945   -1.310626
C   -0.321445    1.160941   -1.226096
H    1.398615    2.086347    1.564649
```

```
H   -0.140897    4.005221    1.392326
H   -1.813114    4.101651   -0.432417
H   -1.928895    2.275787   -2.104662
H   -0.386383    0.353181   -1.947862
C    4.343848   -0.454090   -0.561325
H    2.914526   -0.418322   -2.255940
H    3.134153    1.129758   -1.419009
C    4.183434   -0.036899    0.906630
H    4.402310   -1.545094   -0.628876
H    5.252819   -0.044594   -1.004363
H    4.269061    1.051475    0.985100
H    4.949448   -0.477188    1.546780
H    2.762919   -1.546475    1.599744
H    2.363956    0.058992    2.193041
H    0.050327   -3.149992    1.395429
C   -1.967343   -1.353319    0.293617
C   -2.955956   -1.729324   -0.623176
C   -2.263880   -0.307885    1.177848
C   -4.193631   -1.088952   -0.659089
H   -2.752525   -2.533001   -1.324759
C   -3.499520    0.329513    1.158387
H   -1.504214    0.022306    1.880925
C   -4.467296   -0.057604    0.233201
H   -4.942141   -1.394445   -1.382138
H   -3.705496    1.136043    1.853850
H   -5.428293    0.444322    0.207746
1 imaginary frequency
E = -1328.279576
H = -1327.932792
G = -1327.991526
```

2j

```
Si   0.110436   -2.622169   -0.581208
O   -1.153641   -1.749848    0.084636
P   -1.593110   -0.170490   -0.281838
H   -1.008519   -0.399250   -1.616947
C   -0.380389    1.204546   -0.045779
C   -2.444916   -0.046837    1.426706
C   -3.205295    0.266380   -1.110681
H    0.123745   -3.908036    0.143334
C   -0.059485    2.025477   -1.127078
C    0.897642    3.024746   -0.993901
C    1.586808    3.169488    0.208119
C    1.301192    2.327100    1.277625
C    0.305404    1.360928    1.157973
H   -0.552448    1.873111   -2.083462
H    1.122143    3.675632   -1.831386
H    2.352614    3.930593    0.306126
H    1.851541    2.421167    2.206833
H    0.079978    0.714135    1.999477
C   -3.922696   -0.315273    1.156862
H   -2.009519   -0.722383    2.161776
H   -2.339549    0.983020    1.784516
C   -4.280671    0.541241   -0.067132
H   -4.078198   -1.374894    0.923302
H   -4.554800   -0.071524    2.014010
H   -4.263929    1.597275    0.219740
H   -5.279181    0.317481   -0.448787
H   -3.442026   -0.620626   -1.708865
H   -3.016421    1.082919   -1.812202
H   -0.093060   -2.834095   -2.031308
C    1.700867   -1.684399   -0.289574
```

```
C    2.417787   -1.845703    0.903025
C    2.135249   -0.710176   -1.198448
C    3.530009   -1.056454    1.182432
H    2.104812   -2.593361    1.626369
C    3.240881    0.086389   -0.920718
H    1.592679   -0.558082   -2.127468
C    3.938020   -0.086177    0.272150
H    4.074333   -1.195022    2.109792
H    3.554525    0.844855   -1.629016
H    4.798500    0.535908    0.492089
0 imaginary frequencies
E = -1328.295568
H = -1327.946513
G = -1328.006830
```

TS2j

```
Si   0.376432   -2.581865   -0.538373
O   -0.945765   -1.825893    0.145478
P   -1.660889   -0.350692   -0.296059
H   -1.104797   -0.593831   -1.630242
C   -0.533073    1.073098   -0.022864
C   -2.587577   -0.358308    1.385697
C   -3.247338    0.190635   -1.143613
H    0.527987   -3.859982    0.185391
C   -0.315540    2.004080   -1.037808
C    0.596350    3.039095   -0.859047
C    1.327423    3.125309    0.322646
C    1.138445    2.179868    1.326166
C    0.202577    1.163588    1.158396
H   -0.849237    1.914422   -1.979345
H    0.747023    3.768647   -1.646656
H    2.051399    3.921109    0.456037
H    1.722204    2.229342    2.238176
H    0.060134    0.426530    1.942571
C   -4.080724   -0.371464    1.073063
H   -2.270066   -1.185983    2.015954
H   -2.345706    0.581003    1.892772
C   -4.280784    0.591550   -0.105810
H   -4.396702   -1.377823    0.774897
H   -4.684311   -0.081248    1.936069
H   -4.097475    1.617538    0.230326
H   -5.298241    0.547113   -0.500706
H   -3.575396   -0.690577   -1.707959
H   -2.991537    0.959654   -1.876811
H    0.159396   -2.815735   -1.984327
C    1.897119   -1.520792   -0.297436
C    2.680252   -1.646546    0.856461
C    2.223091   -0.512165   -1.214207
C    3.752656   -0.790372    1.092000
H    2.452109   -2.420295    1.584032
C    3.290609    0.348357   -0.982110
H    1.628182   -0.387656   -2.115119
C    4.055797    0.209492    0.173293
H    4.349498   -0.902363    1.990225
H    3.522118    1.130152   -1.696706
H    4.887122    0.881069    0.356754
1 imaginary frequency
E = -1328.295137
H = -1327.947097
G = -1328.005856
```

3j

Si	-0.963311	-0.504715	2.222741
O	0.631704	-0.564880	1.892436
P	1.857168	-0.299131	0.534392
H	2.743825	-0.252230	1.618605
C	1.002701	1.246398	0.057876
C	3.293461	-0.169957	-0.716422
C	1.344955	-1.920600	-0.194623
C	-2.049756	-0.704889	0.697023
C	-2.492427	-1.967565	0.279189
H	-2.237244	-2.848212	0.862711
C	-3.257760	-2.119002	-0.873880
H	-3.591943	-3.104368	-1.179195
C	-3.597857	-1.001725	-1.632193
H	-4.195465	-1.116057	-2.529689
C	-3.174337	0.262488	-1.231853
H	-3.440203	1.136106	-1.817138
C	-2.410124	0.405870	-0.076951
H	-2.084825	1.399217	0.222506
H	-1.332148	0.795402	2.844660
H	-1.314324	-1.604383	3.157216
C	0.614793	1.448686	-1.267162
C	-0.054297	2.612542	-1.631922
C	-0.310774	3.596579	-0.681993
C	0.083451	3.403767	0.639215
C	0.721582	2.225164	1.013146
H	0.812028	0.689978	-2.017326
H	-0.373328	2.749383	-2.658722
H	-0.821252	4.508743	-0.968724
H	-0.117147	4.165207	1.383962
H	0.992801	2.058869	2.049331
C	3.646290	-1.623773	-1.019325
H	4.115497	0.397982	-0.272991
H	3.002147	0.333651	-1.641723
C	2.302487	-2.301068	-1.323997
H	4.100031	-2.097826	-0.140024
H	4.352318	-1.729482	-1.845988
H	2.395130	-3.385564	-1.408719
H	1.925191	-1.928395	-2.281283
H	1.369173	-2.633851	0.631473
H	0.300598	-1.819633	-0.499455

0 imaginary frequencies
E = -1328.307925
H = -1327.958654
G = -1328.019229

TS3j

Si	-1.824793	0.444655	2.212780
O	-0.386316	-0.113719	2.609375
P	1.570783	-0.662114	0.693891
H	1.246510	-0.593420	2.063750
C	1.387832	0.996427	0.020305
C	3.186307	-1.400283	0.240063
C	0.529217	-1.898891	-0.162534
C	-2.313185	-0.030386	0.432901
C	-2.917266	-1.265024	0.155815
H	-3.210559	-1.912597	0.978440
C	-3.145618	-1.690446	-1.150804
H	-3.615180	-2.650527	-1.337132
C	-2.773215	-0.878756	-2.220380
H	-2.950064	-1.204714	-3.239519
C	-2.187631	0.360646	-1.972430

```
H   -1.908199    1.004411   -2.800168
C   -1.965825    0.775743   -0.660273
H   -1.504405    1.745556   -0.486816
H   -1.929122    1.944477    2.222450
H   -2.954967   -0.059756    3.057459
C    1.512515    1.204101   -1.355236
C    1.325418    2.477691   -1.876689
C    1.021053    3.538642   -1.025681
C    0.901551    3.328890    0.344345
C    1.078747    2.054779    0.875259
H    1.736400    0.375510   -2.020830
H    1.410883    2.642466   -2.944178
H    0.870610    4.530835   -1.435155
H    0.651751    4.152488    1.002355
H    0.933529    1.863465    1.932657
C    2.823958   -2.847000   -0.132485
H    3.901985   -1.314360    1.057360
H    3.579407   -0.858477   -0.624439
C    1.521646   -2.781460   -0.940045
H    2.663535   -3.432814    0.777576
H    3.631793   -3.319190   -0.693318
H    1.099811   -3.772100   -1.113966
H    1.723992   -2.334039   -1.918038
H   -0.000253   -2.454274    0.614859
H   -0.214606   -1.404699   -0.788416
1 imaginary frequency
E = -1328.288727
H = -1327.941949
G = -1328.003553
```

1-phenylphospholane (4j)

```
H   -1.404935    0.741896    1.760048
C   -2.274708    0.811813    1.098125
H   -3.003980    1.475631    1.569881
C   -1.837181    1.330017   -0.272479
H   -2.710592    1.596720   -0.874626
H   -1.196792    2.210859   -0.226861
P   -0.995214   -0.098220   -1.136139
C   -1.817294   -1.353538    0.005497
H   -2.275819   -2.153192   -0.576959
H   -1.058233   -1.799243    0.650885
C   -2.847250   -0.583591    0.849074
H   -3.786207   -0.490643    0.293965
H   -3.067193   -1.113334    1.778840
C    0.702447   -0.027520   -0.404884
C    1.395364   -1.216304   -0.146766
H    0.909159   -2.173221   -0.308514
C    2.709267   -1.196394    0.308327
H    3.222823   -2.130661    0.505655
C    3.363654    0.015614    0.506290
H    4.386707    0.033178    0.863177
C    2.695176    1.203794    0.231729
H    3.197440    2.154474    0.371367
C    1.381169    1.182309   -0.227305
H    0.891968    2.123636   -0.450418
0 imaginary frequencies
E = -730.168311
H = -729.951479
G = -729.994291
```

1k

H	0.769663	-2.022451	0.782442
C	1.660278	-1.395759	0.858548
H	2.324487	-1.828665	1.611598
C	1.370106	0.082854	1.171021
H	0.855608	0.298647	2.106049
P	0.436072	0.628908	-0.320738
C	1.307816	-0.572081	-1.416498
H	1.728208	-0.028635	-2.264686
H	0.623331	-1.332417	-1.799169
C	2.379790	-1.180803	-0.488164
H	2.820099	-2.081837	-0.915110
C	-1.308659	0.136855	-0.130123
C	-2.217428	1.166522	0.127577
H	-1.858544	2.189256	0.162972
C	-3.564747	0.880185	0.318274
H	-4.263583	1.684446	0.516546
C	-4.015151	-0.434323	0.244629
H	-5.065994	-0.657116	0.389355
C	-3.117378	-1.462881	-0.024951
H	-3.467722	-2.486015	-0.095611
C	-1.768673	-1.179563	-0.214602
H	-1.085919	-1.991372	-0.437857
O	0.553895	2.082349	-0.674509
C	2.771548	0.713025	1.028296
H	2.722970	1.779532	0.808310
H	3.319406	0.583942	1.964127
C	3.430973	-0.109090	-0.119047
H	4.350472	-0.584892	0.226325
H	3.684413	0.515523	-0.977900

0 imaginary frequencies
E = -882.826463
H = -882.566797
G = -882.613302

TS1k

Si	-0.473888	-2.213782	0.403488
O	0.874639	-1.552908	-0.615998
P	1.391757	-0.186139	-0.016628
H	0.029728	-0.939553	1.327546
C	0.150576	1.122348	-0.146186
C	2.452156	-0.165647	1.478705
C	2.778147	0.326595	-1.107444
H	-0.686288	-3.251305	-0.679928
C	-0.700677	1.069399	-1.252334
C	-1.707490	2.017244	-1.397794
C	-1.860827	3.020777	-0.447225
C	-1.006328	3.078816	0.650528
C	-0.002601	2.129471	0.806132
H	-0.598543	0.271828	-1.981338
H	-2.379886	1.959482	-2.245414
H	-2.651616	3.753762	-0.556582
H	-1.127591	3.858238	1.393635
H	0.640495	2.170097	1.678104
C	3.836130	0.264386	0.950392
H	2.439494	-1.160555	1.926989
H	2.038042	0.532653	2.208751
C	3.536213	1.283676	-0.166189
H	4.467954	0.640338	1.754600
H	2.944327	2.138601	0.172631
H	4.448770	1.655800	-0.637876
H	2.440564	0.741526	-2.055723

```
C     3.763560   -0.855953   -1.225076
H     4.480364   -0.642578   -2.020458
H     3.259043   -1.789357   -1.473037
C     4.474028   -0.895714    0.159850
H     4.341143   -1.852255    0.668713
H     5.546562   -0.728436    0.047252
C    -2.209892   -1.429967    0.332004
C    -3.117452   -1.827883   -0.656106
C    -2.603282   -0.404951    1.202212
C    -4.368980   -1.225537   -0.776852
H    -2.836791   -2.616389   -1.348408
C    -3.852711    0.195868    1.096776
H    -1.907395   -0.059728    1.961721
C    -4.738197   -0.210876    0.100217
H    -5.053488   -1.546819   -1.554542
H    -4.133540    0.989467    1.781024
H    -5.709288    0.262998    0.007366
H    -0.165353   -3.131811    1.543892
1 imaginary frequency
E = -1405.684165
H = -1405.299987
G = -1405.360438
```

1l

```
C    -0.887249   -1.691836    0.877513
C    -0.249499   -0.337452    1.331118
C    -1.170537   -1.697378   -0.662827
H    -0.214680   -2.507122    1.150262
H    -1.823264   -1.854074    1.411436
H    -0.846171   -2.634472   -1.120077
H    -2.239398   -1.584372   -0.841257
H    -0.728356   -0.007811    2.254383
C     1.103933   -0.874860   -1.356370
H     1.248894   -1.800181   -0.790124
H     1.320971   -1.134723   -2.396004
C     1.290309   -0.403794    1.538603
H     1.504095   -0.103805    2.567496
H     1.604266   -1.448981    1.464444
P    -0.897251    0.729527   -0.019172
O    -2.391024    0.880279    0.084636
C    -0.163499    2.380214   -0.228998
H    -0.115941    2.877427    0.742000
H     0.811195    2.401312   -0.706968
H    -0.879239    2.922244   -0.850884
C    -0.402094   -0.508516   -1.278119
H    -0.800788   -0.228383   -2.254853
C     2.174219    0.116297   -0.885456
H     2.116748    1.035988   -1.474215
H     3.136168   -0.331768   -1.148631
C     2.191221    0.448324    0.632418
H     3.214229    0.326366    0.998206
H     1.957397    1.501213    0.797989
0 imaginary frequencies
E = -769.705105
H = -769.441255
G = -769.485538
```

TS1l

```
Si   -1.354652    1.794499   -0.471885
O     0.185613    1.770887    0.419988
P     1.178846    0.714501   -0.246490
H    -0.462960    0.681249   -1.370649
C     0.732094   -1.026924    0.184655
C     2.499844    0.698153    1.031987
```

```
H   -1.903048    2.769251    0.548363
H   -0.196686   -1.301306   -0.309581
H    2.732777    1.733979    1.282114
C    1.740709    0.037776    2.220593
H    2.432901   -0.579462    2.796138
H    1.362526    0.810158    2.889826
C    0.540865   -0.815474    1.698948
H   -0.403033   -0.305155    1.895568
H    0.497679   -1.788175    2.192838
C    1.875898    1.357412   -1.798011
H    1.938351    0.589100   -2.566998
H    1.191181    2.132305   -2.143911
H    2.855630    1.798007   -1.610715
C    3.951726   -0.738506   -0.738830
H    4.924955   -1.235468   -0.713545
H    4.040304    0.006873   -1.529655
C    2.878375   -1.791236   -1.132861
H    2.366931   -1.494576   -2.053354
H    3.384702   -2.728895   -1.372740
C    1.835018   -2.087120   -0.057324
H    1.321556   -3.019069   -0.305865
H    2.353340   -2.274526    0.887727
C    3.814226   -0.038517    0.631356
H    4.634153    0.682052    0.687227
H    4.024801   -0.777776    1.408768
C   -2.704842    0.463908   -0.268806
C   -3.655709    0.586380    0.751769
C   -2.810043   -0.640275   -1.124535
C   -4.669694   -0.355535    0.916135
H   -3.602504    1.434914    1.427533
C   -3.828234   -1.577317   -0.979799
H   -2.080363   -0.762953   -1.920559
C   -4.758790   -1.438505    0.047749
H   -5.391022   -0.242127    1.718067
H   -3.896515   -2.417055   -1.662912
H   -5.548881   -2.171163    0.169656
H   -1.427898    2.646896   -1.697665
1 imaginary frequency
E = -1292.562561
H = -1292.173616
G = -1292.232016
```

1m

```
C   -0.565027   -1.387525    1.304740
C    0.836247    0.647195   -1.486055
H   -0.582269   -2.476480    1.212140
H   -1.261553   -1.118221    2.104386
H    0.326961    1.153234   -2.311761
H    1.832342    1.080514   -1.384961
C    0.836247   -0.874665    1.688954
H    1.597755   -1.339057    1.058900
H    1.077410   -1.134046    2.721656
C    0.836247    0.647195    1.486055
H    1.832342    1.080514    1.384961
H    0.326961    1.153234    2.311761
C   -0.565027   -1.387525   -1.304740
H   -0.582269   -2.476480   -1.212140
H   -1.261553   -1.118221   -2.104386
C    0.836247   -0.874665   -1.688954
H    1.597755   -1.339057   -1.058900
H    1.077410   -1.134046   -2.721656
C   -1.031239   -0.710434   -0.000000
H   -2.112803   -0.574434   -0.000000
P   -0.194225    0.948024    0.000000
O   -1.007161    2.208092    0.000000
```

0 imaginary frequencies
E = -691.121212
H = -690.918765
G = -690.956070

TS1m

Si	-1.058915	1.632712	0.116357
O	0.502464	1.20427	0.948079
P	1.428489	0.318886	0.028933
H	-0.321967	0.758875	-1.055116
C	2.313157	1.080684	-1.364379
H	-1.463448	2.290699	1.419895
H	2.402576	2.14765	-1.134674
H	1.764189	0.971885	-2.2977
C	4.129428	0.258684	0.122687
H	4.929095	-0.478344	0.22896
H	4.532645	1.222935	0.44189
C	3.678959	0.380681	-1.346048
H	4.407793	0.936205	-1.938404
H	3.583062	-0.608149	-1.802498
C	-2.596195	0.505849	-0.028189
C	-3.617617	0.59663	0.925697
C	-2.767703	-0.40804	-1.075235
C	-4.769288	-0.18154	0.833855
H	-3.508311	1.290062	1.754315
C	-3.9163	-1.187579	-1.179532
H	-1.986623	-0.505911	-1.824257
C	-4.920977	-1.07573	-0.221448
H	-5.546517	-0.092166	1.58506
H	-4.029261	-1.883356	-2.004016
H	-5.81532	-1.684394	-0.296089
H	-1.056409	2.838629	-0.768331
C	2.926292	-0.09613	1.02916
C	2.757474	-1.589252	1.362177
H	3.713782	-2.047024	1.625103
H	2.097659	-1.683268	2.230396
C	2.101741	-2.286174	0.161327
H	2.825363	-2.394603	-0.650607
H	1.75546	-3.288154	0.419989
C	0.926252	-1.407039	-0.298927
H	0.028269	-1.585187	0.300973
H	0.656858	-1.531228	-1.347853
H	2.93753	0.503179	1.938481

1 imaginary frequency
E = -1213.978983
H = -1213.650801
G = -1213.704966

1n (H_2PhP=O)

P	1.901227	-0.409173	-0.000013
H	2.125002	-1.270291	1.093852
H	2.125010	-1.270203	-1.093945
O	2.696002	0.855349	0.000035
C	0.105833	-0.173929	-0.000004
C	-0.763830	-1.265562	0.000007
C	-0.393281	1.125941	-0.000010
C	-2.136509	-1.052707	0.000010
H	-0.374106	-2.279650	0.000014
C	-1.769861	1.334220	-0.000006
H	0.298213	1.961631	-0.000012
C	-2.637914	0.247796	0.000003
H	-2.815391	-1.897276	0.000015
H	-2.162549	2.344126	-0.000015
H	-3.709227	0.411919	0.000007

0 imaginary frequencies
E = -649.373733
H = -649.250819
G = -649.287888

TS1n: $PhSiH_3 + H_2PhP{=}O$

C	3.756062	-1.232648	-0.049222
C	2.790169	-0.225496	-0.002788
C	3.125548	1.047642	0.457552
C	4.427116	1.306461	0.874981
C	5.387951	0.301278	0.832647
C	5.054310	-0.968763	0.369630
P	1.097649	-0.625521	-0.503834
O	0.423189	0.769043	-0.708732
Si	-1.321226	0.562330	-1.274499
C	-2.888277	0.152113	-0.266912
C	-3.716321	1.190402	0.177399
C	-4.895082	0.930927	0.872223
C	-5.267477	-0.382548	1.141433
C	-4.455583	-1.430850	0.715864
C	-3.277738	-1.160604	0.025385
H	-0.829790	-0.993130	-1.107357
H	-3.433271	2.219200	-0.024854
H	-5.520855	1.751529	1.205668
H	-6.183318	-0.588991	1.684043
H	-4.740066	-2.456192	0.925752
H	-2.648062	-1.985082	-0.297010
H	-1.424339	2.063153	-1.149135
H	-1.455762	0.392281	-2.749669
H	2.373485	1.827190	0.476230
H	4.690657	2.295925	1.229158
H	6.401332	0.508093	1.156360
H	5.804498	-1.749421	0.330115
H	3.500104	-2.222653	-0.415994
H	1.276661	-1.455907	-1.612521
H	0.591559	-1.415637	0.530403

1 imaginary frequency
E = -1172.225860
H = -1171.978039
G = -1172.030039

1o ($H_2MeP{=}O$)

P	-0.205200	0.376772	0.000000
H	-0.186034	1.265575	1.094725
H	-0.186035	1.265576	-1.094724
O	-1.334074	-0.602323	-0.000000
C	1.457239	-0.324926	0.000000
H	1.588907	-0.944890	-0.888052
H	2.201343	0.475055	-0.000083
H	1.588969	-0.944764	0.888130

0 imaginary frequencies
E = -457.664995
H = -457.599019
G = -457.627602

TS1o: $PhSiH_3 + H_2MeP{=}O$

Si	-0.436955	-1.019107	-0.746463
O	-1.993571	-0.844990	0.189719
P	-2.629154	0.567182	-0.061404
H	-0.931457	0.502084	-1.172249
C	-4.123094	0.532111	0.953156
H	-4.655224	1.480607	0.856797

```
H   -4.770672   -0.281741    0.624259
H   -3.854957    0.370831    1.998021
C    1.255374   -0.299515   -0.247465
C    2.152274   -1.086523    0.485723
H    1.856453   -2.086528    0.788471
C    3.414957   -0.613290    0.834104
H    4.091910   -1.240857    1.403323
C    3.806708    0.666075    0.452190
H    4.788822    1.038452    0.721632
C    2.929739    1.468151   -0.273783
H    3.230090    2.466401   -0.573173
C    1.667747    0.988466   -0.611404
H    0.988367    1.624008   -1.172267
H   -0.273468   -2.358017   -0.066465
H   -0.569532   -1.457150   -2.166557
H   -3.097550    0.851385   -1.345216
H   -1.921774    1.677357    0.402086
1 imaginary frequency
E = -980.517961
H = -980.327009
G = -980.372023
```

$Et_2PhP{=}O$

```
O   -1.160161   -2.006360   -0.496571
P   -0.936129   -0.558536   -0.169195
C    0.834666   -0.181067    0.044534
C   -1.749307   -0.018355    1.367743
C   -1.547284    0.541278   -1.488671
C    1.308207    0.991105    0.641580
C    2.676455    1.213497    0.755165
C    3.578630    0.266994    0.277037
C    3.112708   -0.904538   -0.311044
C    1.744569   -1.130594   -0.424137
H    0.617231    1.734621    1.023968
H    3.038298    2.122767    1.220904
H    4.644528    0.441688    0.368167
H    3.814042   -1.645870   -0.675989
H    1.366870   -2.046798   -0.865151
C   -3.271761   -0.126218    1.270202
H   -1.359645   -0.672127    2.153560
H   -1.441824    1.001871    1.611059
C   -1.443334    2.041622   -1.222191
H   -2.585547    0.239714   -1.659198
H   -0.988812    0.261283   -2.386844
H   -1.985389    2.331901   -0.318402
H   -1.872810    2.600989   -2.055718
H   -0.403515    2.357332   -1.116375
H   -3.731812    0.089965    2.236080
H   -3.571966   -1.132277    0.970100
H   -3.677724    0.581524    0.543021
0 imaginary frequencies
E = -806.626009
H = -806.381996
G = -806.431270
```

TS: $PhSiH_3$ + $Et_2PhP{=}O$

```
Si  -0.028017   -2.236082   -0.025505
O   -1.331565   -1.404147    0.824839
P   -1.785920   -0.125816   -0.031666
H   -0.550806   -0.959276   -1.118343
C   -3.061308    0.489954    1.150695
C    1.708384   -1.477699   -0.118923
```

```
C    2.627973   -1.753068    0.899980
H    2.340183   -2.409377    1.715937
C    3.905722   -1.195564    0.893061
H    4.598110   -1.416343    1.698059
C    4.291420   -0.358886   -0.148497
H    5.284523    0.076579   -0.158157
C    3.395663   -0.081727   -1.179677
H    3.690054    0.572535   -1.992996
C    2.117999   -0.628560   -1.155379
H    1.415234   -0.376508   -1.944274
H    0.182494   -3.168745    1.137763
H   -0.392117   -3.189345   -1.106597
C   -2.583399    0.695916    2.585870
H   -3.881780   -0.235844    1.124956
H   -3.447857    1.427054    0.735668
H   -2.170512   -0.227265    2.994891
H   -3.415493    1.009168    3.220613
H   -1.816568    1.471724    2.642404
C   -0.602881    1.242988   -0.077158
C   -0.645653    2.199098   -1.092690
C    0.371902    1.325044    0.919171
C    0.290892    3.227198   -1.113904
H   -1.397724    2.143165   -1.872584
C    1.306381    2.354465    0.890763
H    0.416957    0.575752    1.702473
C    1.268355    3.303586   -0.125664
H    0.258510    3.966625   -1.905593
H    2.071297    2.404209    1.656718
H    2.001365    4.101479   -0.150043
C   -3.388348   -1.684125   -1.660259
H   -4.054976   -1.737020   -2.522611
H   -2.589233   -2.412797   -1.804374
H   -3.960980   -1.971912   -0.775559
C   -2.821539   -0.268157   -1.533374
H   -2.206281   -0.025150   -2.399950
H   -3.630216    0.464074   -1.449148
1 imaginary frequency
E = -1329.478090
H = -1329.109141
G = -1329.172023
```

TS: $PhSiH_2(OH) + Me_3P{=}O$

```
Si  -0.065027    1.113742    0.670113
O   -1.500064    1.001682   -0.371236
P   -2.204021   -0.405564   -0.140005
H   -0.682870   -0.404120    1.060879
C   -3.579355   -0.207398   -1.320264
H   -4.209756   -1.099373   -1.323390
C   -3.079174   -0.674696    1.425750
C   -1.360030   -1.880198   -0.772451
H   -2.570629   -1.429549    2.023011
H   -1.031635   -2.516519    0.047737
H   -3.073921    0.265906    1.981158
H   -0.480364   -1.554318   -1.332837
H   -4.112814   -0.968625    1.232970
H   -2.024903   -2.431431   -1.440519
H   -4.184446    0.657726   -1.042366
H   -3.181835   -0.045542   -2.323957
C    1.575019    0.246145    0.269528
C    2.543943    0.867194   -0.531919
H    2.341701    1.857422   -0.921935
C    3.751773    0.237598   -0.822925
```

```
H     4.482167    0.735022   -1.451716
C     4.026993   -1.022813   -0.301733
H     4.969706   -1.511166   -0.522587
C     3.085786   -1.652235    0.508077
H     3.295046   -2.631791    0.923908
C     1.872884   -1.025074    0.777391
H     1.140603   -1.532787    1.398431
H    -0.369230    1.512736    2.070463
O     0.373708    2.627006    0.011095
H    -0.352312    3.226830   -0.168344
1 imaginary frequency
E = -1134.448184
H = -1134.188750
G = -1134.242627
```

References

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian 16, Revisions A.03 and B.01, Gaussian, Inc., Wallingford CT, 2016.
2. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215.
3. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378.
4. (a) C. Gonzalez and H. B. Schlegel, *J. Chem. Phys.*, 1989, **90**, 2154; (b) C. Gonzalez and H. B. Schlegel, *J. Phys. Chem.*, 1990, **94**, 5523.
5. Y. Zhao and D. G. Truhlar, *Phys. Chem. Chem. Phys.*, 2008, **10**, 2813.
6. E. D. Glendening, A. E. Reed, J. E. Carpenter and F. Weinhold, NBO Version 3.1.
7. CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org).
8. M. Fianchini, C. J. O'Brien and G. A. Chass, *J. Org. Chem.* 2019, **84**, 10579.