Electronic Supplementary Material (ESI) for Dalton Transactions.


# *Supplementary Information*

## Evidence for a $S_N2$-Type Pathway in the Exchange of Phosphines at a $[PhSe]^+$ Centre

**Laura C. Forfar,[a] Michael Green,[a] Mairi F. Haddow,[a] Sharifa Hussein,[b] Jason M. Lynam,[b] John M. Slattery[b] and Christopher A. Russell[a]**

[a] *School of Chemistry, University of Bristol, Bristol, BS8 1TS, Email: Chris.Russell@bristol.ac.uk; Web: http://www.inchm.bris.ac.uk/people/russell/Index2.htm*

[b] *Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK, Fax: (+) 44(0)1904 432516. Email: john.slattery@york.ac.uk.*

This document contains the kinetic data for phosphine exchange at **1** and **2**, SCF energies, ZPEs, XYZ coordinates and vibrational frequencies for the stationary points reported in the main section of the publication.

# Contents

## Kinetic Data

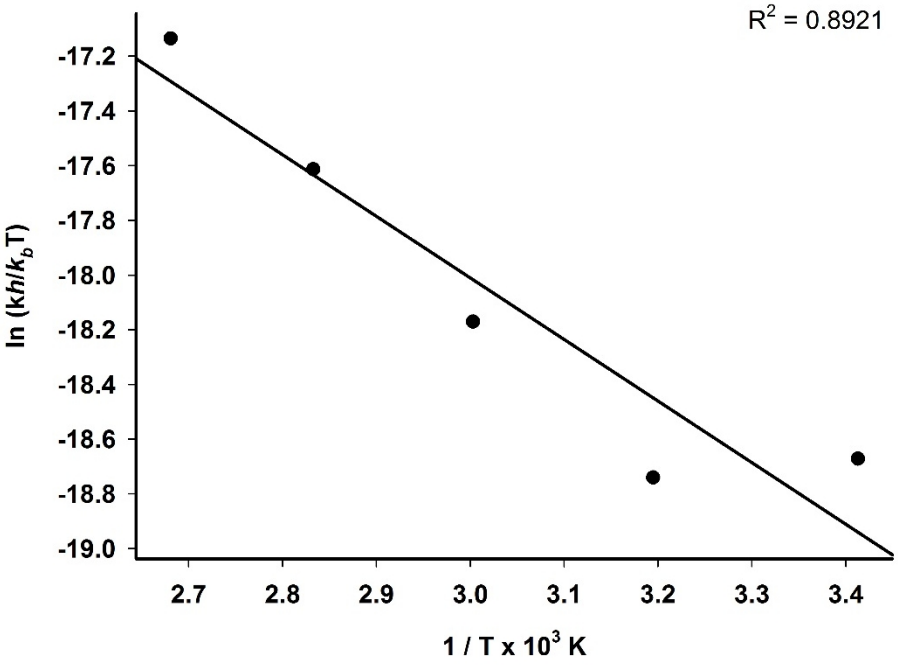


**Figure S1a** Eyring plot for exchange of $[PhSPPh_3]^+[GaCl_4]$ (**1**) with $PPh_3$. Data are derived from analysis of the coordinated $PPh_3$ resonance.

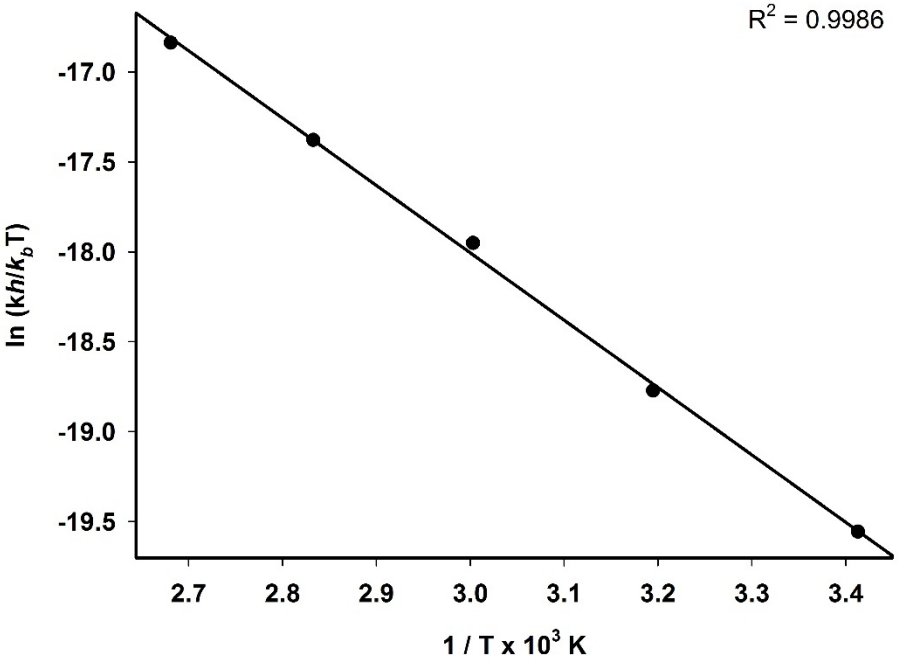


**Figure S1b** Eyring plot for exchange of $[PhSPPh_3]^+[GaCl_4]$ (**1**) with $PPh_3$. Data are derived from analysis of the free $PPh_3$ resonance.

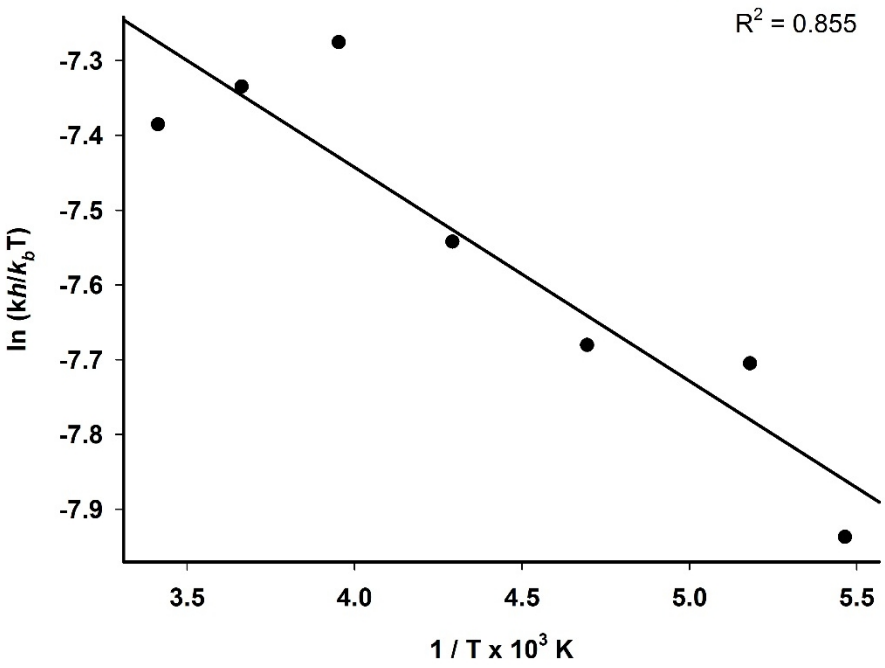


**Figure S2** Eyring plot for exchange of $[PhSePPh_3]^+[GaCl_4]$ (**2**) with $PPh_3$

# Computational details

## General Considerations

Optimisations were performed at the (RI-)BP86/SV(P), (RI-)BP86/def2-TZVPP, (RI-)BP86-D3/SV(P) and (RI-)BP86-D3/def2-TZVPP levels, followed by frequency calculations at the same level. Transition states were located by initially performing a constrained minimisation (by freezing internal coordinates that change most during the reaction) of a structure close to the anticipated transition state. This was followed by a frequency calculation to identify the transition vector to follow during a subsequent transition state optimisation. A final frequency calculation was then performed on the optimised transition-state structure. All minima were confirmed as such by the absence of imaginary frequencies and all transition states were identified by the presence of only one imaginary frequency. Reaction intermediates in the $S_N2$-like phosphine exchange mechanism for $[PhSePR_3]^+$ ions were found to be minima on the potential energy surface at all levels of theory, rather than first-order saddle points. Zero-point energies, thermal energies and entropies were derived from frequency calculations at the level of theory used for each optimisation. Gas-phase entropies from frequency calculations were converted to standard-state concentration of 1 mol $dm^{-3}$. Symmetry constraints were only applied during optimisations of $[GaCl_4]^-$, which was constrained to tetrahedral symmetry. All calculations were performed using the TURBOMOLE V6.40 package using the resolution of identity (RI) approximation.[1-9] Solvation effects were modelled using the COSMO module of TURBOMOLE using the dielectric constant of dichloromethane (8.93 at 298 K).[10]

It was not possible to locate some transition states at certain levels of theory using the approach described above (as the potential energy surface is very flat in some cases). In these cases one S-P bond was constrained to a distance found for a transition state at a related level of theory and a constrained optimisation was performed on this structure in order to approximate the transition state. Details of these constraints and the states modelled in this way are below.

| Structure and level | Fixed S-P distance (Å) |
|---|---|
| TS $[PhS(PPh_3)_2]^+$ BP86/TZVPP | 2.589 (as in BP86/SV(P) optimised structure) |
| TS $[PhS(PPh_3)_2]^+$ BP86-D3/TZVPP | 2.527 (as in BP86-D3/SV(P) optimised structure) |
| TS $[PhS(PPh_3)(P^tBu_3)]^+$ BP86/TZVPP | 2.542 (as in BP86/SV(P) optimised structure) |
| TS $[PhS(PPh_3)(P^tBu_3)]^+$ BP86-D3/SV(P) | 2.542 (as in BP86/SV(P) optimised structure) |
| TS $[PhS(PPh_3)(P^tBu_3)]^+$ BP86-D3/TZVPP | 2.542 (as in BP86/SV(P) optimised structure) |

Single-point calculations on the (RI-)BP86/SV(P) optimised geometries were performed using the hybrid PBE0 functional and the flexible def2-TZVPP basis set. The (RI-)PBE0/def2-TZVPP SCF energies were corrected for their zero point energies, thermal energies and entropies (obtained from the (RI-)BP86/SV(P)-level frequency calculations). Single-point DFT-D3 corrections (on the (RI)-BP86/SV(P) geometries) have been applied at the PBE0-D3 level using Grimme's DFT-D3 V3.0 Rev 2 program (with BJ-damping)[11, 12] and data presented below, where PBE0-D3 is indicated, includes this correction.

The effects of including counter anions explicitly in the calculations was explored for some states in the $[PhSe(PPh_3)][GaCl_4]$ + $PPh_3$ system (where DFT-D3 calculations were seen to disagree more markedly with experimental energy changes). When solvation effects were taken into account using

the COSMO model, this generally resulted in small changes in relative energies compared to modelling the isolated cations. This suggests that the salts in these systems are likely to be relatively ion-separated and that solvation-corrections are a reasonable approximation to the experimental system. Since there is significant potential for the introduction of errors in relative energies when including explicit anions in these types of system, e.g. if there is incomplete sampling of conformational and isomer space, explicit anion calculations were not performed on all states. The only exception to this is in the $S_N1$-like phosphine exchange mechanism, which would proceed via a $[PhE]^+$ (E = S, Se) ion in the cation-only model. In this case inclusion of an explicit $[GaCl_4]^-$ anion leads to halide abstraction by the Lewis-acidic pnictogenium ion and the formation of a $GaCl_3$ adduct of the resulting species (i.e. $PhECl.GaCl_3$) both in the gas phase and solution. As such, an explicit anion was included when modelling the $S_N1$-like phosphine exchange mechanism.

Single-point energy calculations on the BP86/SV(P) optimised structures were performed using Gaussian 09 (at the BP86/SVP level of theory)[13] to prepare input for NBO analysis by the NBO 5.9 package.[14]

## Table 1 – Summary of energetic data (BP86/SV(P) level)

| | BP86/SV(P) | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | BP86/SV(P) Vibrational Frequencies | | | | | | BP86/SV(P) Gas Phase | | | BP86/SV(P) COSMO DCM | | |
| Structure | BP86/SV(P) Opt SCF (a.u.) | BP86/SV(P) COSMO (CH2Cl2) (a.u.) | ZPE (a.u.) | Chem. Pot. (kJ/mol) | Energy (kJ/mol) | Entropy (kJ/K/mol) | ln q(vib) | Entropy at 1 mol/dm3 (kJ/K/mol) | Rel H (kJ/mol) | Rel S (J/K/mol) | Rel G (kJ/mol) | Rel H (kJ/mol) | Rel S (J/K/mol) @ 1moldm-3 | Rel G (kJ/mol) @ 1moldm-3 |
| [PhS]+ | -629.2578512 | -629.3280117 | 0.0881712 | 151.83 | 247.06 | 0.3277 | 2.01 | 0.3010 | 374 | 188 | 320 | 295 | 162 | 247 |
| PhSCl.GaCl3_iso2 | -4395.079756 | -4395.08858 | 0.0944103 | 120.92 | 288.1 | 0.56903 | 16.51 | 0.5423 | -94 | 67 | -115 | 161 | 67 | 141 |
| [PhS(PPh3)]+ | -1665.139043 | -1665.187512 | 0.3581954 | 794.43 | 1001.3 | 0.70216 | 23.06 | 0.6755 | 0 | 0 | 0 | 0 | 0 | 0 |
| [PhS(PPh3).PPh3]+ | -2700.883466 | -2700.929785 | 0.6248255 | 1418.79 | 1750.62 | 1.12127 | 51.20 | 1.0946 | -20 | -144 | 21 | 8 | -117 | 43 |
| TS [PhS(PPh3)2]+ | -2700.882058 | -2700.926259 | 0.6242501 | 1423.72 | 1747.99 | 1.09592 | 48.99 | 1.0692 | -18 | -169 | 29 | 15 | -142 | 57 |
| | | | | | | | | | | | | | | |
| [PhS(PPh3).PtBu3]+_try4 | -2479.554563 | -2479.597542 | 0.7156387 | 1667.24 | 1994.05 | 1.10444 | 47.68 | 1.0777 | -18 | -138 | 21 | 6 | -111 | 39 |
| TS [PhS(PPh3)(PtBu3)]+ | -2479.552992 | -2479.596223 | 0.7153819 | 1681.89 | 1989.36 | 1.03957 | 41.51 | 1.0129 | -19 | -203 | 39 | 4 | -176 | 57 |
| [PhS(PtBu3).PPh3]+ | -2479.554078 | -2479.602365 | 0.7151331 | 1663.07 | 1993.63 | 1.11704 | 48.8 | 1.0903 | -17 | -125 | 18 | -7 | -98 | 22 |
| [PhS(PtBu3)]+ | -1443.812296 | -1443.862305 | 0.4487512 | 1043.31 | 1244.73 | 0.68386 | 19.51 | 0.6572 | -4 | 5 | -5 | -21 | 5 | -22 |
| | | | | | | | | | | | | | | |
| [PhSe]+ | -2632.700198 | -2632.768909 | 0.0876259 | 147.39 | 246.11 | 0.33942 | 2.25 | 0.3127 | 356 | 186 | 303 | 280 | 159 | 233 |
| PhSeCl.GaCl3_iso2 | -6398.525782 | -6398.53507 | 0.0937054 | 116.58 | 287.1 | 0.58023 | 17.15 | 0.5535 | -122 | 64 | -141 | 132 | 64 | 113 |
| [PhSe(PPh3)]+ | -3668.574318 | -3668.622563 | 0.3570935 | 788.5 | 999.69 | 0.71665 | 24.01 | 0.6900 | 0 | 0 | 0 | 0 | 0 | 0 |
| [PhSe(PPh3).PPh3]+ | -4704.326289 | -4704.37042 | 0.6238542 | 1414.95 | 1749.36 | 1.12993 | 51.6 | 1.1032 | -39 | -150 | 3 | -6 | -123 | 30 |
| TS [PhSe(PPh3)2]+ | -4704.326383 | -4704.370538 | 0.6239177 | 1414.96 | 1749.48 | 1.13027 | 51.67 | 1.1036 | -39 | -149 | 3 | -7 | -123 | 30 |
| | | | | | | | | | | | | | | |
| [PhSe(PPh3).PtBu3]+_iso1 | -4482.998476 | -4483.041200 | 0.7146757 | 1665.84 | 1992.84 | 1.10507 | 47.08 | 1.0784 | -40 | -152 | 2 | -17 | -125 | 21 |
| TS [PhSe(PPh3)(PtBu3)]+ | -4482.998382 | -4483.041318 | 0.7148867 | 1665.16 | 1993.29 | 1.10885 | 47.57 | 1.0822 | -40 | -148 | 2 | -16 | -121 | 20 |
| [PhSe(PtBu3).PPh3]+ | -4482.998278 | -4483.041349 | 0.7146983 | 1662.76 | 1993.04 | 1.11609 | 48.34 | 1.0894 | -40 | -141 | 0 | -17 | -114 | 17 |
| [PhSe(PtBu3)]+ | -3447.249276 | -3447.298889 | 0.4477377 | 1038.54 | 1243.18 | 0.69468 | 20.05 | 0.6680 | -8 | 1 | -9 | -25 | 1 | -25 |
| | | | | | | | | | | | | | | |
| PPh3 | -1035.733961 | -1035.742263 | 0.2660713 | 576.05 | 741.41 | 0.56293 | 14.93 | 0.5362 | | | | | | |
| PtBu3 | -814.4052432 | -814.4087242 | 0.3562707 | 825.19 | 983.72 | 0.54003 | 11.46 | 0.5133 | | | | | | |
| [GaCl4]- | -3765.640321 | -3765.706409 | 0.0047151 | -73.09 | 32.51 | 0.3625 | 4.76 | 0.3358 | | | | | | |

## Table 2 – Summary of energetic data (BP86/def-TZVPP level)

| | BP86/def2-TZVPP | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | BP86/TZVPP Vibrational Frequencies | | | | | | BP86/TZVPP Gas Phase | | | BP86/TZVPP COSMO DCM | | |
| Structure | BP86/TZVPP Opt SCF (a.u.) | BP86/TZVPP COSMO (CH2Cl2) (a.u.) | ZPE (a.u.) | Chem. Pot. (kJ/mol) | Energy (kJ/mol) | Gas-Phase Entropy (kJ/K/mol) | ln q(vib) | Entropy at 1 mol/dm3 (kJ/K/mol) | Rel H (kJ/mol) | Rel S (J/K/mol) | Rel G (kJ/mol) | Rel H (kJ/mol) | Rel S (J/K/mol) @ 1moldm-3 | Rel G (kJ/mol) @ 1moldm-3 |
| [PhS]+ | -629.6545305 | -629.7248707 | 0.088063 | 151.38 | 246.9 | 0.32871 | 2.10 | 0.3020 | 382 | 186 | 329 | 302 | 160 | 254 |
| PhSCl.GaCl3_iso2 | -4396.364299 | -4396.373126 | 0.094391 | 120.23 | 288.03 | 0.5711 | 16.77 | 0.5444 | -75 | 64 | -94 | 179 | 64 | 160 |
| [PhS(PPh3)]+ | -1666.433038 | -1666.481798 | 0.357836 | 791.35 | 1000.63 | 0.71026 | 23.93 | 0.6836 | 0 | 0 | 0 | 0 | 0 | 0 |
| [PhS(PPh3).PPh3]+ | -2703.067607 | -2703.11583 | 0.624025 | 1409.32 | 1749.04 | 1.14772 | 54.15 | 1.1210 | -9 | -130 | 27 | 16 | -104 | 47 |
| TS [PhS(PPh3)2]+ | -2703.064302 | -2703.109632 | 0.623969 | 1420.07 | 1746.59 | 1.10346 | 49.85 | 1.0768 | -3 | -175 | 47 | 29 | -148 | 74 |
| | | | | | | | | | | | | | | |
| [PhS(PPh3).PtBu3]+_try4 | -2481.547187 | -2481.592036 | 0.715361 | 1663.56 | 1994.46 | 1.11816 | 48.83 | 1.0915 | -6 | -135 | 32 | 16 | -108 | 48 |
| TS [PhS(PPh3)(PtBu3)]+ | -2481.541724 | -2481.58565 | 0.715524 | 1672.39 | 1992.65 | 1.08248 | 45.53 | 1.0558 | 7 | -171 | 55 | 31 | -144 | 74 |
| [PhS(PtBu3).PPh3]+ | -2481.546399 | -2481.597084 | 0.715444 | 1657.27 | 1995.23 | 1.14184 | 51.41 | 1.1151 | -3 | -111 | 28 | 4 | -85 | 29 |
| [PhS(PtBu3)]+ | -1444.913414 | -1444.963929 | 0.449103 | 1042.38 | 1246.38 | 0.69253 | 20.28 | 0.6658 | 1 | 7 | -1 | -15 | 7 | -17 |
| | | | | | | | | | | | | | | |
| [PhSe]+ | -2633.252337 | -2633.321235 | 0.087496 | 146.88 | 245.89 | 0.3404 | 2.33 | 0.3137 | 361 | 188 | 307 | 285 | 162 | 236 |
| PhSeCl.GaCl3_iso2 | -6399.963657 | -6399.973202 | 0.093566 | 115.53 | 286.83 | 0.58286 | 17.42 | 0.5562 | -100 | 66 | -120 | 152 | 66 | 132 |
| [PhSe(PPh3)]+ | -3670.022868 | -3670.071445 | 0.356842 | 787.04 | 999.19 | 0.71987 | 24.34 | 0.6932 | 0 | 0 | 0 | 0 | 0 | 0 |
| [PhSe(PPh3).PPh3]+ | -4706.664428 | -4706.709329 | 0.623047 | 1408.09 | 1747.81 | 1.14774 | 53.53 | 1.1210 | -27 | -140 | 12 | 6 | -113 | 39 |
| TS [PhSe(PPh3)2]+ | -4706.664431 | -4706.709346 | 0.62308 | 1408.97 | 1747.86 | 1.14497 | 53.21 | 1.1183 | -27 | -143 | 13 | 6 | -116 | 40 |
| | | | | | | | | | | | | | | |
| [PhSe(PPh3).PtBu3]+_iso1 | -4485.144100 | -4485.187291 | 0.714691 | 1663.44 | 1993.88 | 1.11661 | 48.07 | 1.0899 | -24 | -146 | 18 | 2 | -120 | 38 |
| TS [PhSe(PPh3)(PtBu3)]+ | -4485.144104 | -4485.187285 | 0.714693 | 1663.24 | 1993.89 | 1.11732 | 48.15 | 1.0906 | -24 | -146 | 17 | 2 | -119 | 38 |
| [PhSe(PtBu3).PPh3]+ | -4485.144092 | -4485.187282 | 0.714655 | 1662.71 | 1993.83 | 1.11891 | 48.33 | 1.0922 | -24 | -144 | 17 | 2 | -117 | 37 |
| [PhSe(PtBu3)]+ | -3448.505481 | -3448.555716 | 0.448217 | 1037.42 | 1245.17 | 0.70513 | 21.03 | 0.6784 | -4 | 10 | -7 | -20 | 10 | -23 |
| | | | | | | | | | | | | | | |
| PPh3 | -1036.628078 | -1036.636922 | 0.265576 | 573.59 | 740.39 | 0.56778 | 15.41 | 0.5411 | | | | | | |
| PtBu3 | -815.1088131 | -815.1132352 | 0.356844 | 826.25 | 985.65 | 0.54296 | 11.66 | 0.5163 | | | | | | |
| [GaCl4]- | -3766.532423 | -3766.598161 | 0.004571 | -73.86 | 32.35 | 0.36455 | 4.92 | 0.3379 | | | | | | |

## Table 3 – Summary of energetic data (PBE0/def2-TZVPP//BP86/SV(P) level)

| | PBE0/def2-TZVPP//BP86/SV(P) | | | | | | | | PBE0-D3/def2-TZVPP//BP86/SV(P) | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | PBE0/TZVPP//BP86/SV(P) Gas Phase | | | PBE0/TZVPP//BP86/SV(P) COSMO DCM | | | | | | PBE0/TZVPP//BP86/SV(P) Gas Phase | | | PBE0/TZVPP//BP86/SV(P) COSMO DCM | | |
| Structure | PBE0/TZVPP SP SCF (a.u.) | PBE0/TZVPP_SP COSMO (CH2Cl2) (a.u.) | Rel H (kJ/mol) | Rel S (J/K/mol) | Rel G (kJ/mol) | Rel H (kJ/mol) | Rel S (J/K/mol) @ 1moldm-3 | Rel G (kJ/mol) @ 1moldm-3 | PBE0-D3/TZVPP SP SCF (a.u.) | PBE0-D3/TZVPP_SP COSMO (CH2Cl2) (a.u.) | PBE0/TZVPP DFT-D3 correction (a.u.) | Rel H (kJ/mol) | Rel S (J/K/mol) | Rel G (kJ/mol) | Rel H (kJ/mol) | Rel S (J/K/mol) @ 1moldm-3 | Rel G (kJ/mol) @ 1moldm-3 |
| [PhS]+ | -629.1687228 | -629.2388026 | 420 | 188 | 366 | 340 | 162 | 292 | -629.1803211 | -629.250401 | -0.01159836 | 455 | 188 | 401 | 374 | 162 | 326 |
| PhSCl.GaCl3_iso2 | -4394.54498 | -4394.554942 | -42 | 67 | -62 | 208 | 67 | 188 | -4394.569429 | -4394.579391 | -0.02444938 | -23 | 67 | -43 | 227 | 67 | 207 |
| [PhS(PPh3)]+ | -1664.919058 | -1664.968978 | 0 | 0 | 0 | 0 | 0 | 0 | -1664.987991 | -1665.037911 | -0.06893334 | 0 | 0 | 0 | 0 | 0 | 0 |
| [PhS(PPh3).PPh3]+ | -2700.510708 | -2700.560418 | -8 | -144 | 32 | 19 | -117 | 54 | -2700.637093 | -2700.686803 | -0.12638516 | -43 | -144 | -3 | -15 | -117 | 20 |
| TS [PhS(PPh3)2]+ | -2700.499725 | -2700.546769 | 18 | -169 | 66 | 53 | -142 | 95 | -2700.626157 | -2700.673202 | -0.12643234 | -17 | -169 | 31 | 18 | -142 | 60 |
| [PhS(PPh3).PtBu3]+_try4 | -2479.255024 | -2479.300513 | -3 | -138 | 35 | 21 | -111 | 54 | -2479.385268 | -2479.430757 | -0.13024382 | -46 | -138 | -7 | -21 | -111 | 12 |
| TS [PhS(PPh3)(PtBu3)]+ | -2479.247034 | -2479.292627 | 13 | -203 | 71 | 37 | -176 | 89 | -2479.37886 | -2479.424452 | -0.13182564 | -33 | -203 | 24 | -9 | -176 | 43 |
| [PhS(PtBu3).PPh3]+ | -2479.255866 | -2479.307109 | -6 | -125 | 29 | 3 | -98 | 33 | -2479.384881 | -2479.436123 | -0.12901411 | -45 | -125 | -10 | -36 | -98 | -6 |
| [PhS(PtBu3)]+ | -1443.664047 | -1443.715121 | 3 | 5 | 2 | -14 | 5 | -16 | -1443.735099 | -1443.786173 | -0.07105184 | 0 | 5 | -1 | -17 | 5 | -18 |
| [PhSe]+ | -2632.380331 | -2632.449059 | 398 | 186 | 345 | 321 | 159 | 274 | -2632.392284 | -2632.461012 | -0.01195326 | 433 | 186 | 380 | 356 | 159 | 309 |
| PhSeCl.GaCl3_iso2 | -6397.759767 | -6397.770324 | -72 | 64 | -91 | 176 | 64 | 157 | -6397.784858 | -6397.795415 | -0.02509095 | -53 | 64 | -72 | 195 | 64 | 176 |
| [PhSe(PPh3)]+ | -3668.12209 | -3668.171862 | 0 | 0 | 0 | 0 | 0 | 0 | -3668.191602 | -3668.241374 | -0.06951228 | 0 | 0 | 0 | 0 | 0 | 0 |
| [PhSe(PPh3).PPh3]+ | -4703.719884 | -4703.767005 | -24 | -150 | 18 | 10 | -123 | 47 | -4703.847836 | -4703.894957 | -0.12795223 | -62 | -150 | -19 | -27 | -123 | 9 |
| TS [PhSe(PPh3)2]+ | -4703.720204 | -4703.76732 | -25 | -149 | 17 | 9 | -123 | 46 | -4703.848327 | -4703.895444 | -0.1281232 | -63 | -149 | -21 | -29 | -123 | 8 |
| [PhSe(PPh3).PtBu3]+_iso1 | -4482.464474 | -4482.50954 | -20 | -152 | 23 | 5 | -125 | 43 | -4482.596117 | -4482.641183 | -0.1316432 | -64 | -152 | -21 | -39 | -125 | -2 |
| TS [PhSe(PPh3)(PtBu3)]+ | -4482.464473 | -4482.50981 | -19 | -148 | 22 | 5 | -121 | 41 | -4482.595974 | -4482.641311 | -0.13150114 | -63 | -148 | -22 | -39 | -121 | -3 |
| [PhSe(PtBu3).PPh3]+ | -4482.464385 | -4482.50991 | -19 | -141 | 20 | 5 | -114 | 38 | -4482.59583 | -4482.641355 | -0.13144527 | -63 | -141 | -24 | -39 | -114 | -5 |
| [PhSe(PtBu3)]+ | -3446.869744 | -3446.920496 | -4 | 1 | -4 | -21 | 1 | -21 | -3446.941695 | -3446.992447 | -0.07195057 | -7 | 1 | -8 | -24 | 1 | -25 |
| PPh3 | -1035.585414 | -1035.595794 | | | | | | | -1035.629631 | -1035.64001 | -0.04421661 | | | | | | |
| PtBu3 | -814.3312085 | -814.3360985 | | | | | | | -814.376468 | -814.381358 | -0.04525954 | | | | | | |
| [GaCl4]- | -3765.197072 | -3765.262728 | | | | | | | -3765.204054 | -3765.26971 | -0.00698146 | | | | | | |

## Table 4 – Summary of energetic data (BP86-D3/SV(P) level)

| | BP86-D3/SV(P) | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | BP86/SV(P) Vibrational Frequencies | | | | | | BP86/SV(P) Gas Phase | | | BP86/SV(P) COSMO DCM | | |
| Structure | BP86/SV(P) Opt SCF (a.u.) | BP86/SV(P) COSMO (CH2Cl2) (a.u.) | ZPE (a.u.) | Chem. Pot. (kJ/mol) | Energy (kJ/mol) | Entropy (kJ/K/mol) | ln q(vib) | Entropy at 1 mol/dm3 (kJ/K/mol) | Rel H (kJ/mol) | Rel S (J/K/mol) | Rel G (kJ/mol) | Rel H (kJ/mol) | Rel S (J/K/mol) @ 1moldm-3 | Rel G (kJ/mol) @ 1moldm-3 |
| [PhS]+ | -629.2658134 | -629.3359743 | 0.0881591 | 151.8 | 247.03 | 0.32772 | 2.01 | 0.3010 | 426 | 193 | 371 | 348 | 166 | 298 |
| PhSCl.GaCl3_iso2 | -4395.103225 | -4395.111992 | 0.0945176 | 121.37 | 288.23 | 0.56797 | 16.48 | 0.5413 | -66 | 71 | -87 | 191 | 71 | 170 |
| [PhS(PPh3)]+ | -1665.202624 | -1665.251359 | 0.3585327 | 798.64 | 1001.63 | 0.68915 | 21.77 | 0.6625 | 0 | 0 | 0 | 0 | 0 | 0 |
| [PhS(PPh3).PPh3]+ | -2701.003836 | -2701.048585 | 0.6254154 | 1428.62 | 1751.27 | 1.09049 | 47.94 | 1.0638 | -75 | -153 | -31 | -43 | -126 | -5 |
| TS [PhS(PPh3)2]+ | -2701.003813 | -2701.048309 | 0.6253348 | 1434.06 | 1748.75 | 1.0638 | 45.66 | 1.0371 | -77 | -180 | -26 | -44 | -153 | 1 |
| [PhS(PPh3).PtBu3]+ | -2479.7000 | -2479.742682 | 0.7167281 | 1681.27 | 1995.81 | 1.0633 | 43.25 | 1.0366 | -87 | -163 | -41 | -62 | -137 | -21 |
| TS [PhS(PPh3)(PtBu3)]+ | -2479.699756 | -2479.742682 | 0.7166162 | 1679.79 | 1995.84 | 1.06836 | 43.74 | 1.0417 | -86 | -158 | -42 | -62 | -131 | -23 |
| [PhS(PtBu3).PPh3]+ | -2479.700724 | -2479.747923 | 0.7168914 | 1681.15 | 1996.32 | 1.06541 | 43.48 | 1.0387 | -88 | -161 | -43 | -75 | -134 | -35 |
| [PhS(PtBu3)]+ | -1443.897514 | -1443.947662 | 0.4494198 | 1046.08 | 1246.01 | 0.67887 | 19.13 | 0.6522 | -9 | 7 | -11 | -25 | 7 | -27 |
| [PhSe]+ | -2632.708555 | -2632.777263 | 0.0876113 | 147.35 | 246.08 | 0.33945 | 2.25 | 0.3128 | 410 | 193 | 355 | 336 | 166 | 286 |
| PhSeCl.GaCl3_iso2 | -6398.550283 | -6398.559447 | 0.0937974 | 117.57 | 287.18 | 0.57719 | 16.88 | 0.5505 | -93 | 68 | -114 | 162 | 68 | 142 |
| [PhSe(PPh3)]+ | -3668.639266 | -3668.687866 | 0.3575188 | 793.64 | 1000.16 | 0.701 | 22.44 | 0.6743 | 0 | 0 | 0 | 0 | 0 | 0 |
| [PhSe(PPh3).PPh3]+ | -4704.449277 | -4704.493568 | 0.6246469 | 1425.06 | 1750.1 | 1.0985 | 48.41 | 1.0718 | -97 | -157 | -53 | -65 | -130 | -26 |
| TS [PhSe(PPh3)2]+ | -4704.449284 | -4704.493575 | 0.6246426 | 1425.03 | 1750.09 | 1.0986 | 48.42 | 1.0719 | -97 | -157 | -53 | -65 | -130 | -26 |
| [PhSe(PPh3).PtBu3]+_iso1 | -4483.144958 | -4483.187911 | 0.7159353 | 1676.99 | 1994.67 | 1.07382 | 43.97 | 1.0471 | -109 | -165 | -62 | -84 | -138 | -43 |
| TS [PhSe(PPh3)(PtBu3)]+ | -4483.144906 | -4483.187908 | 0.7161509 | 1677.11 | 1995.11 | 1.07491 | 44.14 | 1.0482 | -108 | -163 | -62 | -84 | -137 | -43 |
| [PhSe(PtBu3).PPh3]+ | -4483.14487 | -4483.187825 | 0.7158782 | 1676.02 | 1994.7 | 1.07716 | 44.29 | 1.0505 | -108 | -161 | -63 | -84 | -135 | -44 |
| [PhSe(PtBu3)]+ | -3447.336202 | -3447.385962 | 0.4484289 | 1042.13 | 1244.4 | 0.68672 | 19.36 | 0.6600 | -15 | 3 | -16 | -30 | 3 | -31 |
| PPh3 | -1035.769804 | -1035.777984 | 0.2662863 | 578.91 | 741.69 | 0.55429 | 14.03 | 0.5276 | | | | | | |
| PtBu3 | -814.4604618 | -814.4639838 | 0.3566093 | 826.6 | 984.33 | 0.53736 | 11.26 | 0.5107 | | | | | | |
| [GaCl4]- | -3765.646767 | -3765.712872 | 0.0047297 | -73.01 | 32.53 | 0.3623 | 4.74 | 0.3356 | | | | | | |

## Table 5 – Summary of energetic data (BP86-D3/def2-TZVPP level)

| | BP86-D3/def2-TZVPP | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | BP86/TZVPP Vibrational Frequencies | | | | | | BP86/TZVPP Gas Phase | | | BP86/TZVPP COSMO DCM | | |
| Structure | BP86/TZVPP Opt SCF (a.u.) | BP86/TZVPP COSMO (CH2Cl2) (a.u.) | ZPE (a.u.) | Chem. Pot. (kJ/mol) | Energy (kJ/mol) | Entropy (kJ/K/mol) | ln q(vib) | Entropy at 1 mol/dm3 (kJ/K/mol) | Rel H (kJ/mol) | Rel S (J/K/mol) | Rel G (kJ/mol) | Rel H (kJ/mol) | Rel S (J/K/mol) @ 1moldm-3 | Rel G (kJ/mol) @ 1moldm-3 |
| [PhS]+ | -629.662471 | -629.7328138 | 0.08805 | 151.34 | 246.87 | 0.32874 | 2.10 | 0.3020 | 433 | 191 | 379 | 354 | 165 | 305 |
| PhSCl.GaCl3_iso2 | -4396.390311 | -4396.398586 | 0.094662 | 127.41 | 288.15 | 0.54742 | 14.43 | 0.5207 | -54 | 46 | -65 | 203 | 46 | 189 |
| [PhS(PPh3)]+ | -1666.496612 | -1666.545581 | 0.358172 | 795.94 | 1000.99 | 0.69606 | 22.49 | 0.6694 | 0 | 0 | 0 | 0 | 0 | 0 |
| [PhS(PPh3).PPh3]+ | -2703.187137 | -2703.232997 | 0.625043 | 1427.48 | 1750.33 | 1.09116 | 48.02 | 1.0645 | -61 | -164 | -15 | -30 | -137 | 11 |
| TS [PhS(PPh3)2]+ | -2703.186981 | -2703.232375 | 0.624386 | 1425.62 | 1747.01 | 1.08627 | 48.08 | 1.0596 | -64 | -169 | -16 | -32 | -142 | 11 |
| | | | | | | | | | | | | | | |
| [PhS(PPh3).PtBu3]+ | -2481.691102 | -2481.734823 | 0.717046 | 1678.56 | 1997.01 | 1.07641 | 44.69 | 1.0497 | -69 | -160 | -24 | -44 | -133 | -4 |
| TS [PhS(PPh3)(PtBu3)]+ | -2481.690400 | -2481.734168 | 0.716868 | 1682.58 | 1994.74 | 1.0553 | 42.90 | 1.0286 | -70 | -181 | -18 | -45 | -154 | 1 |
| [PhS(PtBu3).PPh3]+ | -2481.691953 | -2481.740415 | 0.717167 | 1681.61 | 1997.51 | 1.06784 | 43.6 | 1.0411 | -71 | -169 | -23 | -58 | -142 | -16 |
| [PhS(PtBu3)]+ | -1444.999251 | -1445.049865 | 0.449604 | 1043.99 | 1247.44 | 0.69066 | 20.19 | 0.6640 | -5 | 13 | -9 | -21 | 13 | -24 |
| | | | | | | | | | | | | | | |
| [PhSe]+ | -2633.260673 | -2633.329569 | 0.087483 | 146.83 | 245.86 | 0.34047 | 2.33 | 0.3138 | 415 | 189 | 361 | 340 | 162 | 291 |
| PhSeCl.GaCl3_iso2 | -6399.99054 | -6399.999592 | 0.093835 | 122.48 | 286.95 | 0.55997 | 15.09 | 0.5333 | -78 | 44 | -89 | 177 | 44 | 164 |
| [PhSe(PPh3)]+ | -3670.087614 | -3670.136507 | 0.357083 | 790.16 | 999.43 | 0.7102 | 23.39 | 0.6835 | 0 | 0 | 0 | 0 | 0 | 0 |
| [PhSe(PPh3).PPh3]+ | -4706.787428 | -4706.832468 | 0.623718 | 1417.06 | 1748.44 | 1.11976 | 50.67 | 1.0931 | -86 | -149 | -44 | -53 | -123 | -16 |
| TS [PhSe(PPh3)2]+ | -4706.78744 | -4706.832452 | 0.623769 | 1417.98 | 1748.52 | 1.11698 | 50.35 | 1.0903 | -86 | -152 | -43 | -53 | -125 | -15 |
| | | | | | | | | | | | | | | |
| [PhSe(PPh3).PtBu3]+_iso1 | -4485.291076 | -4485.335035 | 0.716029 | 1674.97 | 1995.94 | 1.08484 | 44.89 | 1.0581 | -92 | -166 | -46 | -68 | -139 | -26 |
| TS [PhSe(PPh3)(PtBu3)]+ | -4485.291093 | -4485.335072 | 0.716125 | 1675.68 | 1996.12 | 1.08308 | 44.71 | 1.0564 | -92 | -168 | -45 | -68 | -141 | -26 |
| [PhSe(PtBu3).PPh3]+ | -4485.291079 | -4485.335073 | 0.716031 | 1674.77 | 1995.98 | 1.08565 | 44.97 | 1.0590 | -92 | -165 | -46 | -68 | -138 | -27 |
| [PhSe(PtBu3)]+ | -3448.592873 | -3448.643253 | 0.448762 | 1041.12 | 1246.08 | 0.69574 | 20.13 | 0.6690 | -12 | 4 | -13 | -27 | 4 | -28 |
| | | | | | | | | | | | | | | |
| PPh3 | -1036.663971 | -1036.672685 | 0.265828 | 576.65 | 740.77 | 0.55878 | 14.47 | 0.5321 | | | | | | |
| PtBu3 | -815.164336 | -815.1687591 | 0.357168 | 827.61 | 986.26 | 0.54042 | 11.46 | 0.5137 | | | | | | |
| [GaCl4]- | -3766.538884 | -3766.604637 | 0.004585 | -73.78 | 32.36 | 0.36433 | 4.9 | 0.3376 | | | | | | |

## Table 6 – Summary of key computational data for $PPh_3$ exchange (for comparison with experiment)

| **Summary for $[PhSPPh_3]^+ + PPh_3$** | | | | | | |
|---|---|---|---|---|---|---|
| | | | | | | |
| | **BP86/SV(P) COSMO ($CH_2Cl_2$)** | **BP86/TZVPP COSMO ($CH_2Cl_2$)** | **PBE0/TZVPP//BP86/ SV(P) COSMO ($CH_2Cl_2$)** | **BP86-D3/SV(P) COSMO ($CH_2Cl_2$)** | **BP86-D3/TZVPP COSMO ($CH_2Cl_2$)** | **PBE0-D3/TZVPP//BP86/SV(P) COSMO ($CH_2Cl_2$)** |
| **ΔH Encounter complex (kJ $mol^{-1}$)** | 8 | 16 | 19 | -43 | -30 | -15 |
| **$\Delta H^{\ddagger}$ (kJ $mol^{-1}$)** | 15 | 29 | 53 | -44 | -32 | 18 |
| **$\Delta S^{\ddagger}$ (J $mol^{-1}$ $K^{-1}$ at 1 mol $dm^{-3}$)** | -142 | -148 | -142 | -153 | -142 | -142 |
| **$\Delta G^{\ddagger}$ (298.15 K,1 mol $dm^{-3}$) (kJ $mol^{-1}$)** | 57 | 74 | 95 | 1 | 11 | 60 |
| | | | | | | |
| **Summary for $[PhSePPh_3]^+ + PPh_3$** | | | | | | |
| | | | | | | |
| | **BP86/SV(P) COSMO ($CH_2Cl_2$)** | **BP86/TZVPP COSMO ($CH_2Cl_2$)** | **PBE0/TZVPP//BP86/ SV(P) COSMO ($CH_2Cl_2$)** | **BP86-D3/SV(P) COSMO ($CH_2Cl_2$)** | **BP86-D3/TZVPP COSMO ($CH_2Cl_2$)** | **PBE0-D3/TZVPP//BP86/SV(P) COSMO ($CH_2Cl_2$)** |
| **ΔH Encounter complex (kJ $mol^{-1}$)** | -6 | 6 | 10 | -65 | -53 | -27 |
| **$\Delta H^{\ddagger}$ (kJ $mol^{-1}$)** | -7 | 6 | 9 | -65 | -53 | -29 |
| **$\Delta S^{\ddagger}$ (J $mol^{-1}$ $K^{-1}$ at 1 mol $dm^{-3}$)** | -123 | -116 | -123 | -130 | -125 | -123 |
| **$\Delta G^{\ddagger}$ (298.15 K,1 mol $dm^{-3}$) (kJ $mol^{-1}$)** | 30 | 40 | 46 | -26 | -15 | 8 |

| **Experimental data** | |
|---|---|
| | |
| **$[PhSPPh_3]^+ + PPh_3$** | |
| **$\Delta H^{\ddagger}$ (kJ $mol^{-1}$)** | 18.7 ± 12.0 |
| **$\Delta S^{\ddagger}$ (J $mol^{-1}$ $K^{-1}$)** | -93.6 ± 36.3 |
| **$\Delta G^{\ddagger}$ (298.15 K) (kJ $mol^{-1}$)** | 46 |
| | |
| **$[PhSePPh_3]^+ + PPh_3$** | |
| **$\Delta H^{\ddagger}$ (kJ $mol^{-1}$)** | 2.4 ± 1.1 |

| | |
|---|---|
| **$\Delta S^{\ddagger}$ (J mol$^{-1}$ K$^{-1}$)** | -52.4 ± 5.0 |
| **$\Delta G^{\ddagger}$ (298.15 K) (kJ mol$^{-1}$)** | 18 |

# SCF energies, ZPEs, XYZ coordinates and vibrational frequencies

## BP86/SV(P) level optimisations

**$PPh_3$**

bp86 energy (au): -1035.7339608900

pbe0_def2-tzvpp_sp energy (au): -1035.585414363

Zero point energy (au): 0.2660713
Entropy (kJ mol^-1): 0.56293
Chemical potential (kJ mol^-1): 576.05

XYZ coordinates:

34

| | | | |
|---|---|---|---|
| P | 0.00171 | -1.19430 | -0.00336 |
| C | 1.19684 | -0.37974 | 1.16401 |
| C | -0.11867 | -0.98179 | -2.79066 |
| H | -0.75298 | -1.88097 | -2.70011 |
| C | 1.24473 | 0.74968 | -1.76255 |
| H | 1.67481 | 1.22641 | -0.86652 |
| C | 0.41181 | -0.38225 | -1.62426 |
| C | 3.42198 | -0.45921 | 2.18712 |
| H | 4.40494 | -0.94938 | 2.28773 |
| C | 1.53243 | 1.27278 | -3.03577 |
| H | 2.18742 | 2.15560 | -3.12755 |
| C | 0.90735 | 0.77111 | 1.92963 |
| H | -0.07633 | 1.25976 | 1.83485 |
| C | 0.98790 | 0.67790 | -4.18662 |
| H | 1.21565 | 1.08932 | -5.18411 |
| C | 2.46263 | -0.99339 | 1.31201 |
| H | 2.69505 | -1.90612 | 0.73573 |
| C | 1.86385 | 1.29784 | 2.81554 |
| H | 1.62215 | 2.19573 | 3.40913 |
| C | 3.12315 | 0.68739 | 2.94465 |
| H | 3.87131 | 1.10162 | 3.64096 |
| C | 0.15765 | -0.45038 | -4.06057 |
| H | -0.26772 | -0.92840 | -4.95901 |
| C | -2.18273 | 0.70196 | -0.23984 |
| H | -1.65372 | 1.14604 | -1.09884 |
| C | -1.60750 | -0.38475 | 0.45439 |
| C | -2.31300 | -0.94273 | 1.54660 |
| H | -1.88644 | -1.80668 | 2.08579 |
| C | -3.42895 | 1.22158 | 0.15449 |
| H | -3.86682 | 2.06886 | -0.39976 |
| C | -4.11358 | 0.66916 | 1.25021 |
| H | -5.09042 | 1.07816 | 1.55780 |
| C | -3.54981 | -0.41418 | 1.94848 |
| H | -4.08282 | -0.85903 | 2.80551 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 23.76 | 0.33541 | YES YES |
| 8 | a | 26.73 | 0.33130 | YES YES |
| 9 | a | 41.23 | 0.00375 | YES YES |
| 10 | a | 51.33 | 0.10158 | YES YES |
| 11 | a | 52.07 | 0.09240 | YES YES |
| 12 | a | 65.84 | 0.39812 | YES YES |
| 13 | a | 177.83 | 0.37032 | YES YES |
| 14 | a | 193.30 | 1.24981 | YES YES |
| 15 | a | 196.02 | 1.26312 | YES YES |
| 16 | a | 237.81 | 0.57497 | YES YES |
| 17 | a | 252.20 | 0.30586 | YES YES |
| 18 | a | 254.76 | 0.32301 | YES YES |
| 19 | a | 394.44 | 0.35406 | YES YES |
| 20 | a | 394.95 | 1.31325 | YES YES |
| 21 | a | 396.10 | 1.42281 | YES YES |
| 22 | a | 401.52 | 0.10566 | YES YES |
| 23 | a | 418.79 | 5.79853 | YES YES |
| 24 | a | 420.61 | 6.47973 | YES YES |
| 25 | a | 495.02 | 25.69092 | YES YES |
| 26 | a | 497.58 | 26.50054 | YES YES |
| 27 | a | 504.28 | 12.89446 | YES YES |
| 28 | a | 610.35 | 0.25013 | YES YES |
| 29 | a | 610.52 | 0.22123 | YES YES |
| 30 | a | 610.76 | 0.07554 | YES YES |
| 31 | a | 670.23 | 0.53694 | YES YES |
| 32 | a | 684.84 | 1.33674 | YES YES |
| 33 | a | 685.19 | 1.50753 | YES YES |
| 34 | a | 699.04 | 35.19071 | YES YES |
| 35 | a | 699.28 | 33.95861 | YES YES |
| 36 | a | 700.26 | 31.66711 | YES YES |
| 37 | a | 743.47 | 15.10509 | YES YES |
| 38 | a | 744.02 | 15.53636 | YES YES |
| 39 | a | 745.29 | 14.45767 | YES YES |
| 40 | a | 836.01 | 0.11030 | YES YES |
| 41 | a | 836.91 | 0.13707 | YES YES |
| 42 | a | 839.17 | 0.14680 | YES YES |
| 43 | a | 904.14 | 0.70325 | YES YES |
| 44 | a | 905.49 | 0.68915 | YES YES |
| 45 | a | 906.22 | 0.41315 | YES YES |
| 46 | a | 957.39 | 0.00819 | YES YES |
| 47 | a | 957.92 | 0.03083 | YES YES |
| 48 | a | 959.08 | 0.09644 | YES YES |
| 49 | a | 982.45 | 0.18753 | YES YES |
| 50 | a | 982.76 | 0.78649 | YES YES |

**$P(^tBu)_3$**

bp86 energy (au): -814.4052431920

pbe0_def2-tzvpp_sp energy (au): -814.3312084563

Zero point energy (au): 0.3562707
Entropy (kJ mol^-1): 0.54003
Chemical potential (kJ mol^-1): 825.19

XYZ coordinates:

40

| | | | |
|---|---|---|---|
| P | 0.69066 | -0.00005 | -0.00014 |
| C | -0.02585 | 1.72088 | -0.61588 |
| C | -1.50487 | 1.76254 | -1.05129 |
| H | -1.77928 | 2.80416 | -1.34629 |
| C | 0.87862 | 2.16356 | -1.79616 |
| H | 0.61793 | 3.20892 | -2.08725 |
| H | 0.76320 | 1.53445 | -2.69987 |
| H | 1.95223 | 2.14835 | -1.50606 |
| C | -0.02585 | -1.39396 | -1.18214 |
| C | -1.50465 | -1.79242 | -1.00054 |
| H | -1.77839 | -2.56916 | -1.75472 |
| H | -2.19515 | -0.93523 | -1.14401 |
| H | -1.70704 | -2.23029 | -0.00078 |
| H | 0.76285 | -3.10563 | 0.02069 |
| H | 1.95250 | -2.37747 | -1.10641 |
| H | 0.61910 | -3.41137 | -1.73572 |
| C | 0.19252 | -0.96657 | -2.65232 |
| H | 1.24219 | -0.65136 | -2.84205 |
| H | -0.48553 | -0.14964 | -2.97438 |
| H | -0.01465 | -1.84051 | -3.31375 |
| C | -0.02580 | -0.32704 | 1.79815 |
| C | 0.19249 | -1.81387 | 2.16333 |
| H | -0.01479 | -1.94939 | 3.25093 |
| H | 1.24203 | -2.13550 | 1.98481 |
| H | -0.48557 | -2.50131 | 1.61697 |
| C | -1.50466 | 0.02975 | 2.05230 |
| H | -2.19500 | -0.52336 | 1.38189 |
| H | -1.70714 | 1.11436 | 1.93153 |
| H | -1.77852 | -0.23477 | 3.10215 |
| C | 0.87910 | 0.47364 | 2.77116 |
| H | 0.76294 | 1.57078 | 2.67876 |
| H | 1.95274 | 0.23044 | 2.61203 |
| H | 0.61935 | 0.20295 | 3.82202 |
| H | -1.70747 | 1.11626 | -1.93085 |
| H | -2.19506 | 1.45754 | -0.23727 |
| C | 0.19283 | 2.78054 | 0.48914 |
| H | -0.01360 | 3.79059 | 0.06290 |
| H | -0.48577 | 2.65185 | 1.35747 |
| H | 1.24241 | 2.78632 | 0.85729 |
| C | 0.87903 | -2.63707 | -0.97539 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 90.78 | 0.01132 | YES YES |
| 8 | a | 93.08 | 0.01106 | YES YES |
| 9 | a | 122.53 | 0.00017 | YES YES |
| 10 | a | 171.60 | 0.05700 | YES YES |
| 11 | a | 180.22 | 0.01806 | YES YES |
| 12 | a | 182.58 | 0.00701 | YES YES |
| 13 | a | 196.99 | 0.03585 | YES YES |
| 14 | a | 201.63 | 0.01152 | YES YES |
| 15 | a | 208.08 | 0.03829 | YES YES |
| 16 | a | 240.61 | 0.05602 | YES YES |
| 17 | a | 243.99 | 0.11735 | YES YES |
| 18 | a | 247.03 | 0.16993 | YES YES |
| 19 | a | 257.22 | 0.31294 | YES YES |
| 20 | a | 258.09 | 0.26933 | YES YES |
| 21 | a | 268.93 | 0.02843 | YES YES |
| 22 | a | 277.65 | 0.07710 | YES YES |
| 23 | a | 282.81 | 0.06682 | YES YES |
| 24 | a | 293.03 | 0.01892 | YES YES |
| 25 | a | 331.54 | 0.22205 | YES YES |
| 26 | a | 342.09 | 0.28941 | YES YES |
| 27 | a | 347.72 | 0.30608 | YES YES |
| 28 | a | 351.87 | 0.03473 | YES YES |
| 29 | a | 364.92 | 0.12790 | YES YES |
| 30 | a | 367.25 | 0.18799 | YES YES |
| 31 | a | 397.97 | 0.31752 | YES YES |
| 32 | a | 399.17 | 0.28936 | YES YES |
| 33 | a | 401.08 | 0.34610 | YES YES |
| 34 | a | 450.03 | 3.63619 | YES YES |
| 35 | a | 452.13 | 3.68777 | YES YES |
| 36 | a | 472.45 | 0.66880 | YES YES |
| 37 | a | 530.62 | 0.15721 | YES YES |
| 38 | a | 555.82 | 4.75781 | YES YES |
| 39 | a | 556.99 | 4.78828 | YES YES |
| 40 | a | 793.38 | 10.69000 | YES YES |
| 41 | a | 795.32 | 9.57779 | YES YES |
| 42 | a | 797.78 | 3.50892 | YES YES |
| 43 | a | 910.48 | 1.83637 | YES YES |
| 44 | a | 911.11 | 2.32124 | YES YES |
| 45 | a | 912.28 | 1.81416 | YES YES |
| 46 | a | 918.26 | 0.48107 | YES YES |
| 47 | a | 919.83 | 0.90826 | YES YES |
| 48 | a | 921.27 | 1.21790 | YES YES |
| 49 | a | 925.19 | 0.20480 | YES YES |
| 50 | a | 930.17 | 0.79070 | YES YES |

**$[GaCl_4]^-$**

bp86 energy (au): -3765.6403205050

pbe0_def2-tzvpp_sp energy (au): -3765.197072358

Zero point energy (au): 0.0047151
Entropy (kJ mol^-1): 0.36250
Chemical potential (kJ mol^-1): -73.09

XYZ coordinates:

5

| | | | |
|---|---|---|---|
| Ga | 0.00000 | 0.00000 | 0.00000 |
| Cl | -1.28592 | -1.28592 | -1.28592 |
| Cl | 1.28592 | 1.28592 | -1.28592 |
| Cl | 1.28592 | -1.28592 | 1.28592 |
| Cl | -1.28592 | 1.28592 | 1.28592 |

Vibrational Spectrum:

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | e | 101.43 | 0.00000 | NO YES |
| 8 | e | 101.43 | 0.00000 | NO YES |
| 9 | t2 | 144.32 | 8.04866 | YES YES |
| 10 | t2 | 144.32 | 8.04866 | YES YES |
| 11 | t2 | 144.32 | 8.04866 | YES YES |
| 12 | a1 | 318.59 | 0.00000 | NO YES |
| 13 | t2 | 371.75 | 79.94531 | YES YES |
| 14 | t2 | 371.75 | 79.94531 | YES YES |
| 15 | t2 | 371.75 | 79.94531 | YES YES |

**[PhS]+**

bp86 energy (au): -629.2578512224

pbe0_def2-tzvpp_sp energy (au): -629.1687227827

Zero point energy (au): 0.0881712
Entropy (kJ mol^-1): 0.32770
Chemical potential (kJ mol^-1): 151.83

XYZ coordinates:

12

| | | | |
|---|---|---|---|
| C | -2.27142 | -0.00000 | -0.00154 |
| H | -3.37568 | -0.00032 | -0.00325 |
| C | -0.20146 | 1.26343 | 0.00212 |
| H | 0.37217 | 2.20458 | 0.00319 |
| C | -1.58518 | 1.24917 | -0.00071 |
| H | -2.15958 | 2.18935 | -0.00159 |
| C | 0.53988 | 0.00009 | 0.00197 |
| C | -0.20148 | -1.26341 | 0.00188 |
| H | 0.37247 | -2.20437 | 0.00257 |
| C | -1.58515 | -1.24922 | -0.00045 |
| H | -2.15964 | -2.18933 | -0.00111 |
| S | 2.20567 | -0.00002 | -0.00122 |

Vibrational Spectrum:

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 106.86 | 0.00191 | YES YES |
| 8 | a | 295.74 | 0.00857 | YES YES |
| 9 | a | 312.69 | 0.00004 | YES YES |
| 10 | a | 372.68 | 0.19608 | YES YES |
| 11 | a | 429.59 | 0.14768 | YES YES |
| 12 | a | 566.35 | 2.48383 | YES YES |
| 13 | a | 611.66 | 43.29091 | YES YES |
| 14 | a | 720.04 | 2.98407 | YES YES |
| 15 | a | 784.90 | 27.64036 | YES YES |
| 16 | a | 797.63 | 0.00012 | YES YES |
| 17 | a | 963.37 | 5.45166 | YES YES |
| 18 | a | 979.56 | 0.69445 | YES YES |
| 19 | a | 986.76 | 7.57082 | YES YES |
| 20 | a | 991.51 | 0.00015 | YES YES |
| 21 | a | 1025.07 | 1.76033 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 22 | a | 1072.12 | 4.87161 | YES | YES |
| 23 | a | 1121.32 | 23.94289 | YES | YES |
| 24 | a | 1148.21 | 11.43442 | YES | YES |
| 25 | a | 1177.90 | 0.00958 | YES | YES |
| 26 | a | 1240.52 | 6.87264 | YES | YES |
| 27 | a | 1352.76 | 0.04051 | YES | YES |
| 28 | a | 1412.47 | 17.29113 | YES | YES |
| 29 | a | 1462.82 | 107.94732 | YES | YES |
| 30 | a | 1508.60 | 11.78970 | YES | YES |
| 31 | a | 1607.11 | 129.95451 | YES | YES |
| 32 | a | 3115.94 | 0.78407 | YES | YES |
| 33 | a | 3128.54 | 1.08674 | YES | YES |
| 34 | a | 3130.14 | 11.07445 | YES | YES |
| 35 | a | 3138.62 | 19.60609 | YES | YES |

**PhSCl.GaCl3_iso2**

bp86 energy (au): -4395.0797564920

pbe0_def2-tzvpp_sp energy (au): -4394.544979996

Zero point energy (au): 0.0944103
Entropy (kJ mol^-1): 0.56903
Chemical potential (kJ mol^-1): 120.92

XYZ coordinates:

17

| | | | |
|---|---|---|---|
| S | 0.37738 | 0.34281 | 1.56337 |
| C | -1.10682 | -0.37191 | 0.94495 |
| C | -1.14716 | -0.93927 | -0.35440 |
| H | -0.21686 | -1.01366 | -0.94026 |
| C | -2.36376 | -1.41345 | -0.86020 |
| H | -2.40098 | -1.86083 | -1.86664 |
| C | -3.53828 | -1.31131 | -0.08809 |
| H | -4.49441 | -1.67901 | -0.49606 |
| C | -3.50127 | -0.74715 | 1.20129 |
| H | -4.42347 | -0.67270 | 1.80004 |
| C | -2.28622 | -0.28927 | 1.72846 |
| H | -2.23361 | 0.14313 | 2.74023 |
| Ga | 3.41952 | -1.63045 | 0.63263 |
| Cl | 1.49678 | -1.42097 | 2.27626 |
| Cl | 4.32055 | -3.31835 | 1.65258 |
| Cl | 4.33884 | 0.31654 | 0.83823 |
| Cl | 2.40377 | -2.03719 | -1.25039 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 16.65 | 0.08603 | YES YES |
| 8 | a | 22.63 | 0.05536 | YES YES |
| 9 | a | 42.42 | 1.20154 | YES YES |
| 10 | a | 48.16 | 0.41008 | YES YES |
| 11 | a | 60.08 | 1.24489 | YES YES |
| 12 | a | 85.82 | 0.16055 | YES YES |
| 13 | a | 99.13 | 0.28959 | YES YES |
| 14 | a | 122.26 | 5.11986 | YES YES |
| 15 | a | 125.95 | 4.95776 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 16 | a | 136.63 | 32.92721 | YES | YES |
| 17 | a | 175.81 | 46.55457 | YES | YES |
| 18 | a | 212.53 | 18.74553 | YES | YES |
| 19 | a | 275.81 | 4.14892 | YES | YES |
| 20 | a | 334.63 | 43.46124 | YES | YES |
| 21 | a | 351.03 | 15.82188 | YES | YES |
| 22 | a | 397.72 | 6.97891 | YES | YES |
| 23 | a | 407.54 | 4.93976 | YES | YES |
| 24 | a | 419.29 | 70.54416 | YES | YES |
| 25 | a | 430.74 | 59.88078 | YES | YES |
| 26 | a | 483.53 | 10.67991 | YES | YES |
| 27 | a | 602.44 | 0.25931 | YES | YES |
| 28 | a | 681.61 | 32.17965 | YES | YES |
| 29 | a | 706.59 | 3.57728 | YES | YES |
| 30 | a | 753.58 | 26.66601 | YES | YES |
| 31 | a | 829.34 | 0.12661 | YES | YES |
| 32 | a | 927.08 | 2.32209 | YES | YES |
| 33 | a | 967.97 | 0.19824 | YES | YES |
| 34 | a | 983.63 | 0.71441 | YES | YES |
| 35 | a | 997.37 | 0.21264 | YES | YES |
| 36 | a | 1017.98 | 0.20351 | YES | YES |
| 37 | a | 1067.72 | 58.80252 | YES | YES |
| 38 | a | 1071.08 | 4.54691 | YES | YES |
| 39 | a | 1145.88 | 0.28320 | YES | YES |
| 40 | a | 1160.00 | 4.46829 | YES | YES |
| 41 | a | 1283.09 | 1.07179 | YES | YES |
| 42 | a | 1367.38 | 4.99229 | YES | YES |
| 43 | a | 1433.77 | 16.86381 | YES | YES |
| 44 | a | 1455.51 | 0.64346 | YES | YES |
| 45 | a | 1575.16 | 0.29908 | YES | YES |
| 46 | a | 1590.71 | 38.67749 | YES | YES |
| 47 | a | 3100.91 | 1.07884 | YES | YES |
| 48 | a | 3109.87 | 10.38420 | YES | YES |
| 49 | a | 3115.13 | 0.68609 | YES | YES |
| 50 | a | 3122.07 | 6.70751 | YES | YES |

**[PhSe]+**

bp86 energy (au): -2632.7001982390

pbe0_def2-tzvpp_sp energy (au): -2632.380331126

Zero point energy (au): 0.0876259
Entropy (kJ mol^-1): 0.33942
Chemical potential (kJ mol^-1): 147.39

XYZ coordinates:

12

| | | | |
|---|---|---|---|
| C | -3.00905 | -0.00005 | 0.00011 |
| H | -4.11279 | -0.00031 | 0.00002 |
| C | -0.93379 | 1.25804 | 0.00057 |
| H | -0.36628 | 2.20274 | 0.00097 |
| C | -2.32013 | 1.24532 | -0.00061 |
| H | -2.89055 | 2.18779 | -0.00062 |
| C | -0.20210 | 0.00005 | -0.00002 |
| C | -0.93371 | -1.25797 | -0.00023 |
| H | -0.36632 | -2.20271 | -0.00077 |
| C | -2.32002 | -1.24535 | 0.00024 |
| H | -2.89032 | -2.18786 | 0.00080 |
| Se | 1.61404 | 0.00000 | -0.00001 |

Vibrational Spectrum:

| # | mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|---|
| 1 | | | 0.00 | 0.00000 | - | - |
| 2 | | | 0.00 | 0.00000 | - | - |
| 3 | | | 0.00 | 0.00000 | - | - |
| 4 | | | 0.00 | 0.00000 | - | - |
| 5 | | | 0.00 | 0.00000 | - | - |
| 6 | | | 0.00 | 0.00000 | - | - |
| 7 | | a | 98.47 | 0.03835 | YES | YES |
| 8 | | a | 245.75 | 0.00012 | YES | YES |
| 9 | | a | 320.65 | 0.00001 | YES | YES |
| 10 | | a | 333.00 | 0.01887 | YES | YES |
| 11 | | a | 377.30 | 0.00310 | YES | YES |
| 12 | | a | 569.44 | 1.91231 | YES | YES |
| 13 | | a | 617.00 | 44.17870 | YES | YES |
| 14 | | a | 684.32 | 2.77772 | YES | YES |
| 15 | | a | 774.29 | 28.57703 | YES | YES |
| 16 | | a | 803.26 | 0.00007 | YES | YES |
| 17 | | a | 967.75 | 10.93717 | YES | YES |
| 18 | | a | 970.54 | 0.78330 | YES | YES |
| 19 | | a | 989.20 | 0.00045 | YES | YES |
| 20 | | a | 992.26 | 7.14072 | YES | YES |
| 21 | | a | 1020.86 | 1.14675 | YES | YES |
| 22 | | a | 1062.21 | 27.48814 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 23 | a | 1074.69 | 4.69575 | YES | YES |
| 24 | a | 1148.80 | 8.12238 | YES | YES |
| 25 | a | 1171.12 | 2.66994 | YES | YES |
| 26 | a | 1250.50 | 8.69795 | YES | YES |
| 27 | a | 1356.77 | 0.00021 | YES | YES |
| 28 | a | 1416.33 | 13.81695 | YES | YES |
| 29 | a | 1453.31 | 90.12197 | YES | YES |
| 30 | a | 1506.96 | 5.99416 | YES | YES |
| 31 | a | 1601.96 | 140.31545 | YES | YES |
| 32 | a | 3118.40 | 0.23697 | YES | YES |
| 33 | a | 3128.20 | 1.42248 | YES | YES |
| 34 | a | 3130.17 | 9.22751 | YES | YES |
| 35 | a | 3138.50 | 15.05361 | YES | YES |

**PhSeCl.GaCl3_iso2**

bp86 energy (au): -6398.5257817610

pbe0_def2-tzvpp_sp energy (au): -6397.759766818

Zero point energy (au): 0.0937054
Entropy (kJ mol^-1): 0.58023
Chemical potential (kJ mol^-1): 116.58

XYZ coordinates:

17

| | | | |
|---|---|---|---|
| Se | 0.46654 | 0.42794 | 1.58517 |
| C | -1.14516 | -0.34650 | 0.92889 |
| C | -1.17970 | -0.93274 | -0.35927 |
| H | -0.25227 | -1.01162 | -0.94902 |
| C | -2.39432 | -1.42512 | -0.85632 |
| H | -2.42777 | -1.88884 | -1.85558 |
| C | -3.56843 | -1.32130 | -0.08500 |
| H | -4.52189 | -1.70408 | -0.48524 |
| C | -3.53315 | -0.73694 | 1.19488 |
| H | -4.45400 | -0.66282 | 1.79600 |
| C | -2.32050 | -0.25868 | 1.71307 |
| H | -2.27547 | 0.18575 | 2.72010 |
| Ga | 3.46860 | -1.66181 | 0.64030 |
| Cl | 1.56821 | -1.47985 | 2.29674 |
| Cl | 4.43581 | -3.34134 | 1.60890 |
| Cl | 4.34477 | 0.30751 | 0.86372 |
| Cl | 2.43273 | -2.05258 | -1.23534 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules | |
|---|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR | RAMAN |
| 1 | | 0.00 | 0.00000 | - | - |
| 2 | | 0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 17.89 | 0.06201 | YES | YES |
| 8 | a | 22.09 | 0.03164 | YES | YES |
| 9 | a | 37.94 | 1.03255 | YES | YES |
| 10 | a | 43.11 | 0.05628 | YES | YES |
| 11 | a | 54.26 | 1.03562 | YES | YES |
| 12 | a | 77.47 | 0.49830 | YES | YES |
| 13 | a | 95.44 | 0.17011 | YES | YES |
| 14 | a | 122.44 | 4.70701 | YES | YES |
| 15 | a | 126.28 | 5.25827 | YES | YES |
| 16 | a | 137.05 | 28.37463 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 17 | a | 176.64 | 37.77423 | YES | YES |
| 18 | a | 199.92 | 23.05237 | YES | YES |
| 19 | a | 236.27 | 1.46693 | YES | YES |
| 20 | a | 295.42 | 45.12900 | YES | YES |
| 21 | a | 311.58 | 2.09164 | YES | YES |
| 22 | a | 343.83 | 5.72358 | YES | YES |
| 23 | a | 398.53 | 1.48273 | YES | YES |
| 24 | a | 418.51 | 63.22407 | YES | YES |
| 25 | a | 429.10 | 58.74071 | YES | YES |
| 26 | a | 461.33 | 8.78114 | YES | YES |
| 27 | a | 602.23 | 0.20937 | YES | YES |
| 28 | a | 673.12 | 0.72426 | YES | YES |
| 29 | a | 684.91 | 31.07643 | YES | YES |
| 30 | a | 746.06 | 28.91137 | YES | YES |
| 31 | a | 830.85 | 0.12106 | YES | YES |
| 32 | a | 924.03 | 2.08520 | YES | YES |
| 33 | a | 966.98 | 0.24086 | YES | YES |
| 34 | a | 981.45 | 0.97220 | YES | YES |
| 35 | a | 995.93 | 0.19738 | YES | YES |
| 36 | a | 1015.41 | 1.44357 | YES | YES |
| 37 | a | 1053.07 | 36.94745 | YES | YES |
| 38 | a | 1070.85 | 3.23650 | YES | YES |
| 39 | a | 1145.64 | 0.18666 | YES | YES |
| 40 | a | 1161.98 | 6.57676 | YES | YES |
| 41 | a | 1286.01 | 1.84070 | YES | YES |
| 42 | a | 1365.81 | 3.87043 | YES | YES |
| 43 | a | 1431.66 | 16.55561 | YES | YES |
| 44 | a | 1455.82 | 0.60164 | YES | YES |
| 45 | a | 1577.80 | 0.32117 | YES | YES |
| 46 | a | 1587.31 | 27.14151 | YES | YES |
| 47 | a | 3099.78 | 0.75487 | YES | YES |
| 48 | a | 3108.88 | 8.63984 | YES | YES |
| 49 | a | 3114.57 | 1.28728 | YES | YES |
| 50 | a | 3121.04 | 4.58618 | YES | YES |

**[PhSe(PPh3)]+**

bp86 energy (au): -3668.5743178450

pbe0_def2-tzvpp_sp energy (au): -3668.122090030

Zero point energy (au): 0.3570935
Entropy (kJ mol^-1): 0.71665
Chemical potential (kJ mol^-1): 788.50

XYZ coordinates:

46

| | | | |
|---|---|---|---|
| C | -1.2029585 | 4.9630951 | -1.1887858 |
| H | -1.5053128 | 5.9851064 | -1.4688662 |
| C | 2.9694561 | -1.6896173 | -1.6962984 |
| H | 3.4628223 | -2.6470298 | -1.4638532 |
| Se | -1.8805974 | -0.5074414 | -0.1949047 |
| P | 0.0670997 | 0.6704024 | -0.0102287 |
| C | 2.6979776 | 0.2509933 | -3.1461022 |
| H | 2.9815098 | 0.8174381 | -4.0477052 |
| C | -1.6053777 | 3.8717505 | -1.9796202 |
| H | -2.2218157 | 4.0352252 | -2.8780984 |
| C | -0.4405941 | 2.3570074 | -0.4684725 |
| C | 1.9856913 | -1.1904207 | -0.8297377 |
| H | 1.7188570 | -1.7574850 | 0.0765091 |
| C | 1.6441992 | 0.8032563 | 4.3394812 |
| H | 2.0167499 | 0.8567901 | 5.3752530 |
| C | 1.3563708 | 0.0435728 | -1.1252641 |
| C | -0.5773239 | -4.3880028 | -1.1841395 |
| H | -0.3947140 | -4.9565042 | -2.1104470 |
| C | -1.2289404 | 2.5670734 | -1.6260350 |
| H | -1.5549501 | 1.7163984 | -2.2468332 |
| C | 0.6948635 | 0.6564688 | 1.6994825 |
| C | 0.2616047 | 0.7112410 | 4.0953691 |
| H | -0.4498563 | 0.6938085 | 4.9365236 |
| C | 1.7112703 | 0.7629311 | -2.2893881 |
| H | 1.2309285 | 1.7263152 | -2.5223442 |
| C | 3.3256190 | -0.9720048 | -2.8520777 |
| H | 4.1014175 | -1.3678190 | -3.5274458 |
| C | -0.0399285 | 3.4533987 | 0.3287403 |
| H | 0.5653194 | 3.2956356 | 1.2354366 |
| C | 2.0850302 | 0.7526702 | 1.9435864 |
| H | 2.8031059 | 0.7729481 | 1.1084754 |
| C | -0.2180408 | 0.6368542 | 2.7789887 |
| H | -1.3013090 | 0.5582864 | 2.5885086 |
| C | -1.0738217 | -2.9407800 | 1.1866935 |
| H | -1.2856966 | -2.3802849 | 2.1106655 |
| C | -0.4231488 | 4.7531835 | -0.0383296 |
| H | -0.1121901 | 5.6072722 | 0.5843812 |
| C | 2.5519118 | 0.8250169 | 3.2663057 |
| H | 3.6347662 | 0.8976639 | 3.4570087 |
| C | -0.6753739 | -4.2867293 | 1.2506119 |
| H | -0.5700288 | -4.7770611 | 2.2320643 |
| C | -0.9677235 | -3.0402357 | -1.2632873 |

| | | | |
|---|---|---|---|
| H | -1.0913621 | -2.5526882 | -2.2430025 |
| C | -0.4289884 | -5.0088719 | 0.0686527 |
| H | -0.1279048 | -6.0675193 | 0.1250493 |
| C | -1.2106352 | -2.3230973 | -0.0735956 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 17.48 | 0.11709 | YES YES |
| 8 | a | 28.10 | 0.03472 | YES YES |
| 9 | a | 32.84 | 0.04346 | YES YES |
| 10 | a | 40.54 | 0.01081 | YES YES |
| 11 | a | 45.13 | 0.23538 | YES YES |
| 12 | a | 48.28 | 0.08080 | YES YES |
| 13 | a | 55.84 | 0.18636 | YES YES |
| 14 | a | 59.58 | 0.11391 | YES YES |
| 15 | a | 72.29 | 0.25729 | YES YES |
| 16 | a | 86.98 | 0.44585 | YES YES |
| 17 | a | 98.76 | 0.59693 | YES YES |
| 18 | a | 176.47 | 1.05789 | YES YES |
| 19 | a | 186.49 | 2.37706 | YES YES |
| 20 | a | 204.62 | 1.47131 | YES YES |
| 21 | a | 208.30 | 0.29038 | YES YES |
| 22 | a | 230.64 | 1.06555 | YES YES |
| 23 | a | 238.27 | 0.13391 | YES YES |
| 24 | a | 241.44 | 1.49802 | YES YES |
| 25 | a | 256.40 | 0.35228 | YES YES |
| 26 | a | 267.82 | 0.27564 | YES YES |
| 27 | a | 298.80 | 2.08488 | YES YES |
| 28 | a | 392.69 | 0.07565 | YES YES |
| 29 | a | 395.15 | 0.01917 | YES YES |
| 30 | a | 400.93 | 0.33120 | YES YES |
| 31 | a | 401.39 | 0.08544 | YES YES |
| 32 | a | 417.87 | 7.30067 | YES YES |
| 33 | a | 438.08 | 8.37735 | YES YES |
| 34 | a | 443.88 | 8.29827 | YES YES |
| 35 | a | 465.60 | 6.59278 | YES YES |
| 36 | a | 493.53 | 51.53863 | YES YES |
| 37 | a | 505.33 | 74.58828 | YES YES |
| 38 | a | 519.19 | 71.36798 | YES YES |
| 39 | a | 602.93 | 0.00477 | YES YES |
| 40 | a | 605.12 | 0.34703 | YES YES |
| 41 | a | 605.65 | 0.16925 | YES YES |
| 42 | a | 606.35 | 0.10623 | YES YES |
| 43 | a | 660.71 | 1.85846 | YES YES |
| 44 | a | 676.35 | 5.37229 | YES YES |
| 45 | a | 691.72 | 48.98079 | YES YES |
| 46 | a | 692.14 | 10.31686 | YES YES |
| 47 | a | 693.52 | 24.28370 | YES YES |
| 48 | a | 694.82 | 12.13249 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 49 | a | 708.73 | 22.81948 | YES | YES |
| 50 | a | 709.40 | 25.84263 | YES | YES |

**[PhSe(PPh3).PPh3]+**

bp86 energy (au): -4704.3262892010

pbe0_def2-tzvpp_sp energy (au): -4703.719884263

Zero point energy (au): 0.6238542
Entropy (kJ mol^-1): 1.12993
Chemical potential (kJ mol^-1): 1414.95

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.77031 | 0.75293 | 3.41992 |
| H | -5.84301 | 0.93231 | 3.59946 |
| C | 2.85339 | 2.28945 | 4.08880 |
| H | 3.95379 | 2.26579 | 4.03190 |
| Se | -0.18113 | 0.02287 | -0.01555 |
| P | -0.24779 | 0.02340 | 2.61391 |
| C | 0.80114 | 3.33486 | 4.87541 |
| H | 0.28780 | 4.12961 | 5.44095 |
| C | -4.06923 | 1.54892 | 2.49655 |
| H | -4.58933 | 2.35326 | 1.95122 |
| C | -2.02698 | 0.29134 | 2.96186 |
| C | 2.10472 | 1.29849 | 3.43608 |
| H | 2.62401 | 0.50558 | 2.87361 |
| C | 0.81835 | -4.11797 | 4.44467 |
| H | 1.05867 | -5.10575 | 4.87058 |
| C | 0.69075 | 1.31492 | 3.51115 |
| C | 3.87387 | 1.23313 | -0.11249 |
| H | 4.42276 | 2.18392 | -0.21455 |
| C | -2.70445 | 1.31782 | 2.26129 |
| H | -2.16195 | 1.94140 | 1.53085 |
| C | 0.20689 | -1.59084 | 3.35572 |
| C | 0.18819 | -4.02677 | 3.19031 |
| H | -0.06669 | -4.94211 | 2.63143 |
| C | 0.04255 | 2.34256 | 4.23192 |
| H | -1.05649 | 2.36484 | 4.30030 |
| C | 2.20423 | 3.31053 | 4.80652 |
| H | 2.79570 | 4.08900 | 5.31547 |
| C | -2.73660 | -0.50728 | 3.88639 |
| H | -2.22121 | -1.31241 | 4.43356 |
| C | 0.83901 | -1.68623 | 4.61547 |
| H | 1.09324 | -0.77518 | 5.18003 |
| C | -0.11185 | -2.76975 | 2.64250 |
| H | -0.59691 | -2.70147 | 1.65429 |
| C | 2.46477 | -1.19317 | 0.14138 |
| H | 1.91640 | -2.14315 | 0.23601 |
| C | -4.10344 | -0.27379 | 4.11089 |
| H | -4.65059 | -0.89886 | 4.83516 |
| C | 1.14306 | -2.94838 | 5.15333 |
| H | 1.63502 | -3.01558 | 6.13732 |
| C | 3.87094 | -1.18606 | 0.17036 |
| H | 4.41737 | -2.13577 | 0.29035 |

| | | | |
|---|---|---|---|
| C | 2.46762 | 1.23808 | -0.13013 |
| H | 1.92043 | 2.18781 | -0.23857 |
| C | 4.57578 | 0.02415 | 0.04040 |
| H | 5.67796 | 0.02501 | 0.05840 |
| C | 1.76492 | 0.02189 | -0.00624 |
| C | -4.74711 | -0.77426 | -3.47590 |
| H | -5.81582 | -0.96070 | -3.67030 |
| C | 2.89999 | -2.26961 | -4.02630 |
| H | 3.99998 | -2.20748 | -3.99979 |
| P | -0.23893 | -0.01225 | -2.62086 |
| C | 0.86436 | -3.42592 | -4.69448 |
| H | 0.36472 | -4.27164 | -5.19490 |
| C | -4.07736 | -1.50097 | -2.47598 |
| H | -4.61892 | -2.25658 | -1.88407 |
| C | -2.01369 | -0.29528 | -2.98074 |
| C | 2.13388 | -1.26081 | -3.42334 |
| H | 2.63392 | -0.41123 | -2.93050 |
| C | 0.82006 | 4.09788 | -4.52370 |
| H | 1.05800 | 5.07888 | -4.96592 |
| C | 0.71965 | -1.32346 | -3.46664 |
| C | -2.71693 | -1.26171 | -2.22301 |
| H | -2.19796 | -1.82999 | -1.43295 |
| C | 0.21572 | 1.58825 | -3.39139 |
| C | 0.18460 | 4.02670 | -3.27083 |
| H | -0.07697 | 4.95064 | -2.72971 |
| C | 0.08818 | -2.41619 | -4.10212 |
| H | -1.01099 | -2.47497 | -4.14519 |
| C | 2.26750 | -3.35509 | -4.65977 |
| H | 2.87173 | -4.14782 | -5.13037 |
| C | -2.69280 | 0.43501 | -3.98231 |
| H | -2.15707 | 1.19478 | -4.57372 |
| C | 0.85343 | 1.66368 | -4.65061 |
| H | 1.11370 | 0.74373 | -5.19850 |
| C | -0.11287 | 2.77875 | -2.70168 |
| H | -0.60342 | 2.72567 | -1.71508 |
| C | -4.05461 | 0.19298 | -4.22538 |
| H | -4.57767 | 0.76427 | -5.00925 |
| C | 1.15381 | 2.91761 | -5.20987 |
| H | 1.64973 | 2.96932 | -6.19278 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 8.38 | 0.00330 | YES YES |
| 8 | a | 13.96 | 0.21909 | YES YES |
| 9 | a | 17.06 | 0.13402 | YES YES |
| 10 | a | 19.97 | 3.21321 | YES YES |
| 11 | a | 25.21 | 6.63064 | YES YES |
| 12 | a | 26.99 | 0.75691 | YES YES |
| 13 | a | 32.07 | 22.52319 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 14 | a | 33.69 | 1.45398 | YES | YES |
| 15 | a | 37.44 | 0.11430 | YES | YES |
| 16 | a | 39.05 | 0.13234 | YES | YES |
| 17 | a | 42.09 | 4.63996 | YES | YES |
| 18 | a | 47.08 | 11.00608 | YES | YES |
| 19 | a | 47.57 | 0.85720 | YES | YES |
| 20 | a | 51.42 | 12.03972 | YES | YES |
| 21 | a | 54.58 | 0.18856 | YES | YES |
| 22 | a | 56.48 | 0.03530 | YES | YES |
| 23 | a | 58.64 | 0.01961 | YES | YES |
| 24 | a | 64.29 | 11.54196 | YES | YES |
| 25 | a | 67.17 | 1.49846 | YES | YES |
| 26 | a | 68.51 | 0.28158 | YES | YES |
| 27 | a | 76.35 | 72.97126 | YES | YES |
| 28 | a | 94.31 | 0.03737 | YES | YES |
| 29 | a | 112.97 | 0.54051 | YES | YES |
| 30 | a | 113.31 | 0.62153 | YES | YES |
| 31 | a | 183.80 | 1.81234 | YES | YES |
| 32 | a | 184.16 | 1.25158 | YES | YES |
| 33 | a | 191.36 | 0.47157 | YES | YES |
| 34 | a | 192.61 | 3.60493 | YES | YES |
| 35 | a | 199.44 | 8.77504 | YES | YES |
| 36 | a | 202.79 | 1.16955 | YES | YES |
| 37 | a | 210.42 | 19.12125 | YES | YES |
| 38 | a | 236.77 | 4.11701 | YES | YES |
| 39 | a | 237.30 | 1.01172 | YES | YES |
| 40 | a | 239.54 | 0.49570 | YES | YES |
| 41 | a | 253.51 | 0.50027 | YES | YES |
| 42 | a | 254.26 | 0.80020 | YES | YES |
| 43 | a | 261.98 | 0.66047 | YES | YES |
| 44 | a | 263.72 | 0.44246 | YES | YES |
| 45 | a | 301.81 | 0.42153 | YES | YES |
| 46 | a | 392.57 | 0.96983 | YES | YES |
| 47 | a | 394.04 | 0.66378 | YES | YES |
| 48 | a | 394.75 | 1.55261 | YES | YES |
| 49 | a | 395.32 | 1.34503 | YES | YES |
| 50 | a | 395.91 | 0.50461 | YES | YES |

**[PhSe(PtBu3).PPh3]+**

bp86 energy (au): -4482.9982779610

pbe0_def2-tzvpp_sp energy (au): -4482.464384557

Zero point energy (au): 0.7146983
Entropy (kJ mol^-1): 1.11609
Chemical potential (kJ mol^-1): 1662.76

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.12184 | 0.30541 | 0.02314 |
| Se | 0.57281 | 0.05258 | 0.02895 |
| C | 0.37823 | -1.88760 | 0.04190 |
| C | 0.02739 | -2.55181 | -1.15286 |
| H | -0.08840 | -1.98338 | -2.08892 |
| C | -0.18788 | -3.94111 | -1.14394 |
| H | -0.46855 | -4.45360 | -2.07861 |
| C | -0.04376 | -4.67262 | 0.04850 |
| H | -0.20713 | -5.76257 | 0.05085 |
| C | 0.30304 | -4.00907 | 1.23834 |
| H | 0.40740 | -4.57529 | 2.17852 |
| C | 0.50559 | -2.61722 | 1.24113 |
| H | 0.74806 | -2.10102 | 2.18212 |
| C | -3.18322 | -0.51350 | 1.27879 |
| C | -3.09890 | -1.91836 | 1.42827 |
| H | -2.39114 | -2.50580 | 0.82046 |
| C | -3.90851 | -2.57530 | 2.36846 |
| H | -3.83919 | -3.67020 | 2.47561 |
| C | -4.79615 | -1.84162 | 3.17581 |
| H | -5.42670 | -2.36082 | 3.91583 |
| C | -4.87488 | -0.44529 | 3.03901 |
| H | -5.56908 | 0.13521 | 3.66824 |
| C | -4.07425 | 0.21994 | 2.09524 |
| H | -4.14936 | 1.31393 | 1.99056 |
| C | -2.31218 | 2.11323 | 0.28617 |
| C | -3.07258 | 2.93149 | -0.57780 |
| H | -3.59357 | 2.49003 | -1.44237 |
| C | -3.17211 | 4.31200 | -0.33354 |
| H | -3.77061 | 4.94248 | -1.01123 |
| C | -2.51992 | 4.88556 | 0.77118 |
| H | -2.60321 | 5.96819 | 0.96057 |
| C | -1.76135 | 4.07573 | 1.63557 |
| H | -1.25181 | 4.52102 | 2.50581 |
| C | -1.64969 | 2.69747 | 1.39243 |
| H | -1.05338 | 2.06835 | 2.07514 |
| C | -2.86661 | -0.06097 | -1.61540 |
| C | -4.12005 | -0.69816 | -1.74970 |
| H | -4.69100 | -0.99150 | -0.85446 |
| C | -4.64557 | -0.95362 | -3.02806 |
| H | -5.62568 | -1.44871 | -3.12363 |
| C | -3.93068 | -0.57605 | -4.17720 |
| H | -4.34724 | -0.77700 | -5.17765 |

| | | | |
|---|---|---|---|
| C | -2.68083 | 0.05742 | -4.04894 |
| H | -2.11658 | 0.35444 | -4.94825 |
| C | -2.14540 | 0.30755 | -2.77597 |
| H | -1.16021 | 0.79497 | -2.68112 |
| P | 3.19520 | 0.26535 | 0.01351 |
| C | 3.44797 | 1.78812 | -1.18394 |
| C | 4.80145 | 2.50442 | -0.97542 |
| H | 4.89848 | 3.30124 | -1.74847 |
| C | 2.29624 | 2.80530 | -0.98225 |
| H | 2.45787 | 3.64883 | -1.69172 |
| H | 2.25172 | 3.24070 | 0.03309 |
| H | 1.30537 | 2.36456 | -1.22309 |
| C | 3.67433 | 0.75722 | 1.84206 |
| C | 5.19904 | 0.77446 | 2.09051 |
| H | 5.38146 | 1.13420 | 3.12934 |
| H | 5.74194 | 1.45863 | 1.40712 |
| H | 5.65774 | -0.23262 | 2.01576 |
| H | 3.33098 | -1.28667 | 2.68221 |
| H | 1.89221 | -0.20283 | 2.71650 |
| H | 3.25565 | 0.06011 | 3.85486 |
| C | 3.09228 | 2.14978 | 2.17674 |
| H | 1.99865 | 2.20554 | 1.98640 |
| H | 3.59695 | 2.97698 | 1.63807 |
| H | 3.24525 | 2.33168 | 3.26488 |
| C | 4.24912 | -1.26533 | -0.59166 |
| C | 4.27291 | -2.33965 | 0.51975 |
| H | 4.75788 | -3.25120 | 0.10271 |
| H | 3.25207 | -2.63211 | 0.84485 |
| H | 4.86577 | -2.03733 | 1.40663 |
| C | 5.70014 | -0.89175 | -0.96792 |
| H | 6.25740 | -0.41082 | -0.13890 |
| H | 5.75516 | -0.23371 | -1.85888 |
| H | 6.24217 | -1.83045 | -1.22782 |
| C | 3.54962 | -1.90237 | -1.81646 |
| H | 3.52309 | -1.24345 | -2.70398 |
| H | 2.51424 | -2.22230 | -1.58087 |
| H | 4.12235 | -2.81397 | -2.10330 |
| H | 4.87273 | 3.00578 | 0.01153 |
| H | 5.67307 | 1.82944 | -1.08981 |
| C | 3.34851 | 1.30520 | -2.64941 |
| H | 3.32997 | 2.20382 | -3.30708 |
| H | 4.21675 | 0.69297 | -2.96681 |
| H | 2.41329 | 0.73603 | -2.84064 |
| C | 2.99808 | -0.23974 | 2.81333 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 6.38 | 0.12370 | YES YES |
| 8 | a | 11.83 | 0.19303 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 9 | a | 14.04 | 4.06532 | YES | YES |
| 10 | a | 18.22 | 2.00489 | YES | YES |
| 11 | a | 30.74 | 21.14088 | YES | YES |
| 12 | a | 35.83 | 1.16523 | YES | YES |
| 13 | a | 39.43 | 0.14943 | YES | YES |
| 14 | a | 46.18 | 18.11460 | YES | YES |
| 15 | a | 46.90 | 6.32022 | YES | YES |
| 16 | a | 49.27 | 3.27949 | YES | YES |
| 17 | a | 58.15 | 9.66417 | YES | YES |
| 18 | a | 61.59 | 0.07761 | YES | YES |
| 19 | a | 66.02 | 34.74150 | YES | YES |
| 20 | a | 68.13 | 9.47966 | YES | YES |
| 21 | a | 76.06 | 0.81299 | YES | YES |
| 22 | a | 93.10 | 3.08027 | YES | YES |
| 23 | a | 93.84 | 0.55625 | YES | YES |
| 24 | a | 95.67 | 0.84851 | YES | YES |
| 25 | a | 117.16 | 0.48202 | YES | YES |
| 26 | a | 121.40 | 1.19394 | YES | YES |
| 27 | a | 125.19 | 0.39740 | YES | YES |
| 28 | a | 183.48 | 0.23327 | YES | YES |
| 29 | a | 184.41 | 0.83914 | YES | YES |
| 30 | a | 192.05 | 0.66939 | YES | YES |
| 31 | a | 192.49 | 0.40431 | YES | YES |
| 32 | a | 196.09 | 0.00841 | YES | YES |
| 33 | a | 197.49 | 2.10276 | YES | YES |
| 34 | a | 199.12 | 1.04248 | YES | YES |
| 35 | a | 205.00 | 0.07508 | YES | YES |
| 36 | a | 213.29 | 7.38431 | YES | YES |
| 37 | a | 215.35 | 16.13645 | YES | YES |
| 38 | a | 235.66 | 4.52405 | YES | YES |
| 39 | a | 237.53 | 1.09086 | YES | YES |
| 40 | a | 245.17 | 0.22004 | YES | YES |
| 41 | a | 249.16 | 0.38469 | YES | YES |
| 42 | a | 253.97 | 1.13750 | YES | YES |
| 43 | a | 255.95 | 0.13185 | YES | YES |
| 44 | a | 257.14 | 0.35606 | YES | YES |
| 45 | a | 257.76 | 0.99793 | YES | YES |
| 46 | a | 263.22 | 0.10720 | YES | YES |
| 47 | a | 269.62 | 1.03222 | YES | YES |
| 48 | a | 286.67 | 0.31186 | YES | YES |
| 49 | a | 292.12 | 0.94970 | YES | YES |
| 50 | a | 302.84 | 0.35265 | YES | YES |

**[PhSe(PPh3).PtBu3]+_iso1**

bp86 energy (au): -4482.9984762200

pbe0_def2-tzvpp_sp energy (au): -4482.464473821

Zero point energy (au): 0.7146757
Entropy (kJ mol^-1): 1.10507
Chemical potential (kJ mol^-1): 1665.84

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.11637 | 0.33002 | 0.02126 |
| Se | 0.50930 | 0.08214 | 0.00169 |
| C | 0.31188 | -1.85897 | 0.00085 |
| C | -0.00456 | -2.52113 | -1.20450 |
| H | -0.10448 | -1.94939 | -2.14045 |
| C | -0.20409 | -3.91308 | -1.20558 |
| H | -0.45503 | -4.42547 | -2.14879 |
| C | -0.07939 | -4.64739 | -0.01279 |
| H | -0.22871 | -5.73939 | -0.01894 |
| C | 0.22975 | -3.98531 | 1.18826 |
| H | 0.31804 | -4.55433 | 2.12827 |
| C | 0.41700 | -2.59146 | 1.20019 |
| H | 0.63759 | -2.07388 | 2.14598 |
| C | -3.09368 | -0.57026 | 1.28298 |
| C | -3.11797 | -1.98534 | 1.23493 |
| H | -2.58222 | -2.52572 | 0.43727 |
| C | -3.83666 | -2.70845 | 2.19902 |
| H | -3.85875 | -3.80921 | 2.14907 |
| C | -4.52025 | -2.03393 | 3.22670 |
| H | -5.08001 | -2.60537 | 3.98492 |
| C | -4.48847 | -0.63032 | 3.28471 |
| H | -5.02655 | -0.09656 | 4.08496 |
| C | -3.78079 | 0.10324 | 2.31776 |
| H | -3.77182 | 1.20347 | 2.36653 |
| C | -2.33088 | 2.12412 | 0.33860 |
| C | -3.17511 | 2.92949 | -0.45740 |
| H | -3.73942 | 2.48407 | -1.29220 |
| C | -3.29999 | 4.30203 | -0.18427 |
| H | -3.96244 | 4.92289 | -0.80915 |
| C | -2.58882 | 4.88012 | 0.88121 |
| H | -2.69099 | 5.95696 | 1.09285 |
| C | -1.74627 | 4.08330 | 1.67679 |
| H | -1.18865 | 4.53343 | 2.51434 |
| C | -1.60958 | 2.71241 | 1.40531 |
| H | -0.94243 | 2.09537 | 2.03094 |
| C | -2.88899 | -0.01140 | -1.60788 |
| C | -4.18354 | -0.56546 | -1.72599 |
| H | -4.76097 | -0.82414 | -0.82416 |
| C | -4.73927 | -0.78575 | -2.99788 |
| H | -5.74982 | -1.21764 | -3.08183 |
| C | -4.01559 | -0.45168 | -4.15540 |
| H | -4.45575 | -0.62534 | -5.15072 |

| | | | |
|---|---|---|---|
| C | -2.72682 | 0.10099 | -4.04237 |
| H | -2.15600 | 0.36248 | -4.94837 |
| C | -2.16061 | 0.31482 | -2.77591 |
| H | -1.14524 | 0.73739 | -2.69118 |
| P | 3.20034 | 0.26237 | -0.00763 |
| C | 3.47561 | 1.83988 | -1.12788 |
| C | 4.83447 | 2.53456 | -0.88807 |
| H | 4.93301 | 3.37298 | -1.61560 |
| C | 2.33062 | 2.85273 | -0.87130 |
| H | 2.49128 | 3.73023 | -1.53857 |
| H | 2.29386 | 3.23571 | 0.16536 |
| H | 1.33695 | 2.42785 | -1.12868 |
| C | 3.70422 | 0.65459 | 1.83896 |
| C | 5.23037 | 0.65260 | 2.07872 |
| H | 5.42200 | 0.94406 | 3.13729 |
| H | 5.77062 | 1.37683 | 1.43601 |
| H | 5.68505 | -0.34919 | 1.93558 |
| H | 3.38210 | -1.42644 | 2.59254 |
| H | 1.92639 | -0.36869 | 2.64915 |
| H | 3.26943 | -0.13014 | 3.81836 |
| C | 3.12892 | 2.02853 | 2.25490 |
| H | 2.03447 | 2.09973 | 2.07294 |
| H | 3.63382 | 2.88129 | 1.75715 |
| H | 3.29077 | 2.15244 | 3.34994 |
| C | 4.23085 | -1.24882 | -0.69646 |
| C | 4.25056 | -2.37668 | 0.36076 |
| H | 4.71678 | -3.27450 | -0.10481 |
| H | 3.22863 | -2.66847 | 0.68507 |
| H | 4.85794 | -2.12621 | 1.25392 |
| C | 5.68393 | -0.88118 | -1.07148 |
| H | 6.25614 | -0.44987 | -0.22514 |
| H | 5.74070 | -0.17910 | -1.92823 |
| H | 6.20933 | -1.81319 | -1.38431 |
| C | 3.50430 | -1.81488 | -1.93965 |
| H | 3.48413 | -1.11661 | -2.79720 |
| H | 2.46373 | -2.11876 | -1.70533 |
| H | 4.04963 | -2.72675 | -2.27465 |
| H | 4.91505 | 2.97838 | 0.12537 |
| H | 5.69933 | 1.85937 | -1.04515 |
| C | 3.37022 | 1.43508 | -2.61650 |
| H | 3.36510 | 2.36602 | -3.22751 |
| H | 4.22865 | 0.82616 | -2.96506 |
| H | 2.42662 | 0.89075 | -2.83709 |
| C | 3.03169 | -0.39069 | 2.76182 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 10.97 | 1.60285 | YES YES |
| 8 | a | 14.65 | 1.70208 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 9 | a | 16.16 | 0.69938 | YES | YES |
| 10 | a | 22.87 | 1.23102 | YES | YES |
| 11 | a | 32.69 | 27.28928 | YES | YES |
| 12 | a | 38.68 | 1.60387 | YES | YES |
| 13 | a | 41.27 | 9.80152 | YES | YES |
| 14 | a | 45.82 | 7.19138 | YES | YES |
| 15 | a | 46.77 | 6.95772 | YES | YES |
| 16 | a | 51.60 | 1.05305 | YES | YES |
| 17 | a | 58.35 | 11.70294 | YES | YES |
| 18 | a | 60.69 | 28.84364 | YES | YES |
| 19 | a | 62.66 | 0.02234 | YES | YES |
| 20 | a | 69.58 | 2.35076 | YES | YES |
| 21 | a | 75.62 | 0.16108 | YES | YES |
| 22 | a | 91.07 | 0.11138 | YES | YES |
| 23 | a | 96.59 | 4.12222 | YES | YES |
| 24 | a | 98.34 | 12.30386 | YES | YES |
| 25 | a | 115.09 | 0.31138 | YES | YES |
| 26 | a | 118.44 | 0.81277 | YES | YES |
| 27 | a | 125.20 | 0.23306 | YES | YES |
| 28 | a | 180.33 | 0.09707 | YES | YES |
| 29 | a | 185.14 | 1.19264 | YES | YES |
| 30 | a | 189.04 | 0.28600 | YES | YES |
| 31 | a | 193.84 | 1.20323 | YES | YES |
| 32 | a | 194.88 | 1.16101 | YES | YES |
| 33 | a | 201.38 | 2.14212 | YES | YES |
| 34 | a | 205.84 | 0.44655 | YES | YES |
| 35 | a | 206.43 | 0.33737 | YES | YES |
| 36 | a | 213.37 | 19.45904 | YES | YES |
| 37 | a | 216.53 | 1.31963 | YES | YES |
| 38 | a | 236.49 | 5.31347 | YES | YES |
| 39 | a | 237.21 | 0.39190 | YES | YES |
| 40 | a | 246.37 | 0.77188 | YES | YES |
| 41 | a | 246.80 | 0.05835 | YES | YES |
| 42 | a | 254.16 | 0.29515 | YES | YES |
| 43 | a | 254.70 | 0.79620 | YES | YES |
| 44 | a | 256.39 | 0.23530 | YES | YES |
| 45 | a | 261.24 | 0.48869 | YES | YES |
| 46 | a | 263.28 | 0.29899 | YES | YES |
| 47 | a | 268.64 | 0.54321 | YES | YES |
| 48 | a | 284.59 | 0.30234 | YES | YES |
| 49 | a | 291.01 | 1.09071 | YES | YES |
| 50 | a | 301.93 | 0.56323 | YES | YES |

**[PhSe(PPh3).PtBu3]+/encounter/startpoint/iso2**

bp86 energy (au): -4482.9966782020

Single point data not present for this isomer

Zero point energy (au): 0.7140836
Entropy (kJ mol^-1): 1.08308
Chemical potential (kJ mol^-1): 1669.28

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -1.67235 | 0.39576 | 0.00446 |
| Se | 0.87674 | 0.11343 | 0.10374 |
| C | 0.66585 | -1.82264 | 0.03093 |
| C | 0.66298 | -2.49718 | -1.20693 |
| H | 0.77496 | -1.93557 | -2.14730 |
| C | 0.50226 | -3.89379 | -1.24172 |
| H | 0.50187 | -4.41704 | -2.21203 |
| C | 0.34341 | -4.61795 | -0.04675 |
| H | 0.22456 | -5.71320 | -0.07830 |
| C | 0.32962 | -3.94201 | 1.18558 |
| H | 0.19466 | -4.50294 | 2.12434 |
| C | 0.48502 | -2.54551 | 1.22846 |
| H | 0.45833 | -2.01536 | 2.19355 |
| C | -2.65814 | -0.52774 | 1.23932 |
| C | -2.80883 | -1.92750 | 1.08496 |
| H | -2.38334 | -2.44139 | 0.20815 |
| C | -3.51475 | -2.66754 | 2.04542 |
| H | -3.63356 | -3.75517 | 1.91305 |
| C | -4.06197 | -2.02809 | 3.17202 |
| H | -4.61061 | -2.61432 | 3.92706 |
| C | -3.90977 | -0.64011 | 3.33153 |
| H | -4.34614 | -0.13206 | 4.20687 |
| C | -3.21190 | 0.11154 | 2.37184 |
| H | -3.11097 | 1.20076 | 2.50142 |
| C | -1.90959 | 2.18503 | 0.32376 |
| C | -2.78760 | 2.96368 | -0.46311 |
| H | -3.34550 | 2.50289 | -1.29386 |
| C | -2.95301 | 4.33056 | -0.18565 |
| H | -3.64182 | 4.93033 | -0.80243 |
| C | -2.24739 | 4.92973 | 0.87211 |
| H | -2.38040 | 6.00268 | 1.08604 |
| C | -1.36924 | 4.16029 | 1.65558 |
| H | -0.81369 | 4.62785 | 2.48483 |
| C | -1.19384 | 2.79364 | 1.38229 |
| H | -0.50252 | 2.19559 | 1.99960 |
| C | -2.39326 | 0.04672 | -1.64415 |
| C | -3.71935 | -0.42044 | -1.79216 |
| H | -4.34251 | -0.61676 | -0.90520 |
| C | -4.24840 | -0.63174 | -3.07631 |
| H | -5.28310 | -0.99548 | -3.18467 |
| C | -3.46608 | -0.37644 | -4.21574 |
| H | -3.88536 | -0.54455 | -5.22108 |

| | | | |
|---|---|---|---|
| C | -2.14792 | 0.09235 | -4.07195 |
| H | -1.53213 | 0.29429 | -4.96335 |
| C | -1.60825 | 0.29897 | -2.79256 |
| H | -0.57179 | 0.65961 | -2.68172 |
| P | 3.68727 | 0.22619 | 0.15855 |
| C | 3.92367 | 2.16391 | 0.29113 |
| C | 5.35018 | 2.59721 | 0.69693 |
| H | 5.40486 | 3.70991 | 0.66161 |
| C | 2.91098 | 2.72080 | 1.32387 |
| H | 3.04985 | 3.82466 | 1.38652 |
| H | 3.04219 | 2.31478 | 2.34436 |
| H | 1.85955 | 2.54213 | 1.01339 |
| C | 4.53335 | -0.64896 | 1.68751 |
| C | 6.07519 | -0.70542 | 1.61338 |
| H | 6.45586 | -1.15290 | 2.56068 |
| H | 6.54717 | 0.29208 | 1.51063 |
| H | 6.43659 | -1.35205 | 0.78721 |
| H | 4.26744 | -2.74631 | 0.95942 |
| H | 2.87303 | -2.10150 | 1.87841 |
| H | 4.38789 | -2.54617 | 2.73091 |
| C | 4.10839 | 0.08208 | 2.98174 |
| H | 3.00351 | 0.17355 | 3.06614 |
| H | 4.56486 | 1.08677 | 3.08717 |
| H | 4.45529 | -0.52188 | 3.85096 |
| C | 4.47715 | -0.41789 | -1.50742 |
| C | 4.57739 | -1.96021 | -1.45680 |
| H | 4.87172 | -2.32137 | -2.46850 |
| H | 3.60748 | -2.43954 | -1.20267 |
| H | 5.35233 | -2.32009 | -0.75058 |
| C | 5.87567 | 0.16574 | -1.80692 |
| H | 6.61079 | -0.04171 | -1.00264 |
| H | 5.85413 | 1.25982 | -1.98806 |
| H | 6.26440 | -0.30683 | -2.73860 |
| C | 3.51476 | -0.07431 | -2.67123 |
| H | 3.43277 | 1.01036 | -2.87200 |
| H | 2.49278 | -0.46835 | -2.48866 |
| H | 3.90341 | -0.55072 | -3.60032 |
| H | 5.61088 | 2.29652 | 1.73221 |
| H | 6.13148 | 2.20885 | 0.01273 |
| C | 3.56650 | 2.82498 | -1.06107 |
| H | 3.53346 | 3.92800 | -0.90874 |
| H | 4.31807 | 2.63302 | -1.85310 |
| H | 2.56615 | 2.51478 | -1.43196 |
| C | 3.97859 | -2.08899 | 1.80061 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | a | -16.37 | 0.00000 | YES YES |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | | 0.00 | 0.00000 | - - |
| 8 | a | 12.25 | 0.96407 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 9 | a | 19.41 | 2.89243 | YES | YES |
| 10 | a | 21.79 | 3.12238 | YES | YES |
| 11 | a | 30.03 | 45.88806 | YES | YES |
| 12 | a | 37.23 | 24.43158 | YES | YES |
| 13 | a | 39.99 | 1.39072 | YES | YES |
| 14 | a | 43.43 | 0.08621 | YES | YES |
| 15 | a | 48.14 | 3.21850 | YES | YES |
| 16 | a | 49.17 | 0.33289 | YES | YES |
| 17 | a | 53.89 | 0.18971 | YES | YES |
| 18 | a | 56.16 | 0.48403 | YES | YES |
| 19 | a | 64.85 | 0.42876 | YES | YES |
| 20 | a | 69.35 | 0.03564 | YES | YES |
| 21 | a | 80.88 | 0.00558 | YES | YES |
| 22 | a | 86.46 | 0.07013 | YES | YES |
| 23 | a | 96.89 | 0.87965 | YES | YES |
| 24 | a | 100.03 | 1.11725 | YES | YES |
| 25 | a | 105.05 | 28.62702 | YES | YES |
| 26 | a | 106.80 | 3.32494 | YES | YES |
| 27 | a | 115.14 | 0.84237 | YES | YES |
| 28 | a | 167.79 | 0.27405 | YES | YES |
| 29 | a | 169.80 | 0.66654 | YES | YES |
| 30 | a | 174.16 | 0.02304 | YES | YES |
| 31 | a | 187.49 | 0.92407 | YES | YES |
| 32 | a | 193.66 | 1.68665 | YES | YES |
| 33 | a | 195.48 | 1.06590 | YES | YES |
| 34 | a | 200.25 | 0.26725 | YES | YES |
| 35 | a | 200.76 | 3.25027 | YES | YES |
| 36 | a | 206.45 | 2.59515 | YES | YES |
| 37 | a | 215.99 | 16.06259 | YES | YES |
| 38 | a | 229.98 | 0.28722 | YES | YES |
| 39 | a | 235.42 | 0.35956 | YES | YES |
| 40 | a | 238.93 | 2.00022 | YES | YES |
| 41 | a | 239.06 | 0.20566 | YES | YES |
| 42 | a | 244.21 | 0.66268 | YES | YES |
| 43 | a | 252.37 | 0.12922 | YES | YES |
| 44 | a | 252.83 | 0.51476 | YES | YES |
| 45 | a | 256.01 | 0.58339 | YES | YES |
| 46 | a | 264.75 | 0.49370 | YES | YES |
| 47 | a | 268.79 | 0.78949 | YES | YES |
| 48 | a | 277.16 | 0.08545 | YES | YES |
| 49 | a | 281.76 | 0.08019 | YES | YES |
| 50 | a | 295.18 | 0.50994 | YES | YES |

**[PhSe(PtBu3)]+**

bp86 energy (au): -3447.2492755360

pbe0_def2-tzvpp_sp energy (au): -3446.869744332

Zero point energy (au): 0.4477377
Entropy (kJ mol^-1): 0.69468
Chemical potential (kJ mol^-1): 1038.54

XYZ coordinates:

52

| | | | |
|---|---|---|---|
| P | 1.14783 | 0.12796 | -0.13267 |
| C | -4.92953 | 0.41993 | -0.36710 |
| H | -5.96270 | 0.69572 | -0.63307 |
| C | 1.69819 | 1.59794 | 1.03081 |
| C | -2.85557 | 0.91140 | 0.81935 |
| H | -2.28332 | 1.55949 | 1.49875 |
| C | 2.34679 | 1.03257 | 2.31485 |
| H | 2.52119 | 1.88760 | 3.00589 |
| H | 3.33171 | 0.55542 | 2.14007 |
| H | 1.67944 | 0.32048 | 2.84613 |
| C | -4.16997 | 1.26104 | 0.46544 |
| H | -4.60731 | 2.19255 | 0.85998 |
| C | 2.14755 | -2.29648 | -1.30925 |
| H | 2.85104 | -3.15439 | -1.21844 |
| H | 2.28646 | -1.87423 | -2.32474 |
| H | 1.11921 | -2.70520 | -1.21641 |
| C | -2.29597 | -0.27982 | 0.31457 |
| C | 2.48675 | -1.29697 | -0.18042 |
| C | -3.05872 | -1.13528 | -0.50979 |
| H | -2.63338 | -2.08366 | -0.87461 |
| C | -0.21380 | 2.02046 | -1.80426 |
| H | -0.55899 | 2.27875 | -2.83065 |
| H | 0.35501 | 2.89450 | -1.42852 |
| H | -1.12185 | 1.87610 | -1.18243 |
| C | 3.89781 | -0.71063 | -0.41674 |
| H | 4.60457 | -1.56413 | -0.52608 |
| H | 4.26134 | -0.10145 | 0.43544 |
| H | 3.97207 | -0.10730 | -1.34358 |
| C | -0.21375 | -0.33627 | -2.62391 |
| H | -1.16603 | -0.52975 | -2.09251 |
| H | 0.31191 | -1.29638 | -2.77840 |
| H | -0.47359 | 0.06098 | -3.63092 |
| C | 0.45163 | 2.39220 | 1.47965 |
| H | 0.80051 | 3.23717 | 2.11494 |
| H | -0.21751 | 1.76419 | 2.10443 |
| H | -0.13336 | 2.82745 | 0.64746 |
| C | 2.69503 | 2.53643 | 0.31306 |
| H | 2.23110 | 3.09878 | -0.52260 |
| H | 3.59644 | 2.01363 | -0.06601 |
| H | 3.04418 | 3.29134 | 1.05318 |
| C | 0.64143 | 0.73738 | -1.91426 |
| C | 2.46881 | -2.09334 | 1.14849 |

| | | | |
|---|---|---|---|
| H | 1.51024 | -2.63302 | 1.30299 |
| H | 2.68820 | -1.48597 | 2.04563 |
| H | 3.26230 | -2.87151 | 1.07832 |
| C | 1.90622 | 1.02996 | -2.75446 |
| H | 1.56934 | 1.45785 | -3.72582 |
| H | 2.48581 | 0.11500 | -2.99170 |
| H | 2.58462 | 1.77332 | -2.29021 |
| C | -4.37656 | -0.78007 | -0.84588 |
| H | -4.97384 | -1.45227 | -1.48316 |
| Se | -0.58514 | -0.96608 | 0.94179 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 32.21 | 0.22020 | YES YES |
| 8 | a | 52.40 | 0.17604 | YES YES |
| 9 | a | 61.50 | 0.30432 | YES YES |
| 10 | a | 85.23 | 0.18602 | YES YES |
| 11 | a | 94.63 | 0.40405 | YES YES |
| 12 | a | 115.31 | 0.21672 | YES YES |
| 13 | a | 119.24 | 0.27832 | YES YES |
| 14 | a | 125.40 | 0.04203 | YES YES |
| 15 | a | 151.54 | 0.61807 | YES YES |
| 16 | a | 162.93 | 0.09100 | YES YES |
| 17 | a | 190.39 | 1.10708 | YES YES |
| 18 | a | 193.98 | 0.76177 | YES YES |
| 19 | a | 197.41 | 0.96171 | YES YES |
| 20 | a | 203.73 | 0.30836 | YES YES |
| 21 | a | 207.57 | 0.34786 | YES YES |
| 22 | a | 224.74 | 0.10045 | YES YES |
| 23 | a | 231.54 | 0.29662 | YES YES |
| 24 | a | 241.44 | 0.50420 | YES YES |
| 25 | a | 246.79 | 0.32396 | YES YES |
| 26 | a | 251.42 | 0.20979 | YES YES |
| 27 | a | 254.72 | 0.33246 | YES YES |
| 28 | a | 259.32 | 0.09970 | YES YES |
| 29 | a | 275.71 | 0.13487 | YES YES |
| 30 | a | 280.63 | 0.06955 | YES YES |
| 31 | a | 288.96 | 0.65132 | YES YES |
| 32 | a | 297.33 | 0.09969 | YES YES |
| 33 | a | 303.46 | 1.77696 | YES YES |
| 34 | a | 328.19 | 0.46993 | YES YES |
| 35 | a | 346.56 | 0.58521 | YES YES |
| 36 | a | 351.83 | 0.52483 | YES YES |
| 37 | a | 365.80 | 1.17446 | YES YES |
| 38 | a | 373.62 | 0.16197 | YES YES |
| 39 | a | 377.29 | 0.21705 | YES YES |
| 40 | a | 401.03 | 0.33137 | YES YES |
| 41 | a | 403.27 | 0.57173 | YES YES |
| 42 | a | 405.35 | 0.41960 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 43 | a | 408.78 | 0.59008 | YES | YES |
| 44 | a | 456.27 | 11.11421 | YES | YES |
| 45 | a | 458.27 | 9.21389 | YES | YES |
| 46 | a | 470.98 | 6.98247 | YES | YES |
| 47 | a | 491.63 | 26.96240 | YES | YES |
| 48 | a | 527.82 | 8.04084 | YES | YES |
| 49 | a | 555.16 | 2.74144 | YES | YES |
| 50 | a | 560.51 | 0.62071 | YES | YES |

**[PhS(PPh3)]+**

bp86 energy (au): -1665.1390434500

pbe0_def2-tzvpp_sp energy (au): -1664.919057810

Zero point energy (au): 0.3581954
Entropy (kJ mol^-1): 0.70216
Chemical potential (kJ mol^-1): 794.43

XYZ coordinates:

46

| | | | |
|---|---|---|---|
| P | 0.1392601 | 0.5738565 | 0.0229572 |
| S | 1.9998524 | -0.4661656 | 0.1192764 |
| C | 1.5122026 | -2.1986323 | 0.0403477 |
| C | 1.3740572 | -2.8383642 | -1.2095328 |
| H | 1.4995025 | -2.2678853 | -2.1429921 |
| C | 1.0896681 | -4.2131663 | -1.2493444 |
| H | 0.9847487 | -4.7194194 | -2.2226429 |
| C | 0.9579510 | -4.9435621 | -0.0541676 |
| H | 0.7468035 | -6.0245024 | -0.0921786 |
| C | 1.1084022 | -4.3017150 | 1.1878265 |
| H | 1.0172282 | -4.8761983 | 2.1238145 |
| C | 1.3845171 | -2.9256015 | 1.2426657 |
| H | 1.5120968 | -2.4177425 | 2.2113933 |
| C | -1.0868459 | -0.1132557 | 1.1694660 |
| C | -1.7057354 | -1.3514225 | 0.8688980 |
| H | -1.4707073 | -1.8885104 | -0.0639941 |
| C | -2.6372027 | -1.8942893 | 1.7665236 |
| H | -3.1224892 | -2.8550133 | 1.5308385 |
| C | -2.9504891 | -1.2165263 | 2.9582254 |
| H | -3.6856000 | -1.6465640 | 3.6577494 |
| C | -2.3326430 | 0.0102901 | 3.2577132 |
| H | -2.5827997 | 0.5449385 | 4.1881257 |
| C | -1.3987585 | 0.5660317 | 2.3698360 |
| H | -0.9252809 | 1.5319025 | 2.6071682 |
| C | 0.6124288 | 2.2649011 | 0.4904251 |
| C | 0.0878664 | 3.3622081 | -0.2302914 |
| H | -0.5840188 | 3.2001969 | -1.0879969 |
| C | 0.4339906 | 4.6684470 | 0.1496243 |
| H | 0.0272166 | 5.5240052 | -0.4128629 |
| C | 1.2997866 | 4.8831575 | 1.2361757 |
| H | 1.5725095 | 5.9106899 | 1.5264249 |
| C | 1.8255993 | 3.7909125 | 1.9495732 |
| H | 2.5100397 | 3.9592501 | 2.7964122 |
| C | 1.4862871 | 2.4794966 | 1.5835510 |
| H | 1.9090372 | 1.6278958 | 2.1408524 |
| C | -0.5300351 | 0.5594357 | -1.6679514 |
| C | -1.9273993 | 0.5983333 | -1.8832573 |
| H | -2.6289354 | 0.5716603 | -1.0343880 |
| C | -2.4228379 | 0.6741562 | -3.1954041 |
| H | -3.5112972 | 0.7018233 | -3.3648228 |
| C | -1.5359728 | 0.7128846 | -4.2853459 |
| H | -1.9307889 | 0.7695246 | -5.3127020 |

| | | | |
|---|---|---|---|
| C | -0.1459232 | 0.6789043 | -4.0694075 |
| H | 0.5487075 | 0.7100765 | -4.9240947 |
| C | 0.3624527 | 0.6020163 | -2.7642572 |
| H | 1.4513400 | 0.5709817 | -2.5948388 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 20.28 | 0.08755 | YES YES |
| 8 | a | 27.88 | 0.00810 | YES YES |
| 9 | a | 33.36 | 0.06606 | YES YES |
| 10 | a | 39.18 | 0.02010 | YES YES |
| 11 | a | 46.49 | 0.16347 | YES YES |
| 12 | a | 50.36 | 0.04573 | YES YES |
| 13 | a | 56.93 | 0.11035 | YES YES |
| 14 | a | 60.70 | 0.08646 | YES YES |
| 15 | a | 73.63 | 0.31691 | YES YES |
| 16 | a | 100.93 | 0.58271 | YES YES |
| 17 | a | 116.98 | 0.89837 | YES YES |
| 18 | a | 185.48 | 1.14471 | YES YES |
| 19 | a | 189.86 | 2.10379 | YES YES |
| 20 | a | 209.53 | 1.36231 | YES YES |
| 21 | a | 214.52 | 0.35815 | YES YES |
| 22 | a | 240.02 | 0.58162 | YES YES |
| 23 | a | 256.66 | 0.39745 | YES YES |
| 24 | a | 266.34 | 0.44498 | YES YES |
| 25 | a | 283.07 | 1.65099 | YES YES |
| 26 | a | 314.34 | 3.15946 | YES YES |
| 27 | a | 393.19 | 0.23918 | YES YES |
| 28 | a | 394.55 | 0.12588 | YES YES |
| 29 | a | 400.61 | 6.47780 | YES YES |
| 30 | a | 401.29 | 0.13196 | YES YES |
| 31 | a | 403.78 | 1.63041 | YES YES |
| 32 | a | 436.16 | 5.14157 | YES YES |
| 33 | a | 440.37 | 6.23189 | YES YES |
| 34 | a | 449.15 | 7.00389 | YES YES |
| 35 | a | 481.29 | 15.44570 | YES YES |
| 36 | a | 497.61 | 57.90493 | YES YES |
| 37 | a | 513.58 | 76.15323 | YES YES |
| 38 | a | 544.98 | 63.67789 | YES YES |
| 39 | a | 604.29 | 0.01925 | YES YES |
| 40 | a | 605.35 | 0.32121 | YES YES |
| 41 | a | 605.55 | 0.26694 | YES YES |
| 42 | a | 606.65 | 0.50988 | YES YES |
| 43 | a | 677.64 | 7.52248 | YES YES |
| 44 | a | 686.14 | 2.36627 | YES YES |
| 45 | a | 692.21 | 39.29860 | YES YES |
| 46 | a | 693.05 | 18.36036 | YES YES |
| 47 | a | 694.01 | 35.33904 | YES YES |
| 48 | a | 694.73 | 7.98434 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 49 | a | 711.00 | 26.27979 | YES | YES |
| 50 | a | 711.64 | 30.90159 | YES | YES |

**[PhS(PPh3).PPh3]+**

bp86 energy (au): -2700.8834663460

pbe0_def2-tzvpp_sp energy (au): -2700.510707785

Zero point energy (au): 0.6248255
Entropy (kJ mol^-1): 1.12127
Chemical potential (kJ mol^-1): 1418.79

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.75761 | 0.43244 | 3.37906 |
| H | -5.84038 | 0.54000 | 3.55572 |
| C | 2.64634 | 2.63161 | 4.05460 |
| H | 3.73317 | 2.77248 | 3.93354 |
| S | -0.08435 | 0.01129 | -0.38243 |
| P | -0.17857 | 0.02624 | 2.56367 |
| C | 0.52566 | 3.31000 | 5.03323 |
| H | -0.05650 | 3.98309 | 5.68385 |
| C | -4.12168 | 1.21724 | 2.40066 |
| H | -4.70407 | 1.94174 | 1.80793 |
| C | -1.98124 | 0.15674 | 2.93192 |
| C | 1.99916 | 1.59060 | 3.37048 |
| H | 2.58373 | 0.92601 | 2.71193 |
| C | 1.15307 | -3.98704 | 4.54539 |
| H | 1.46303 | -4.94486 | 4.99445 |
| C | 0.60700 | 1.38796 | 3.52687 |
| C | 3.82246 | 1.25677 | -0.31495 |
| H | 4.37087 | 2.20810 | -0.41187 |
| C | -2.74369 | 1.07431 | 2.17142 |
| H | -2.25181 | 1.68677 | 1.39636 |
| C | 0.35790 | -1.52958 | 3.39794 |
| C | 0.43745 | -3.97460 | 3.33434 |
| H | 0.18348 | -4.92303 | 2.83251 |
| C | -0.12532 | 2.26038 | 4.36216 |
| H | -1.21011 | 2.11904 | 4.49278 |
| C | 1.91029 | 3.49672 | 4.88440 |
| H | 2.41809 | 4.31837 | 5.41543 |
| C | -2.62804 | -0.62837 | 3.91257 |
| H | -2.04867 | -1.34945 | 4.51130 |
| C | 1.07667 | -1.55050 | 4.61303 |
| H | 1.32628 | -0.60610 | 5.12253 |
| C | 0.05008 | -2.75427 | 2.75895 |
| H | -0.50480 | -2.75137 | 1.80490 |
| C | 2.41560 | -1.17006 | -0.05854 |
| H | 1.85976 | -2.11459 | 0.04579 |
| C | -4.00927 | -0.48972 | 4.13113 |
| H | -4.50366 | -1.10547 | 4.90043 |
| C | 1.47204 | -2.77470 | 5.18005 |
| H | 2.03026 | -2.77876 | 6.13082 |
| C | 3.81513 | -1.15140 | 0.05460 |
| H | 4.35697 | -2.09144 | 0.24894 |
| C | 2.42096 | 1.25178 | -0.41410 |

| | | | |
|---|---|---|---|
| H | 1.87195 | 2.19225 | -0.57613 |
| C | 4.52011 | 0.05833 | -0.07886 |
| H | 5.61883 | 0.06845 | 0.00786 |
| C | 1.71969 | 0.03409 | -0.29389 |
| C | -4.78110 | -0.85107 | -3.20425 |
| H | -5.85474 | -1.05442 | -3.34810 |
| C | 2.86455 | -2.20108 | -4.13235 |
| H | 3.96064 | -2.10500 | -4.19133 |
| P | -0.26241 | -0.01184 | -2.60313 |
| C | 0.82607 | -3.45199 | -4.59487 |
| H | 0.32094 | -4.33368 | -5.02123 |
| C | -4.06355 | -1.53987 | -2.21048 |
| H | -4.57200 | -2.28051 | -1.57245 |
| C | -2.04224 | -0.32909 | -2.83610 |
| C | 2.11491 | -1.18984 | -3.51271 |
| H | 2.62808 | -0.31049 | -3.09146 |
| C | 0.62282 | 4.14116 | -4.46387 |
| H | 0.81580 | 5.13347 | -4.90286 |
| C | 0.70509 | -1.30686 | -3.44092 |
| C | -2.69602 | -1.28377 | -2.02158 |
| H | -2.14077 | -1.82170 | -1.23634 |
| C | 0.13866 | 1.60823 | -3.33958 |
| C | 0.00682 | 4.03859 | -3.20285 |
| H | -0.28420 | 4.94833 | -2.65325 |
| C | 0.06377 | -2.44607 | -3.98023 |
| H | -1.03241 | -2.54323 | -3.93306 |
| C | 2.22426 | -3.33110 | -4.67211 |
| H | 2.81925 | -4.12214 | -5.15675 |
| C | -2.76617 | 0.36493 | -3.83213 |
| H | -2.26510 | 1.11439 | -4.46519 |
| C | 0.75162 | 1.71181 | -4.60911 |
| H | 1.03950 | 0.80681 | -5.16739 |
| C | -0.23487 | 2.77786 | -2.63723 |
| H | -0.70917 | 2.69928 | -1.64521 |
| C | -4.13260 | 0.09864 | -4.01306 |
| H | -4.69438 | 0.64092 | -4.79043 |
| C | 0.99293 | 2.98014 | -5.16387 |
| H | 1.47258 | 3.05777 | -6.15294 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 8.91 | 0.00853 | YES YES |
| 8 | a | 10.28 | 0.01662 | YES YES |
| 9 | a | 15.04 | 0.01446 | YES YES |
| 10 | a | 20.06 | 0.15562 | YES YES |
| 11 | a | 24.87 | 0.36964 | YES YES |
| 12 | a | 27.04 | 4.13689 | YES YES |
| 13 | a | 29.56 | 4.39775 | YES YES |
| 14 | a | 32.92 | 0.12713 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 15 | a | 33.45 | 0.10094 | YES | YES |
| 16 | a | 41.29 | 0.05059 | YES | YES |
| 17 | a | 42.52 | 0.14980 | YES | YES |
| 18 | a | 43.32 | 0.05403 | YES | YES |
| 19 | a | 49.55 | 0.07086 | YES | YES |
| 20 | a | 51.61 | 1.86015 | YES | YES |
| 21 | a | 54.69 | 0.10829 | YES | YES |
| 22 | a | 55.99 | 0.10047 | YES | YES |
| 23 | a | 57.73 | 0.03562 | YES | YES |
| 24 | a | 62.29 | 1.01023 | YES | YES |
| 25 | a | 63.04 | 3.15374 | YES | YES |
| 26 | a | 73.04 | 1.18964 | YES | YES |
| 27 | a | 81.16 | 33.88866 | YES | YES |
| 28 | a | 109.52 | 0.08470 | YES | YES |
| 29 | a | 133.81 | 1.34940 | YES | YES |
| 30 | a | 169.92 | 63.77951 | YES | YES |
| 31 | a | 181.91 | 0.16209 | YES | YES |
| 32 | a | 188.47 | 0.87705 | YES | YES |
| 33 | a | 191.05 | 1.00501 | YES | YES |
| 34 | a | 196.49 | 1.18372 | YES | YES |
| 35 | a | 205.49 | 1.77216 | YES | YES |
| 36 | a | 210.49 | 4.64363 | YES | YES |
| 37 | a | 235.90 | 12.08249 | YES | YES |
| 38 | a | 239.24 | 0.62946 | YES | YES |
| 39 | a | 249.15 | 102.80359 | YES | YES |
| 40 | a | 253.79 | 2.38221 | YES | YES |
| 41 | a | 256.90 | 20.01326 | YES | YES |
| 42 | a | 258.14 | 0.54766 | YES | YES |
| 43 | a | 266.53 | 7.46505 | YES | YES |
| 44 | a | 296.65 | 12.50641 | YES | YES |
| 45 | a | 391.18 | 2.85725 | YES | YES |
| 46 | a | 394.64 | 0.42482 | YES | YES |
| 47 | a | 394.94 | 0.09809 | YES | YES |
| 48 | a | 395.47 | 0.77244 | YES | YES |
| 49 | a | 395.94 | 0.14994 | YES | YES |
| 50 | a | 400.74 | 1.89072 | YES | YES |

**[PhS(PtBu3).PPh3]+**

bp86 energy (au): -2479.5540780740

pbe0_def2-tzvpp_sp energy (au): -2479.255866431

Zero point energy (au): 0.7151331
Entropy (kJ mol^-1): 1.11704
Chemical potential (kJ mol^-1): 1663.07

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.09958 | 0.19799 | 0.05376 |
| S | 1.05840 | -0.10995 | 0.18665 |
| C | 0.78936 | -1.89806 | 0.17717 |
| C | 0.72098 | -2.63099 | -1.02497 |
| H | 0.89077 | -2.13557 | -1.99245 |
| C | 0.39866 | -3.99887 | -0.99055 |
| H | 0.34699 | -4.56799 | -1.93293 |
| C | 0.12641 | -4.63315 | 0.23396 |
| H | -0.12788 | -5.70523 | 0.25519 |
| C | 0.15985 | -3.89245 | 1.42890 |
| H | -0.07721 | -4.37744 | 2.38972 |
| C | 0.48605 | -2.52692 | 1.40423 |
| H | 0.48960 | -1.94054 | 2.33650 |
| C | -3.41360 | -0.69117 | 1.00480 |
| C | -3.35975 | -2.10511 | 1.02076 |
| H | -2.56168 | -2.63078 | 0.46887 |
| C | -4.31851 | -2.84696 | 1.72881 |
| H | -4.27098 | -3.94856 | 1.72517 |
| C | -5.33127 | -2.18707 | 2.44787 |
| H | -6.07963 | -2.76906 | 3.01040 |
| C | -5.38431 | -0.78286 | 2.44781 |
| H | -6.17709 | -0.25970 | 3.00769 |
| C | -4.43423 | -0.03648 | 1.72888 |
| H | -4.49198 | 1.06382 | 1.72965 |
| C | -2.35608 | 1.97474 | 0.50390 |
| C | -2.96751 | 2.91957 | -0.34869 |
| H | -3.35172 | 2.60542 | -1.33246 |
| C | -3.09788 | 4.26088 | 0.05376 |
| H | -3.58097 | 4.98692 | -0.62098 |
| C | -2.62820 | 4.67387 | 1.31196 |
| H | -2.73935 | 5.72431 | 1.62730 |
| C | -2.01887 | 3.73961 | 2.16940 |
| H | -1.65343 | 4.05494 | 3.16095 |
| C | -1.87320 | 2.40310 | 1.76391 |
| H | -1.39252 | 1.67648 | 2.44224 |
| C | -2.68084 | 0.09703 | -1.70070 |
| C | -3.96202 | -0.36744 | -2.07089 |
| H | -4.68197 | -0.67319 | -1.29483 |
| C | -4.32690 | -0.43990 | -3.42670 |
| H | -5.33088 | -0.80339 | -3.70149 |
| C | -3.42284 | -0.04548 | -4.42760 |
| H | -3.71372 | -0.10087 | -5.48944 |

| | | | |
|---|---|---|---|
| C | -2.14445 | 0.41863 | -4.06898 |
| H | -1.43070 | 0.72954 | -4.85003 |
| C | -1.77280 | 0.47898 | -2.71630 |
| H | -0.76468 | 0.83465 | -2.44065 |
| P | 3.23039 | 0.29128 | 0.07703 |
| C | 3.92556 | -0.15174 | -1.69559 |
| C | 5.19878 | 0.66074 | -2.02749 |
| H | 5.58205 | 0.30395 | -3.01055 |
| C | 2.84428 | 0.13362 | -2.76360 |
| H | 3.22702 | -0.23713 | -3.74090 |
| H | 2.62151 | 1.20962 | -2.88647 |
| H | 1.89059 | -0.38897 | -2.54982 |
| C | 3.11873 | 2.23039 | 0.33179 |
| C | 4.50728 | 2.82710 | 0.65894 |
| H | 4.40255 | 3.93546 | 0.67769 |
| H | 5.28200 | 2.58661 | -0.09656 |
| H | 4.87856 | 2.52417 | 1.65910 |
| H | 2.40618 | 2.12892 | 2.45200 |
| H | 1.08828 | 2.30056 | 1.24252 |
| H | 2.16068 | 3.68370 | 1.60658 |
| C | 2.56663 | 2.89879 | -0.94964 |
| H | 1.59155 | 2.47302 | -1.26635 |
| H | 3.27562 | 2.86500 | -1.80088 |
| H | 2.39307 | 3.97335 | -0.71703 |
| C | 4.25686 | -0.56511 | 1.50018 |
| C | 3.81138 | 0.01711 | 2.86023 |
| H | 4.29335 | -0.58655 | 3.66179 |
| H | 2.71280 | -0.05367 | 3.00724 |
| H | 4.13085 | 1.06769 | 3.01169 |
| C | 5.77520 | -0.34534 | 1.30725 |
| H | 6.06588 | 0.72158 | 1.23913 |
| H | 6.17393 | -0.88060 | 0.42134 |
| H | 6.29300 | -0.76944 | 2.19761 |
| C | 3.96870 | -2.08420 | 1.53641 |
| H | 4.25984 | -2.61790 | 0.61341 |
| H | 2.90510 | -2.30782 | 1.74633 |
| H | 4.57104 | -2.51579 | 2.36760 |
| H | 5.00163 | 1.74645 | -2.13560 |
| H | 6.01432 | 0.51907 | -1.29011 |
| C | 4.26205 | -1.66019 | -1.75618 |
| H | 4.52209 | -1.90680 | -2.81012 |
| H | 5.14166 | -1.93121 | -1.13833 |
| H | 3.40489 | -2.30423 | -1.46826 |
| C | 2.13598 | 2.57804 | 1.47854 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 5.34 | 0.00269 | YES YES |
| 8 | a | 10.86 | 0.03648 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 9 | a | 13.44 | 0.03608 | YES | YES |
| 10 | a | 17.67 | 0.12527 | YES | YES |
| 11 | a | 28.40 | 5.66079 | YES | YES |
| 12 | a | 30.54 | 1.19580 | YES | YES |
| 13 | a | 36.17 | 0.54334 | YES | YES |
| 14 | a | 38.10 | 0.51034 | YES | YES |
| 15 | a | 42.28 | 0.08852 | YES | YES |
| 16 | a | 51.65 | 2.06433 | YES | YES |
| 17 | a | 56.48 | 0.20839 | YES | YES |
| 18 | a | 57.39 | 2.62142 | YES | YES |
| 19 | a | 59.42 | 0.28183 | YES | YES |
| 20 | a | 68.77 | 0.81859 | YES | YES |
| 21 | a | 73.81 | 9.26106 | YES | YES |
| 22 | a | 95.26 | 0.30151 | YES | YES |
| 23 | a | 95.96 | 0.53606 | YES | YES |
| 24 | a | 115.97 | 0.21843 | YES | YES |
| 25 | a | 129.96 | 0.97131 | YES | YES |
| 26 | a | 135.16 | 0.64665 | YES | YES |
| 27 | a | 152.62 | 13.62361 | YES | YES |
| 28 | a | 164.70 | 10.26302 | YES | YES |
| 29 | a | 180.14 | 3.71531 | YES | YES |
| 30 | a | 182.05 | 0.10245 | YES | YES |
| 31 | a | 192.51 | 0.24626 | YES | YES |
| 32 | a | 193.60 | 1.13422 | YES | YES |
| 33 | a | 194.70 | 1.41420 | YES | YES |
| 34 | a | 201.16 | 1.09892 | YES | YES |
| 35 | a | 205.81 | 0.46852 | YES | YES |
| 36 | a | 212.00 | 0.23867 | YES | YES |
| 37 | a | 236.94 | 5.34937 | YES | YES |
| 38 | a | 239.02 | 1.20228 | YES | YES |
| 39 | a | 242.43 | 1.86718 | YES | YES |
| 40 | a | 244.51 | 2.60839 | YES | YES |
| 41 | a | 250.76 | 8.94675 | YES | YES |
| 42 | a | 254.27 | 0.45098 | YES | YES |
| 43 | a | 256.54 | 0.64234 | YES | YES |
| 44 | a | 257.06 | 0.79187 | YES | YES |
| 45 | a | 263.01 | 10.99157 | YES | YES |
| 46 | a | 275.23 | 16.05915 | YES | YES |
| 47 | a | 283.66 | 6.50935 | YES | YES |
| 48 | a | 283.87 | 1.74967 | YES | YES |
| 49 | a | 291.61 | 20.61850 | YES | YES |
| 50 | a | 302.11 | 1.36833 | YES | YES |

**[PhS(PPh3).PtBu3]+_try4**

Optimisation data present for this isomer

pbe0_def2-tzvpp_sp energy (au): -2479.255024102

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.06849 | 0.34547 | 0.03073 |
| S | 0.15760 | 0.05451 | -0.00059 |
| C | 0.11557 | -1.74962 | -0.05539 |
| C | -0.04878 | -2.41859 | -1.28611 |
| H | -0.15535 | -1.84123 | -2.21769 |
| C | -0.06673 | -3.82360 | -1.31697 |
| H | -0.19492 | -4.34594 | -2.27913 |
| C | 0.09266 | -4.55953 | -0.12899 |
| H | 0.08776 | -5.66126 | -0.15875 |
| C | 0.26388 | -3.88946 | 1.09549 |
| H | 0.39105 | -4.46337 | 2.02785 |
| C | 0.26970 | -2.48495 | 1.13811 |
| H | 0.39336 | -1.95529 | 2.09554 |
| C | -2.97530 | -0.63438 | 1.26939 |
| C | -3.12592 | -2.02966 | 1.07543 |
| H | -2.72587 | -2.51639 | 0.17161 |
| C | -3.79685 | -2.79845 | 2.03795 |
| H | -3.91697 | -3.88228 | 1.87951 |
| C | -4.31015 | -2.19190 | 3.19847 |
| H | -4.83527 | -2.80096 | 3.95208 |
| C | -4.15606 | -0.80886 | 3.39588 |
| H | -4.56310 | -0.32933 | 4.30071 |
| C | -3.49092 | -0.02717 | 2.43796 |
| H | -3.38614 | 1.05767 | 2.59642 |
| C | -2.21037 | 2.11837 | 0.43237 |
| C | -3.08950 | 2.95257 | -0.29406 |
| H | -3.69067 | 2.54264 | -1.12113 |
| C | -3.19612 | 4.31248 | 0.03925 |
| H | -3.88299 | 4.95935 | -0.52999 |
| C | -2.43079 | 4.84553 | 1.09071 |
| H | -2.51642 | 5.91389 | 1.34736 |
| C | -1.55401 | 4.01773 | 1.81414 |
| H | -0.95184 | 4.43464 | 2.63754 |
| C | -1.43734 | 2.65712 | 1.48850 |
| H | -0.74462 | 2.01526 | 2.05668 |
| C | -2.81521 | 0.06432 | -1.61037 |
| C | -4.12237 | -0.45706 | -1.74557 |
| H | -4.70647 | -0.74071 | -0.85585 |
| C | -4.68259 | -0.60926 | -3.02497 |
| H | -5.70151 | -1.01651 | -3.12661 |
| C | -3.95073 | -0.24185 | -4.16714 |
| H | -4.39483 | -0.36384 | -5.16842 |
| C | -2.65161 | 0.28171 | -4.03360 |
| H | -2.07698 | 0.57171 | -4.92810 |
| C | -2.07992 | 0.43260 | -2.76134 |
| H | -1.05882 | 0.83565 | -2.65894 |
| P | 3.19525 | 0.21531 | -0.03032 |
| C | 3.61148 | 1.37048 | -1.55481 |

| | | | |
|---|---|---|---|
| C | 4.92204 | 2.17759 | -1.43894 |
| H | 5.07667 | 2.75671 | -2.37963 |
| C | 2.42160 | 2.34567 | -1.74684 |
| H | 2.59452 | 2.93990 | -2.67376 |
| H | 2.30003 | 3.06814 | -0.91704 |
| H | 1.46295 | 1.79642 | -1.86884 |
| C | 3.54681 | 1.19571 | 1.62531 |
| C | 5.03413 | 1.33989 | 2.01321 |
| H | 5.10897 | 1.95369 | 2.94113 |
| H | 5.63185 | 1.85117 | 1.23109 |
| H | 5.51539 | 0.36485 | 2.23361 |
| H | 3.16875 | -0.54718 | 2.97400 |
| H | 1.69823 | 0.38210 | 2.52437 |
| H | 2.88097 | 1.06022 | 3.69903 |
| C | 2.92353 | 2.60777 | 1.52798 |
| H | 1.85400 | 2.57618 | 1.22627 |
| H | 3.46837 | 3.27651 | 0.83171 |
| H | 2.97085 | 3.08253 | 2.53528 |
| C | 4.35700 | -1.36150 | -0.09158 |
| C | 4.29506 | -2.09392 | 1.26912 |
| H | 4.81813 | -3.07218 | 1.16367 |
| H | 3.24997 | -2.31231 | 1.57798 |
| H | 4.80471 | -1.54448 | 2.08634 |
| C | 5.83415 | -1.08082 | -0.44048 |
| H | 6.31721 | -0.37621 | 0.26687 |
| H | 5.96218 | -0.68209 | -1.46785 |
| H | 6.40320 | -2.03846 | -0.39424 |
| C | 3.75520 | -2.34099 | -1.13035 |
| H | 3.79772 | -1.96460 | -2.17013 |
| H | 2.69825 | -2.58734 | -0.89495 |
| H | 4.33766 | -3.29061 | -1.10215 |
| H | 4.89664 | 2.91535 | -0.61004 |
| H | 5.81238 | 1.53189 | -1.29881 |
| C | 3.66484 | 0.51000 | -2.83859 |
| H | 3.71562 | 1.19208 | -3.71858 |
| H | 4.55894 | -0.14420 | -2.88871 |
| H | 2.75596 | -0.11922 | -2.95980 |
| C | 2.78157 | 0.46750 | 2.76008 |

**[PhS(PtBu3)]+**

bp86 energy (au): -1443.8122964960

pbe0_def2-tzvpp_sp energy (au): -1443.664047188

Zero point energy (au): 0.4487512
Entropy (kJ mol^-1): 0.68386
Chemical potential (kJ mol^-1): 1043.31

XYZ coordinates:

52

| | | | |
|---|---|---|---|
| P | -1.00074 | 0.02552 | 0.00057 |
| C | 2.24653 | -0.65845 | 0.09607 |
| C | 4.34329 | -0.10279 | 1.20499 |
| H | 4.92752 | 0.01764 | 2.13154 |
| C | 4.94126 | 0.12975 | -0.04581 |
| H | 5.99713 | 0.43935 | -0.10314 |
| C | 4.19716 | -0.05141 | -1.22492 |
| H | 4.66956 | 0.10645 | -2.20802 |
| C | 2.85355 | -0.45757 | -1.16115 |
| H | 2.29464 | -0.63841 | -2.09151 |
| C | -0.84565 | 1.50267 | 1.26156 |
| C | -1.90786 | 2.58681 | 0.96499 |
| H | -1.83709 | 3.35396 | 1.76943 |
| C | 0.56479 | 2.13317 | 1.18301 |
| H | 0.59214 | 2.96886 | 1.91836 |
| H | 0.81138 | 2.56232 | 0.19493 |
| H | 1.36318 | 1.41996 | 1.46395 |
| C | -1.07527 | 0.62602 | -1.85472 |
| C | -2.49110 | 1.14077 | -2.20668 |
| H | -2.45420 | 1.54433 | -3.24370 |
| H | -2.83635 | 1.96477 | -1.54983 |
| H | -3.25585 | 0.33762 | -2.20316 |
| H | -1.43479 | -1.36741 | -2.79471 |
| H | 0.29495 | -0.96986 | -2.56547 |
| H | -0.66578 | -0.13649 | -3.83406 |
| C | -0.05299 | 1.76499 | -2.07514 |
| H | 0.97963 | 1.48157 | -1.78311 |
| H | -0.33183 | 2.70301 | -1.55463 |
| H | -0.03645 | 1.99439 | -3.16396 |
| C | -2.47933 | -1.18430 | 0.44281 |
| C | -2.73228 | -2.16237 | -0.72870 |
| H | -3.49103 | -2.90038 | -0.38529 |
| H | -1.82441 | -2.73625 | -1.01079 |
| H | -3.15037 | -1.66938 | -1.62883 |
| C | -3.76531 | -0.37117 | 0.72045 |
| H | -4.05462 | 0.29711 | -0.11540 |
| H | -3.70387 | 0.22582 | 1.65312 |
| H | -4.59753 | -1.09731 | 0.86015 |
| C | -2.13644 | -2.04265 | 1.68649 |
| H | -1.90941 | -1.45197 | 2.59304 |
| H | -1.29560 | -2.74152 | 1.50141 |
| H | -3.03409 | -2.66112 | 1.91196 |

| | | | |
|---|---|---|---|
| S | 0.60305 | -1.38783 | 0.26236 |
| C | 2.99782 | -0.49759 | 1.28175 |
| H | 2.53346 | -0.69757 | 2.26058 |
| H | -1.72633 | 3.11334 | 0.00596 |
| H | -2.94761 | 2.20386 | 0.97148 |
| C | -1.02988 | 0.96457 | 2.69802 |
| H | -0.80012 | 1.79663 | 3.40087 |
| H | -2.06665 | 0.63769 | 2.91509 |
| H | -0.32939 | 0.13457 | 2.92878 |
| C | -0.70050 | -0.54038 | -2.79760 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR | RAMAN |
| 1 | | 0.00 | 0.00000 | - | - |
| 2 | | 0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 27.79 | 0.15426 | YES | YES |
| 8 | a | 55.95 | 0.07687 | YES | YES |
| 9 | a | 59.61 | 0.08344 | YES | YES |
| 10 | a | 86.75 | 0.52811 | YES | YES |
| 11 | a | 97.96 | 0.16022 | YES | YES |
| 12 | a | 119.34 | 0.14072 | YES | YES |
| 13 | a | 128.92 | 0.81837 | YES | YES |
| 14 | a | 129.70 | 0.14458 | YES | YES |
| 15 | a | 163.98 | 0.09934 | YES | YES |
| 16 | a | 176.39 | 0.99974 | YES | YES |
| 17 | a | 187.85 | 0.01568 | YES | YES |
| 18 | a | 195.08 | 0.22831 | YES | YES |
| 19 | a | 201.42 | 1.45397 | YES | YES |
| 20 | a | 209.04 | 0.62751 | YES | YES |
| 21 | a | 209.83 | 0.82123 | YES | YES |
| 22 | a | 233.37 | 0.56312 | YES | YES |
| 23 | a | 241.09 | 1.03914 | YES | YES |
| 24 | a | 249.00 | 0.29624 | YES | YES |
| 25 | a | 256.64 | 0.18184 | YES | YES |
| 26 | a | 257.58 | 0.25279 | YES | YES |
| 27 | a | 265.09 | 0.22925 | YES | YES |
| 28 | a | 273.35 | 0.72106 | YES | YES |
| 29 | a | 285.61 | 0.39240 | YES | YES |
| 30 | a | 292.17 | 0.24219 | YES | YES |
| 31 | a | 302.91 | 0.03741 | YES | YES |
| 32 | a | 315.95 | 0.30287 | YES | YES |
| 33 | a | 326.81 | 0.35369 | YES | YES |
| 34 | a | 339.00 | 0.37775 | YES | YES |
| 35 | a | 345.56 | 0.66223 | YES | YES |
| 36 | a | 366.21 | 1.47850 | YES | YES |
| 37 | a | 375.90 | 0.33479 | YES | YES |
| 38 | a | 382.23 | 0.47435 | YES | YES |
| 39 | a | 397.32 | 0.57857 | YES | YES |
| 40 | a | 402.36 | 1.97378 | YES | YES |
| 41 | a | 405.55 | 1.20592 | YES | YES |
| 42 | a | 410.26 | 0.03896 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 43 | a | 416.64 | 3.40347 | YES | YES |
| 44 | a | 458.38 | 12.46442 | YES | YES |
| 45 | a | 461.23 | 9.34973 | YES | YES |
| 46 | a | 487.78 | 7.95595 | YES | YES |
| 47 | a | 508.03 | 11.69427 | YES | YES |
| 48 | a | 537.86 | 12.99659 | YES | YES |
| 49 | a | 561.63 | 3.73592 | YES | YES |
| 50 | a | 568.51 | 7.13609 | YES | YES |

**TS [PhS(PPh3)2]+**

bp86 energy (au): -2700.8820576920

Zero point energy (au): 0.6242501
Entropy (kJ mol^-1): 1.09592
Chemical potential (kJ mol^-1): 1423.72

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.77608 | 0.45972 | 2.92641 |
| H | -5.86081 | 0.57141 | 3.08749 |
| C | 2.70508 | 2.53078 | 3.68856 |
| H | 3.80464 | 2.59122 | 3.64238 |
| S | -0.11555 | -0.00057 | -0.29467 |
| P | -0.20447 | 0.02213 | 2.21292 |
| C | 0.57052 | 3.42299 | 4.44474 |
| H | -0.00774 | 4.18132 | 4.99710 |
| C | -4.12350 | 1.24877 | 1.96267 |
| H | -4.69401 | 1.97892 | 1.36595 |
| C | -2.00258 | 0.17251 | 2.51723 |
| C | 2.04143 | 1.47848 | 3.03979 |
| H | 2.62597 | 0.72418 | 2.48810 |
| C | 1.11278 | -4.04370 | 4.04408 |
| H | 1.41563 | -5.01544 | 4.46691 |
| C | 0.62945 | 1.38560 | 3.10293 |
| C | 3.74088 | 1.37494 | -0.52375 |
| H | 4.24467 | 2.34343 | -0.67677 |
| C | -2.74273 | 1.10476 | 1.75229 |
| H | -2.23718 | 1.72063 | 0.99019 |
| C | 0.33984 | -1.55705 | 2.96365 |
| C | 0.37974 | -3.99589 | 2.84417 |
| H | 0.10633 | -4.92921 | 2.32533 |
| C | -0.10320 | 2.36918 | 3.80551 |
| H | -1.20143 | 2.30788 | 3.86310 |
| C | 1.97231 | 3.50576 | 4.38936 |
| H | 2.49683 | 4.33283 | 4.89491 |
| C | -2.66326 | -0.61989 | 3.48297 |
| H | -2.09702 | -1.35116 | 4.08152 |
| C | 1.07473 | -1.60939 | 4.16905 |
| H | 1.34399 | -0.68094 | 4.69715 |
| C | -0.00022 | -2.75977 | 2.29975 |
| H | -0.56512 | -2.72612 | 1.35330 |
| C | 2.44757 | -1.09738 | -0.14079 |
| H | 1.93813 | -2.06370 | -0.00311 |
| C | -4.04555 | -0.47321 | 3.68333 |
| H | -4.55498 | -1.09198 | 4.43982 |
| C | 1.45879 | -2.85153 | 4.70249 |
| H | 2.02970 | -2.88495 | 5.64475 |
| C | 3.85140 | -1.02880 | -0.14581 |
| H | 4.44170 | -1.94879 | -0.00414 |
| C | 2.33671 | 1.31877 | -0.50216 |
| H | 1.74166 | 2.23606 | -0.63100 |
| C | 4.49922 | 0.20433 | -0.34105 |
| H | 5.60049 | 0.25365 | -0.35109 |

| | | | |
|---|---|---|---|
| C | 1.68839 | 0.07949 | -0.31427 |
| C | -4.77223 | -0.91739 | -3.44810 |
| H | -5.84313 | -1.13299 | -3.59531 |
| C | 2.85478 | -2.27094 | -4.32405 |
| H | 3.95553 | -2.21747 | -4.31141 |
| P | -0.25296 | -0.04467 | -2.80069 |
| C | 0.80223 | -3.39423 | -4.99499 |
| H | 0.28942 | -4.22040 | -5.51403 |
| C | -4.04171 | -1.61795 | -2.47210 |
| H | -4.53797 | -2.38179 | -1.85165 |
| C | -2.03369 | -0.36600 | -3.07499 |
| C | 2.10561 | -1.27815 | -3.67476 |
| H | 2.62494 | -0.45557 | -3.15644 |
| C | 0.62787 | 4.10616 | -4.70302 |
| H | 0.82465 | 5.09705 | -5.14360 |
| C | 0.69030 | -1.33209 | -3.69493 |
| C | -2.67822 | -1.34289 | -2.27983 |
| H | -2.11182 | -1.89039 | -1.50857 |
| C | 0.12619 | 1.57067 | -3.57678 |
| C | -0.03326 | 4.00500 | -3.46527 |
| H | -0.35571 | 4.91556 | -2.93432 |
| C | 0.04259 | -2.40085 | -4.35515 |
| H | -1.05738 | -2.45315 | -4.37965 |
| C | 2.20606 | -3.33120 | -4.98257 |
| H | 2.79803 | -4.11098 | -5.48890 |
| C | -2.77315 | 0.33823 | -4.05197 |
| H | -2.28169 | 1.10399 | -4.67326 |
| C | 0.78975 | 1.67649 | -4.81984 |
| H | 1.10879 | 0.77011 | -5.35877 |
| C | -0.27887 | 2.74491 | -2.89886 |
| H | -0.78868 | 2.66990 | -1.92388 |
| C | -4.13744 | 0.05978 | -4.23489 |
| H | -4.70750 | 0.61014 | -5.00094 |
| C | 1.03809 | 2.94290 | -5.37630 |
| H | 1.55344 | 3.01769 | -6.34770 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | a | -81.48 | 0.00000 | YES YES |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | | 0.00 | 0.00000 | - - |
| 8 | a | 8.57 | 0.00206 | YES YES |
| 9 | a | 12.82 | 0.02413 | YES YES |
| 10 | a | 17.54 | 0.30214 | YES YES |
| 11 | a | 20.00 | 0.52866 | YES YES |
| 12 | a | 25.24 | 0.37270 | YES YES |
| 13 | a | 27.13 | 0.24745 | YES YES |
| 14 | a | 34.46 | 0.00784 | YES YES |
| 15 | a | 37.02 | 0.04849 | YES YES |
| 16 | a | 38.97 | 0.02294 | YES YES |
| 17 | a | 41.74 | 1.34928 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 18 | a | 44.75 | 1.60566 | YES | YES |
| 19 | a | 48.82 | 1.45984 | YES | YES |
| 20 | a | 50.92 | 1.22854 | YES | YES |
| 21 | a | 55.87 | 0.06533 | YES | YES |
| 22 | a | 57.14 | 0.00195 | YES | YES |
| 23 | a | 61.79 | 2.42033 | YES | YES |
| 24 | a | 64.01 | 12.81610 | YES | YES |
| 25 | a | 69.70 | 0.34500 | YES | YES |
| 26 | a | 72.59 | 2.45440 | YES | YES |
| 27 | a | 74.12 | 0.00748 | YES | YES |
| 28 | a | 108.51 | 0.00468 | YES | YES |
| 29 | a | 115.27 | 0.03504 | YES | YES |
| 30 | a | 139.96 | 1.05682 | YES | YES |
| 31 | a | 183.87 | 0.78001 | YES | YES |
| 32 | a | 184.17 | 1.81765 | YES | YES |
| 33 | a | 191.82 | 0.42239 | YES | YES |
| 34 | a | 196.41 | 2.94729 | YES | YES |
| 35 | a | 202.99 | 1.18335 | YES | YES |
| 36 | a | 203.21 | 2.11338 | YES | YES |
| 37 | a | 229.30 | 69.27300 | YES | YES |
| 38 | a | 236.86 | 0.30194 | YES | YES |
| 39 | a | 237.41 | 0.17634 | YES | YES |
| 40 | a | 254.09 | 1.15717 | YES | YES |
| 41 | a | 255.21 | 2.76479 | YES | YES |
| 42 | a | 261.58 | 0.71999 | YES | YES |
| 43 | a | 262.00 | 0.22846 | YES | YES |
| 44 | a | 298.89 | 4.61042 | YES | YES |
| 45 | a | 390.39 | 0.60369 | YES | YES |
| 46 | a | 392.65 | 2.94670 | YES | YES |
| 47 | a | 394.33 | 0.58181 | YES | YES |
| 48 | a | 394.71 | 0.31279 | YES | YES |
| 49 | a | 395.88 | 0.10135 | YES | YES |
| 50 | a | 396.17 | 0.03548 | YES | YES |

**TS [PhS(PPh3)(PtBu3)]+**

bp86 energy (au): -2479.5529924680

pbe0_def2-tzvpp_sp energy (au): -2479.247034127

Zero point energy (au): 0.7153819
Entropy (kJ mol^-1): 1.03957
Chemical potential (kJ mol^-1): 1681.89

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.33740 | 0.33435 | 0.02787 |
| S | 0.24253 | 0.02625 | -0.01367 |
| C | 0.03835 | -1.76710 | 0.01578 |
| C | -0.25811 | -2.45104 | -1.18351 |
| H | -0.32754 | -1.89028 | -2.12874 |
| C | -0.46386 | -3.84060 | -1.16680 |
| H | -0.69795 | -4.36779 | -2.10602 |
| C | -0.36346 | -4.55602 | 0.04031 |
| H | -0.51629 | -5.64735 | 0.04940 |
| C | -0.07328 | -3.87507 | 1.23569 |
| H | -0.00491 | -4.42954 | 2.18593 |
| C | 0.11716 | -2.48213 | 1.22937 |
| H | 0.31725 | -1.94677 | 2.17016 |
| C | -3.34071 | -0.57919 | 1.26058 |
| C | -3.39601 | -1.99153 | 1.17024 |
| H | -2.86957 | -2.51896 | 0.35711 |
| C | -4.12994 | -2.72847 | 2.11216 |
| H | -4.17459 | -3.82666 | 2.02852 |
| C | -4.79910 | -2.07155 | 3.16074 |
| H | -5.37016 | -2.65396 | 3.90199 |
| C | -4.73811 | -0.67129 | 3.26058 |
| H | -5.26391 | -0.15139 | 4.07722 |
| C | -4.01435 | 0.07612 | 2.31642 |
| H | -3.98391 | 1.17389 | 2.39770 |
| C | -2.51179 | 2.11919 | 0.40865 |
| C | -3.32878 | 2.97706 | -0.36075 |
| H | -3.89780 | 2.57961 | -1.21637 |
| C | -3.42285 | 4.34015 | -0.03312 |
| H | -4.06568 | 5.00141 | -0.63696 |
| C | -2.70816 | 4.85752 | 1.06089 |
| H | -2.78675 | 5.92699 | 1.31567 |
| C | -1.89303 | 4.00843 | 1.83078 |
| H | -1.33296 | 4.41024 | 2.69126 |
| C | -1.78680 | 2.64692 | 1.50395 |
| H | -1.14438 | 1.98689 | 2.11090 |
| C | -3.12292 | 0.06982 | -1.60911 |
| C | -4.42170 | -0.46927 | -1.74869 |
| H | -5.00174 | -0.75685 | -0.85743 |
| C | -4.98051 | -0.63314 | -3.02762 |
| H | -5.99549 | -1.05123 | -3.12751 |
| C | -4.25475 | -0.26082 | -4.17208 |

| | | | |
|---|---|---|---|
| H | -4.69802 | -0.38974 | -5.17297 |
| C | -2.96129 | 0.27582 | -4.03858 |
| H | -2.38899 | 0.56872 | -4.93399 |
| C | -2.39286 | 0.43409 | -2.76508 |
| H | -1.37502 | 0.84731 | -2.66532 |
| P | 2.77779 | 0.21091 | -0.02648 |
| C | 3.08325 | 1.42020 | -1.52944 |
| C | 4.40322 | 2.21534 | -1.41403 |
| H | 4.53616 | 2.81138 | -2.34635 |
| C | 1.90229 | 2.41595 | -1.64943 |
| H | 2.08416 | 3.05276 | -2.54477 |
| H | 1.79947 | 3.09748 | -0.78394 |
| H | 0.93544 | 1.89172 | -1.79946 |
| C | 3.10357 | 1.12678 | 1.66524 |
| C | 4.60348 | 1.27705 | 2.00436 |
| H | 4.69168 | 1.86952 | 2.94372 |
| H | 5.17175 | 1.81855 | 1.22096 |
| H | 5.10250 | 0.30403 | 2.19058 |
| H | 2.78650 | -0.67673 | 2.94809 |
| H | 1.29714 | 0.27395 | 2.60310 |
| H | 2.53343 | 0.90046 | 3.74893 |
| C | 2.45774 | 2.53140 | 1.62570 |
| H | 1.38252 | 2.49619 | 1.34854 |
| H | 2.98318 | 3.23274 | 0.94704 |
| H | 2.51994 | 2.96570 | 2.64963 |
| C | 3.92157 | -1.37504 | -0.17760 |
| C | 3.90531 | -2.15095 | 1.15932 |
| H | 4.45145 | -3.10927 | 1.00410 |
| H | 2.87501 | -2.41143 | 1.48094 |
| H | 4.42133 | -1.61758 | 1.98260 |
| C | 5.38141 | -1.02516 | -0.54263 |
| H | 5.85709 | -0.32636 | 0.17470 |
| H | 5.47798 | -0.60290 | -1.56358 |
| H | 5.97541 | -1.96781 | -0.52704 |
| C | 3.33776 | -2.32489 | -1.25020 |
| H | 3.33487 | -1.89593 | -2.26990 |
| H | 2.30673 | -2.64753 | -1.00250 |
| H | 3.97535 | -3.23762 | -1.28121 |
| H | 4.39257 | 2.93773 | -0.57168 |
| H | 5.29617 | 1.56786 | -1.30795 |
| C | 3.09293 | 0.59578 | -2.83747 |
| H | 3.10151 | 1.30690 | -3.69477 |
| H | 3.99112 | -0.04533 | -2.94336 |
| H | 2.18390 | -0.03531 | -2.94137 |
| C | 2.38867 | 0.34458 | 2.79449 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | a | -67.01 | 0.00000 | YES YES |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | | 0.00 | 0.00000 | - - |

| | | | | | |
|---|---|---|---|---|---|
| 8 | a | 7.90 | 0.12855 | YES | YES |
| 9 | a | 18.82 | 0.37200 | YES | YES |
| 10 | a | 22.05 | 0.77639 | YES | YES |
| 11 | a | 22.34 | 0.34579 | YES | YES |
| 12 | a | 39.04 | 0.33226 | YES | YES |
| 13 | a | 42.33 | 6.86947 | YES | YES |
| 14 | a | 46.43 | 0.03274 | YES | YES |
| 15 | a | 50.50 | 0.41462 | YES | YES |
| 16 | a | 53.54 | 0.46323 | YES | YES |
| 17 | a | 60.38 | 0.41480 | YES | YES |
| 18 | a | 62.97 | 1.76200 | YES | YES |
| 19 | a | 66.81 | 0.86359 | YES | YES |
| 20 | a | 71.44 | 1.13924 | YES | YES |
| 21 | a | 78.06 | 2.41563 | YES | YES |
| 22 | a | 92.83 | 3.48993 | YES | YES |
| 23 | a | 98.60 | 0.26824 | YES | YES |
| 24 | a | 102.55 | 0.14317 | YES | YES |
| 25 | a | 116.82 | 1.20342 | YES | YES |
| 26 | a | 125.58 | 0.47803 | YES | YES |
| 27 | a | 150.26 | 1.17558 | YES | YES |
| 28 | a | 174.91 | 0.73080 | YES | YES |
| 29 | a | 180.75 | 0.08562 | YES | YES |
| 30 | a | 185.19 | 0.94201 | YES | YES |
| 31 | a | 192.68 | 0.27832 | YES | YES |
| 32 | a | 194.64 | 2.08036 | YES | YES |
| 33 | a | 198.75 | 0.24907 | YES | YES |
| 34 | a | 200.41 | 2.42998 | YES | YES |
| 35 | a | 204.84 | 0.46677 | YES | YES |
| 36 | a | 207.43 | 1.03486 | YES | YES |
| 37 | a | 232.94 | 51.57880 | YES | YES |
| 38 | a | 236.37 | 0.76634 | YES | YES |
| 39 | a | 237.58 | 0.36506 | YES | YES |
| 40 | a | 243.17 | 9.20242 | YES | YES |
| 41 | a | 251.79 | 1.95015 | YES | YES |
| 42 | a | 252.52 | 0.48327 | YES | YES |
| 43 | a | 255.37 | 1.83292 | YES | YES |
| 44 | a | 260.18 | 0.09489 | YES | YES |
| 45 | a | 260.96 | 0.51058 | YES | YES |
| 46 | a | 269.51 | 0.97323 | YES | YES |
| 47 | a | 279.69 | 0.08317 | YES | YES |
| 48 | a | 285.13 | 1.02862 | YES | YES |
| 49 | a | 294.10 | 7.40102 | YES | YES |
| 50 | a | 303.86 | 0.04710 | YES | YES |

**TS [PhSe(PPh3)2]+**

bp86 energy (au): -4704.3263826960

pbe0_def2-tzvpp_sp energy (au): -4703.720204176

Zero point energy (au): 0.6239177
Entropy (kJ mol^-1): 1.13027
Chemical potential (kJ mol^-1): 1414.96

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.76992 | 0.70800 | 3.43471 |
| H | -5.84337 | 0.87852 | 3.61828 |
| C | 2.83941 | 2.35321 | 4.02022 |
| H | 3.93867 | 2.35258 | 3.94101 |
| Se | -0.18477 | 0.00064 | -0.00090 |
| P | -0.24425 | 0.01741 | 2.61624 |
| C | 0.78184 | 3.35647 | 4.84677 |
| H | 0.26354 | 4.14150 | 5.42117 |
| C | -4.08090 | 1.50384 | 2.50228 |
| H | -4.61144 | 2.29856 | 1.95308 |
| C | -2.02453 | 0.27039 | 2.96827 |
| C | 2.09870 | 1.34503 | 3.38490 |
| H | 2.62340 | 0.56280 | 2.81221 |
| C | 0.88147 | -4.09662 | 4.47233 |
| H | 1.13756 | -5.07820 | 4.90324 |
| C | 0.68661 | 1.33114 | 3.48933 |
| C | 3.86795 | 1.19987 | -0.21708 |
| H | 4.41535 | 2.14161 | -0.38635 |
| C | -2.71491 | 1.28479 | 2.26284 |
| H | -2.18170 | 1.90850 | 1.52582 |
| C | 0.23008 | -1.58523 | 3.37018 |
| C | 0.20061 | -4.02360 | 3.24348 |
| H | -0.07861 | -4.94681 | 2.70987 |
| C | 0.03146 | 2.34684 | 4.22108 |
| H | -1.06613 | 2.34597 | 4.31227 |
| C | 2.18357 | 3.36169 | 4.74922 |
| H | 2.76835 | 4.15423 | 5.24398 |
| C | -2.72198 | -0.52822 | 3.90196 |
| H | -2.19581 | -1.32358 | 4.45348 |
| C | 0.91261 | -1.66273 | 4.60479 |
| H | 1.19015 | -0.74365 | 5.14518 |
| C | -0.11952 | -2.77468 | 2.68884 |
| H | -0.64351 | -2.72083 | 1.71972 |
| C | 2.46225 | -1.20422 | 0.20924 |
| H | 1.91282 | -2.14580 | 0.36479 |
| C | -4.09006 | -0.30659 | 4.13087 |
| H | -4.62785 | -0.93154 | 4.86225 |
| C | 1.23649 | -2.91717 | 5.14906 |
| H | 1.76800 | -2.97040 | 6.11317 |
| C | 3.86842 | -1.19692 | 0.21814 |
| H | 4.41620 | -2.13837 | 0.38784 |
| C | 2.46177 | 1.20632 | -0.20960 |

| | | | |
|---|---|---|---|
| H | 1.91191 | 2.14757 | -0.36559 |
| C | 4.57160 | 0.00168 | 0.00091 |
| H | 5.67389 | 0.00203 | 0.00151 |
| C | 1.76105 | 0.00087 | -0.00036 |
| C | -4.76008 | -0.72534 | -3.45474 |
| H | -5.83165 | -0.90044 | -3.64474 |
| C | 2.85335 | -2.33908 | -4.01616 |
| H | 3.95280 | -2.33153 | -3.94002 |
| P | -0.24159 | -0.01690 | -2.61360 |
| C | 0.79957 | -3.35775 | -4.83333 |
| H | 0.28450 | -4.14793 | -5.40354 |
| C | -4.07844 | -1.50398 | -2.50265 |
| H | -4.61292 | -2.28977 | -1.94450 |
| C | -2.01986 | -0.27559 | -2.97129 |
| C | 2.10838 | -1.33300 | -3.38247 |
| H | 2.62995 | -0.54549 | -2.81416 |
| C | 0.86653 | 4.10199 | -4.46903 |
| H | 1.11723 | 5.08483 | -4.90027 |
| C | 0.69597 | -1.32774 | -3.48369 |
| C | -2.71476 | -1.27916 | -2.25515 |
| H | -2.18703 | -1.88960 | -1.50328 |
| C | 0.22907 | 1.58756 | -3.36570 |
| C | 0.18331 | 4.02573 | -3.24166 |
| H | -0.10339 | 4.94764 | -2.70973 |
| C | 0.04481 | -2.35036 | -4.20933 |
| H | -1.05302 | -2.35627 | -4.29757 |
| C | 2.20158 | -3.35397 | -4.73988 |
| H | 2.78976 | -4.14466 | -5.23353 |
| C | -2.70984 | 0.50571 | -3.92514 |
| H | -2.17967 | 1.29233 | -4.48531 |
| C | 0.91376 | 1.66822 | -4.59902 |
| H | 1.19817 | 0.75047 | -5.13807 |
| C | -0.13023 | 2.77537 | -2.68661 |
| H | -0.65660 | 2.71916 | -1.71893 |
| C | -4.07540 | 0.27803 | -4.16252 |
| H | -4.60756 | 0.88937 | -4.90933 |
| C | 1.23077 | 2.92430 | -5.14377 |
| H | 1.76405 | 2.98004 | -6.10675 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules | |
|---|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR | RAMAN |
| 1 | | 0.00 | 0.00000 | - | - |
| 2 | | 0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 7.86 | 0.00459 | YES | YES |
| 8 | a | 12.66 | 1.35900 | YES | YES |
| 9 | a | 17.61 | 0.01432 | YES | YES |
| 10 | a | 19.25 | 2.64155 | YES | YES |
| 11 | a | 25.29 | 0.34701 | YES | YES |
| 12 | a | 25.58 | 3.05287 | YES | YES |
| 13 | a | 33.17 | 25.55879 | YES | YES |
| 14 | a | 34.89 | 0.34858 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 15 | a | 37.42 | 0.09188 | YES | YES |
| 16 | a | 39.39 | 0.08998 | YES | YES |
| 17 | a | 41.69 | 1.72286 | YES | YES |
| 18 | a | 46.41 | 14.29265 | YES | YES |
| 19 | a | 47.83 | 0.23930 | YES | YES |
| 20 | a | 51.37 | 9.84061 | YES | YES |
| 21 | a | 54.71 | 0.06887 | YES | YES |
| 22 | a | 57.86 | 0.00911 | YES | YES |
| 23 | a | 59.66 | 0.00749 | YES | YES |
| 24 | a | 66.87 | 1.56060 | YES | YES |
| 25 | a | 67.67 | 0.60604 | YES | YES |
| 26 | a | 68.12 | 10.69895 | YES | YES |
| 27 | a | 76.95 | 79.35749 | YES | YES |
| 28 | a | 94.96 | 0.00947 | YES | YES |
| 29 | a | 112.40 | 0.98917 | YES | YES |
| 30 | a | 113.48 | 0.03239 | YES | YES |
| 31 | a | 184.04 | 2.56118 | YES | YES |
| 32 | a | 184.38 | 0.70388 | YES | YES |
| 33 | a | 192.26 | 0.40070 | YES | YES |
| 34 | a | 193.96 | 3.09935 | YES | YES |
| 35 | a | 200.30 | 5.65050 | YES | YES |
| 36 | a | 202.03 | 0.65149 | YES | YES |
| 37 | a | 210.77 | 20.48164 | YES | YES |
| 38 | a | 236.53 | 4.85933 | YES | YES |
| 39 | a | 236.96 | 0.68821 | YES | YES |
| 40 | a | 239.78 | 1.38006 | YES | YES |
| 41 | a | 254.94 | 0.18614 | YES | YES |
| 42 | a | 255.13 | 1.24157 | YES | YES |
| 43 | a | 261.35 | 0.76578 | YES | YES |
| 44 | a | 262.41 | 0.35690 | YES | YES |
| 45 | a | 301.69 | 0.34976 | YES | YES |
| 46 | a | 392.53 | 1.27789 | YES | YES |
| 47 | a | 394.14 | 0.13507 | YES | YES |
| 48 | a | 394.52 | 2.54741 | YES | YES |
| 49 | a | 394.70 | 0.84260 | YES | YES |
| 50 | a | 395.83 | 0.08473 | YES | YES |

**TS [PhSe(PPh3)(PtBu3)]+**

bp86 energy (au): -4482.9983823930

pbe0_def2-tzvpp_sp energy (au): -4482.464472514

Zero point energy (au): 0.7148867
Entropy (kJ mol^-1): 1.10885
Chemical potential (kJ mol^-1): 1665.16

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.12051 | 0.32729 | 0.02113 |
| Se | 0.54354 | 0.07517 | 0.02827 |
| C | 0.33041 | -1.86522 | 0.03153 |
| C | 0.05154 | -2.53014 | -1.18165 |
| H | -0.01485 | -1.96004 | -2.12172 |
| C | -0.16118 | -3.91981 | -1.18595 |
| H | -0.38317 | -4.43298 | -2.13592 |
| C | -0.08462 | -4.65099 | 0.01277 |
| H | -0.24252 | -5.74173 | 0.00541 |
| C | 0.18076 | -3.98575 | 1.22216 |
| H | 0.22510 | -4.55076 | 2.16774 |
| C | 0.38090 | -2.59345 | 1.23730 |
| H | 0.55163 | -2.07624 | 2.19344 |
| C | -3.12825 | -0.56484 | 1.26669 |
| C | -3.15232 | -1.98002 | 1.22473 |
| H | -2.59949 | -2.52385 | 0.44121 |
| C | -3.89128 | -2.69890 | 2.17668 |
| H | -3.91226 | -3.79996 | 2.13119 |
| C | -4.59750 | -2.01974 | 3.18591 |
| H | -5.17387 | -2.58767 | 3.93426 |
| C | -4.56764 | -0.61589 | 3.23728 |
| H | -5.12399 | -0.07821 | 4.02227 |
| C | -3.83778 | 0.11306 | 2.28330 |
| H | -3.83083 | 1.21358 | 2.32623 |
| C | -2.34311 | 2.12245 | 0.33060 |
| C | -3.17466 | 2.92712 | -0.47937 |
| H | -3.72371 | 2.48143 | -1.32410 |
| C | -3.30644 | 4.29926 | -0.20743 |
| H | -3.95864 | 4.91959 | -0.84356 |
| C | -2.61574 | 4.87796 | 0.87117 |
| H | -2.72357 | 5.95449 | 1.08176 |
| C | -1.78563 | 4.08204 | 1.68063 |
| H | -1.24298 | 4.53255 | 2.52783 |
| C | -1.64212 | 2.71164 | 1.41003 |
| H | -0.98154 | 2.09492 | 2.04286 |
| C | -2.87264 | -0.01569 | -1.61837 |
| C | -4.17383 | -0.54933 | -1.75460 |
| H | -4.77114 | -0.79047 | -0.86089 |
| C | -4.71172 | -0.77010 | -3.03401 |
| H | -5.72835 | -1.18454 | -3.13205 |

| | | | |
|---|---|---|---|
| C | -3.96251 | -0.45905 | -4.18166 |
| H | -4.38918 | -0.63254 | -5.18302 |
| C | -2.66653 | 0.07196 | -4.05096 |
| H | -2.07565 | 0.31618 | -4.94900 |
| C | -2.11888 | 0.28689 | -2.77645 |
| H | -1.09860 | 0.69453 | -2.67733 |
| P | 3.20404 | 0.26694 | 0.00342 |
| C | 3.43625 | 1.91059 | -1.02577 |
| C | 4.80284 | 2.59057 | -0.78496 |
| H | 4.88280 | 3.46839 | -1.46653 |
| C | 2.30092 | 2.90387 | -0.66880 |
| H | 2.44776 | 3.82626 | -1.27586 |
| H | 2.28987 | 3.21258 | 0.39294 |
| H | 1.29882 | 2.50264 | -0.93118 |
| C | 3.76772 | 0.54627 | 1.85122 |
| C | 5.30096 | 0.51703 | 2.03952 |
| H | 5.52907 | 0.75339 | 3.10437 |
| H | 5.82830 | 1.26771 | 1.41680 |
| H | 5.73890 | -0.48114 | 1.83246 |
| H | 3.40964 | -1.57824 | 2.45428 |
| H | 2.00516 | -0.47551 | 2.68575 |
| H | 3.42098 | -0.38235 | 3.78366 |
| C | 3.21939 | 1.89602 | 2.37022 |
| H | 2.11930 | 1.98104 | 2.23595 |
| H | 3.71002 | 2.77670 | 1.90878 |
| H | 3.42195 | 1.94978 | 3.46435 |
| C | 4.20954 | -1.19840 | -0.80994 |
| C | 4.24515 | -2.39525 | 0.16851 |
| H | 4.68315 | -3.26535 | -0.37126 |
| H | 3.23023 | -2.69589 | 0.50586 |
| H | 4.88378 | -2.21378 | 1.05659 |
| C | 5.65440 | -0.80894 | -1.19333 |
| H | 6.24765 | -0.43124 | -0.33619 |
| H | 5.69317 | -0.05549 | -2.00678 |
| H | 6.17013 | -1.72020 | -1.57542 |
| C | 3.45427 | -1.67989 | -2.07200 |
| H | 3.40676 | -0.92484 | -2.87910 |
| H | 2.42278 | -2.00736 | -1.83148 |
| H | 3.99638 | -2.56278 | -2.48104 |
| H | 4.91286 | 2.97605 | 0.24924 |
| H | 5.66226 | 1.92554 | -1.00342 |
| C | 3.28488 | 1.60110 | -2.53295 |
| H | 3.26235 | 2.56885 | -3.08273 |
| H | 4.13264 | 1.01752 | -2.94484 |
| H | 2.33498 | 1.06978 | -2.75827 |
| C | 3.11230 | -0.54805 | 2.72617 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |

| | | | | | |
|---|---|---|---|---|---|
| 7 | a | 8.02 | 0.10843 | YES | YES |
| 8 | a | 12.40 | 1.53054 | YES | YES |
| 9 | a | 16.26 | 0.55798 | YES | YES |
| 10 | a | 22.03 | 3.28677 | YES | YES |
| 11 | a | 31.04 | 25.52181 | YES | YES |
| 12 | a | 37.10 | 1.64608 | YES | YES |
| 13 | a | 41.04 | 2.42926 | YES | YES |
| 14 | a | 45.90 | 2.33219 | YES | YES |
| 15 | a | 46.81 | 15.25501 | YES | YES |
| 16 | a | 51.03 | 5.25771 | YES | YES |
| 17 | a | 56.61 | 12.18422 | YES | YES |
| 18 | a | 61.46 | 32.82781 | YES | YES |
| 19 | a | 62.24 | 1.42182 | YES | YES |
| 20 | a | 70.14 | 2.61750 | YES | YES |
| 21 | a | 80.84 | 0.29815 | YES | YES |
| 22 | a | 93.87 | 0.11471 | YES | YES |
| 23 | a | 94.97 | 9.32824 | YES | YES |
| 24 | a | 99.33 | 0.79343 | YES | YES |
| 25 | a | 113.31 | 0.70666 | YES | YES |
| 26 | a | 117.53 | 0.73744 | YES | YES |
| 27 | a | 126.05 | 0.18886 | YES | YES |
| 28 | a | 182.17 | 0.05234 | YES | YES |
| 29 | a | 184.62 | 1.20037 | YES | YES |
| 30 | a | 189.76 | 0.58150 | YES | YES |
| 31 | a | 193.15 | 1.54039 | YES | YES |
| 32 | a | 195.68 | 0.50597 | YES | YES |
| 33 | a | 201.57 | 1.77390 | YES | YES |
| 34 | a | 202.77 | 0.29551 | YES | YES |
| 35 | a | 209.66 | 0.98187 | YES | YES |
| 36 | a | 214.70 | 19.84247 | YES | YES |
| 37 | a | 217.56 | 1.78811 | YES | YES |
| 38 | a | 236.29 | 3.95516 | YES | YES |
| 39 | a | 237.22 | 0.79110 | YES | YES |
| 40 | a | 243.26 | 0.39641 | YES | YES |
| 41 | a | 248.51 | 0.47270 | YES | YES |
| 42 | a | 252.82 | 0.52254 | YES | YES |
| 43 | a | 254.24 | 0.68967 | YES | YES |
| 44 | a | 257.60 | 0.29281 | YES | YES |
| 45 | a | 261.05 | 0.27334 | YES | YES |
| 46 | a | 262.37 | 0.50981 | YES | YES |
| 47 | a | 271.24 | 0.91203 | YES | YES |
| 48 | a | 286.09 | 0.55276 | YES | YES |
| 49 | a | 289.48 | 0.16435 | YES | YES |
| 50 | a | 301.24 | 0.93987 | YES | YES |

## BP86/def2-TZVPP level optimisations

**$PPh_3$**

bp86_def2-tzvpp energy (au): -1036.6280780380

Zero point energy (au): 0.2655762
Entropy (kJ mol^-1): 0.56778
Chemical potential (kJ mol^-1): 573.59

XYZ coordinates:

34

| | | | |
|---|---|---|---|
| P | 0.00255 | -1.17284 | -0.00199 |
| C | 1.19139 | -0.37003 | 1.16124 |
| C | -0.11433 | -0.97560 | -2.77323 |
| H | -0.73909 | -1.86600 | -2.67800 |
| C | 1.23854 | 0.75228 | -1.76014 |
| H | 1.66464 | 1.22792 | -0.87660 |
| C | 0.41223 | -0.37348 | -1.61588 |
| C | 3.40431 | -0.45808 | 2.17739 |
| H | 4.37467 | -0.94604 | 2.27577 |
| C | 1.52368 | 1.26659 | -3.02845 |
| H | 2.17085 | 2.13943 | -3.12356 |
| C | 0.90866 | 0.77336 | 1.92530 |
| H | -0.06321 | 1.25893 | 1.83391 |
| C | 0.98153 | 0.66991 | -4.16920 |
| H | 1.20557 | 1.07255 | -5.15739 |
| C | 2.44801 | -0.98477 | 1.30793 |
| H | 2.67277 | -1.88824 | 0.73738 |
| C | 1.86142 | 1.29231 | 2.80668 |
| H | 1.62523 | 2.17960 | 3.39554 |
| C | 3.11157 | 0.68171 | 2.93238 |
| H | 3.85288 | 1.08750 | 3.62133 |
| C | 0.15782 | -0.45238 | -4.03811 |
| H | -0.26288 | -0.92953 | -4.92396 |
| C | -2.17443 | 0.70733 | -0.23378 |
| H | -1.65053 | 1.15217 | -1.07995 |
| C | -1.60050 | -0.37535 | 0.45110 |
| C | -2.30457 | -0.93829 | 1.53161 |
| H | -1.88191 | -1.79569 | 2.05928 |
| C | -3.41555 | 1.21881 | 0.15792 |
| H | -3.84932 | 2.05800 | -0.38739 |
| C | -4.09681 | 0.66258 | 1.24299 |
| H | -5.06441 | 1.06294 | 1.54676 |
| C | -3.53539 | -0.41717 | 1.93226 |
| H | -4.06349 | -0.86286 | 2.77592 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 20.61 | 0.35411 | YES YES |
| 8 | a | 23.32 | 0.37352 | YES YES |
| 9 | a | 39.87 | 0.00853 | YES YES |
| 10 | a | 48.22 | 0.07288 | YES YES |
| 11 | a | 50.79 | 0.09938 | YES YES |
| 12 | a | 63.29 | 0.37296 | YES YES |
| 13 | a | 174.18 | 0.34206 | YES YES |
| 14 | a | 190.45 | 1.30932 | YES YES |
| 15 | a | 193.20 | 1.34084 | YES YES |
| 16 | a | 236.27 | 0.69361 | YES YES |
| 17 | a | 249.79 | 0.30630 | YES YES |
| 18 | a | 251.29 | 0.33286 | YES YES |
| 19 | a | 389.78 | 1.34843 | YES YES |
| 20 | a | 390.25 | 0.90345 | YES YES |
| 21 | a | 391.24 | 0.88146 | YES YES |
| 22 | a | 396.70 | 0.12589 | YES YES |
| 23 | a | 416.22 | 5.32980 | YES YES |
| 24 | a | 418.30 | 6.01308 | YES YES |
| 25 | a | 489.77 | 27.77965 | YES YES |
| 26 | a | 492.37 | 28.41900 | YES YES |
| 27 | a | 499.29 | 15.25823 | YES YES |
| 28 | a | 611.18 | 0.15836 | YES YES |
| 29 | a | 612.46 | 0.20297 | YES YES |
| 30 | a | 612.78 | 0.06189 | YES YES |
| 31 | a | 671.20 | 0.74592 | YES YES |
| 32 | a | 685.61 | 1.61912 | YES YES |
| 33 | a | 686.64 | 1.75468 | YES YES |
| 34 | a | 692.40 | 34.31979 | YES YES |
| 35 | a | 693.09 | 36.88420 | YES YES |
| 36 | a | 693.77 | 31.32465 | YES YES |
| 37 | a | 737.98 | 24.86374 | YES YES |
| 38 | a | 738.70 | 23.12285 | YES YES |
| 39 | a | 739.46 | 23.77117 | YES YES |
| 40 | a | 835.46 | 0.09627 | YES YES |
| 41 | a | 836.43 | 0.10392 | YES YES |
| 42 | a | 839.24 | 0.12623 | YES YES |
| 43 | a | 904.97 | 0.76949 | YES YES |
| 44 | a | 906.30 | 0.78603 | YES YES |
| 45 | a | 907.40 | 0.26704 | YES YES |
| 46 | a | 956.13 | 0.00640 | YES YES |
| 47 | a | 956.78 | 0.02453 | YES YES |
| 48 | a | 958.23 | 0.11303 | YES YES |
| 49 | a | 971.17 | 0.01184 | YES YES |
| 50 | a | 972.48 | 0.02498 | YES YES |

**$P(^tBu)_3$**

bp86_def2-tzvpp energy (au): -815.1088131371

Zero point energy (au): 0.3568443
Entropy (kJ mol^-1): 0.54296
Chemical potential (kJ mol^-1): 826.25

XYZ coordinates:

40

| | | | |
|---|---|---|---|
| P | 0.68550 | 0.00078 | -0.00069 |
| C | -0.02432 | 1.70515 | -0.61191 |
| C | -1.50107 | 1.75305 | -1.03929 |
| H | -1.76291 | 2.78255 | -1.33708 |
| C | 0.86759 | 2.15106 | -1.79451 |
| H | 0.60341 | 3.18503 | -2.07003 |
| H | 0.74513 | 1.53255 | -2.68821 |
| H | 1.93005 | 2.13614 | -1.51555 |
| C | -0.02308 | -1.38193 | -1.17130 |
| C | -1.49883 | -1.77950 | -0.99842 |
| H | -1.75777 | -2.55492 | -1.73906 |
| H | -2.18025 | -0.93496 | -1.15652 |
| H | -1.70622 | -2.20103 | -0.00743 |
| H | 0.75168 | -3.09159 | 0.01727 |
| H | 1.93375 | -2.37504 | -1.09344 |
| H | 0.60860 | -3.38412 | -1.72219 |
| C | 0.19827 | -0.95781 | -2.63704 |
| H | 1.23576 | -0.64611 | -2.82025 |
| H | -0.47099 | -0.15074 | -2.95567 |
| H | -0.00547 | -1.82486 | -3.28585 |
| C | -0.02517 | -0.32207 | 1.78180 |
| C | 0.19413 | -1.80414 | 2.14746 |
| H | -0.01249 | -1.93298 | 3.22238 |
| H | 1.23211 | -2.11776 | 1.97151 |
| H | -0.47384 | -2.48350 | 1.60606 |
| C | -1.50099 | 0.02793 | 2.03933 |
| H | -2.18203 | -0.52822 | 1.38425 |
| H | -1.70728 | 1.09765 | 1.91373 |
| H | -1.76064 | -0.22965 | 3.08000 |
| C | 0.87087 | 0.47537 | 2.75881 |
| H | 0.75501 | 1.55942 | 2.66865 |
| H | 1.93187 | 0.23433 | 2.60710 |
| H | 0.60452 | 0.20052 | 3.79262 |
| H | -1.70856 | 1.10796 | -1.90148 |
| H | -2.18020 | 1.46346 | -0.22847 |
| C | 0.19912 | 2.76159 | 0.48880 |
| H | -0.00883 | 3.75740 | 0.06505 |
| H | -0.46635 | 2.63172 | 1.34985 |
| H | 1.23794 | 2.76607 | 0.84588 |
| C | 0.87207 | -2.62694 | -0.96591 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 89.23 | 0.01690 | YES YES |
| 8 | a | 92.33 | 0.01584 | YES YES |
| 9 | a | 125.32 | 0.00178 | YES YES |
| 10 | a | 168.32 | 0.10368 | YES YES |
| 11 | a | 180.02 | 0.01230 | YES YES |
| 12 | a | 182.14 | 0.00610 | YES YES |
| 13 | a | 194.06 | 0.02100 | YES YES |
| 14 | a | 199.15 | 0.00678 | YES YES |
| 15 | a | 207.41 | 0.01990 | YES YES |
| 16 | a | 233.39 | 0.10087 | YES YES |
| 17 | a | 239.69 | 0.16219 | YES YES |
| 18 | a | 241.36 | 0.04735 | YES YES |
| 19 | a | 254.59 | 0.28294 | YES YES |
| 20 | a | 255.88 | 0.22683 | YES YES |
| 21 | a | 263.56 | 0.02394 | YES YES |
| 22 | a | 271.54 | 0.01149 | YES YES |
| 23 | a | 277.14 | 0.01924 | YES YES |
| 24 | a | 284.77 | 0.00262 | YES YES |
| 25 | a | 322.76 | 0.07550 | YES YES |
| 26 | a | 332.35 | 0.20913 | YES YES |
| 27 | a | 341.42 | 0.24713 | YES YES |
| 28 | a | 346.79 | 0.01405 | YES YES |
| 29 | a | 360.46 | 0.21324 | YES YES |
| 30 | a | 363.13 | 0.27428 | YES YES |
| 31 | a | 393.75 | 0.41595 | YES YES |
| 32 | a | 395.51 | 0.17576 | YES YES |
| 33 | a | 397.48 | 0.35974 | YES YES |
| 34 | a | 445.37 | 3.87887 | YES YES |
| 35 | a | 447.74 | 3.94365 | YES YES |
| 36 | a | 468.93 | 0.92062 | YES YES |
| 37 | a | 525.85 | 0.27230 | YES YES |
| 38 | a | 553.46 | 5.72614 | YES YES |
| 39 | a | 555.00 | 5.80944 | YES YES |
| 40 | a | 785.99 | 8.55442 | YES YES |
| 41 | a | 787.97 | 8.87783 | YES YES |
| 42 | a | 789.95 | 2.85750 | YES YES |
| 43 | a | 904.79 | 0.68575 | YES YES |
| 44 | a | 906.21 | 1.56775 | YES YES |
| 45 | a | 906.40 | 1.78698 | YES YES |
| 46 | a | 911.46 | 0.35847 | YES YES |
| 47 | a | 913.84 | 0.80155 | YES YES |
| 48 | a | 915.59 | 1.14546 | YES YES |
| 49 | a | 924.87 | 0.09329 | YES YES |
| 50 | a | 929.90 | 0.75201 | YES YES |

**$[GaCl_4]^-$**

bp86_def2-tzvpp energy (au): -3766.5324232560

Zero point energy (au): 0.0045708
Entropy (kJ mol^-1): 0.36455
Chemical potential (kJ mol^-1): -73.86

XYZ coordinates:

5

| | | | |
|---|---|---|---|
| Ga | 0.00000 | 0.00000 | 0.00000 |
| Cl | -1.28337 | -1.28337 | -1.28337 |
| Cl | 1.28337 | 1.28337 | -1.28337 |
| Cl | 1.28337 | -1.28337 | 1.28337 |
| Cl | -1.28337 | 1.28337 | 1.28337 |

Vibrational Spectrum:

| # mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|
| 1 | | 0.00 | 0.00000 | - | - |
| 2 | | 0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | e | 97.80 | 0.00000 | NO | YES |
| 8 | e | 97.80 | 0.00000 | NO | YES |
| 9 | t2 | 139.98 | 8.76876 | YES | YES |
| 10 | t2 | 139.98 | 8.76876 | YES | YES |
| 11 | t2 | 139.98 | 8.76876 | YES | YES |
| 12 | a1 | 317.51 | 0.00000 | NO | YES |
| 13 | t2 | 357.76 | 91.42040 | YES | YES |
| 14 | t2 | 357.76 | 91.42040 | YES | YES |
| 15 | t2 | 357.76 | 91.42040 | YES | YES |

**[PhS]+**

bp86_def2-tzvpp energy (au): -629.6545304899

Zero point energy (au): 0.0880630
Entropy (kJ mol^-1): 0.32871
Chemical potential (kJ mol^-1): 151.38

XYZ coordinates:

12

| | | | |
|---|---|---|---|
| C | -2.26206 | -0.00005 | -0.00136 |
| H | -3.35390 | -0.00009 | -0.00289 |
| C | -0.20711 | 1.25720 | 0.00121 |
| H | 0.36333 | 2.18581 | 0.00208 |
| C | -1.58085 | 1.24268 | -0.00039 |
| H | -2.15042 | 2.17120 | -0.00096 |
| C | 0.53058 | 0.00004 | 0.00147 |
| C | -0.20704 | -1.25716 | 0.00115 |
| H | 0.36349 | -2.18573 | 0.00185 |
| C | -1.58078 | -1.24274 | -0.00034 |
| H | -2.15029 | -2.17128 | -0.00085 |
| S | 2.18563 | 0.00008 | 0.00089 |

Vibrational Spectrum:

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 100.18 | 0.00178 | YES YES |
| 8 | a | 291.01 | 0.00136 | YES YES |
| 9 | a | 303.24 | 0.00000 | YES YES |
| 10 | a | 358.02 | 0.29260 | YES YES |
| 11 | a | 428.21 | 0.20408 | YES YES |
| 12 | a | 566.17 | 2.42236 | YES YES |
| 13 | a | 602.54 | 41.92228 | YES YES |
| 14 | a | 718.45 | 3.66257 | YES YES |
| 15 | a | 785.94 | 31.57815 | YES YES |
| 16 | a | 799.72 | 0.00000 | YES YES |
| 17 | a | 967.90 | 6.42885 | YES YES |
| 18 | a | 983.91 | 7.90641 | YES YES |
| 19 | a | 987.18 | 0.86919 | YES YES |
| 20 | a | 996.43 | 0.00001 | YES YES |
| 21 | a | 1018.69 | 1.84399 | YES YES |
| 22 | a | 1075.24 | 3.36393 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 23 | a | 1123.35 | 21.82881 | YES | YES |
| 24 | a | 1154.17 | 13.45895 | YES | YES |
| 25 | a | 1188.36 | 0.83582 | YES | YES |
| 26 | a | 1244.30 | 4.57448 | YES | YES |
| 27 | a | 1353.23 | 1.43277 | YES | YES |
| 28 | a | 1418.07 | 17.39326 | YES | YES |
| 29 | a | 1437.11 | 97.70096 | YES | YES |
| 30 | a | 1502.95 | 13.88875 | YES | YES |
| 31 | a | 1591.19 | 130.04503 | YES | YES |
| 32 | a | 3113.94 | 0.92279 | YES | YES |
| 33 | a | 3129.92 | 0.99331 | YES | YES |
| 34 | a | 3131.61 | 8.60443 | YES | YES |
| 35 | a | 3140.82 | 15.47455 | YES | YES |
| 36 | a | 3143.31 | 0.09839 | YES | YES |

**PhSCl.GaCl3_iso2**

bp86_def2-tzvpp energy (au): -4396.3642993750

Zero point energy (au): 0.0943912
Entropy (kJ mol^-1): 0.57110
Chemical potential (kJ mol^-1): 120.23

XYZ coordinates:

17

| | | | |
|---|---|---|---|
| S | 1.04292 | 1.38494 | 0.97662 |
| C | -0.44424 | 0.67293 | 0.36687 |
| C | -0.50209 | 0.13817 | -0.93457 |
| H | 0.40576 | 0.09146 | -1.53531 |
| C | -1.71645 | -0.33204 | -1.42829 |
| H | -1.76593 | -0.75197 | -2.43261 |
| C | -2.87146 | -0.25734 | -0.64008 |
| H | -3.82053 | -0.62009 | -1.03539 |
| C | -2.81731 | 0.27930 | 0.65062 |
| H | -3.71964 | 0.33653 | 1.25887 |
| C | -1.60396 | 0.73474 | 1.16336 |
| H | -1.53995 | 1.14733 | 2.16956 |
| Ga | 4.10640 | -0.59065 | 0.08636 |
| Cl | 2.13716 | -0.30247 | 1.68607 |
| Cl | 4.97075 | -2.24731 | 1.17067 |
| Cl | 5.03139 | 1.34933 | 0.26123 |
| Cl | 3.10717 | -1.03286 | -1.78397 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 14.28 | 0.10465 | YES YES |
| 8 | a | 20.62 | 0.03294 | YES YES |
| 9 | a | 40.09 | 0.98027 | YES YES |
| 10 | a | 48.57 | 0.30166 | YES YES |
| 11 | a | 62.03 | 0.65646 | YES YES |
| 12 | a | 84.96 | 0.15447 | YES YES |
| 13 | a | 100.33 | 0.22223 | YES YES |
| 14 | a | 120.38 | 3.98287 | YES YES |
| 15 | a | 123.67 | 5.03448 | YES YES |
| 16 | a | 136.06 | 39.90869 | YES YES |
| 17 | a | 167.15 | 34.90904 | YES YES |
| 18 | a | 221.91 | 12.38542 | YES YES |
| 19 | a | 273.15 | 1.71381 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 20 | a | 342.19 | 15.61539 | YES | YES |
| 21 | a | 387.10 | 37.94688 | YES | YES |
| 22 | a | 394.87 | 6.15405 | YES | YES |
| 23 | a | 404.90 | 11.88669 | YES | YES |
| 24 | a | 413.59 | 88.48624 | YES | YES |
| 25 | a | 421.21 | 68.94336 | YES | YES |
| 26 | a | 487.85 | 11.97013 | YES | YES |
| 27 | a | 605.18 | 0.20532 | YES | YES |
| 28 | a | 679.10 | 32.57357 | YES | YES |
| 29 | a | 703.01 | 3.99429 | YES | YES |
| 30 | a | 753.80 | 33.71137 | YES | YES |
| 31 | a | 831.53 | 0.03215 | YES | YES |
| 32 | a | 929.07 | 2.12009 | YES | YES |
| 33 | a | 967.88 | 0.05599 | YES | YES |
| 34 | a | 987.33 | 0.92338 | YES | YES |
| 35 | a | 989.95 | 0.29340 | YES | YES |
| 36 | a | 1016.79 | 0.08614 | YES | YES |
| 37 | a | 1062.86 | 42.73208 | YES | YES |
| 38 | a | 1072.55 | 3.13459 | YES | YES |
| 39 | a | 1154.83 | 0.34603 | YES | YES |
| 40 | a | 1169.60 | 5.05673 | YES | YES |
| 41 | a | 1291.13 | 0.56955 | YES | YES |
| 42 | a | 1335.73 | 5.67002 | YES | YES |
| 43 | a | 1430.08 | 13.94716 | YES | YES |
| 44 | a | 1456.67 | 0.70594 | YES | YES |
| 45 | a | 1560.45 | 0.46906 | YES | YES |
| 46 | a | 1571.27 | 23.84590 | YES | YES |
| 47 | a | 3104.38 | 0.55306 | YES | YES |
| 48 | a | 3114.47 | 6.14624 | YES | YES |
| 49 | a | 3120.63 | 1.78443 | YES | YES |
| 50 | a | 3127.79 | 4.21963 | YES | YES |

**[PhSe]+**

bp86_def2-tzvpp energy (au): -2633.2523372090

Zero point energy (au): 0.0874961
Entropy (kJ mol^-1): 0.34040
Chemical potential (kJ mol^-1): 146.88

XYZ coordinates:

12

| | | | |
|---|---|---|---|
| C | -3.00029 | -0.00007 | -0.00005 |
| H | -4.09168 | -0.00013 | -0.00030 |
| C | -0.93954 | 1.25160 | -0.00007 |
| H | -0.37528 | 2.18373 | -0.00029 |
| C | -2.31622 | 1.23882 | 0.00024 |
| H | -2.88148 | 2.16989 | 0.00067 |
| C | -0.21351 | 0.00002 | 0.00007 |
| C | -0.93945 | -1.25161 | 0.00025 |
| H | -0.37516 | -2.18372 | 0.00032 |
| C | -2.31613 | -1.23891 | -0.00009 |
| H | -2.88134 | -2.17003 | -0.00024 |
| Se | 1.59908 | 0.00008 | -0.00006 |

Vibrational Spectrum:

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 93.16 | 0.00562 | YES YES |
| 8 | a | 240.15 | 0.00059 | YES YES |
| 9 | a | 312.26 | 0.00000 | YES YES |
| 10 | a | 331.10 | 0.03716 | YES YES |
| 11 | a | 364.25 | 0.04001 | YES YES |
| 12 | a | 569.49 | 1.81708 | YES YES |
| 13 | a | 608.13 | 41.47548 | YES YES |
| 14 | a | 682.55 | 3.22124 | YES YES |
| 15 | a | 773.72 | 33.50259 | YES YES |
| 16 | a | 805.11 | 0.00002 | YES YES |
| 17 | a | 971.89 | 14.41339 | YES YES |
| 18 | a | 976.67 | 0.88845 | YES YES |
| 19 | a | 989.48 | 5.84231 | YES YES |
| 20 | a | 994.04 | 0.00049 | YES YES |
| 21 | a | 1015.15 | 1.23348 | YES YES |
| 22 | a | 1057.75 | 24.92509 | YES YES |
| 23 | a | 1077.87 | 3.88736 | YES YES |
| 24 | a | 1156.02 | 9.33838 | YES YES |
| 25 | a | 1182.75 | 4.92094 | YES YES |
| 26 | a | 1253.96 | 5.90009 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 27 | a | 1354.76 | 3.08619 | YES | YES |
| 28 | a | 1421.14 | 13.42113 | YES | YES |
| 29 | a | 1428.47 | 77.30915 | YES | YES |
| 30 | a | 1500.23 | 9.52522 | YES | YES |
| 31 | a | 1584.74 | 140.76685 | YES | YES |
| 32 | a | 3116.44 | 0.46948 | YES | YES |
| 33 | a | 3129.63 | 0.98603 | YES | YES |
| 34 | a | 3131.60 | 7.29925 | YES | YES |
| 35 | a | 3140.58 | 12.06787 | YES | YES |
| 36 | a | 3143.28 | 0.07826 | YES | YES |

**PhSeCl.GaCl3_iso2**

bp86_def2-tzvpp energy (au): -6399.9636572000

Zero point energy (au): 0.0935660
Entropy (kJ mol^-1): 0.58286
Chemical potential (kJ mol^-1): 115.53

XYZ coordinates:

17

| | | | |
|---|---|---|---|
| Se | 0.45126 | 0.44597 | 1.56594 |
| C | -1.15728 | -0.34788 | 0.91322 |
| C | -1.20271 | -0.89359 | -0.38127 |
| H | -0.29623 | -0.93485 | -0.98424 |
| C | -2.41110 | -1.38755 | -0.87021 |
| H | -2.45347 | -1.81771 | -1.87060 |
| C | -3.56655 | -1.32418 | -0.08245 |
| H | -4.51001 | -1.70537 | -0.47383 |
| C | -3.51940 | -0.77710 | 1.20391 |
| H | -4.42132 | -0.73105 | 1.81388 |
| C | -2.31263 | -0.29664 | 1.71232 |
| H | -2.25799 | 0.12070 | 2.71703 |
| Ga | 3.48135 | -1.67717 | 0.65741 |
| Cl | 1.57049 | -1.39132 | 2.29249 |
| Cl | 4.40974 | -3.32947 | 1.69373 |
| Cl | 4.40741 | 0.26902 | 0.80066 |
| Cl | 2.43245 | -2.12482 | -1.18600 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 14.84 | 0.10641 | YES YES |
| 8 | a | 20.57 | 0.02926 | YES YES |
| 9 | a | 37.53 | 0.82333 | YES YES |
| 10 | a | 42.83 | 0.01825 | YES YES |
| 11 | a | 56.34 | 0.75082 | YES YES |
| 12 | a | 77.52 | 0.31842 | YES YES |
| 13 | a | 96.87 | 0.16651 | YES YES |
| 14 | a | 120.42 | 3.88784 | YES YES |
| 15 | a | 124.38 | 5.12084 | YES YES |
| 16 | a | 136.48 | 35.11938 | YES YES |
| 17 | a | 170.89 | 36.55572 | YES YES |
| 18 | a | 201.38 | 12.57343 | YES YES |
| 19 | a | 231.11 | 1.07172 | YES YES |
| 20 | a | 299.54 | 30.43154 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 21 | a | 318.44 | 23.14265 | YES | YES |
| 22 | a | 344.38 | 5.10419 | YES | YES |
| 23 | a | 395.69 | 0.97527 | YES | YES |
| 24 | a | 411.53 | 70.69273 | YES | YES |
| 25 | a | 419.18 | 68.15158 | YES | YES |
| 26 | a | 458.70 | 8.48885 | YES | YES |
| 27 | a | 604.22 | 0.16765 | YES | YES |
| 28 | a | 670.50 | 0.98253 | YES | YES |
| 29 | a | 680.87 | 29.99781 | YES | YES |
| 30 | a | 743.88 | 38.08813 | YES | YES |
| 31 | a | 831.50 | 0.05243 | YES | YES |
| 32 | a | 924.36 | 1.80516 | YES | YES |
| 33 | a | 966.15 | 0.08686 | YES | YES |
| 34 | a | 985.15 | 1.28647 | YES | YES |
| 35 | a | 988.72 | 0.37897 | YES | YES |
| 36 | a | 1012.20 | 1.04038 | YES | YES |
| 37 | a | 1049.81 | 28.60182 | YES | YES |
| 38 | a | 1071.68 | 3.13124 | YES | YES |
| 39 | a | 1154.73 | 0.24426 | YES | YES |
| 40 | a | 1170.81 | 6.86490 | YES | YES |
| 41 | a | 1293.13 | 1.17484 | YES | YES |
| 42 | a | 1334.38 | 5.16480 | YES | YES |
| 43 | a | 1428.52 | 13.79348 | YES | YES |
| 44 | a | 1455.59 | 0.75962 | YES | YES |
| 45 | a | 1561.89 | 0.59962 | YES | YES |
| 46 | a | 1566.92 | 18.50889 | YES | YES |
| 47 | a | 3103.77 | 0.50035 | YES | YES |
| 48 | a | 3113.81 | 5.93128 | YES | YES |
| 49 | a | 3120.53 | 2.04549 | YES | YES |
| 50 | a | 3127.55 | 3.09697 | YES | YES |

**[PhSe(PPh3)]+**

bp86_def2-tzvpp energy (au): -3670.0228676270

Zero point energy (au): 0.3568415
Entropy (kJ mol^-1): 0.71987
Chemical potential (kJ mol^-1): 787.04

XYZ coordinates:

46

| | | | |
|---|---|---|---|
| C | -1.20823 | 4.92910 | -1.18234 |
| H | -1.51309 | 5.93814 | -1.45853 |
| C | 2.98848 | -1.65694 | -1.68362 |
| H | 3.47986 | -2.60241 | -1.45672 |
| Se | -1.84736 | -0.50881 | -0.19992 |
| P | 0.08259 | 0.66903 | -0.01074 |
| C | 2.71662 | 0.27866 | -3.11663 |
| H | 2.99870 | 0.84438 | -4.00393 |
| C | -1.61050 | 3.84154 | -1.96354 |
| H | -2.22785 | 3.99930 | -2.84721 |
| C | -0.43416 | 2.34115 | -0.46814 |
| C | 2.00537 | -1.16861 | -0.82409 |
| H | 1.73788 | -1.73328 | 0.06837 |
| C | 1.64982 | 0.81614 | 4.31406 |
| H | 2.01818 | 0.87136 | 5.33816 |
| C | 1.37369 | 0.05650 | -1.11382 |
| C | -0.63144 | -4.40349 | -1.17987 |
| H | -0.47261 | -4.97238 | -2.09563 |
| C | -1.22816 | 2.54714 | -1.61274 |
| H | -1.54994 | 1.70258 | -2.22209 |
| C | 0.70594 | 0.66275 | 1.68881 |
| C | 0.27628 | 0.71284 | 4.07182 |
| H | -0.42681 | 0.68948 | 4.90375 |
| C | 1.73015 | 0.77859 | -2.26604 |
| H | 1.25151 | 1.73055 | -2.49116 |
| C | 3.34358 | -0.93631 | -2.82813 |
| H | 4.11472 | -1.32149 | -3.49481 |
| C | -0.03368 | 3.43541 | 0.31789 |
| H | 0.57220 | 3.28207 | 1.20985 |
| C | 2.08705 | 0.77071 | 1.93291 |
| H | 2.79499 | 0.79667 | 1.10562 |
| C | -0.19967 | 0.63476 | 2.76357 |
| H | -1.27000 | 0.54791 | 2.57480 |
| C | -1.07048 | -2.94670 | 1.17591 |
| H | -1.26192 | -2.38444 | 2.08861 |
| C | -0.42177 | 4.72545 | -0.04570 |
| H | -0.11186 | 5.57223 | 0.56565 |
| C | 2.55149 | 0.84621 | 3.24717 |
| H | 3.62158 | 0.92723 | 3.43520 |
| C | -0.70131 | -4.29245 | 1.24056 |
| H | -0.59713 | -4.77568 | 2.21173 |
| C | -0.99262 | -3.05612 | -1.25937 |
| H | -1.11655 | -2.57420 | -2.22813 |
| C | -0.48321 | -5.01895 | 0.06603 |

| | | | |
|---|---|---|---|
| H | -0.20642 | -6.07139 | 0.12256 |
| C | -1.20591 | -2.33600 | -0.07722 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 16.58 | 0.10660 | YES YES |
| 8 | a | 26.84 | 0.01915 | YES YES |
| 9 | a | 30.67 | 0.06919 | YES YES |
| 10 | a | 38.15 | 0.00943 | YES YES |
| 11 | a | 45.23 | 0.19370 | YES YES |
| 12 | a | 46.74 | 0.09141 | YES YES |
| 13 | a | 55.24 | 0.10087 | YES YES |
| 14 | a | 58.06 | 0.09766 | YES YES |
| 15 | a | 70.34 | 0.33184 | YES YES |
| 16 | a | 87.69 | 0.39030 | YES YES |
| 17 | a | 98.52 | 0.57526 | YES YES |
| 18 | a | 175.47 | 0.98754 | YES YES |
| 19 | a | 184.89 | 2.07089 | YES YES |
| 20 | a | 204.20 | 1.32143 | YES YES |
| 21 | a | 208.57 | 0.21773 | YES YES |
| 22 | a | 229.10 | 0.91397 | YES YES |
| 23 | a | 237.47 | 0.02261 | YES YES |
| 24 | a | 241.47 | 1.43002 | YES YES |
| 25 | a | 254.94 | 0.35038 | YES YES |
| 26 | a | 267.74 | 0.26030 | YES YES |
| 27 | a | 296.80 | 1.91016 | YES YES |
| 28 | a | 388.50 | 0.06014 | YES YES |
| 29 | a | 389.94 | 0.01331 | YES YES |
| 30 | a | 396.14 | 0.39696 | YES YES |
| 31 | a | 397.35 | 0.09635 | YES YES |
| 32 | a | 416.18 | 7.03519 | YES YES |
| 33 | a | 435.57 | 7.64682 | YES YES |
| 34 | a | 441.01 | 8.21349 | YES YES |
| 35 | a | 461.56 | 6.62179 | YES YES |
| 36 | a | 492.67 | 54.06028 | YES YES |
| 37 | a | 504.65 | 72.00558 | YES YES |
| 38 | a | 519.86 | 79.98313 | YES YES |
| 39 | a | 605.35 | 0.00937 | YES YES |
| 40 | a | 608.27 | 0.25478 | YES YES |
| 41 | a | 608.65 | 0.16084 | YES YES |
| 42 | a | 609.23 | 0.11196 | YES YES |
| 43 | a | 660.42 | 2.25214 | YES YES |
| 44 | a | 678.15 | 5.43300 | YES YES |
| 45 | a | 686.33 | 15.02281 | YES YES |
| 46 | a | 686.84 | 47.99613 | YES YES |
| 47 | a | 687.97 | 20.68255 | YES YES |
| 48 | a | 689.33 | 11.82128 | YES YES |
| 49 | a | 710.42 | 24.81373 | YES YES |
| 50 | a | 711.10 | 27.60995 | YES YES |

**[PhSe(PPh3).PPh3]+**

bp86_def2-tzvpp energy (au): -4706.6644284590

Zero point energy (au): 0.6230472
Entropy (kJ mol^-1): 1.14774
Chemical potential (kJ mol^-1): 1408.09

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.76621 | 0.64976 | 3.29180 |
| H | -5.83385 | 0.80756 | 3.44345 |
| C | 2.75978 | 2.38463 | 4.07122 |
| H | 3.84758 | 2.40708 | 4.00854 |
| Se | -0.13126 | -0.00253 | -0.01164 |
| P | -0.23647 | 0.01286 | 2.60695 |
| C | 0.68388 | 3.32787 | 4.87963 |
| H | 0.14792 | 4.08516 | 5.45158 |
| C | -4.05961 | 1.45982 | 2.39831 |
| H | -4.57356 | 2.24995 | 1.85120 |
| C | -2.01834 | 0.24359 | 2.90605 |
| C | 2.05230 | 1.37672 | 3.41688 |
| H | 2.59312 | 0.62181 | 2.84556 |
| C | 0.88626 | -4.06001 | 4.49265 |
| H | 1.14163 | -5.02624 | 4.92731 |
| C | 0.64754 | 1.33094 | 3.50088 |
| C | 3.90555 | 1.20021 | -0.22023 |
| H | 4.44450 | 2.13106 | -0.39672 |
| C | -2.69351 | 1.25633 | 2.19933 |
| H | -2.14866 | 1.88883 | 1.49739 |
| C | 0.23232 | -1.57286 | 3.37506 |
| C | 0.23124 | -3.99902 | 3.25859 |
| H | -0.02616 | -4.91653 | 2.72958 |
| C | -0.03247 | 2.31717 | 4.23463 |
| H | -1.11869 | 2.29185 | 4.31080 |
| C | 2.07777 | 3.36352 | 4.80080 |
| H | 2.63331 | 4.15217 | 5.30785 |
| C | -2.73496 | -0.56840 | 3.80047 |
| H | -2.22488 | -1.35855 | 4.35020 |
| C | 0.88922 | -1.64012 | 4.61481 |
| H | 1.14358 | -0.72614 | 5.15000 |
| C | -0.08886 | -2.76292 | 2.69717 |
| H | -0.59040 | -2.71866 | 1.72939 |
| C | 2.51333 | -1.18747 | 0.22689 |
| H | 1.97117 | -2.11755 | 0.39026 |
| C | -4.10314 | -0.36314 | 3.98924 |
| H | -4.65090 | -0.99614 | 4.68714 |
| C | 1.21452 | -2.88141 | 5.16672 |
| H | 1.72285 | -2.92497 | 6.12983 |
| C | 3.91117 | -1.17600 | 0.24283 |
| H | 4.45454 | -2.10285 | 0.42654 |
| C | 2.50752 | 1.20160 | -0.22184 |
| H | 1.96086 | 2.12796 | -0.39134 |
| C | 4.60751 | 0.01461 | 0.01564 |
| H | 5.69738 | 0.01857 | 0.02269 |
| C | 1.81417 | 0.00453 | -0.00198 |

| | | | |
|---|---|---|---|
| C | -4.73501 | -0.67924 | -3.33847 |
| H | -5.80010 | -0.84146 | -3.50267 |
| C | 2.80969 | -2.37239 | -4.03851 |
| H | 3.89783 | -2.37934 | -3.97854 |
| P | -0.21702 | -0.02077 | -2.60420 |
| C | 0.74438 | -3.35619 | -4.82574 |
| H | 0.21711 | -4.12970 | -5.38382 |
| C | -4.04038 | -1.47232 | -2.42081 |
| H | -4.56092 | -2.25392 | -1.86779 |
| C | -1.99444 | -0.26074 | -2.91922 |
| C | 2.09080 | -1.36324 | -3.39871 |
| H | 2.62310 | -0.59196 | -2.84144 |
| C | 0.90257 | 4.05449 | -4.48429 |
| H | 1.15617 | 5.02136 | -4.91852 |
| C | 0.68522 | -1.33778 | -3.47967 |
| C | -2.67762 | -1.26298 | -2.20534 |
| H | -2.14202 | -1.88219 | -1.48474 |
| C | 0.25294 | 1.56611 | -3.36798 |
| C | 0.23428 | 3.99218 | -3.25742 |
| H | -0.03487 | 4.90920 | -2.73346 |
| C | 0.01625 | -2.34491 | -4.19514 |
| H | -1.07043 | -2.33532 | -4.26852 |
| C | 2.13882 | -3.37186 | -4.75027 |
| H | 2.70355 | -4.16091 | -5.24639 |
| C | -2.69901 | 0.53444 | -3.83819 |
| H | -2.18243 | 1.31672 | -4.39314 |
| C | 0.92297 | 1.63445 | -4.60072 |
| H | 1.18902 | 0.72092 | -5.13104 |
| C | -0.08426 | 2.75547 | -2.69660 |
| H | -0.59660 | 2.70998 | -1.73456 |
| C | -4.06365 | 0.32270 | -4.04385 |
| H | -4.60218 | 0.94224 | -4.76071 |
| C | 1.24607 | 2.87662 | -5.15196 |
| H | 1.76480 | 2.92127 | -6.10943 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 6.08 | 0.09461 | YES YES |
| 8 | a | 11.11 | 7.19963 | YES YES |
| 9 | a | 14.27 | 10.06967 | YES YES |
| 10 | a | 15.53 | 0.59740 | YES YES |
| 11 | a | 21.56 | 9.82076 | YES YES |
| 12 | a | 22.77 | 0.05179 | YES YES |
| 13 | a | 28.23 | 32.26922 | YES YES |
| 14 | a | 34.67 | 0.04111 | YES YES |
| 15 | a | 35.61 | 0.03691 | YES YES |
| 16 | a | 37.34 | 0.42975 | YES YES |
| 17 | a | 38.37 | 7.88556 | YES YES |
| 18 | a | 42.68 | 7.57749 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 19 | a | 46.90 | 0.78206 | YES | YES |
| 20 | a | 51.60 | 7.43524 | YES | YES |
| 21 | a | 53.20 | 0.04919 | YES | YES |
| 22 | a | 55.09 | 0.02209 | YES | YES |
| 23 | a | 58.91 | 0.15273 | YES | YES |
| 24 | a | 60.55 | 21.75511 | YES | YES |
| 25 | a | 63.66 | 1.57883 | YES | YES |
| 26 | a | 66.30 | 1.60906 | YES | YES |
| 27 | a | 73.74 | 36.35131 | YES | YES |
| 28 | a | 93.98 | 0.05958 | YES | YES |
| 29 | a | 112.14 | 0.94481 | YES | YES |
| 30 | a | 113.25 | 0.21556 | YES | YES |
| 31 | a | 182.47 | 1.60086 | YES | YES |
| 32 | a | 182.96 | 1.07486 | YES | YES |
| 33 | a | 190.51 | 0.59545 | YES | YES |
| 34 | a | 191.49 | 4.55441 | YES | YES |
| 35 | a | 199.22 | 5.31814 | YES | YES |
| 36 | a | 201.28 | 0.64124 | YES | YES |
| 37 | a | 207.55 | 19.85077 | YES | YES |
| 38 | a | 235.96 | 6.04379 | YES | YES |
| 39 | a | 236.56 | 0.47257 | YES | YES |
| 40 | a | 237.77 | 0.36749 | YES | YES |
| 41 | a | 253.54 | 0.41535 | YES | YES |
| 42 | a | 253.77 | 0.98035 | YES | YES |
| 43 | a | 259.26 | 0.70527 | YES | YES |
| 44 | a | 260.54 | 0.43216 | YES | YES |
| 45 | a | 299.20 | 0.35002 | YES | YES |
| 46 | a | 388.46 | 0.63715 | YES | YES |
| 47 | a | 389.46 | 0.13005 | YES | YES |
| 48 | a | 389.97 | 0.99158 | YES | YES |
| 49 | a | 390.35 | 1.60349 | YES | YES |
| 50 | a | 390.78 | 0.40697 | YES | YES |

**[PhSe(PtBu3).PPh3]+**

bp86_def2-tzvpp energy (au): -4485.1440918810

Zero point energy (au): 0.7146552
Entropy (kJ mol^-1): 1.11891
Chemical potential (kJ mol^-1): 1662.71

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.15882 | 0.34286 | -0.04329 |
| Se | 0.34435 | 0.08567 | -0.00482 |
| C | 0.20386 | -1.85775 | 0.05758 |
| C | -0.02527 | -2.57529 | -1.12426 |
| H | -0.10638 | -2.05067 | -2.07528 |
| C | -0.15353 | -3.96662 | -1.07755 |
| H | -0.33431 | -4.52155 | -1.99813 |
| C | -0.04242 | -4.64229 | 0.14104 |
| H | -0.13451 | -5.72773 | 0.17318 |
| C | 0.18500 | -3.92398 | 1.31786 |
| H | 0.26588 | -4.44538 | 2.27166 |
| C | 0.30037 | -2.53108 | 1.28145 |
| H | 0.45668 | -1.97274 | 2.20262 |
| C | -3.12345 | -0.51839 | 1.23499 |
| C | -3.19538 | -1.92452 | 1.20063 |
| H | -2.70155 | -2.48176 | 0.40445 |
| C | -3.90953 | -2.61083 | 2.18205 |
| H | -3.96849 | -3.69828 | 2.14283 |
| C | -4.54491 | -1.90929 | 3.21134 |
| H | -5.10044 | -2.44950 | 3.97760 |
| C | -4.46929 | -0.51534 | 3.25416 |
| H | -4.96853 | 0.03645 | 4.05036 |
| C | -3.76278 | 0.18187 | 2.27219 |
| H | -3.72078 | 1.26956 | 2.30758 |
| C | -2.35405 | 2.13422 | 0.20910 |
| C | -3.18065 | 2.90769 | -0.62239 |
| H | -3.72642 | 2.43918 | -1.44042 |
| C | -3.30542 | 4.28062 | -0.40118 |
| H | -3.94970 | 4.87356 | -1.04994 |
| C | -2.61163 | 4.89092 | 0.64660 |
| H | -2.71305 | 5.96260 | 0.81643 |
| C | -1.78650 | 4.12669 | 1.47669 |
| H | -1.24516 | 4.59959 | 2.29584 |
| C | -1.65111 | 2.75503 | 1.25865 |
| H | -1.00397 | 2.16367 | 1.90735 |
| C | -2.89427 | -0.06370 | -1.65893 |
| C | -4.18822 | -0.60048 | -1.76981 |
| H | -4.77541 | -0.80627 | -0.87585 |
| C | -4.72675 | -0.86734 | -3.03047 |
| H | -5.73115 | -1.28295 | -3.10885 |
| C | -3.98584 | -0.59922 | -4.18403 |
| H | -4.41030 | -0.80917 | -5.16557 |
| C | -2.69891 | -0.06252 | -4.07881 |
| H | -2.11871 | 0.14829 | -4.97697 |
| C | -2.15067 | 0.19975 | -2.82327 |

| | | | |
|---|---|---|---|
| H | -1.14271 | 0.60856 | -2.74284 |
| P | 3.18205 | 0.27481 | 0.02282 |
| C | 3.49828 | 1.80056 | -1.12679 |
| C | 4.84769 | 2.50657 | -0.89474 |
| H | 4.94587 | 3.31886 | -1.63208 |
| C | 2.35464 | 2.82103 | -0.92767 |
| H | 2.52345 | 3.66014 | -1.61984 |
| H | 2.30508 | 3.23696 | 0.08166 |
| H | 1.37696 | 2.38781 | -1.17515 |
| C | 3.67418 | 0.72401 | 1.84017 |
| C | 5.18966 | 0.71803 | 2.11564 |
| H | 5.35455 | 1.02987 | 3.15896 |
| H | 5.73993 | 1.41591 | 1.47490 |
| H | 5.63514 | -0.27670 | 2.00501 |
| H | 3.29646 | -1.31269 | 2.64312 |
| H | 1.88582 | -0.22907 | 2.67251 |
| H | 3.21687 | 0.00315 | 3.82310 |
| C | 3.11217 | 2.11232 | 2.20700 |
| H | 2.03317 | 2.18367 | 2.01715 |
| H | 3.61959 | 2.93385 | 1.69066 |
| H | 3.26584 | 2.26414 | 3.28622 |
| C | 4.23646 | -1.22964 | -0.58963 |
| C | 4.23825 | -2.32730 | 0.49344 |
| H | 4.71219 | -3.22300 | 0.06428 |
| H | 3.22266 | -2.60982 | 0.79907 |
| H | 4.81537 | -2.05356 | 1.38301 |
| C | 5.69363 | -0.88627 | -0.95160 |
| H | 6.25055 | -0.44993 | -0.11536 |
| H | 5.76599 | -0.20686 | -1.80821 |
| H | 6.20642 | -1.81830 | -1.23713 |
| C | 3.53884 | -1.84121 | -1.82400 |
| H | 3.53290 | -1.17996 | -2.69410 |
| H | 2.50631 | -2.13373 | -1.60061 |
| H | 4.08718 | -2.75225 | -2.10865 |
| H | 4.91875 | 2.96538 | 0.09773 |
| H | 5.70558 | 1.83873 | -1.02773 |
| C | 3.41899 | 1.35769 | -2.60171 |
| H | 3.42853 | 2.26249 | -3.22820 |
| H | 4.27074 | 0.74313 | -2.91150 |
| H | 2.49010 | 0.81510 | -2.82120 |
| C | 2.97646 | -0.27721 | 2.78621 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 7.49 | 0.14336 | YES YES |
| 8 | a | 13.21 | 0.20366 | YES YES |
| 9 | a | 18.54 | 5.56232 | YES YES |
| 10 | a | 21.98 | 0.37869 | YES YES |
| 11 | a | 30.74 | 63.26513 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 37.50 | 0.20351 | YES | YES |
| 13 | a | 39.21 | 1.76727 | YES | YES |
| 14 | a | 41.15 | 0.89197 | YES | YES |
| 15 | a | 44.58 | 0.11908 | YES | YES |
| 16 | a | 50.94 | 0.20297 | YES | YES |
| 17 | a | 54.44 | 2.52867 | YES | YES |
| 18 | a | 57.65 | 0.33141 | YES | YES |
| 19 | a | 63.77 | 0.07562 | YES | YES |
| 20 | a | 67.80 | 2.15376 | YES | YES |
| 21 | a | 73.04 | 0.04869 | YES | YES |
| 22 | a | 90.87 | 0.04077 | YES | YES |
| 23 | a | 96.06 | 1.08575 | YES | YES |
| 24 | a | 105.20 | 10.42144 | YES | YES |
| 25 | a | 109.06 | 22.14297 | YES | YES |
| 26 | a | 114.87 | 1.52484 | YES | YES |
| 27 | a | 126.64 | 0.20277 | YES | YES |
| 28 | a | 176.13 | 0.02574 | YES | YES |
| 29 | a | 184.21 | 0.57548 | YES | YES |
| 30 | a | 184.81 | 0.84464 | YES | YES |
| 31 | a | 189.97 | 0.13719 | YES | YES |
| 32 | a | 193.50 | 1.10174 | YES | YES |
| 33 | a | 195.25 | 0.60379 | YES | YES |
| 34 | a | 199.45 | 6.73320 | YES | YES |
| 35 | a | 201.52 | 0.56508 | YES | YES |
| 36 | a | 205.51 | 0.75253 | YES | YES |
| 37 | a | 210.59 | 16.69181 | YES | YES |
| 38 | a | 230.78 | 0.18022 | YES | YES |
| 39 | a | 235.60 | 3.02244 | YES | YES |
| 40 | a | 237.44 | 1.48011 | YES | YES |
| 41 | a | 238.16 | 0.19746 | YES | YES |
| 42 | a | 244.27 | 0.14446 | YES | YES |
| 43 | a | 251.53 | 0.27531 | YES | YES |
| 44 | a | 253.63 | 0.66988 | YES | YES |
| 45 | a | 254.52 | 0.09107 | YES | YES |
| 46 | a | 261.85 | 0.60123 | YES | YES |
| 47 | a | 264.56 | 0.39711 | YES | YES |
| 48 | a | 272.99 | 0.07882 | YES | YES |
| 49 | a | 276.16 | 0.05550 | YES | YES |
| 50 | a | 284.14 | 0.61775 | YES | YES |

**[PhSe(PPh3).PtBu3]+_iso1**

bp86_def2-tzvpp energy (au): -4485.1440996000

Zero point energy (au): 0.7146910
Entropy (kJ mol^-1): 1.11661
Chemical potential (kJ mol^-1): 1663.44

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.14653 | 0.33823 | 0.00679 |
| Se | 0.36088 | 0.08042 | 0.00094 |
| C | 0.21724 | -1.86383 | -0.00150 |
| C | -0.04095 | -2.53832 | -1.20255 |
| H | -0.14010 | -1.98012 | -2.13248 |
| C | -0.17568 | -3.92980 | -1.20203 |
| H | -0.37971 | -4.45099 | -2.13734 |
| C | -0.04148 | -4.64861 | -0.01074 |
| H | -0.13891 | -5.73407 | -0.01471 |
| C | 0.21606 | -3.97335 | 1.18519 |
| H | 0.31539 | -4.52845 | 2.11801 |
| C | 0.33744 | -2.58049 | 1.19536 |
| H | 0.51706 | -2.05612 | 2.13212 |
| C | -3.09174 | -0.56662 | 1.26944 |
| C | -3.16050 | -1.97110 | 1.19048 |
| H | -2.67663 | -2.50069 | 0.36968 |
| C | -3.85861 | -2.69112 | 2.15921 |
| H | -3.91523 | -3.77691 | 2.08554 |
| C | -4.48085 | -2.02531 | 3.21978 |
| H | -5.02374 | -2.59182 | 3.97604 |
| C | -4.40835 | -0.63327 | 3.30669 |
| H | -4.89750 | -0.10913 | 4.12745 |
| C | -3.71796 | 0.09761 | 2.33782 |
| H | -3.67820 | 1.18370 | 2.40796 |
| C | -2.33972 | 2.11978 | 0.32295 |
| C | -3.17926 | 2.92029 | -0.46908 |
| H | -3.73670 | 2.47946 | -1.29461 |
| C | -3.30213 | 4.28460 | -0.19882 |
| H | -3.95651 | 4.89857 | -0.81721 |
| C | -2.59367 | 4.85944 | 0.85916 |
| H | -2.69372 | 5.92446 | 1.06742 |
| C | -1.75567 | 4.06823 | 1.65017 |
| H | -1.20290 | 4.51337 | 2.47722 |
| C | -1.62207 | 2.70514 | 1.38283 |
| H | -0.96500 | 2.09271 | 2.00131 |
| C | -2.90675 | -0.01297 | -1.61051 |
| C | -4.20042 | -0.55055 | -1.72046 |
| H | -4.77267 | -0.79069 | -0.82537 |
| C | -4.75801 | -0.77375 | -2.98133 |
| H | -5.76215 | -1.19012 | -3.05887 |
| C | -4.03653 | -0.46101 | -4.13594 |
| H | -4.47592 | -0.63672 | -5.11764 |
| C | -2.74985 | 0.07652 | -4.03162 |
| H | -2.18471 | 0.32207 | -4.93057 |
| C | -2.18259 | 0.29520 | -2.77618 |

| | | | |
|---|---|---|---|
| H | -1.17485 | 0.70485 | -2.69695 |
| P | 3.19197 | 0.26482 | -0.00362 |
| C | 3.49242 | 1.82885 | -1.10473 |
| C | 4.84650 | 2.52469 | -0.86904 |
| H | 4.93497 | 3.36143 | -1.57975 |
| C | 2.35389 | 2.84343 | -0.85317 |
| H | 2.51443 | 3.70587 | -1.51807 |
| H | 2.31993 | 3.22402 | 0.17065 |
| H | 1.37177 | 2.42077 | -1.10132 |
| C | 3.71164 | 0.65064 | 1.82054 |
| C | 5.23117 | 0.63410 | 2.07231 |
| H | 5.41215 | 0.90943 | 3.12320 |
| H | 5.77241 | 1.35346 | 1.44787 |
| H | 5.67370 | -0.35651 | 1.92048 |
| H | 3.34509 | -1.41220 | 2.55892 |
| H | 1.93535 | -0.33032 | 2.64590 |
| H | 3.28321 | -0.13735 | 3.78418 |
| C | 3.15687 | 2.02583 | 2.24354 |
| H | 2.07506 | 2.10413 | 2.07351 |
| H | 3.65690 | 2.86436 | 1.74773 |
| H | 3.32784 | 2.14038 | 3.32475 |
| C | 4.23368 | -1.21919 | -0.68371 |
| C | 4.25094 | -2.35319 | 0.36107 |
| H | 4.71718 | -3.23392 | -0.10585 |
| H | 3.23991 | -2.64546 | 0.67253 |
| H | 4.84213 | -2.11036 | 1.25039 |
| C | 5.68555 | -0.86490 | -1.05637 |
| H | 6.25605 | -0.45813 | -0.21438 |
| H | 5.74564 | -0.15661 | -1.89022 |
| H | 6.19230 | -1.78718 | -1.38160 |
| C | 3.51583 | -1.78728 | -1.92723 |
| H | 3.49720 | -1.09648 | -2.77387 |
| H | 2.48653 | -2.08648 | -1.69790 |
| H | 4.05848 | -2.68842 | -2.25151 |
| H | 4.93314 | 2.94942 | 0.13726 |
| H | 5.70110 | 1.86066 | -1.03755 |
| C | 3.38994 | 1.43698 | -2.59259 |
| H | 3.39149 | 2.36282 | -3.18759 |
| H | 4.23582 | 0.83246 | -2.93627 |
| H | 2.45689 | 0.90338 | -2.81635 |
| C | 3.02750 | -0.38226 | 2.74200 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 8.87 | 0.71784 | YES YES |
| 8 | a | 13.42 | 0.70158 | YES YES |
| 9 | a | 18.74 | 4.59345 | YES YES |
| 10 | a | 22.42 | 0.08849 | YES YES |
| 11 | a | 30.73 | 64.32789 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 37.59 | 0.28542 | YES | YES |
| 13 | a | 39.52 | 2.55588 | YES | YES |
| 14 | a | 41.41 | 0.39700 | YES | YES |
| 15 | a | 44.57 | 0.09361 | YES | YES |
| 16 | a | 51.14 | 0.18361 | YES | YES |
| 17 | a | 54.71 | 2.53213 | YES | YES |
| 18 | a | 57.73 | 0.28712 | YES | YES |
| 19 | a | 63.84 | 0.06367 | YES | YES |
| 20 | a | 68.17 | 2.13936 | YES | YES |
| 21 | a | 73.32 | 0.07012 | YES | YES |
| 22 | a | 91.07 | 0.03359 | YES | YES |
| 23 | a | 95.98 | 1.18819 | YES | YES |
| 24 | a | 105.37 | 13.19014 | YES | YES |
| 25 | a | 108.82 | 18.73286 | YES | YES |
| 26 | a | 115.06 | 1.25645 | YES | YES |
| 27 | a | 127.29 | 0.26014 | YES | YES |
| 28 | a | 176.94 | 0.02229 | YES | YES |
| 29 | a | 184.15 | 0.53105 | YES | YES |
| 30 | a | 184.76 | 0.90187 | YES | YES |
| 31 | a | 189.91 | 0.14173 | YES | YES |
| 32 | a | 193.66 | 1.12041 | YES | YES |
| 33 | a | 195.01 | 0.59321 | YES | YES |
| 34 | a | 199.35 | 5.99257 | YES | YES |
| 35 | a | 201.08 | 0.81379 | YES | YES |
| 36 | a | 205.28 | 0.70415 | YES | YES |
| 37 | a | 210.75 | 17.27589 | YES | YES |
| 38 | a | 231.93 | 0.19008 | YES | YES |
| 39 | a | 235.82 | 3.16165 | YES | YES |
| 40 | a | 237.40 | 1.36021 | YES | YES |
| 41 | a | 238.90 | 0.22666 | YES | YES |
| 42 | a | 243.91 | 0.11613 | YES | YES |
| 43 | a | 251.51 | 0.30857 | YES | YES |
| 44 | a | 253.56 | 0.63929 | YES | YES |
| 45 | a | 254.40 | 0.10936 | YES | YES |
| 46 | a | 261.73 | 0.59384 | YES | YES |
| 47 | a | 264.95 | 0.40537 | YES | YES |
| 48 | a | 273.42 | 0.09159 | YES | YES |
| 49 | a | 276.48 | 0.04289 | YES | YES |
| 50 | a | 284.61 | 0.57559 | YES | YES |

**[PhSe(PtBu3)]+**

bp86_def2-tzvpp energy (au): -3448.5054806150

Zero point energy (au): 0.4482169
Entropy (kJ mol^-1): 0.70513
Chemical potential (kJ mol^-1): 1037.42

XYZ coordinates:

52

| | | | |
|---|---|---|---|
| P | 1.14252 | 0.12348 | -0.13668 |
| C | -4.91912 | 0.42786 | -0.33685 |
| H | -5.94275 | 0.70392 | -0.58779 |
| C | 1.68349 | 1.58059 | 1.01053 |
| C | -2.85084 | 0.89643 | 0.83864 |
| H | -2.28058 | 1.52333 | 1.52011 |
| C | 2.32774 | 1.02630 | 2.29682 |
| H | 2.50026 | 1.87948 | 2.96890 |
| H | 3.29845 | 0.54987 | 2.12707 |
| H | 1.66597 | 0.32846 | 2.82570 |
| C | -4.16006 | 1.24932 | 0.50120 |
| H | -4.59112 | 2.16231 | 0.91126 |
| C | 2.14997 | -2.28119 | -1.30670 |
| H | 2.85976 | -3.11607 | -1.21371 |
| H | 2.28038 | -1.85965 | -2.30874 |
| H | 1.14008 | -2.69900 | -1.21532 |
| C | -2.29855 | -0.27612 | 0.30964 |
| C | 2.47330 | -1.27979 | -0.18047 |
| C | -3.05878 | -1.11224 | -0.52004 |
| H | -2.63699 | -2.04184 | -0.90021 |
| C | -0.19844 | 2.00938 | -1.80666 |
| H | -0.51956 | 2.26116 | -2.82795 |
| H | 0.35907 | 2.87068 | -1.42461 |
| H | -1.10503 | 1.86812 | -1.20672 |
| C | 3.88209 | -0.69608 | -0.41130 |
| H | 4.57954 | -1.54276 | -0.49375 |
| H | 4.22902 | -0.07652 | 0.42248 |
| H | 3.96344 | -0.11783 | -1.33747 |
| C | -0.19438 | -0.33843 | -2.62165 |
| H | -1.13890 | -0.53073 | -2.10421 |
| H | 0.32647 | -1.28665 | -2.77188 |
| H | -0.44011 | 0.06264 | -3.61590 |
| C | 0.44373 | 2.38033 | 1.45508 |
| H | 0.79627 | 3.21015 | 2.08462 |
| H | -0.22167 | 1.76264 | 2.06983 |
| H | -0.12858 | 2.81322 | 0.63056 |
| C | 2.68109 | 2.51930 | 0.30184 |
| H | 2.22985 | 3.06394 | -0.53440 |
| H | 3.57961 | 2.00530 | -0.05650 |
| H | 3.00750 | 3.27077 | 1.03548 |
| C | 0.65397 | 0.72800 | -1.90161 |
| C | 2.46053 | -2.07690 | 1.14300 |
| H | 1.51206 | -2.60520 | 1.30002 |
| H | 2.68360 | -1.47672 | 2.02767 |
| H | 3.24245 | -2.84658 | 1.06252 |

| | | | |
|---|---|---|---|
| C | 1.91740 | 1.02066 | -2.73712 |
| H | 1.58179 | 1.43076 | -3.70115 |
| H | 2.49712 | 0.11808 | -2.95782 |
| H | 2.57938 | 1.76419 | -2.28144 |
| C | -4.37160 | -0.75507 | -0.83873 |
| H | -4.96536 | -1.40895 | -1.47695 |
| Se | -0.58164 | -0.97295 | 0.91399 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 20.28 | 0.14930 | YES YES |
| 8 | a | 49.93 | 0.08310 | YES YES |
| 9 | a | 53.46 | 0.36533 | YES YES |
| 10 | a | 75.06 | 0.12615 | YES YES |
| 11 | a | 94.80 | 0.41808 | YES YES |
| 12 | a | 113.68 | 0.29365 | YES YES |
| 13 | a | 116.75 | 0.31896 | YES YES |
| 14 | a | 129.03 | 0.06919 | YES YES |
| 15 | a | 149.06 | 0.60830 | YES YES |
| 16 | a | 158.66 | 0.04415 | YES YES |
| 17 | a | 185.62 | 0.99546 | YES YES |
| 18 | a | 191.75 | 0.51334 | YES YES |
| 19 | a | 195.27 | 0.90931 | YES YES |
| 20 | a | 202.58 | 0.17307 | YES YES |
| 21 | a | 204.85 | 0.54648 | YES YES |
| 22 | a | 219.37 | 0.05779 | YES YES |
| 23 | a | 226.16 | 0.35048 | YES YES |
| 24 | a | 231.77 | 0.42344 | YES YES |
| 25 | a | 240.98 | 0.23020 | YES YES |
| 26 | a | 249.72 | 0.23856 | YES YES |
| 27 | a | 252.74 | 0.34719 | YES YES |
| 28 | a | 257.28 | 0.06621 | YES YES |
| 29 | a | 272.15 | 0.12673 | YES YES |
| 30 | a | 276.89 | 0.06294 | YES YES |
| 31 | a | 281.00 | 0.28806 | YES YES |
| 32 | a | 286.46 | 0.07628 | YES YES |
| 33 | a | 299.42 | 1.82355 | YES YES |
| 34 | a | 314.23 | 0.29664 | YES YES |
| 35 | a | 336.26 | 0.43252 | YES YES |
| 36 | a | 341.65 | 0.47179 | YES YES |
| 37 | a | 361.10 | 0.94395 | YES YES |
| 38 | a | 369.93 | 0.31840 | YES YES |
| 39 | a | 373.84 | 0.33640 | YES YES |
| 40 | a | 396.22 | 0.40134 | YES YES |
| 41 | a | 397.27 | 0.29662 | YES YES |
| 42 | a | 400.67 | 0.67941 | YES YES |
| 43 | a | 405.11 | 0.93166 | YES YES |
| 44 | a | 452.44 | 11.03291 | YES YES |
| 45 | a | 453.65 | 9.21231 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 46 | a | 466.24 | 6.64555 | YES | YES |
| 47 | a | 487.66 | 28.29108 | YES | YES |
| 48 | a | 525.74 | 14.69404 | YES | YES |
| 49 | a | 556.95 | 5.12160 | YES | YES |
| 50 | a | 563.61 | 1.79411 | YES | YES |

**[PhS(PPh3)]+**

bp86_def2-tzvpp energy (au): -1666.4330382650

Zero point energy (au): 0.3578356
Entropy (kJ mol^-1): 0.71026
Chemical potential (kJ mol^-1): 791.35

XYZ coordinates:

46

| | | | |
|---|---|---|---|
| P | 0.12937 | 0.56504 | 0.03564 |
| S | 1.96395 | -0.46918 | 0.14549 |
| C | 1.50659 | -2.20016 | 0.04296 |
| C | 1.36348 | -2.81927 | -1.20707 |
| H | 1.46206 | -2.23686 | -2.12178 |
| C | 1.11138 | -4.19106 | -1.26540 |
| H | 1.00356 | -4.67787 | -2.23433 |
| C | 1.01632 | -4.93916 | -0.08788 |
| H | 0.83174 | -6.01179 | -0.13979 |
| C | 1.17150 | -4.31815 | 1.15451 |
| H | 1.10961 | -4.90300 | 2.07175 |
| C | 1.41556 | -2.94530 | 1.22735 |
| H | 1.54609 | -2.45563 | 2.19132 |
| C | -1.10448 | -0.10096 | 1.17052 |
| C | -1.72268 | -1.33299 | 0.88149 |
| H | -1.48044 | -1.87482 | -0.03224 |
| C | -2.65944 | -1.85902 | 1.76985 |
| H | -3.14022 | -2.81015 | 1.54373 |
| C | -2.98289 | -1.16833 | 2.94150 |
| H | -3.71943 | -1.58203 | 3.62989 |
| C | -2.36932 | 0.05337 | 3.22971 |
| H | -2.62666 | 0.59552 | 4.13901 |
| C | -1.42854 | 0.59019 | 2.35088 |
| H | -0.95974 | 1.54699 | 2.57666 |
| C | 0.60955 | 2.24529 | 0.49529 |
| C | 0.11057 | 3.33638 | -0.23719 |
| H | -0.54367 | 3.17414 | -1.09271 |
| C | 0.46327 | 4.63469 | 0.13214 |
| H | 0.07735 | 5.47934 | -0.43747 |
| C | 1.31233 | 4.84949 | 1.22087 |
| H | 1.58931 | 5.86529 | 1.50161 |
| C | 1.81299 | 3.76516 | 1.94771 |
| H | 2.47939 | 3.93234 | 2.79314 |
| C | 1.46600 | 2.46223 | 1.59163 |
| H | 1.86441 | 1.62046 | 2.15744 |
| C | -0.53663 | 0.55461 | -1.64548 |
| C | -1.92594 | 0.59716 | -1.85936 |
| H | -2.61641 | 0.57521 | -1.01733 |
| C | -2.42171 | 0.67044 | -3.16231 |
| H | -3.49826 | 0.70089 | -3.32718 |
| C | -1.54250 | 0.70299 | -4.24760 |
| H | -1.93465 | 0.75630 | -5.26292 |
| C | -0.16047 | 0.66603 | -4.03552 |
| H | 0.52468 | 0.69282 | -4.88212 |
| C | 0.34682 | 0.59192 | -2.73901 |

H 1.42399 0.56091 -2.57403

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|
| 1 | | 0.00 | 0.00000 | - | - |
| 2 | | 0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 12.46 | 0.08012 | YES | YES |
| 8 | a | 26.78 | 0.01150 | YES | YES |
| 9 | a | 30.17 | 0.05791 | YES | YES |
| 10 | a | 37.45 | 0.01996 | YES | YES |
| 11 | a | 45.43 | 0.11446 | YES | YES |
| 12 | a | 48.97 | 0.06635 | YES | YES |
| 13 | a | 52.37 | 0.04437 | YES | YES |
| 14 | a | 59.33 | 0.10381 | YES | YES |
| 15 | a | 71.88 | 0.27208 | YES | YES |
| 16 | a | 99.84 | 0.41980 | YES | YES |
| 17 | a | 115.98 | 0.76749 | YES | YES |
| 18 | a | 181.78 | 1.25005 | YES | YES |
| 19 | a | 187.78 | 1.54191 | YES | YES |
| 20 | a | 209.19 | 1.19405 | YES | YES |
| 21 | a | 213.48 | 0.34342 | YES | YES |
| 22 | a | 238.84 | 0.66435 | YES | YES |
| 23 | a | 255.35 | 0.40394 | YES | YES |
| 24 | a | 262.37 | 0.39225 | YES | YES |
| 25 | a | 281.12 | 1.45515 | YES | YES |
| 26 | a | 315.76 | 2.85484 | YES | YES |
| 27 | a | 388.12 | 0.17207 | YES | YES |
| 28 | a | 389.71 | 0.07659 | YES | YES |
| 29 | a | 395.98 | 0.78423 | YES | YES |
| 30 | a | 397.28 | 3.55608 | YES | YES |
| 31 | a | 400.43 | 4.72162 | YES | YES |
| 32 | a | 434.22 | 6.18343 | YES | YES |
| 33 | a | 438.54 | 6.33447 | YES | YES |
| 34 | a | 447.61 | 5.29078 | YES | YES |
| 35 | a | 478.43 | 16.12966 | YES | YES |
| 36 | a | 496.24 | 58.67422 | YES | YES |
| 37 | a | 513.14 | 72.76973 | YES | YES |
| 38 | a | 549.19 | 72.11901 | YES | YES |
| 39 | a | 606.09 | 0.31747 | YES | YES |
| 40 | a | 606.24 | 0.03151 | YES | YES |
| 41 | a | 608.08 | 0.11865 | YES | YES |
| 42 | a | 609.25 | 0.64579 | YES | YES |
| 43 | a | 678.56 | 6.79028 | YES | YES |
| 44 | a | 682.70 | 10.60311 | YES | YES |
| 45 | a | 686.97 | 43.53009 | YES | YES |
| 46 | a | 688.14 | 23.77483 | YES | YES |
| 47 | a | 689.11 | 10.24141 | YES | YES |
| 48 | a | 689.59 | 16.31962 | YES | YES |
| 49 | a | 711.48 | 29.46269 | YES | YES |
| 50 | a | 712.43 | 30.67794 | YES | YES |

**[PhS(PPh3).PPh3]+**

bp86_def2-tzvpp energy (au): -2703.0676071170

Zero point energy (au): 0.6240249
Entropy (kJ mol^-1): 1.14772
Chemical potential (kJ mol^-1): 1409.32

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.73516 | 0.55697 | 3.39294 |
| H | -5.80605 | 0.68369 | 3.55182 |
| C | 2.58798 | 2.67269 | 4.23300 |
| H | 3.63510 | 2.90799 | 4.04112 |
| S | -0.01114 | 0.08319 | -0.54092 |
| P | -0.17069 | 0.08952 | 2.64424 |
| C | 0.54774 | 3.04395 | 5.47621 |
| H | -0.00151 | 3.56824 | 6.25855 |
| C | -4.04976 | 1.40754 | 2.51998 |
| H | -4.58452 | 2.20054 | 1.99652 |
| C | -1.97001 | 0.23159 | 2.99096 |
| C | 1.94315 | 1.70099 | 3.46658 |
| H | 2.48946 | 1.18548 | 2.67461 |
| C | 1.05148 | -4.00687 | 4.47513 |
| H | 1.33612 | -4.97686 | 4.88259 |
| C | 0.59574 | 1.37670 | 3.70856 |
| C | 3.86778 | 1.34149 | -0.44662 |
| H | 4.41020 | 2.27870 | -0.56983 |
| C | -2.68010 | 1.23937 | 2.31263 |
| H | -2.15190 | 1.90231 | 1.62462 |
| C | 0.31455 | -1.50099 | 3.42814 |
| C | 0.35412 | -3.93106 | 3.26512 |
| H | 0.09188 | -4.84254 | 2.72718 |
| C | -0.09716 | 2.06193 | 4.71950 |
| H | -1.14290 | 1.82786 | 4.91744 |
| C | 1.88989 | 3.34920 | 5.23793 |
| H | 2.39043 | 4.11424 | 5.83140 |
| C | -2.66773 | -0.61729 | 3.86506 |
| H | -2.13553 | -1.40485 | 4.39805 |
| C | 1.01498 | -1.58841 | 4.64141 |
| H | 1.27220 | -0.68083 | 5.18689 |
| C | -0.00149 | -2.68798 | 2.74095 |
| H | -0.53947 | -2.63567 | 1.79215 |
| C | 2.46780 | -1.06127 | -0.11306 |
| H | 1.91703 | -1.99003 | 0.02703 |
| C | -4.04218 | -0.45552 | 4.06071 |
| H | -4.57053 | -1.11976 | 4.74507 |
| C | 1.38250 | -2.83446 | 5.15778 |
| H | 1.92460 | -2.88673 | 6.10225 |
| C | 3.85577 | -1.03171 | 0.03700 |
| H | 4.38830 | -1.94754 | 0.29219 |
| C | 2.47786 | 1.32577 | -0.58619 |
| H | 1.93668 | 2.24472 | -0.80518 |
| C | 4.55665 | 0.16542 | -0.13519 |
| H | 5.63995 | 0.18409 | -0.01772 |

| | | | |
|---|---|---|---|
| C | 1.78159 | 0.11945 | -0.42832 |
| C | -4.73397 | -0.90359 | -3.16615 |
| H | -5.79577 | -1.11783 | -3.28555 |
| C | 2.87115 | -2.19251 | -4.18162 |
| H | 3.94987 | -2.07727 | -4.28241 |
| P | -0.24073 | -0.00852 | -2.67584 |
| C | 0.85903 | -3.50045 | -4.50837 |
| H | 0.36626 | -4.40318 | -4.86808 |
| C | -4.00153 | -1.54586 | -2.16406 |
| H | -4.48878 | -2.25879 | -1.49979 |
| C | -2.01103 | -0.34804 | -2.85587 |
| C | 2.12234 | -1.17262 | -3.59593 |
| H | 2.62119 | -0.27059 | -3.24308 |
| C | 0.56203 | 4.04238 | -4.72031 |
| H | 0.73303 | 5.00405 | -5.20353 |
| C | 0.72671 | -1.31434 | -3.46951 |
| C | -2.64247 | -1.27379 | -2.00493 |
| H | -2.07715 | -1.77408 | -1.21940 |
| C | 0.13103 | 1.57449 | -3.47681 |
| C | -0.00126 | 3.99456 | -3.44084 |
| H | -0.27123 | 4.91633 | -2.92632 |
| C | 0.09808 | -2.48607 | -3.92595 |
| H | -0.98135 | -2.60136 | -3.83803 |
| C | 2.24257 | -3.35564 | -4.63672 |
| H | 2.83265 | -4.14896 | -5.09500 |
| C | -2.75120 | 0.29957 | -3.85991 |
| H | -2.27181 | 1.02460 | -4.51648 |
| C | 0.69116 | 1.62445 | -4.76495 |
| H | 0.95609 | 0.70637 | -5.28744 |
| C | -0.21617 | 2.76678 | -2.81640 |
| H | -0.64917 | 2.73038 | -1.81642 |
| C | -4.10893 | 0.01648 | -4.01199 |
| H | -4.67958 | 0.52063 | -4.79127 |
| C | 0.90582 | 2.85992 | -5.37961 |
| H | 1.34224 | 2.89529 | -6.37736 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 4.07 | 0.00586 | YES YES |
| 8 | a | 6.87 | 0.01582 | YES YES |
| 9 | a | 10.71 | 0.10594 | YES YES |
| 10 | a | 17.64 | 0.13053 | YES YES |
| 11 | a | 22.33 | 5.73505 | YES YES |
| 12 | a | 24.19 | 0.02272 | YES YES |
| 13 | a | 25.13 | 0.99935 | YES YES |
| 14 | a | 26.87 | 0.21514 | YES YES |
| 15 | a | 29.08 | 0.66387 | YES YES |
| 16 | a | 36.54 | 0.41306 | YES YES |
| 17 | a | 38.01 | 0.12325 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 18 | a | 41.30 | 0.02575 | YES | YES |
| 19 | a | 46.25 | 0.68682 | YES | YES |
| 20 | a | 49.71 | 0.21586 | YES | YES |
| 21 | a | 53.64 | 0.08973 | YES | YES |
| 22 | a | 54.34 | 0.05006 | YES | YES |
| 23 | a | 55.00 | 0.29392 | YES | YES |
| 24 | a | 58.70 | 0.21482 | YES | YES |
| 25 | a | 60.85 | 1.34848 | YES | YES |
| 26 | a | 70.79 | 5.16112 | YES | YES |
| 27 | a | 74.09 | 5.91530 | YES | YES |
| 28 | a | 107.14 | 0.06376 | YES | YES |
| 29 | a | 127.31 | 1.47251 | YES | YES |
| 30 | a | 177.72 | 1.16053 | YES | YES |
| 31 | a | 183.79 | 8.24358 | YES | YES |
| 32 | a | 188.01 | 1.78363 | YES | YES |
| 33 | a | 191.10 | 1.33686 | YES | YES |
| 34 | a | 193.14 | 0.77269 | YES | YES |
| 35 | a | 207.83 | 1.24390 | YES | YES |
| 36 | a | 212.98 | 0.82082 | YES | YES |
| 37 | a | 235.80 | 5.21046 | YES | YES |
| 38 | a | 239.26 | 0.52625 | YES | YES |
| 39 | a | 251.68 | 0.44706 | YES | YES |
| 40 | a | 254.53 | 0.97703 | YES | YES |
| 41 | a | 254.59 | 0.46805 | YES | YES |
| 42 | a | 263.28 | 18.46716 | YES | YES |
| 43 | a | 272.06 | 57.44221 | YES | YES |
| 44 | a | 298.06 | 33.09583 | YES | YES |
| 45 | a | 387.94 | 3.70337 | YES | YES |
| 46 | a | 389.17 | 0.17042 | YES | YES |
| 47 | a | 390.12 | 0.78514 | YES | YES |
| 48 | a | 390.31 | 0.12286 | YES | YES |
| 49 | a | 390.51 | 0.67031 | YES | YES |
| 50 | a | 396.17 | 1.99477 | YES | YES |

**[PhS(PtBu3).PPh3]+**

bp86_def2-tzvpp energy (au): -2481.5463992060

Zero point energy (au): 0.7154442
Entropy (kJ mol^-1): 1.14184
Chemical potential (kJ mol^-1): 1657.27

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.27526 | 0.17958 | 0.05090 |
| S | 1.24688 | -0.23265 | 0.13212 |
| C | 0.99302 | -2.01436 | 0.11412 |
| C | 0.98288 | -2.75211 | -1.07638 |
| H | 1.21419 | -2.27444 | -2.02586 |
| C | 0.64039 | -4.10614 | -1.04900 |
| H | 0.63410 | -4.67650 | -1.97756 |
| C | 0.28782 | -4.71989 | 0.15552 |
| H | 0.01759 | -5.77537 | 0.17089 |
| C | 0.26313 | -3.97328 | 1.33672 |
| H | -0.03429 | -4.43940 | 2.27572 |
| C | 0.61126 | -2.62179 | 1.31986 |
| H | 0.56907 | -2.03205 | 2.23464 |
| C | -3.60146 | -0.68323 | 0.99492 |
| C | -3.54935 | -2.08837 | 1.03319 |
| H | -2.74463 | -2.61242 | 0.51385 |
| C | -4.51830 | -2.81852 | 1.72298 |
| H | -4.46994 | -3.90775 | 1.73641 |
| C | -5.54334 | -2.15414 | 2.40316 |
| H | -6.29585 | -2.72277 | 2.94950 |
| C | -5.59715 | -0.75846 | 2.38233 |
| H | -6.39480 | -0.23445 | 2.90959 |
| C | -4.63569 | -0.02596 | 1.68044 |
| H | -4.69214 | 1.06235 | 1.66641 |
| C | -2.46187 | 1.93818 | 0.57191 |
| C | -2.98746 | 2.94882 | -0.24814 |
| H | -3.35587 | 2.70297 | -1.24393 |
| C | -3.05104 | 4.27040 | 0.20532 |
| H | -3.46684 | 5.04220 | -0.44310 |
| C | -2.60018 | 4.60013 | 1.48502 |
| H | -2.66089 | 5.62900 | 1.83983 |
| C | -2.07527 | 3.60104 | 2.31183 |
| H | -1.72850 | 3.84827 | 3.31581 |
| C | -1.99554 | 2.28516 | 1.85451 |
| H | -1.58207 | 1.51212 | 2.50597 |
| C | -2.91311 | 0.17318 | -1.67830 |
| C | -4.24174 | -0.12457 | -2.02074 |
| H | -4.96507 | -0.35508 | -1.23874 |
| C | -4.64449 | -0.12953 | -3.35898 |
| H | -5.67931 | -0.36452 | -3.60937 |
| C | -3.73018 | 0.16937 | -4.37208 |
| H | -4.04782 | 0.16545 | -5.41476 |
| C | -2.40437 | 0.46678 | -4.04328 |
| H | -1.68515 | 0.69700 | -4.83002 |
| C | -1.99810 | 0.45731 | -2.70780 |

| | | | |
|---|---|---|---|
| H | -0.95765 | 0.67262 | -2.45538 |
| P | 3.33086 | 0.26709 | 0.04651 |
| C | 4.10858 | -0.23116 | -1.65207 |
| C | 5.36901 | 0.60171 | -1.96645 |
| H | 5.78883 | 0.22004 | -2.90911 |
| C | 3.08177 | -0.02590 | -2.78467 |
| H | 3.51676 | -0.44603 | -3.70294 |
| H | 2.85904 | 1.02577 | -2.97911 |
| H | 2.13546 | -0.54134 | -2.59311 |
| C | 3.13643 | 2.18947 | 0.19584 |
| C | 4.48437 | 2.84931 | 0.55337 |
| H | 4.33251 | 3.93832 | 0.52707 |
| H | 5.28567 | 2.61656 | -0.15597 |
| H | 4.82413 | 2.59839 | 1.56390 |
| H | 2.32608 | 2.16605 | 2.26767 |
| H | 1.07881 | 2.25382 | 1.00662 |
| H | 2.09317 | 3.65871 | 1.34956 |
| C | 2.62797 | 2.78148 | -1.13497 |
| H | 1.69430 | 2.31673 | -1.47243 |
| H | 3.36921 | 2.73241 | -1.93920 |
| H | 2.41693 | 3.84566 | -0.95602 |
| C | 4.31730 | -0.46861 | 1.53261 |
| C | 3.82057 | 0.17108 | 2.84391 |
| H | 4.30114 | -0.36675 | 3.67401 |
| H | 2.73569 | 0.06895 | 2.96981 |
| H | 4.09552 | 1.22631 | 2.94109 |
| C | 5.83297 | -0.22415 | 1.38355 |
| H | 6.09772 | 0.83264 | 1.27566 |
| H | 6.26944 | -0.78451 | 0.54950 |
| H | 6.31604 | -0.58950 | 2.30202 |
| C | 4.06493 | -1.98585 | 1.65034 |
| H | 4.37763 | -2.55731 | 0.77349 |
| H | 3.01599 | -2.21510 | 1.85785 |
| H | 4.65758 | -2.34545 | 2.50452 |
| H | 5.14866 | 1.66327 | -2.12129 |
| H | 6.14990 | 0.51099 | -1.20428 |
| C | 4.49605 | -1.72447 | -1.63196 |
| H | 4.81949 | -1.99372 | -2.64795 |
| H | 5.33588 | -1.93629 | -0.96205 |
| H | 3.65644 | -2.37922 | -1.37075 |
| C | 2.09527 | 2.56130 | 1.27589 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 4.35 | 0.01350 | YES YES |
| 8 | a | 8.46 | 0.07543 | YES YES |
| 9 | a | 9.99 | 0.04772 | YES YES |
| 10 | a | 16.14 | 0.11935 | YES YES |
| 11 | a | 19.15 | 3.87376 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 24.96 | 0.42350 | YES | YES |
| 13 | a | 25.84 | 1.22058 | YES | YES |
| 14 | a | 29.54 | 0.28120 | YES | YES |
| 15 | a | 32.76 | 0.04359 | YES | YES |
| 16 | a | 45.08 | 0.54935 | YES | YES |
| 17 | a | 52.86 | 0.38263 | YES | YES |
| 18 | a | 55.83 | 0.23753 | YES | YES |
| 19 | a | 57.57 | 0.18437 | YES | YES |
| 20 | a | 62.98 | 0.28841 | YES | YES |
| 21 | a | 68.31 | 2.35611 | YES | YES |
| 22 | a | 93.25 | 0.29596 | YES | YES |
| 23 | a | 100.85 | 0.13579 | YES | YES |
| 24 | a | 120.88 | 0.19424 | YES | YES |
| 25 | a | 131.00 | 0.39607 | YES | YES |
| 26 | a | 133.10 | 0.60034 | YES | YES |
| 27 | a | 158.66 | 0.75302 | YES | YES |
| 28 | a | 174.49 | 1.82512 | YES | YES |
| 29 | a | 177.40 | 0.54318 | YES | YES |
| 30 | a | 182.20 | 0.57755 | YES | YES |
| 31 | a | 189.16 | 1.04403 | YES | YES |
| 32 | a | 193.79 | 0.26922 | YES | YES |
| 33 | a | 194.84 | 1.35703 | YES | YES |
| 34 | a | 200.52 | 0.92507 | YES | YES |
| 35 | a | 205.08 | 0.83241 | YES | YES |
| 36 | a | 210.33 | 0.61360 | YES | YES |
| 37 | a | 232.35 | 0.73814 | YES | YES |
| 38 | a | 236.49 | 2.79233 | YES | YES |
| 39 | a | 237.10 | 0.40677 | YES | YES |
| 40 | a | 240.59 | 2.71949 | YES | YES |
| 41 | a | 248.51 | 0.73225 | YES | YES |
| 42 | a | 249.27 | 0.44246 | YES | YES |
| 43 | a | 254.70 | 0.26708 | YES | YES |
| 44 | a | 256.12 | 0.37554 | YES | YES |
| 45 | a | 262.48 | 0.89015 | YES | YES |
| 46 | a | 273.84 | 1.51589 | YES | YES |
| 47 | a | 277.75 | 0.16660 | YES | YES |
| 48 | a | 280.34 | 0.43547 | YES | YES |
| 49 | a | 290.50 | 0.43518 | YES | YES |
| 50 | a | 300.18 | 13.45056 | YES | YES |

**[PhS(PPh3).PtBu3]+_try4**

bp86_def2-tzvpp energy (au): -2481.5471872580

Zero point energy (au): 0.7153606
Entropy (kJ mol^-1): 1.11816
Chemical potential (kJ mol^-1): 1663.56

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.20246 | 0.32915 | 0.03148 |
| S | -0.07845 | 0.00606 | 0.01244 |
| C | -0.05006 | -1.78811 | -0.06757 |
| C | -0.16395 | -2.44491 | -1.30051 |
| H | -0.29421 | -1.86953 | -2.21562 |
| C | -0.09722 | -3.83944 | -1.34681 |
| H | -0.18450 | -4.35104 | -2.30509 |
| C | 0.09600 | -4.57355 | -0.17291 |
| H | 0.15709 | -5.66076 | -0.21487 |
| C | 0.22130 | -3.91348 | 1.05281 |
| H | 0.37981 | -4.48289 | 1.96837 |
| C | 0.14499 | -2.52031 | 1.11144 |
| H | 0.24077 | -2.00012 | 2.06332 |
| C | -3.10165 | -0.66001 | 1.24955 |
| C | -3.29027 | -2.03809 | 1.02651 |
| H | -2.92100 | -2.50661 | 0.11482 |
| C | -3.96019 | -2.80781 | 1.97649 |
| H | -4.10904 | -3.87222 | 1.79767 |
| C | -4.43811 | -2.21837 | 3.15091 |
| H | -4.96218 | -2.82450 | 3.88949 |
| C | -4.24860 | -0.85277 | 3.37658 |
| H | -4.62634 | -0.38975 | 4.28764 |
| C | -3.58200 | -0.07091 | 2.43243 |
| H | -3.44843 | 0.99516 | 2.61036 |
| C | -2.31727 | 2.08761 | 0.45038 |
| C | -3.21218 | 2.92037 | -0.24253 |
| H | -3.82362 | 2.52011 | -1.05019 |
| C | -3.31350 | 4.26867 | 0.10256 |
| H | -4.00745 | 4.91154 | -0.43796 |
| C | -2.52669 | 4.79172 | 1.13182 |
| H | -2.60692 | 5.84599 | 1.39565 |
| C | -1.63390 | 3.96634 | 1.82141 |
| H | -1.01785 | 4.37363 | 2.62241 |
| C | -1.52444 | 2.61665 | 1.48582 |
| H | -0.82411 | 1.97813 | 2.02371 |
| C | -2.94356 | 0.06772 | -1.60167 |
| C | -4.25995 | -0.40819 | -1.73253 |
| H | -4.84095 | -0.67377 | -0.85055 |
| C | -4.82692 | -0.53773 | -3.00199 |
| H | -5.84655 | -0.90916 | -3.09990 |
| C | -4.09236 | -0.19201 | -4.13880 |
| H | -4.53867 | -0.29674 | -5.12743 |
| C | -2.78502 | 0.28826 | -4.01045 |
| H | -2.21206 | 0.56062 | -4.89632 |
| C | -2.20764 | 0.41754 | -2.74796 |

| | | | |
|---|---|---|---|
| H | -1.18650 | 0.78643 | -2.64903 |
| P | 3.30844 | 0.23273 | -0.02306 |
| C | 3.75042 | 1.34640 | -1.55053 |
| C | 5.05411 | 2.15907 | -1.45753 |
| H | 5.19741 | 2.71653 | -2.39748 |
| C | 2.56245 | 2.31092 | -1.77161 |
| H | 2.72999 | 2.86797 | -2.70697 |
| H | 2.44255 | 3.04642 | -0.97124 |
| H | 1.61827 | 1.75871 | -1.87266 |
| C | 3.68220 | 1.24083 | 1.59280 |
| C | 5.16240 | 1.39573 | 1.98458 |
| H | 5.23031 | 2.00933 | 2.89771 |
| H | 5.75108 | 1.89772 | 1.20841 |
| H | 5.64141 | 0.43583 | 2.20830 |
| H | 3.30646 | -0.44537 | 2.98806 |
| H | 1.84988 | 0.44747 | 2.50604 |
| H | 3.00613 | 1.16629 | 3.65129 |
| C | 3.06207 | 2.64731 | 1.46987 |
| H | 2.00481 | 2.60674 | 1.17370 |
| H | 3.59703 | 3.29265 | 0.76479 |
| H | 3.11189 | 3.13466 | 2.45633 |
| C | 4.46868 | -1.32312 | -0.04941 |
| C | 4.40319 | -2.02904 | 1.31993 |
| H | 4.91020 | -3.00234 | 1.23027 |
| H | 3.36847 | -2.22645 | 1.63120 |
| H | 4.91140 | -1.47383 | 2.11573 |
| C | 5.94630 | -1.07278 | -0.39936 |
| H | 6.43271 | -0.37962 | 0.29631 |
| H | 6.07846 | -0.68523 | -1.41599 |
| H | 6.49269 | -2.02850 | -0.34699 |
| C | 3.86527 | -2.32292 | -1.06234 |
| H | 3.91341 | -1.97565 | -2.09809 |
| H | 2.81724 | -2.54803 | -0.82465 |
| H | 4.43263 | -3.26527 | -1.00602 |
| H | 5.03313 | 2.89790 | -0.64809 |
| H | 5.93580 | 1.52391 | -1.31632 |
| C | 3.81084 | 0.46752 | -2.81625 |
| H | 3.86773 | 1.12935 | -3.69454 |
| H | 4.69137 | -0.18305 | -2.84596 |
| H | 2.91181 | -0.15371 | -2.92932 |
| C | 2.91802 | 0.54734 | 2.74433 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 3.97 | 0.00898 | YES YES |
| 8 | a | 12.13 | 0.00571 | YES YES |
| 9 | a | 19.84 | 0.71456 | YES YES |
| 10 | a | 22.00 | 0.04567 | YES YES |
| 11 | a | 27.41 | 7.40869 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 32.44 | 0.13688 | YES | YES |
| 13 | a | 34.77 | 0.44341 | YES | YES |
| 14 | a | 39.68 | 0.35710 | YES | YES |
| 15 | a | 40.56 | 0.12496 | YES | YES |
| 16 | a | 45.57 | 0.56837 | YES | YES |
| 17 | a | 51.32 | 0.22215 | YES | YES |
| 18 | a | 57.54 | 0.10053 | YES | YES |
| 19 | a | 59.80 | 0.08987 | YES | YES |
| 20 | a | 61.91 | 1.56206 | YES | YES |
| 21 | a | 73.81 | 0.53605 | YES | YES |
| 22 | a | 93.54 | 0.03900 | YES | YES |
| 23 | a | 95.07 | 0.08504 | YES | YES |
| 24 | a | 104.33 | 0.26428 | YES | YES |
| 25 | a | 125.54 | 0.09839 | YES | YES |
| 26 | a | 126.45 | 1.11983 | YES | YES |
| 27 | a | 172.15 | 0.61819 | YES | YES |
| 28 | a | 180.94 | 0.06703 | YES | YES |
| 29 | a | 182.96 | 0.51100 | YES | YES |
| 30 | a | 184.77 | 6.50689 | YES | YES |
| 31 | a | 189.64 | 1.36365 | YES | YES |
| 32 | a | 197.66 | 0.04326 | YES | YES |
| 33 | a | 198.57 | 0.08523 | YES | YES |
| 34 | a | 200.11 | 0.00540 | YES | YES |
| 35 | a | 207.46 | 1.29544 | YES | YES |
| 36 | a | 212.94 | 1.30664 | YES | YES |
| 37 | a | 236.02 | 0.14853 | YES | YES |
| 38 | a | 236.26 | 0.34395 | YES | YES |
| 39 | a | 237.09 | 0.17160 | YES | YES |
| 40 | a | 239.41 | 0.60537 | YES | YES |
| 41 | a | 254.79 | 1.07737 | YES | YES |
| 42 | a | 254.86 | 0.18315 | YES | YES |
| 43 | a | 255.41 | 0.22823 | YES | YES |
| 44 | a | 262.76 | 7.09013 | YES | YES |
| 45 | a | 263.21 | 9.85302 | YES | YES |
| 46 | a | 271.61 | 1.02194 | YES | YES |
| 47 | a | 272.77 | 38.19460 | YES | YES |
| 48 | a | 274.54 | 12.01168 | YES | YES |
| 49 | a | 283.33 | 0.05750 | YES | YES |
| 50 | a | 298.47 | 30.60146 | YES | YES |

**[PhS(PtBu3)]+**

bp86_def2-tzvpp energy (au): -1444.9134141350

Zero point energy (au): 0.4491026
Entropy (kJ mol^-1): 0.69253
Chemical potential (kJ mol^-1): 1042.38

XYZ coordinates:

52

| | | | |
|---|---|---|---|
| P | -0.98807 | 0.02122 | 0.01385 |
| C | 2.24120 | -0.64834 | 0.09867 |
| C | 4.34210 | -0.08241 | 1.16070 |
| H | 4.93293 | 0.05187 | 2.06629 |
| C | 4.91921 | 0.12472 | -0.09476 |
| H | 5.96290 | 0.42748 | -0.17174 |
| C | 4.16301 | -0.07665 | -1.25248 |
| H | 4.61652 | 0.05883 | -2.23394 |
| C | 2.82768 | -0.47520 | -1.16214 |
| H | 2.26073 | -0.67056 | -2.06979 |
| C | -0.86165 | 1.48828 | 1.25732 |
| C | -1.91394 | 2.57338 | 0.94976 |
| H | -1.84162 | 3.33279 | 1.74270 |
| C | 0.54474 | 2.12083 | 1.20648 |
| H | 0.54941 | 2.94838 | 1.93122 |
| H | 0.80879 | 2.53981 | 0.23317 |
| H | 1.32620 | 1.41724 | 1.50635 |
| C | -1.05599 | 0.61985 | -1.82077 |
| C | -2.46297 | 1.14117 | -2.18288 |
| H | -2.41483 | 1.52706 | -3.21167 |
| H | -2.79863 | 1.96464 | -1.54368 |
| H | -3.22429 | 0.35350 | -2.17240 |
| H | -1.42798 | -1.34126 | -2.78591 |
| H | 0.28527 | -0.97891 | -2.54145 |
| H | -0.63905 | -0.11968 | -3.78869 |
| C | -0.03477 | 1.75498 | -2.03967 |
| H | 0.98609 | 1.47071 | -1.75906 |
| H | -0.30561 | 2.67743 | -1.51602 |
| H | -0.02759 | 1.98543 | -3.11458 |
| C | -2.45614 | -1.17387 | 0.43621 |
| C | -2.70905 | -2.14905 | -0.73240 |
| H | -3.46441 | -2.87157 | -0.39208 |
| H | -1.81372 | -2.71918 | -1.00837 |
| H | -3.11455 | -1.65784 | -1.62265 |
| C | -3.74336 | -0.36619 | 0.70327 |
| H | -4.02807 | 0.28640 | -0.12877 |
| H | -3.68706 | 0.23150 | 1.61946 |
| H | -4.55966 | -1.08958 | 0.84351 |
| C | -2.13595 | -2.03482 | 1.67933 |
| H | -1.90861 | -1.45327 | 2.57552 |
| H | -1.31511 | -2.73756 | 1.50147 |
| H | -3.03566 | -2.63050 | 1.89165 |
| S | 0.60301 | -1.36246 | 0.30187 |
| C | 3.00470 | -0.46897 | 1.26305 |
| H | 2.55733 | -0.64722 | 2.24029 |

| | | | |
|---|---|---|---|
| H | -1.72620 | 3.08632 | 0.00026 |
| H | -2.94233 | 2.19822 | 0.95184 |
| C | -1.06807 | 0.96292 | 2.69151 |
| H | -0.86149 | 1.79653 | 3.37823 |
| H | -2.09302 | 0.63138 | 2.88736 |
| H | -0.37314 | 0.15202 | 2.94070 |
| C | -0.68894 | -0.53647 | -2.77272 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|
| 1 | | 0.00 | 0.00000 | - | - |
| 2 | | 0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 21.32 | 0.09950 | YES | YES |
| 8 | a | 52.33 | 0.06636 | YES | YES |
| 9 | a | 53.98 | 0.05236 | YES | YES |
| 10 | a | 80.03 | 0.45949 | YES | YES |
| 11 | a | 98.79 | 0.14108 | YES | YES |
| 12 | a | 118.98 | 0.10920 | YES | YES |
| 13 | a | 127.13 | 0.21353 | YES | YES |
| 14 | a | 128.95 | 0.72629 | YES | YES |
| 15 | a | 162.84 | 0.06282 | YES | YES |
| 16 | a | 168.72 | 0.28102 | YES | YES |
| 17 | a | 181.69 | 0.35260 | YES | YES |
| 18 | a | 191.44 | 0.28613 | YES | YES |
| 19 | a | 200.21 | 1.22173 | YES | YES |
| 20 | a | 203.60 | 0.23090 | YES | YES |
| 21 | a | 207.69 | 1.02927 | YES | YES |
| 22 | a | 215.00 | 0.83507 | YES | YES |
| 23 | a | 237.34 | 0.93506 | YES | YES |
| 24 | a | 246.85 | 0.21122 | YES | YES |
| 25 | a | 252.15 | 0.46223 | YES | YES |
| 26 | a | 254.04 | 0.01726 | YES | YES |
| 27 | a | 263.39 | 0.18632 | YES | YES |
| 28 | a | 270.85 | 0.50163 | YES | YES |
| 29 | a | 276.90 | 0.44525 | YES | YES |
| 30 | a | 286.17 | 0.15534 | YES | YES |
| 31 | a | 296.58 | 0.03153 | YES | YES |
| 32 | a | 308.10 | 0.22735 | YES | YES |
| 33 | a | 319.57 | 0.36136 | YES | YES |
| 34 | a | 327.70 | 0.13902 | YES | YES |
| 35 | a | 341.48 | 0.36540 | YES | YES |
| 36 | a | 359.54 | 1.27720 | YES | YES |
| 37 | a | 371.20 | 0.45922 | YES | YES |
| 38 | a | 375.07 | 0.44788 | YES | YES |
| 39 | a | 392.23 | 0.57186 | YES | YES |
| 40 | a | 396.27 | 1.89344 | YES | YES |
| 41 | a | 400.69 | 0.98015 | YES | YES |
| 42 | a | 404.38 | 0.57906 | YES | YES |
| 43 | a | 414.03 | 4.76171 | YES | YES |
| 44 | a | 452.13 | 12.00616 | YES | YES |
| 45 | a | 455.85 | 9.53671 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 46 | a | 484.02 | 8.02157 | YES | YES |
| 47 | a | 502.98 | 9.50350 | YES | YES |
| 48 | a | 538.10 | 20.50810 | YES | YES |
| 49 | a | 562.89 | 5.86667 | YES | YES |
| 50 | a | 572.31 | 12.13008 | YES | YES |

**TS [PhS(PPh3)2]+**

bp86_def2-tzvpp energy (au): -2703.0643015890

Zero point energy (au): 0.6239692
Entropy (kJ mol^-1): 1.10346
Chemical potential (kJ mol^-1): 1420.07

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.73210 | 0.43368 | 2.70878 |
| H | -5.80928 | 0.53559 | 2.83993 |
| C | 2.49683 | 2.72468 | 3.84398 |
| H | 3.55392 | 2.96262 | 3.72560 |
| S | -0.01600 | 0.08300 | -0.44100 |
| P | -0.14600 | 0.08900 | 2.14500 |
| C | 0.37004 | 3.10146 | 4.93224 |
| H | -0.23628 | 3.63146 | 5.66689 |
| C | -4.03986 | 1.32380 | 1.88265 |
| H | -4.57539 | 2.12048 | 1.36641 |
| C | -1.95449 | 0.17902 | 2.38635 |
| C | 1.91710 | 1.73648 | 3.04719 |
| H | 2.52529 | 1.21620 | 2.30654 |
| C | 1.16610 | -3.95983 | 3.98965 |
| H | 1.46934 | -4.91824 | 4.41073 |
| C | 0.55625 | 1.41202 | 3.19747 |
| C | 3.86202 | 1.34730 | -0.57760 |
| H | 4.39116 | 2.28645 | -0.73864 |
| C | -2.66025 | 1.19502 | 1.71572 |
| H | -2.12607 | 1.89545 | 1.07228 |
| C | 0.37903 | -1.48809 | 2.91005 |
| C | 0.43927 | -3.91713 | 2.79543 |
| H | 0.17332 | -4.84222 | 2.28378 |
| C | -0.21469 | 2.10744 | 4.14436 |
| H | -1.26971 | 1.86847 | 4.27238 |
| C | 1.72471 | 3.40995 | 4.78659 |
| H | 2.17808 | 4.18428 | 5.40529 |
| C | -2.65825 | -0.71363 | 3.21159 |
| H | -2.12583 | -1.50434 | 3.73889 |
| C | 1.11064 | -1.53977 | 4.10763 |
| H | 1.37017 | -0.61938 | 4.62904 |
| C | 0.05470 | -2.69049 | 2.25370 |
| H | -0.50856 | -2.66564 | 1.31967 |
| C | 2.49626 | -1.05977 | -0.16136 |
| H | 1.96106 | -1.99420 | -0.00047 |
| C | -4.04005 | -0.58458 | 3.36914 |
| H | -4.57482 | -1.27833 | 4.01794 |
| C | 1.50117 | -2.77088 | 4.64085 |
| H | 2.06402 | -2.79787 | 5.57395 |
| C | 3.89128 | -1.02613 | -0.10236 |
| H | 4.44295 | -1.94224 | 0.10775 |
| C | 2.46557 | 1.32559 | -0.62275 |
| H | 1.90746 | 2.24221 | -0.80726 |
| C | 4.57551 | 0.17434 | -0.31374 |
| H | 5.66421 | 0.19681 | -0.26903 |

| | | | |
|---|---|---|---|
| C | 1.78069 | 0.11890 | -0.41814 |
| C | -4.76168 | -0.79360 | -3.07220 |
| H | -5.83336 | -0.97861 | -3.14282 |
| C | 2.78460 | -2.35511 | -4.24280 |
| H | 3.87171 | -2.30563 | -4.29906 |
| P | -0.22141 | -0.02258 | -2.74421 |
| C | 0.71017 | -3.52122 | -4.68389 |
| H | 0.17528 | -4.38015 | -5.08848 |
| C | -3.98685 | -1.51713 | -2.16180 |
| H | -4.45121 | -2.26402 | -1.51843 |
| C | -2.00670 | -0.31751 | -2.89330 |
| C | 2.07809 | -1.30984 | -3.64947 |
| H | 2.61880 | -0.45506 | -3.24336 |
| C | 0.67822 | 4.02141 | -4.78004 |
| H | 0.88236 | 4.98285 | -5.25068 |
| C | 0.67218 | -1.36143 | -3.57949 |
| C | -2.61481 | -1.28143 | -2.06728 |
| H | -2.01685 | -1.84474 | -1.35129 |
| C | 0.15892 | 1.54972 | -3.56942 |
| C | 0.05567 | 3.97428 | -3.52841 |
| H | -0.22757 | 4.89692 | -3.02219 |
| C | -0.00773 | -2.47676 | -4.09871 |
| H | -1.09487 | -2.52590 | -4.05437 |
| C | 2.10375 | -3.46279 | -4.75761 |
| H | 2.66026 | -4.27896 | -5.21773 |
| C | -2.79113 | 0.40850 | -3.80520 |
| H | -2.33194 | 1.16133 | -4.44470 |
| C | 0.77965 | 1.60128 | -4.82845 |
| H | 1.05650 | 0.68165 | -5.34216 |
| C | -0.19972 | 2.74585 | -2.92052 |
| H | -0.67635 | 2.71170 | -1.94027 |
| C | -4.16322 | 0.16747 | -3.89121 |
| H | -4.76565 | 0.73420 | -4.60060 |
| C | 1.03824 | 2.83668 | -5.42650 |
| H | 1.51980 | 2.87044 | -6.40342 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | a | -37.26 | 0.00000 | YES YES |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | | 0.00 | 0.00000 | - - |
| 8 | a | 5.92 | 0.20829 | YES YES |
| 9 | a | 10.87 | 0.60281 | YES YES |
| 10 | a | 16.28 | 0.46690 | YES YES |
| 11 | a | 18.87 | 2.62764 | YES YES |
| 12 | a | 23.24 | 0.07408 | YES YES |
| 13 | a | 26.37 | 5.90171 | YES YES |
| 14 | a | 34.20 | 0.32905 | YES YES |
| 15 | a | 36.43 | 1.54009 | YES YES |
| 16 | a | 39.40 | 3.12504 | YES YES |
| 17 | a | 42.76 | 5.44562 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 18 | a | 44.90 | 13.21965 | YES | YES |
| 19 | a | 46.84 | 1.59235 | YES | YES |
| 20 | a | 53.32 | 4.01714 | YES | YES |
| 21 | a | 55.38 | 0.10037 | YES | YES |
| 22 | a | 56.51 | 4.40176 | YES | YES |
| 23 | a | 59.65 | 1.87348 | YES | YES |
| 24 | a | 60.64 | 5.33166 | YES | YES |
| 25 | a | 64.92 | 4.53160 | YES | YES |
| 26 | a | 70.22 | 1.75660 | YES | YES |
| 27 | a | 73.55 | 10.87669 | YES | YES |
| 28 | a | 113.59 | 0.84465 | YES | YES |
| 29 | a | 126.32 | 25.13252 | YES | YES |
| 30 | a | 142.61 | 1.10424 | YES | YES |
| 31 | a | 182.48 | 1.16376 | YES | YES |
| 32 | a | 185.19 | 1.17285 | YES | YES |
| 33 | a | 191.06 | 0.86663 | YES | YES |
| 34 | a | 196.91 | 2.03577 | YES | YES |
| 35 | a | 202.87 | 1.50389 | YES | YES |
| 36 | a | 207.18 | 1.41907 | YES | YES |
| 37 | a | 232.16 | 78.66780 | YES | YES |
| 38 | a | 236.49 | 0.31996 | YES | YES |
| 39 | a | 237.95 | 4.52844 | YES | YES |
| 40 | a | 252.92 | 1.22521 | YES | YES |
| 41 | a | 255.02 | 2.37449 | YES | YES |
| 42 | a | 256.90 | 2.05566 | YES | YES |
| 43 | a | 261.63 | 0.91239 | YES | YES |
| 44 | a | 300.01 | 6.77761 | YES | YES |
| 45 | a | 389.34 | 0.26924 | YES | YES |
| 46 | a | 389.58 | 1.46141 | YES | YES |
| 47 | a | 390.17 | 1.21143 | YES | YES |
| 48 | a | 390.54 | 0.20915 | YES | YES |
| 49 | a | 390.89 | 0.21748 | YES | YES |
| 50 | a | 393.80 | 2.38398 | YES | YES |

**TS [PhS(PPh3)(PtBu3)]+**

bp86_def2-tzvpp energy (au): -2481.5417241010

Zero point energy (au): 0.7155244
Entropy (kJ mol^-1): 1.08248
Chemical potential (kJ mol^-1): 1672.39

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.25270 | 0.31672 | 0.01975 |
| S | 0.24253 | 0.02625 | -0.01367 |
| C | 0.07231 | -1.76245 | 0.03392 |
| C | -0.22339 | -2.46321 | -1.14584 |
| H | -0.32015 | -1.92124 | -2.08564 |
| C | -0.39250 | -3.84948 | -1.11196 |
| H | -0.62379 | -4.38632 | -2.03192 |
| C | -0.25510 | -4.54536 | 0.09313 |
| H | -0.37665 | -5.62813 | 0.11548 |
| C | 0.03464 | -3.84859 | 1.26927 |
| H | 0.13135 | -4.38403 | 2.21371 |
| C | 0.18858 | -2.45981 | 1.24474 |
| H | 0.38858 | -1.91533 | 2.16620 |
| C | -3.25541 | -0.57695 | 1.25058 |
| C | -3.33158 | -1.98084 | 1.16678 |
| H | -2.82091 | -2.51130 | 0.36271 |
| C | -4.06826 | -2.69997 | 2.10720 |
| H | -4.12872 | -3.78523 | 2.02801 |
| C | -4.72216 | -2.03396 | 3.14842 |
| H | -5.29341 | -2.59912 | 3.88450 |
| C | -4.64268 | -0.64278 | 3.24210 |
| H | -5.15555 | -0.11775 | 4.04782 |
| C | -3.91456 | 0.08647 | 2.29967 |
| H | -3.87007 | 1.17194 | 2.37578 |
| C | -2.40332 | 2.09412 | 0.38598 |
| C | -3.19230 | 2.95393 | -0.39552 |
| H | -3.74479 | 2.56336 | -1.24926 |
| C | -3.27486 | 4.31131 | -0.07762 |
| H | -3.89225 | 4.97007 | -0.68804 |
| C | -2.57663 | 4.82185 | 1.01939 |
| H | -2.64668 | 5.88110 | 1.26610 |
| C | -1.78915 | 3.97197 | 1.80164 |
| H | -1.24626 | 4.36558 | 2.66093 |
| C | -1.69543 | 2.61613 | 1.48482 |
| H | -1.07979 | 1.95737 | 2.09838 |
| C | -3.02392 | 0.04456 | -1.60932 |
| C | -4.31650 | -0.48794 | -1.74887 |
| H | -4.89387 | -0.76104 | -0.86655 |
| C | -4.86732 | -0.66268 | -3.02049 |
| H | -5.87133 | -1.07492 | -3.11909 |
| C | -4.14034 | -0.30620 | -4.15887 |
| H | -4.57469 | -0.44292 | -5.14900 |
| C | -2.85408 | 0.22610 | -4.02647 |
| H | -2.28389 | 0.50660 | -4.91201 |
| C | -2.29424 | 0.39471 | -2.76012 |

| | | | |
|---|---|---|---|
| H | -1.28704 | 0.80149 | -2.66177 |
| P | 2.77779 | 0.21091 | -0.02648 |
| C | 3.07339 | 1.43334 | -1.50065 |
| C | 4.38656 | 2.23319 | -1.39256 |
| H | 4.49273 | 2.84084 | -2.30467 |
| C | 1.89805 | 2.43144 | -1.60721 |
| H | 2.08984 | 3.07715 | -2.47741 |
| H | 1.79028 | 3.08321 | -0.73663 |
| H | 0.94405 | 1.92018 | -1.77862 |
| C | 3.13037 | 1.10529 | 1.65155 |
| C | 4.62878 | 1.26855 | 1.97199 |
| H | 4.71863 | 1.83249 | 2.91338 |
| H | 5.16957 | 1.82980 | 1.20232 |
| H | 5.13729 | 0.31053 | 2.12392 |
| H | 2.85809 | -0.69384 | 2.92346 |
| H | 1.36784 | 0.23210 | 2.62396 |
| H | 2.60772 | 0.85939 | 3.72871 |
| C | 2.47785 | 2.50268 | 1.64661 |
| H | 1.41065 | 2.46586 | 1.39413 |
| H | 2.97886 | 3.20704 | 0.97429 |
| H | 2.56107 | 2.91335 | 2.66419 |
| C | 3.94533 | -1.33397 | -0.20691 |
| C | 3.96751 | -2.12421 | 1.11636 |
| H | 4.52162 | -3.05767 | 0.93657 |
| H | 2.96080 | -2.40370 | 1.45012 |
| H | 4.48142 | -1.59669 | 1.92643 |
| C | 5.39298 | -0.97035 | -0.59065 |
| H | 5.86964 | -0.28618 | 0.11935 |
| H | 5.46751 | -0.53952 | -1.59507 |
| H | 5.98328 | -1.90011 | -0.59677 |
| C | 3.36782 | -2.28595 | -1.27512 |
| H | 3.32630 | -1.84802 | -2.27564 |
| H | 2.36646 | -2.63906 | -1.00839 |
| H | 4.02650 | -3.16593 | -1.33078 |
| H | 4.38600 | 2.92756 | -0.54484 |
| H | 5.27439 | 1.59709 | -1.31906 |
| C | 3.07816 | 0.63621 | -2.82105 |
| H | 3.08185 | 1.35846 | -3.65113 |
| H | 3.96487 | 0.00496 | -2.93976 |
| H | 2.18048 | 0.01378 | -2.93174 |
| C | 2.44959 | 0.31114 | 2.78779 |

Vibrational Spectrum (first 50 lines):

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|---|
| # | | | cm**(-1) | km/mol | IR RAMAN |
| | 1 | a | -105.13 | 0.00000 | YES YES |
| | 2 | | 0.00 | 0.00000 | - - |
| | 3 | | 0.00 | 0.00000 | - - |
| | 4 | | 0.00 | 0.00000 | - - |
| | 5 | | 0.00 | 0.00000 | - - |
| | 6 | | 0.00 | 0.00000 | - - |
| | 7 | | 0.00 | 0.00000 | - - |
| | 8 | a | 4.41 | 0.09151 | YES YES |
| | 9 | a | 15.16 | 0.14058 | YES YES |
| | 10 | a | 20.26 | 0.02065 | YES YES |
| | 11 | a | 21.50 | 0.17716 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 38.04 | 0.15963 | YES | YES |
| 13 | a | 40.29 | 1.13567 | YES | YES |
| 14 | a | 44.79 | 0.02871 | YES | YES |
| 15 | a | 47.47 | 0.06975 | YES | YES |
| 16 | a | 53.34 | 0.15940 | YES | YES |
| 17 | a | 59.51 | 0.06070 | YES | YES |
| 18 | a | 63.77 | 0.39381 | YES | YES |
| 19 | a | 66.50 | 0.20239 | YES | YES |
| 20 | a | 72.87 | 0.51145 | YES | YES |
| 21 | a | 75.79 | 0.28929 | YES | YES |
| 22 | a | 94.41 | 2.53930 | YES | YES |
| 23 | a | 97.34 | 0.01362 | YES | YES |
| 24 | a | 102.87 | 0.13526 | YES | YES |
| 25 | a | 117.24 | 0.61976 | YES | YES |
| 26 | a | 127.92 | 0.26599 | YES | YES |
| 27 | a | 150.95 | 0.81404 | YES | YES |
| 28 | a | 179.38 | 0.15911 | YES | YES |
| 29 | a | 183.69 | 0.93329 | YES | YES |
| 30 | a | 188.39 | 0.22895 | YES | YES |
| 31 | a | 191.57 | 0.08246 | YES | YES |
| 32 | a | 193.85 | 1.66083 | YES | YES |
| 33 | a | 196.58 | 0.67236 | YES | YES |
| 34 | a | 201.98 | 0.57376 | YES | YES |
| 35 | a | 203.77 | 1.74605 | YES | YES |
| 36 | a | 206.81 | 0.69400 | YES | YES |
| 37 | a | 228.36 | 40.03558 | YES | YES |
| 38 | a | 234.14 | 8.36631 | YES | YES |
| 39 | a | 237.08 | 0.42205 | YES | YES |
| 40 | a | 240.49 | 2.25699 | YES | YES |
| 41 | a | 244.71 | 1.30295 | YES | YES |
| 42 | a | 249.78 | 1.42594 | YES | YES |
| 43 | a | 253.86 | 1.45398 | YES | YES |
| 44 | a | 254.99 | 0.06047 | YES | YES |
| 45 | a | 259.56 | 0.51575 | YES | YES |
| 46 | a | 266.94 | 1.10574 | YES | YES |
| 47 | a | 275.48 | 0.16143 | YES | YES |
| 48 | a | 278.80 | 0.07496 | YES | YES |
| 49 | a | 286.71 | 0.50619 | YES | YES |
| 50 | a | 296.27 | 6.81316 | YES | YES |

**TS [PhSe(PPh3)2]+**

bp86_def2-tzvpp energy (au): -4706.6644306490

Zero point energy (au): 0.6230801
Entropy (kJ mol^-1): 1.14497
Chemical potential (kJ mol^-1): 1408.97

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.75073 | 0.66993 | 3.32819 |
| H | -5.81641 | 0.83179 | 3.48905 |
| C | 2.78999 | 2.36186 | 4.06305 |
| H | 3.87825 | 2.37051 | 4.00520 |
| Se | -0.13599 | 0.00026 | -0.00261 |
| P | -0.22961 | 0.01465 | 2.60713 |
| C | 0.72202 | 3.33800 | 4.85264 |
| H | 0.19273 | 4.10727 | 5.41470 |
| C | -4.05244 | 1.46632 | 2.41618 |
| H | -4.57089 | 2.24985 | 1.86385 |
| C | -2.00828 | 0.25294 | 2.91822 |
| C | 2.07344 | 1.35622 | 3.41517 |
| H | 2.60767 | 0.58938 | 2.85359 |
| C | 0.88463 | -4.06519 | 4.48187 |
| H | 1.13727 | -5.03308 | 4.91441 |
| C | 0.66778 | 1.32833 | 3.49318 |
| C | 3.90257 | 1.19460 | -0.21987 |
| H | 4.44298 | 2.12573 | -0.39022 |
| C | -2.68883 | 1.25768 | 2.20544 |
| H | -2.15027 | 1.87951 | 1.48928 |
| C | 0.23762 | -1.57400 | 3.36969 |
| C | 0.22730 | -3.99982 | 3.24929 |
| H | -0.03448 | -4.91552 | 2.71930 |
| C | -0.00365 | 2.33003 | 4.21389 |
| H | -1.09046 | 2.31859 | 4.28514 |
| C | 2.11659 | 3.35579 | 4.78021 |
| H | 2.67941 | 4.14211 | 5.28279 |
| C | -2.71660 | -0.54560 | 3.83129 |
| H | -2.20211 | -1.32974 | 4.38554 |
| C | 0.89665 | -1.64558 | 4.60816 |
| H | 1.15530 | -0.73342 | 5.14441 |
| C | -0.08963 | -2.76168 | 2.69059 |
| H | -0.59302 | -2.71383 | 1.72392 |
| C | 2.50673 | -1.19395 | 0.21110 |
| H | 1.96303 | -2.12423 | 0.36818 |
| C | -4.08211 | -0.33474 | 4.03230 |
| H | -4.62355 | -0.95711 | 4.74454 |
| C | 1.21846 | -2.88896 | 5.15735 |
| H | 1.72858 | -2.93594 | 6.11933 |
| C | 3.90468 | -1.18617 | 0.21917 |
| H | 4.44675 | -2.11619 | 0.39030 |
| C | 2.50459 | 1.19949 | -0.21385 |
| H | 1.95920 | 2.12869 | -0.37153 |
| C | 4.60275 | 0.00494 | 0.00022 |
| H | 5.69265 | 0.00608 | 0.00119 |

| | | | |
|---|---|---|---|
| C | 1.80938 | 0.00204 | -0.00191 |
| C | -4.74339 | -0.68610 | -3.34350 |
| H | -5.80795 | -0.85147 | -3.50812 |
| C | 2.80512 | -2.34897 | -4.05844 |
| H | 3.89353 | -2.35053 | -4.00290 |
| P | -0.22720 | -0.01481 | -2.60755 |
| C | 0.74159 | -3.34226 | -4.83828 |
| H | 0.21595 | -4.11785 | -5.39505 |
| C | -4.04899 | -1.47027 | -2.41809 |
| H | -4.56931 | -2.24780 | -1.85912 |
| C | -2.00410 | -0.25956 | -2.92321 |
| C | 2.08376 | -1.34422 | -3.41454 |
| H | 2.61447 | -0.57097 | -2.85845 |
| C | 0.87592 | 4.06988 | -4.47786 |
| H | 1.12596 | 5.03893 | -4.90930 |
| C | 0.67776 | -1.32553 | -3.48973 |
| C | -2.68683 | -1.25698 | -2.20240 |
| H | -2.15117 | -1.86949 | -1.47614 |
| C | 0.23609 | 1.57577 | -3.36818 |
| C | 0.21440 | 4.00145 | -3.24768 |
| H | -0.05341 | 4.91592 | -2.71859 |
| C | 0.01103 | -2.33537 | -4.20347 |
| H | -1.07599 | -2.33102 | -4.27250 |
| C | 2.13640 | -3.35099 | -4.76867 |
| H | 2.70305 | -4.13666 | -5.26797 |
| C | -2.70851 | 0.52669 | -3.84997 |
| H | -2.19222 | 1.30519 | -4.41053 |
| C | 0.89909 | 1.65037 | -4.60438 |
| H | 1.16354 | 0.73945 | -5.13993 |
| C | -0.09908 | 2.76190 | -2.69023 |
| H | -0.60587 | 2.71173 | -1.72546 |
| C | -4.07246 | 0.31107 | -4.05611 |
| H | -4.61096 | 0.92388 | -4.77879 |
| C | 1.21731 | 2.89524 | -5.15232 |
| H | 1.73055 | 2.94461 | -6.11252 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 6.98 | 0.00874 | YES YES |
| 8 | a | 11.78 | 6.74251 | YES YES |
| 9 | a | 14.79 | 14.13999 | YES YES |
| 10 | a | 15.94 | 0.17845 | YES YES |
| 11 | a | 21.80 | 11.92777 | YES YES |
| 12 | a | 23.48 | 0.03073 | YES YES |
| 13 | a | 27.97 | 30.97163 | YES YES |
| 14 | a | 34.66 | 0.00841 | YES YES |
| 15 | a | 36.04 | 0.03166 | YES YES |
| 16 | a | 37.43 | 0.07089 | YES YES |
| 17 | a | 38.38 | 7.85350 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 18 | a | 42.86 | 6.96687 | YES | YES |
| 19 | a | 47.20 | 0.43758 | YES | YES |
| 20 | a | 51.43 | 7.32219 | YES | YES |
| 21 | a | 53.42 | 0.03007 | YES | YES |
| 22 | a | 55.14 | 0.03419 | YES | YES |
| 23 | a | 58.95 | 0.02637 | YES | YES |
| 24 | a | 60.78 | 22.65174 | YES | YES |
| 25 | a | 63.87 | 0.05345 | YES | YES |
| 26 | a | 66.66 | 1.06814 | YES | YES |
| 27 | a | 73.61 | 35.68194 | YES | YES |
| 28 | a | 93.96 | 0.00656 | YES | YES |
| 29 | a | 112.23 | 0.93814 | YES | YES |
| 30 | a | 113.07 | 0.02208 | YES | YES |
| 31 | a | 182.63 | 2.08559 | YES | YES |
| 32 | a | 182.74 | 0.55094 | YES | YES |
| 33 | a | 190.44 | 0.52263 | YES | YES |
| 34 | a | 191.52 | 4.58471 | YES | YES |
| 35 | a | 199.11 | 5.91609 | YES | YES |
| 36 | a | 201.48 | 0.51860 | YES | YES |
| 37 | a | 207.61 | 19.55412 | YES | YES |
| 38 | a | 236.08 | 5.97702 | YES | YES |
| 39 | a | 236.69 | 0.44570 | YES | YES |
| 40 | a | 237.75 | 0.22737 | YES | YES |
| 41 | a | 253.29 | 0.35217 | YES | YES |
| 42 | a | 253.49 | 1.01558 | YES | YES |
| 43 | a | 259.64 | 0.71820 | YES | YES |
| 44 | a | 260.80 | 0.41027 | YES | YES |
| 45 | a | 299.24 | 0.35525 | YES | YES |
| 46 | a | 388.79 | 0.51184 | YES | YES |
| 47 | a | 389.58 | 0.07956 | YES | YES |
| 48 | a | 390.14 | 0.97301 | YES | YES |
| 49 | a | 390.54 | 1.66298 | YES | YES |
| 50 | a | 390.85 | 0.29472 | YES | YES |

**TS [PhSe(PPh3)(PtBu3)]+**

bp86_def2-tzvpp energy (au): -4485.1441041940

Zero point energy (au): 0.7146932
Entropy (kJ mol^-1): 1.11732
Chemical potential (kJ mol^-1): 1663.24

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.15356 | 0.34112 | 0.00997 |
| Se | 0.35045 | 0.08028 | 0.00742 |
| C | 0.20676 | -1.86383 | -0.02562 |
| C | -0.04315 | -2.52108 | -1.23794 |
| H | -0.13945 | -1.94957 | -2.16005 |
| C | -0.17369 | -3.91282 | -1.25879 |
| H | -0.37098 | -4.42066 | -2.20285 |
| C | -0.04436 | -4.64884 | -0.07753 |
| H | -0.13833 | -5.73441 | -0.09825 |
| C | 0.20327 | -3.99060 | 1.12994 |
| H | 0.29816 | -4.55912 | 2.05510 |
| C | 0.32093 | -2.59776 | 1.16132 |
| H | 0.49268 | -2.08645 | 2.10668 |
| C | -3.10624 | -0.57434 | 1.25918 |
| C | -3.17327 | -1.97827 | 1.16956 |
| H | -2.68292 | -2.50158 | 0.34861 |
| C | -3.87777 | -2.70578 | 2.12804 |
| H | -3.93275 | -3.79107 | 2.04633 |
| C | -4.50845 | -2.04812 | 3.18871 |
| H | -5.05636 | -2.62049 | 3.93689 |
| C | -4.43793 | -0.65665 | 3.28608 |
| H | -4.93364 | -0.13883 | 4.10692 |
| C | -3.74097 | 0.08171 | 2.32766 |
| H | -3.70265 | 1.16729 | 2.40590 |
| C | -2.34383 | 2.11971 | 0.34327 |
| C | -3.17960 | 2.92967 | -0.44311 |
| H | -3.73583 | 2.49807 | -1.27431 |
| C | -3.30016 | 4.29155 | -0.15989 |
| H | -3.95163 | 4.91299 | -0.77387 |
| C | -2.59301 | 4.85447 | 0.90537 |
| H | -2.69105 | 5.91768 | 1.12356 |
| C | -1.75887 | 4.05376 | 1.69088 |
| H | -1.20719 | 4.48965 | 2.52355 |
| C | -1.62771 | 2.69301 | 1.41078 |
| H | -0.97374 | 2.07306 | 2.02504 |
| C | -2.90502 | 0.00717 | -1.61483 |
| C | -4.19479 | -0.53683 | -1.73769 |
| H | -4.77015 | -0.79100 | -0.84851 |
| C | -4.74455 | -0.74864 | -3.00399 |
| H | -5.74565 | -1.17031 | -3.09158 |
| C | -4.01921 | -0.41785 | -4.15111 |
| H | -4.45247 | -0.58477 | -5.13705 |
| C | -2.73654 | 0.12659 | -4.03385 |
| H | -2.16855 | 0.38657 | -4.92693 |
| C | -2.17694 | 0.33371 | -2.77310 |

| | | | |
|---|---|---|---|
| H | -1.17218 | 0.74855 | -2.68387 |
| P | 3.18697 | 0.26570 | -0.00059 |
| C | 3.48147 | 1.86484 | -1.05204 |
| C | 4.83859 | 2.55070 | -0.80488 |
| H | 4.92212 | 3.41118 | -1.48731 |
| C | 2.34652 | 2.87172 | -0.75710 |
| H | 2.50194 | 3.75549 | -1.39465 |
| H | 2.32232 | 3.21828 | 0.27899 |
| H | 1.36157 | 2.45855 | -1.01015 |
| C | 3.72327 | 0.59087 | 1.83073 |
| C | 5.24482 | 0.56105 | 2.06900 |
| H | 5.43572 | 0.80193 | 3.12658 |
| H | 5.78338 | 1.29821 | 1.46326 |
| H | 5.68250 | -0.42565 | 1.88175 |
| H | 3.34970 | -1.49429 | 2.50066 |
| H | 1.94980 | -0.40570 | 2.64262 |
| H | 3.31229 | -0.26283 | 3.77060 |
| C | 3.17710 | 1.95327 | 2.30331 |
| H | 2.09430 | 2.04093 | 2.14450 |
| H | 3.67647 | 2.80603 | 1.83168 |
| H | 3.35682 | 2.03131 | 3.38636 |
| C | 4.22092 | -1.19643 | -0.73784 |
| C | 4.24300 | -2.36498 | 0.26811 |
| H | 4.70385 | -3.23058 | -0.23134 |
| H | 3.23348 | -2.66535 | 0.57694 |
| H | 4.84092 | -2.15344 | 1.16093 |
| C | 5.67077 | -0.83299 | -1.10958 |
| H | 6.24867 | -0.45603 | -0.25881 |
| H | 5.72610 | -0.09701 | -1.91948 |
| H | 6.17292 | -1.74475 | -1.46974 |
| C | 3.49256 | -1.72100 | -1.99431 |
| H | 3.46965 | -1.00238 | -2.81734 |
| H | 2.46414 | -2.02491 | -1.76728 |
| H | 4.03016 | -2.61231 | -2.35235 |
| H | 4.93507 | 2.94054 | 0.21454 |
| H | 5.69056 | 1.89167 | -1.00376 |
| C | 3.36609 | 1.52299 | -2.55123 |
| H | 3.36394 | 2.46814 | -3.11507 |
| H | 4.20835 | 0.92939 | -2.92182 |
| H | 2.43054 | 0.99809 | -2.78489 |
| C | 3.04255 | -0.46903 | 2.72356 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 8.48 | 1.17542 | YES YES |
| 8 | a | 13.23 | 0.91487 | YES YES |
| 9 | a | 18.79 | 3.69991 | YES YES |
| 10 | a | 22.00 | 0.00420 | YES YES |
| 11 | a | 31.42 | 63.55966 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 37.35 | 0.25456 | YES | YES |
| 13 | a | 39.48 | 2.49895 | YES | YES |
| 14 | a | 41.24 | 0.34000 | YES | YES |
| 15 | a | 44.02 | 0.10519 | YES | YES |
| 16 | a | 51.00 | 0.22987 | YES | YES |
| 17 | a | 54.43 | 2.28576 | YES | YES |
| 18 | a | 57.59 | 0.28908 | YES | YES |
| 19 | a | 63.69 | 0.09133 | YES | YES |
| 20 | a | 68.22 | 2.15612 | YES | YES |
| 21 | a | 73.94 | 0.05894 | YES | YES |
| 22 | a | 90.98 | 0.01817 | YES | YES |
| 23 | a | 96.35 | 1.20451 | YES | YES |
| 24 | a | 105.22 | 9.94324 | YES | YES |
| 25 | a | 109.08 | 22.56805 | YES | YES |
| 26 | a | 114.57 | 1.59598 | YES | YES |
| 27 | a | 127.62 | 0.27708 | YES | YES |
| 28 | a | 176.59 | 0.02614 | YES | YES |
| 29 | a | 183.62 | 0.43155 | YES | YES |
| 30 | a | 184.75 | 0.99157 | YES | YES |
| 31 | a | 190.20 | 0.09874 | YES | YES |
| 32 | a | 193.86 | 1.12672 | YES | YES |
| 33 | a | 195.94 | 0.58679 | YES | YES |
| 34 | a | 197.60 | 1.40683 | YES | YES |
| 35 | a | 199.95 | 5.30642 | YES | YES |
| 36 | a | 203.63 | 0.94013 | YES | YES |
| 37 | a | 210.81 | 17.35136 | YES | YES |
| 38 | a | 233.22 | 0.23167 | YES | YES |
| 39 | a | 235.78 | 2.95039 | YES | YES |
| 40 | a | 237.37 | 1.33481 | YES | YES |
| 41 | a | 239.64 | 0.23901 | YES | YES |
| 42 | a | 242.15 | 0.11022 | YES | YES |
| 43 | a | 251.79 | 0.35250 | YES | YES |
| 44 | a | 253.56 | 0.42028 | YES | YES |
| 45 | a | 254.17 | 0.31978 | YES | YES |
| 46 | a | 261.71 | 0.58318 | YES | YES |
| 47 | a | 265.26 | 0.39003 | YES | YES |
| 48 | a | 274.01 | 0.08699 | YES | YES |
| 49 | a | 276.10 | 0.06460 | YES | YES |
| 50 | a | 284.68 | 0.55118 | YES | YES |

## BP86-D3/SV(P) level optimisations

**$PPh_3$**

bp86-d3 energy (au): -1035.7698037320

Zero point energy (au): 0.2662863
Entropy (kJ mol^-1): 0.55429
Chemical potential (kJ mol^-1): 578.91

XYZ coordinates:

34

| | | | |
|---|---|---|---|
| P | 0.00429 | -1.28036 | -0.00149 |
| C | 1.17303 | -0.43712 | 1.16927 |
| C | -0.13259 | -0.99132 | -2.78107 |
| H | -0.78031 | -1.88287 | -2.71300 |
| C | 1.26754 | 0.68600 | -1.71036 |
| H | 1.71428 | 1.12466 | -0.80317 |
| C | 0.42941 | -0.44517 | -1.60428 |
| C | 3.41832 | -0.40569 | 2.14504 |
| H | 4.42528 | -0.84777 | 2.22845 |
| C | 1.53200 | 1.25980 | -2.96622 |
| H | 2.19001 | 2.14234 | -3.03499 |
| C | 0.84540 | 0.70768 | 1.92787 |
| H | -0.15913 | 1.15353 | 1.84232 |
| C | 0.95797 | 0.71775 | -4.12906 |
| H | 1.16647 | 1.17024 | -5.11278 |
| C | 2.46733 | -0.99154 | 1.29432 |
| H | 2.73225 | -1.89348 | 0.71506 |
| C | 1.79415 | 1.28532 | 2.78930 |
| H | 1.52437 | 2.17829 | 3.37805 |
| C | 3.08235 | 0.73369 | 2.89812 |
| H | 3.82505 | 1.18945 | 3.57388 |
| C | 0.12095 | -0.40865 | -4.03304 |
| H | -0.32993 | -0.84276 | -4.94116 |
| C | -2.13926 | 0.64751 | -0.28027 |
| H | -1.60261 | 1.05689 | -1.15165 |
| C | -1.59708 | -0.44547 | 0.42986 |
| C | -2.30369 | -0.95357 | 1.54425 |
| H | -1.89606 | -1.81517 | 2.10166 |
| C | -3.35847 | 1.22176 | 0.12089 |
| H | -3.77196 | 2.07414 | -0.44402 |
| C | -4.04597 | 0.71933 | 1.23891 |
| H | -5.00074 | 1.17286 | 1.55303 |
| C | -3.51304 | -0.36958 | 1.95261 |
| H | -4.04773 | -0.77314 | 2.82874 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 32.15 | 0.31290 | YES YES |
| 8 | a | 35.29 | 0.32629 | YES YES |
| 9 | a | 50.49 | 0.00857 | YES YES |
| 10 | a | 54.16 | 0.09991 | YES YES |
| 11 | a | 55.44 | 0.06705 | YES YES |
| 12 | a | 67.00 | 0.40275 | YES YES |
| 13 | a | 182.11 | 0.27329 | YES YES |
| 14 | a | 197.33 | 1.07961 | YES YES |
| 15 | a | 198.97 | 1.07236 | YES YES |
| 16 | a | 242.23 | 0.69850 | YES YES |
| 17 | a | 254.55 | 0.40265 | YES YES |
| 18 | a | 256.55 | 0.42132 | YES YES |
| 19 | a | 394.71 | 1.31338 | YES YES |
| 20 | a | 394.94 | 1.44041 | YES YES |
| 21 | a | 396.90 | 0.20985 | YES YES |
| 22 | a | 401.71 | 0.18059 | YES YES |
| 23 | a | 419.87 | 5.71722 | YES YES |
| 24 | a | 421.73 | 6.27512 | YES YES |
| 25 | a | 494.26 | 22.69662 | YES YES |
| 26 | a | 496.57 | 23.64416 | YES YES |
| 27 | a | 506.72 | 13.88280 | YES YES |
| 28 | a | 610.28 | 0.24716 | YES YES |
| 29 | a | 610.33 | 0.25081 | YES YES |
| 30 | a | 610.55 | 0.07652 | YES YES |
| 31 | a | 672.07 | 0.73607 | YES YES |
| 32 | a | 685.27 | 1.09568 | YES YES |
| 33 | a | 685.92 | 1.21718 | YES YES |
| 34 | a | 699.43 | 33.82440 | YES YES |
| 35 | a | 699.73 | 33.97641 | YES YES |
| 36 | a | 700.49 | 30.90217 | YES YES |
| 37 | a | 743.91 | 18.17083 | YES YES |
| 38 | a | 744.21 | 14.41482 | YES YES |
| 39 | a | 744.88 | 16.92334 | YES YES |
| 40 | a | 836.78 | 0.06642 | YES YES |
| 41 | a | 837.46 | 0.10913 | YES YES |
| 42 | a | 839.36 | 0.21448 | YES YES |
| 43 | a | 904.10 | 1.05262 | YES YES |
| 44 | a | 905.04 | 0.87668 | YES YES |
| 45 | a | 906.19 | 0.37407 | YES YES |
| 46 | a | 957.58 | 0.03406 | YES YES |
| 47 | a | 957.79 | 0.07613 | YES YES |
| 48 | a | 958.71 | 0.10424 | YES YES |
| 49 | a | 982.06 | 0.02845 | YES YES |
| 50 | a | 982.27 | 0.01096 | YES YES |

**$P(^tBu)_3$**

bp86-d3 energy (au): -814.4604618103

Zero point energy (au): 0.3566093
Entropy (kJ mol^-1): 0.53736
Chemical potential (kJ mol^-1): 826.60

XYZ coordinates:

40

| | | | |
|---|---|---|---|
| P | 0.70838 | 0.00056 | -0.00076 |
| C | -0.01952 | 1.71052 | -0.61558 |
| C | -1.49897 | 1.73631 | -1.04902 |
| H | -1.78730 | 2.77602 | -1.33634 |
| C | 0.87505 | 2.16416 | -1.79932 |
| H | 0.60788 | 3.21013 | -2.08122 |
| H | 0.75380 | 1.54313 | -2.70725 |
| H | 1.95132 | 2.15095 | -1.51897 |
| C | -0.01850 | -1.38778 | -1.17430 |
| C | -1.49733 | -1.77774 | -0.97944 |
| H | -1.78346 | -2.54945 | -1.73378 |
| H | -2.18385 | -0.91636 | -1.10987 |
| H | -1.68929 | -2.21851 | 0.02070 |
| H | 0.75630 | -3.11404 | 0.01812 |
| H | 1.95434 | -2.38576 | -1.10049 |
| H | 0.61421 | -3.40644 | -1.73822 |
| C | 0.18981 | -0.95909 | -2.64533 |
| H | 1.23889 | -0.64609 | -2.84268 |
| H | -0.48819 | -0.13888 | -2.95746 |
| H | -0.02672 | -1.82889 | -3.30900 |
| C | -0.01936 | -0.32219 | 1.78843 |
| C | 0.18616 | -1.81126 | 2.15280 |
| H | -0.03039 | -1.95085 | 3.23812 |
| H | 1.23465 | -2.13946 | 1.97961 |
| H | -0.49325 | -2.49071 | 1.59901 |
| C | -1.49797 | 0.04323 | 2.02928 |
| H | -2.18443 | -0.49732 | 1.34627 |
| H | -1.68896 | 1.13052 | 1.91602 |
| H | -1.78412 | -0.22814 | 3.07368 |
| C | 0.87917 | 0.47331 | 2.77203 |
| H | 0.76542 | 1.57089 | 2.68491 |
| H | 1.95388 | 0.22893 | 2.62207 |
| H | 0.60905 | 0.20005 | 3.81976 |
| H | -1.69015 | 1.09401 | -1.93352 |
| H | -2.18448 | 1.41429 | -0.23864 |
| C | 0.18901 | 2.76945 | 0.49209 |
| H | -0.03214 | 3.77918 | 0.07308 |
| H | -0.48635 | 2.62725 | 1.36048 |
| H | 1.23891 | 2.78597 | 0.85868 |
| C | 0.87854 | -2.63807 | -0.97372 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 94.98 | 0.01118 | YES YES |
| 8 | a | 97.85 | 0.01011 | YES YES |
| 9 | a | 125.86 | 0.00042 | YES YES |
| 10 | a | 174.06 | 0.05013 | YES YES |
| 11 | a | 182.43 | 0.01514 | YES YES |
| 12 | a | 184.20 | 0.01973 | YES YES |
| 13 | a | 202.74 | 0.03690 | YES YES |
| 14 | a | 203.68 | 0.00756 | YES YES |
| 15 | a | 209.96 | 0.05360 | YES YES |
| 16 | a | 241.04 | 0.19185 | YES YES |
| 17 | a | 243.06 | 0.02876 | YES YES |
| 18 | a | 250.69 | 0.14086 | YES YES |
| 19 | a | 258.79 | 0.29993 | YES YES |
| 20 | a | 261.10 | 0.27941 | YES YES |
| 21 | a | 272.39 | 0.02564 | YES YES |
| 22 | a | 278.53 | 0.04371 | YES YES |
| 23 | a | 285.30 | 0.07696 | YES YES |
| 24 | a | 297.72 | 0.02508 | YES YES |
| 25 | a | 330.90 | 0.23616 | YES YES |
| 26 | a | 340.44 | 0.30393 | YES YES |
| 27 | a | 345.74 | 0.32420 | YES YES |
| 28 | a | 354.94 | 0.00399 | YES YES |
| 29 | a | 367.64 | 0.18594 | YES YES |
| 30 | a | 369.55 | 0.22521 | YES YES |
| 31 | a | 401.27 | 0.43498 | YES YES |
| 32 | a | 402.35 | 0.30160 | YES YES |
| 33 | a | 405.20 | 0.18501 | YES YES |
| 34 | a | 452.51 | 3.40440 | YES YES |
| 35 | a | 454.90 | 3.46408 | YES YES |
| 36 | a | 475.44 | 0.73520 | YES YES |
| 37 | a | 534.12 | 0.18770 | YES YES |
| 38 | a | 560.14 | 4.95399 | YES YES |
| 39 | a | 561.38 | 4.97673 | YES YES |
| 40 | a | 794.83 | 11.23698 | YES YES |
| 41 | a | 796.62 | 8.94612 | YES YES |
| 42 | a | 799.33 | 4.93817 | YES YES |
| 43 | a | 909.62 | 2.15722 | YES YES |
| 44 | a | 910.64 | 2.12114 | YES YES |
| 45 | a | 912.82 | 2.01517 | YES YES |
| 46 | a | 917.98 | 0.29397 | YES YES |
| 47 | a | 919.89 | 1.03659 | YES YES |
| 48 | a | 921.16 | 1.32819 | YES YES |
| 49 | a | 923.04 | 0.25391 | YES YES |
| 50 | a | 929.07 | 0.84492 | YES YES |

**$[GaCl_4]^-$**

bp86-d3 energy (au): -3765.6467668620

Zero point energy (au): 0.0047297
Entropy (kJ mol^-1): 0.36230
Chemical potential (kJ mol^-1): -73.01

XYZ coordinates:

5

| | | | |
|---|---|---|---|
| Ga | 0.00000 | 0.00000 | 0.00000 |
| Cl | -1.28496 | -1.28496 | -1.28496 |
| Cl | 1.28496 | 1.28496 | -1.28496 |
| Cl | 1.28496 | -1.28496 | 1.28496 |
| Cl | -1.28496 | 1.28496 | 1.28496 |

Vibrational Spectrum:

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | e | 101.76 | 0.00000 | NO YES |
| 8 | e | 101.76 | 0.00000 | NO YES |
| 9 | t2 | 144.55 | 8.12793 | YES YES |
| 10 | t2 | 144.55 | 8.12793 | YES YES |
| 11 | t2 | 144.55 | 8.12793 | YES YES |
| 12 | a1 | 320.38 | 0.00000 | NO YES |
| 13 | t2 | 372.84 | 79.84398 | YES YES |
| 14 | t2 | 372.84 | 79.84398 | YES YES |
| 15 | t2 | 372.84 | 79.84398 | YES YES |

**[PhS]+**

bp86-d3 energy (au): -629.2658134425

Zero point energy (au): 0.0881591
Entropy (kJ mol^-1): 0.32772
Chemical potential (kJ mol^-1): 151.80

XYZ coordinates:

12

| | | | |
|---|---|---|---|
| C | -2.27113 | -0.00004 | -0.00119 |
| H | -3.37521 | -0.00010 | -0.00238 |
| C | -0.20150 | 1.26401 | 0.00060 |
| H | 0.37069 | 2.20616 | 0.00074 |
| C | -1.58504 | 1.24925 | 0.00005 |
| H | -2.15956 | 2.18920 | -0.00010 |
| C | 0.54061 | 0.00004 | 0.00145 |
| C | -0.20142 | -1.26399 | 0.00136 |
| H | 0.37087 | -2.20609 | 0.00260 |
| C | -1.58496 | -1.24931 | -0.00094 |
| H | -2.15947 | -2.18927 | -0.00197 |
| S | 2.20671 | 0.00009 | 0.00163 |

Vibrational Spectrum:

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 106.84 | 0.00164 | YES YES |
| 8 | a | 295.77 | 0.00879 | YES YES |
| 9 | a | 312.55 | 0.00000 | YES YES |
| 10 | a | 372.83 | 0.20396 | YES YES |
| 11 | a | 429.46 | 0.14956 | YES YES |
| 12 | a | 565.99 | 2.46135 | YES YES |
| 13 | a | 612.09 | 43.38502 | YES YES |
| 14 | a | 719.20 | 3.02552 | YES YES |
| 15 | a | 785.02 | 27.55994 | YES YES |
| 16 | a | 797.81 | 0.00004 | YES YES |
| 17 | a | 962.66 | 5.37220 | YES YES |
| 18 | a | 979.45 | 0.73765 | YES YES |
| 19 | a | 986.36 | 7.67765 | YES YES |
| 20 | a | 991.02 | 0.00134 | YES YES |
| 21 | a | 1024.22 | 1.74026 | YES YES |
| 22 | a | 1072.36 | 4.86080 | YES YES |
| 23 | a | 1120.56 | 23.94002 | YES YES |
| 24 | a | 1148.19 | 11.54427 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 25 | a | 1178.11 | 0.00238 | YES | YES |
| 26 | a | 1238.93 | 6.56263 | YES | YES |
| 27 | a | 1351.07 | 0.02878 | YES | YES |
| 28 | a | 1411.53 | 17.22923 | YES | YES |
| 29 | a | 1463.16 | 107.88925 | YES | YES |
| 30 | a | 1508.13 | 12.06342 | YES | YES |
| 31 | a | 1607.27 | 129.92595 | YES | YES |
| 32 | a | 3117.38 | 0.54578 | YES | YES |
| 33 | a | 3128.36 | 2.15047 | YES | YES |
| 34 | a | 3130.09 | 10.98934 | YES | YES |
| 35 | a | 3139.19 | 18.64368 | YES | YES |
| 36 | a | 3141.76 | 0.54627 | YES | YES |

**PhSCl.GaCl3_iso2**

bp86-d3 energy (au): -4395.1032251820

Zero point energy (au): 0.0945176
Entropy (kJ mol^-1): 0.56797
Chemical potential (kJ mol^-1): 121.37

XYZ coordinates:

17

| | | | |
|---|---|---|---|
| S | 0.40571 | 0.37937 | 1.56638 |
| C | -1.07418 | -0.33503 | 0.94011 |
| C | -1.10588 | -0.87162 | -0.37209 |
| H | -0.17760 | -0.90818 | -0.96298 |
| C | -2.31224 | -1.36639 | -0.88308 |
| H | -2.34341 | -1.78831 | -1.90057 |
| C | -3.48229 | -1.32186 | -0.09941 |
| H | -4.43008 | -1.70821 | -0.50965 |
| C | -3.45237 | -0.79156 | 1.20536 |
| H | -4.37152 | -0.76310 | 1.81252 |
| C | -2.24929 | -0.30653 | 1.73394 |
| H | -2.20210 | 0.10226 | 2.75565 |
| Ga | 3.30625 | -1.66686 | 0.64709 |
| Cl | 1.46190 | -1.39158 | 2.35225 |
| Cl | 4.30998 | -3.28908 | 1.66981 |
| Cl | 4.17308 | 0.31268 | 0.71137 |
| Cl | 2.18806 | -2.18899 | -1.14470 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 12.46 | 0.14365 | YES YES |
| 8 | a | 20.28 | 0.05025 | YES YES |
| 9 | a | 48.44 | 0.82016 | YES YES |
| 10 | a | 58.06 | 0.52122 | YES YES |
| 11 | a | 63.36 | 0.57575 | YES YES |
| 12 | a | 88.97 | 0.09527 | YES YES |
| 13 | a | 100.97 | 0.14568 | YES YES |
| 14 | a | 122.21 | 5.20121 | YES YES |
| 15 | a | 126.31 | 5.81994 | YES YES |
| 16 | a | 137.92 | 32.07820 | YES YES |
| 17 | a | 179.90 | 47.80343 | YES YES |
| 18 | a | 215.79 | 18.84567 | YES YES |
| 19 | a | 278.47 | 2.03664 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 20 | a | 335.39 | 45.73264 | YES | YES |
| 21 | a | 352.08 | 15.33068 | YES | YES |
| 22 | a | 398.66 | 5.81921 | YES | YES |
| 23 | a | 407.89 | 5.32813 | YES | YES |
| 24 | a | 420.01 | 72.60686 | YES | YES |
| 25 | a | 432.95 | 59.15668 | YES | YES |
| 26 | a | 482.92 | 11.37661 | YES | YES |
| 27 | a | 602.64 | 0.29355 | YES | YES |
| 28 | a | 680.66 | 35.02066 | YES | YES |
| 29 | a | 707.77 | 3.13431 | YES | YES |
| 30 | a | 753.81 | 27.40125 | YES | YES |
| 31 | a | 827.42 | 0.60697 | YES | YES |
| 32 | a | 925.67 | 3.33422 | YES | YES |
| 33 | a | 966.01 | 0.54052 | YES | YES |
| 34 | a | 984.55 | 0.62993 | YES | YES |
| 35 | a | 996.62 | 0.26781 | YES | YES |
| 36 | a | 1017.72 | 0.22026 | YES | YES |
| 37 | a | 1068.50 | 54.61205 | YES | YES |
| 38 | a | 1072.05 | 9.65245 | YES | YES |
| 39 | a | 1146.62 | 0.31120 | YES | YES |
| 40 | a | 1160.79 | 4.13916 | YES | YES |
| 41 | a | 1282.84 | 1.06542 | YES | YES |
| 42 | a | 1368.23 | 5.34013 | YES | YES |
| 43 | a | 1434.09 | 17.41831 | YES | YES |
| 44 | a | 1455.52 | 0.59157 | YES | YES |
| 45 | a | 1575.00 | 0.11215 | YES | YES |
| 46 | a | 1591.45 | 41.42320 | YES | YES |
| 47 | a | 3101.22 | 0.74324 | YES | YES |
| 48 | a | 3112.38 | 6.72857 | YES | YES |
| 49 | a | 3118.74 | 4.25033 | YES | YES |
| 50 | a | 3126.18 | 0.91898 | YES | YES |

**[PhSe]+**

bp86-d3 energy (au): -2632.7085547570

Zero point energy (au): 0.0876113
Entropy (kJ mol^-1): 0.33945
Chemical potential (kJ mol^-1): 147.35

XYZ coordinates:

12

| | | | |
|---|---|---|---|
| C | -3.00873 | -0.00007 | -0.00008 |
| H | -4.11243 | -0.00013 | -0.00037 |
| C | -0.93370 | 1.25859 | 0.00000 |
| H | -0.36827 | 2.20459 | -0.00005 |
| C | -2.31983 | 1.24540 | 0.00017 |
| H | -2.89039 | 2.18771 | 0.00048 |
| C | -0.20121 | 0.00001 | -0.00004 |
| C | -0.93361 | -1.25861 | 0.00002 |
| H | -0.36815 | -2.20460 | 0.00003 |
| C | -2.31975 | -1.24550 | 0.00014 |
| H | -2.89025 | -2.18784 | 0.00009 |
| Se | 1.61530 | 0.00010 | 0.00006 |

Vibrational Spectrum:

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 98.48 | 0.03634 | YES YES |
| 8 | a | 245.70 | 0.00012 | YES YES |
| 9 | a | 320.25 | 0.00000 | YES YES |
| 10 | a | 332.82 | 0.01790 | YES YES |
| 11 | a | 377.28 | 0.00470 | YES YES |
| 12 | a | 569.14 | 1.90212 | YES YES |
| 13 | a | 617.24 | 44.10139 | YES YES |
| 14 | a | 683.75 | 2.81686 | YES YES |
| 15 | a | 774.51 | 28.66936 | YES YES |
| 16 | a | 803.40 | 0.00001 | YES YES |
| 17 | a | 966.99 | 10.95317 | YES YES |
| 18 | a | 970.61 | 0.79099 | YES YES |
| 19 | a | 988.95 | 0.00006 | YES YES |
| 20 | a | 991.67 | 7.35393 | YES YES |
| 21 | a | 1020.49 | 1.14774 | YES YES |
| 22 | a | 1061.17 | 27.33189 | YES YES |
| 23 | a | 1074.93 | 4.69664 | YES YES |
| 24 | a | 1149.25 | 8.25896 | YES YES |
| 25 | a | 1171.71 | 2.67890 | YES YES |
| 26 | a | 1248.63 | 8.37431 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 27 | a | 1355.09 | 0.00104 | YES | YES |
| 28 | a | 1415.42 | 13.73272 | YES | YES |
| 29 | a | 1453.76 | 90.14781 | YES | YES |
| 30 | a | 1506.65 | 6.12037 | YES | YES |
| 31 | a | 1602.18 | 140.24812 | YES | YES |
| 32 | a | 3118.51 | 0.16997 | YES | YES |
| 33 | a | 3127.97 | 1.81433 | YES | YES |
| 34 | a | 3129.99 | 9.15290 | YES | YES |
| 35 | a | 3138.82 | 14.73619 | YES | YES |
| 36 | a | 3141.57 | 0.42953 | YES | YES |

**PhSeCl.GaCl3_iso2**

bp86-d3 energy (au): -6398.5502833220

Zero point energy (au): 0.0937974
Entropy (kJ mol^-1): 0.57719
Chemical potential (kJ mol^-1): 117.57

XYZ coordinates:

17

| | | | |
|---|---|---|---|
| Se | 0.48437 | 0.48930 | 1.58748 |
| C | -1.11604 | -0.29949 | 0.92371 |
| C | -1.13764 | -0.85742 | -0.37720 |
| H | -0.21191 | -0.89268 | -0.97255 |
| C | -2.33749 | -1.38149 | -0.87797 |
| H | -2.36147 | -1.82199 | -1.88785 |
| C | -3.50719 | -1.34334 | -0.09450 |
| H | -4.44865 | -1.75321 | -0.49621 |
| C | -3.48346 | -0.79030 | 1.20015 |
| H | -4.40098 | -0.76831 | 1.81020 |
| C | -2.28731 | -0.27447 | 1.71893 |
| H | -2.25145 | 0.14896 | 2.73529 |
| Ga | 3.35550 | -1.70092 | 0.65145 |
| Cl | 1.53215 | -1.42031 | 2.36951 |
| Cl | 4.37500 | -3.34229 | 1.62448 |
| Cl | 4.23466 | 0.27649 | 0.74205 |
| Cl | 2.20592 | -2.17153 | -1.13498 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 14.91 | 0.10925 | YES YES |
| 8 | a | 22.42 | 0.01546 | YES YES |
| 9 | a | 41.79 | 0.42634 | YES YES |
| 10 | a | 54.75 | 0.94806 | YES YES |
| 11 | a | 57.96 | 0.06013 | YES YES |
| 12 | a | 78.90 | 0.50431 | YES YES |
| 13 | a | 98.50 | 0.15225 | YES YES |
| 14 | a | 122.41 | 4.75279 | YES YES |
| 15 | a | 126.65 | 5.94796 | YES YES |
| 16 | a | 138.27 | 28.81732 | YES YES |
| 17 | a | 180.66 | 37.22236 | YES YES |
| 18 | a | 202.40 | 22.14102 | YES YES |
| 19 | a | 236.61 | 0.79937 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 20 | a | 295.36 | 44.49963 | YES | YES |
| 21 | a | 312.39 | 2.15356 | YES | YES |
| 22 | a | 345.55 | 5.41908 | YES | YES |
| 23 | a | 398.17 | 1.94074 | YES | YES |
| 24 | a | 419.53 | 63.86076 | YES | YES |
| 25 | a | 431.41 | 59.20638 | YES | YES |
| 26 | a | 461.41 | 9.11098 | YES | YES |
| 27 | a | 602.33 | 0.25795 | YES | YES |
| 28 | a | 674.17 | 0.69432 | YES | YES |
| 29 | a | 683.72 | 33.49550 | YES | YES |
| 30 | a | 746.19 | 29.33471 | YES | YES |
| 31 | a | 829.07 | 0.50347 | YES | YES |
| 32 | a | 922.57 | 2.94806 | YES | YES |
| 33 | a | 964.93 | 0.53085 | YES | YES |
| 34 | a | 982.28 | 0.89963 | YES | YES |
| 35 | a | 994.99 | 0.27844 | YES | YES |
| 36 | a | 1015.37 | 1.34465 | YES | YES |
| 37 | a | 1053.17 | 37.41026 | YES | YES |
| 38 | a | 1071.16 | 3.29044 | YES | YES |
| 39 | a | 1146.33 | 0.21730 | YES | YES |
| 40 | a | 1162.27 | 6.06721 | YES | YES |
| 41 | a | 1285.02 | 1.84704 | YES | YES |
| 42 | a | 1366.01 | 4.02916 | YES | YES |
| 43 | a | 1431.81 | 16.96160 | YES | YES |
| 44 | a | 1455.29 | 0.51206 | YES | YES |
| 45 | a | 1577.36 | 0.11179 | YES | YES |
| 46 | a | 1587.91 | 29.29802 | YES | YES |
| 47 | a | 3100.36 | 0.66925 | YES | YES |
| 48 | a | 3110.80 | 6.47512 | YES | YES |
| 49 | a | 3117.43 | 4.37290 | YES | YES |
| 50 | a | 3124.19 | 0.75212 | YES | YES |

**[PhSe(PPh3)]+**

bp86-d3 energy (au): -3668.6392661930

Zero point energy (au): 0.3575188
Entropy (kJ mol^-1): 0.70100
Chemical potential (kJ mol^-1): 793.64

XYZ coordinates:

46

| | | | |
|---|---|---|---|
| C | -1.03016 | 5.03770 | -1.15434 |
| H | -1.25897 | 6.08166 | -1.42269 |
| C | 2.75060 | -1.82211 | -1.68876 |
| H | 3.22085 | -2.78446 | -1.43147 |
| Se | -2.01254 | -0.46924 | -0.25725 |
| P | -0.05258 | 0.66535 | -0.03839 |
| C | 2.48545 | 0.06477 | -3.21099 |
| H | 2.75622 | 0.58414 | -4.14413 |
| C | -1.48983 | 3.98836 | -1.97136 |
| H | -2.07821 | 4.20729 | -2.87663 |
| C | -0.45282 | 2.38084 | -0.46745 |
| C | 1.81236 | -1.25807 | -0.81281 |
| H | 1.55694 | -1.77896 | 0.12407 |
| C | 1.46821 | 0.62196 | 4.32358 |
| H | 1.82934 | 0.63259 | 5.36459 |
| C | 1.20775 | -0.02070 | -1.14321 |
| C | -0.27068 | -4.20252 | -1.13315 |
| H | -0.03536 | -4.78052 | -2.04129 |
| C | -1.20631 | 2.65681 | -1.63355 |
| H | -1.57328 | 1.83731 | -2.27356 |
| C | 0.54822 | 0.58075 | 1.67325 |
| C | 0.08548 | 0.60380 | 4.06166 |
| H | -0.63638 | 0.60295 | 4.89393 |
| C | 1.54335 | 0.64131 | -2.34598 |
| H | 1.08445 | 1.60921 | -2.60287 |
| C | 3.08599 | -1.16489 | -2.88575 |
| H | 3.82575 | -1.61201 | -3.56933 |
| C | 0.00558 | 3.43254 | 0.35727 |
| H | 0.58358 | 3.21774 | 1.27035 |
| C | 1.93772 | 0.60739 | 1.93306 |
| H | 2.66468 | 0.61495 | 1.10544 |
| C | -0.37993 | 0.58369 | 2.73879 |
| H | -1.46277 | 0.56249 | 2.53267 |
| C | -0.88737 | -2.72888 | 1.19306 |
| H | -1.13077 | -2.15250 | 2.09918 |
| C | -0.28629 | 4.75991 | 0.00595 |
| H | 0.06749 | 5.58248 | 0.64768 |
| C | 2.39033 | 0.62626 | 3.26229 |
| H | 3.47260 | 0.64369 | 3.46787 |
| C | -0.24792 | -3.97559 | 1.29543 |
| H | 0.00310 | -4.37834 | 2.28992 |
| C | -0.89657 | -2.95022 | -1.25142 |
| H | -1.13580 | -2.53791 | -2.24403 |
| C | 0.06006 | -4.71039 | 0.13538 |
| H | 0.55527 | -5.69103 | 0.22245 |

C -1.19883 -2.22141 -0.08451

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|
| 1 | | 0.00 | 0.00000 | - | - |
| 2 | | 0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 21.18 | 0.08224 | YES | YES |
| 8 | a | 33.59 | 0.01209 | YES | YES |
| 9 | a | 41.66 | 0.22718 | YES | YES |
| 10 | a | 47.53 | 0.15231 | YES | YES |
| 11 | a | 50.70 | 0.06720 | YES | YES |
| 12 | a | 57.65 | 0.21090 | YES | YES |
| 13 | a | 63.24 | 0.08592 | YES | YES |
| 14 | a | 71.20 | 0.13913 | YES | YES |
| 15 | a | 86.57 | 0.09558 | YES | YES |
| 16 | a | 91.85 | 0.48615 | YES | YES |
| 17 | a | 103.08 | 0.32158 | YES | YES |
| 18 | a | 187.28 | 1.61935 | YES | YES |
| 19 | a | 191.72 | 1.65262 | YES | YES |
| 20 | a | 207.58 | 1.49461 | YES | YES |
| 21 | a | 216.01 | 0.35408 | YES | YES |
| 22 | a | 230.71 | 1.29565 | YES | YES |
| 23 | a | 241.29 | 0.55658 | YES | YES |
| 24 | a | 245.39 | 0.79255 | YES | YES |
| 25 | a | 256.98 | 0.39735 | YES | YES |
| 26 | a | 270.49 | 0.27397 | YES | YES |
| 27 | a | 298.93 | 0.65272 | YES | YES |
| 28 | a | 393.50 | 0.13428 | YES | YES |
| 29 | a | 394.75 | 0.03223 | YES | YES |
| 30 | a | 399.06 | 0.09599 | YES | YES |
| 31 | a | 404.39 | 0.21739 | YES | YES |
| 32 | a | 420.22 | 7.19357 | YES | YES |
| 33 | a | 437.71 | 8.04960 | YES | YES |
| 34 | a | 446.17 | 7.42868 | YES | YES |
| 35 | a | 466.04 | 6.24596 | YES | YES |
| 36 | a | 492.91 | 49.04195 | YES | YES |
| 37 | a | 507.33 | 76.41560 | YES | YES |
| 38 | a | 520.46 | 69.82763 | YES | YES |
| 39 | a | 602.48 | 0.00747 | YES | YES |
| 40 | a | 605.07 | 0.49298 | YES | YES |
| 41 | a | 605.88 | 0.11882 | YES | YES |
| 42 | a | 606.53 | 0.07640 | YES | YES |
| 43 | a | 661.14 | 1.96540 | YES | YES |
| 44 | a | 678.50 | 4.19703 | YES | YES |
| 45 | a | 690.41 | 20.87784 | YES | YES |
| 46 | a | 693.04 | 44.31371 | YES | YES |
| 47 | a | 694.62 | 24.96476 | YES | YES |
| 48 | a | 697.59 | 8.43865 | YES | YES |
| 49 | a | 712.06 | 20.48446 | YES | YES |
| 50 | a | 712.92 | 30.78314 | YES | YES |

**[PhSe(PPh3).PPh3]+**

bp86-d3 energy (au): -4704.4492770190

Zero point energy (au): 0.6246469
Entropy (kJ mol^-1): 1.09850
Chemical potential (kJ mol^-1): 1425.06

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.72540 | 0.76239 | 3.98994 |
| H | -5.76085 | 0.94851 | 4.31849 |
| C | 2.93990 | 2.20322 | 3.57757 |
| H | 4.02853 | 2.11255 | 3.43273 |
| Se | -0.52237 | 0.00469 | -0.00390 |
| P | -0.37983 | 0.01228 | 2.56345 |
| C | 1.01348 | 3.42881 | 4.42386 |
| H | 0.58982 | 4.29886 | 4.95121 |
| C | -4.16892 | 1.53279 | 2.95308 |
| H | -4.76520 | 2.32234 | 2.46766 |
| C | -2.08257 | 0.28445 | 3.15326 |
| C | 2.09349 | 1.19625 | 3.09214 |
| H | 2.52480 | 0.32367 | 2.57501 |
| C | 0.95506 | -4.13914 | 4.14291 |
| H | 1.26210 | -5.13278 | 4.50766 |
| C | 0.69361 | 1.30061 | 3.27859 |
| C | 3.52138 | 1.20239 | -0.22700 |
| H | 4.06847 | 2.14110 | -0.41097 |
| C | -2.85315 | 1.29229 | 2.52759 |
| H | -2.42101 | 1.89138 | 1.70798 |
| C | 0.17802 | -1.60050 | 3.20959 |
| C | 0.14199 | -4.03023 | 2.99966 |
| H | -0.19004 | -4.93679 | 2.46800 |
| C | 0.15650 | 2.42374 | 3.94593 |
| H | -0.93059 | 2.51044 | 4.10340 |
| C | 2.40303 | 3.32205 | 4.24051 |
| H | 3.07153 | 4.11219 | 4.61925 |
| C | -2.64405 | -0.48980 | 4.19201 |
| H | -2.05011 | -1.28117 | 4.67734 |
| C | 0.98856 | -1.71168 | 4.36016 |
| H | 1.31723 | -0.80818 | 4.89830 |
| C | -0.24310 | -2.76589 | 2.52921 |
| H | -0.86769 | -2.67847 | 1.62423 |
| C | 2.11606 | -1.19448 | 0.24221 |
| H | 1.56515 | -2.13210 | 0.41211 |
| C | -3.96420 | -0.24762 | 4.60491 |
| H | -4.40118 | -0.85206 | 5.41626 |
| C | 1.37560 | -2.98145 | 4.82029 |
| H | 2.00824 | -3.06529 | 5.71882 |
| C | 3.52117 | -1.18545 | 0.25999 |
| H | 4.06811 | -2.12311 | 0.44952 |
| C | 2.11609 | 1.20858 | -0.22395 |
| H | 1.56516 | 2.14516 | -0.39957 |
| C | 4.22394 | 0.00919 | 0.02035 |

| | | | |
|---|---|---|---|
| H | 5.32603 | 0.01039 | 0.02665 |
| C | 1.41823 | 0.00635 | 0.00555 |
| C | -4.68399 | -0.79262 | -4.03056 |
| H | -5.71456 | -0.98588 | -4.37004 |
| C | 2.98400 | -2.19242 | -3.52937 |
| H | 4.07160 | -2.08904 | -3.38539 |
| P | -0.35757 | -0.01319 | -2.56182 |
| C | 1.06959 | -3.45262 | -4.35183 |
| H | 0.65422 | -4.33751 | -4.86074 |
| C | -4.14034 | -1.54550 | -2.97431 |
| H | -4.74231 | -2.32736 | -2.48353 |
| C | -2.05280 | -0.29802 | -3.16734 |
| C | 2.12814 | -1.18326 | -3.06550 |
| H | 2.55096 | -0.29694 | -2.56483 |
| C | 0.97655 | 4.12867 | -4.16610 |
| H | 1.28320 | 5.12000 | -4.53730 |
| C | 0.72950 | -1.30373 | -3.25158 |
| C | -2.83023 | -1.29706 | -2.53593 |
| H | -2.40814 | -1.88280 | -1.70154 |
| C | 0.20095 | 1.59604 | -3.21591 |
| C | 0.16421 | 4.02692 | -3.02175 |
| H | -0.16745 | 4.93676 | -2.49558 |
| C | 0.20317 | -2.44545 | -3.89582 |
| H | -0.88305 | -2.54542 | -4.05210 |
| C | 2.45797 | -3.32941 | -4.16967 |
| H | 3.13407 | -4.12073 | -4.53203 |
| C | -2.60171 | 0.45902 | -4.22548 |
| H | -2.00258 | 1.24372 | -4.71543 |
| C | 1.01068 | 1.69996 | -4.36796 |
| H | 1.33949 | 0.79299 | -4.90036 |
| C | -0.22062 | 2.76557 | -2.54309 |
| H | -0.84542 | 2.68369 | -1.63770 |
| C | -3.91608 | 0.20861 | -4.65151 |
| H | -4.34346 | 0.80014 | -5.47734 |
| C | 1.39701 | 2.96685 | -4.83648 |
| H | 2.02922 | 3.04513 | -5.73584 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 9.82 | 0.00185 | YES YES |
| 8 | a | 11.67 | 0.12784 | YES YES |
| 9 | a | 19.78 | 0.00869 | YES YES |
| 10 | a | 27.45 | 0.02841 | YES YES |
| 11 | a | 28.69 | 0.00051 | YES YES |
| 12 | a | 30.32 | 0.03207 | YES YES |
| 13 | a | 37.88 | 0.02763 | YES YES |
| 14 | a | 40.87 | 0.12217 | YES YES |
| 15 | a | 41.80 | 2.56135 | YES YES |
| 16 | a | 46.17 | 0.07199 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 17 | a | 47.81 | 2.98025 | YES | YES |
| 18 | a | 50.13 | 2.48620 | YES | YES |
| 19 | a | 53.89 | 0.46315 | YES | YES |
| 20 | a | 58.17 | 0.04022 | YES | YES |
| 21 | a | 59.82 | 0.01247 | YES | YES |
| 22 | a | 64.64 | 16.65256 | YES | YES |
| 23 | a | 74.62 | 0.03550 | YES | YES |
| 24 | a | 80.14 | 0.03730 | YES | YES |
| 25 | a | 85.45 | 37.01558 | YES | YES |
| 26 | a | 94.97 | 0.04067 | YES | YES |
| 27 | a | 100.94 | 89.07462 | YES | YES |
| 28 | a | 104.59 | 0.12209 | YES | YES |
| 29 | a | 115.95 | 1.18782 | YES | YES |
| 30 | a | 125.10 | 0.10082 | YES | YES |
| 31 | a | 184.44 | 2.50071 | YES | YES |
| 32 | a | 185.27 | 0.47879 | YES | YES |
| 33 | a | 194.69 | 0.08360 | YES | YES |
| 34 | a | 195.77 | 4.73525 | YES | YES |
| 35 | a | 204.49 | 1.26848 | YES | YES |
| 36 | a | 205.95 | 3.35746 | YES | YES |
| 37 | a | 220.68 | 12.14932 | YES | YES |
| 38 | a | 238.08 | 7.33413 | YES | YES |
| 39 | a | 238.97 | 0.45796 | YES | YES |
| 40 | a | 240.00 | 0.05790 | YES | YES |
| 41 | a | 253.78 | 0.10006 | YES | YES |
| 42 | a | 254.49 | 1.57173 | YES | YES |
| 43 | a | 265.90 | 0.98981 | YES | YES |
| 44 | a | 266.67 | 0.14756 | YES | YES |
| 45 | a | 306.93 | 0.01850 | YES | YES |
| 46 | a | 393.17 | 0.07531 | YES | YES |
| 47 | a | 393.51 | 0.10457 | YES | YES |
| 48 | a | 394.32 | 1.07868 | YES | YES |
| 49 | a | 394.79 | 0.21548 | YES | YES |
| 50 | a | 395.96 | 0.38292 | YES | YES |

**[PhSe(PtBu3).PPh3]+**

bp86-d3 energy (au): -4483.1448695850

Zero point energy (au): 0.7158782
Entropy (kJ mol^-1): 1.07716
Chemical potential (kJ mol^-1): 1676.02

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.06000 | 0.39231 | -0.02955 |
| Se | 0.51943 | 0.24659 | -0.01159 |
| C | 0.27007 | -1.68248 | 0.02236 |
| C | -0.08794 | -2.34263 | -1.17199 |
| H | -0.17195 | -1.77672 | -2.11293 |
| C | -0.35487 | -3.72195 | -1.15300 |
| H | -0.64229 | -4.23231 | -2.08643 |
| C | -0.25260 | -4.44573 | 0.04890 |
| H | -0.45580 | -5.52874 | 0.05931 |
| C | 0.09962 | -3.78372 | 1.23735 |
| H | 0.16499 | -4.34240 | 2.18502 |
| C | 0.34916 | -2.40008 | 1.23063 |
| H | 0.58803 | -1.88202 | 2.17006 |
| C | -2.95798 | -0.53658 | 1.25498 |
| C | -2.94580 | -1.95109 | 1.19225 |
| H | -2.45500 | -2.46790 | 0.35152 |
| C | -3.57225 | -2.70087 | 2.19785 |
| H | -3.56329 | -3.80126 | 2.13932 |
| C | -4.20261 | -2.05296 | 3.27585 |
| H | -4.69166 | -2.64541 | 4.06611 |
| C | -4.21167 | -0.64877 | 3.34237 |
| H | -4.71200 | -0.13777 | 4.18095 |
| C | -3.59284 | 0.11235 | 2.33700 |
| H | -3.61363 | 1.21269 | 2.39108 |
| C | -2.37260 | 2.17255 | 0.21874 |
| C | -3.27156 | 2.89546 | -0.59521 |
| H | -3.82604 | 2.38260 | -1.39778 |
| C | -3.45700 | 4.27090 | -0.37964 |
| H | -4.16003 | 4.83246 | -1.01590 |
| C | -2.75352 | 4.92885 | 0.64488 |
| H | -2.90404 | 6.00800 | 0.81079 |
| C | -1.85680 | 4.21158 | 1.45749 |
| H | -1.30538 | 4.72608 | 2.26116 |
| C | -1.65842 | 2.83861 | 1.24328 |
| H | -0.95086 | 2.27844 | 1.87822 |
| C | -2.76097 | -0.06518 | -1.65113 |
| C | -3.99141 | -0.74440 | -1.78273 |
| H | -4.57226 | -1.02033 | -0.88795 |
| C | -4.47758 | -1.06685 | -3.06113 |
| H | -5.43879 | -1.59692 | -3.15978 |
| C | -3.74718 | -0.71047 | -4.20795 |
| H | -4.13326 | -0.96489 | -5.20833 |
| C | -2.52295 | -0.02830 | -4.07909 |
| H | -1.94957 | 0.25362 | -4.97718 |
| C | -2.02605 | 0.28926 | -2.80625 |
| H | -1.05946 | 0.81138 | -2.70374 |

| | | | |
|---|---|---|---|
| P | 3.12206 | 0.28747 | 0.02610 |
| C | 3.49229 | 1.79299 | -1.14384 |
| C | 4.87964 | 2.42486 | -0.89698 |
| H | 5.05285 | 3.21120 | -1.66676 |
| C | 2.39781 | 2.87928 | -0.97161 |
| H | 2.64728 | 3.72607 | -1.65069 |
| H | 2.32760 | 3.29533 | 0.04963 |
| H | 1.39340 | 2.51111 | -1.27164 |
| C | 3.58619 | 0.73471 | 1.85613 |
| C | 5.10149 | 0.65151 | 2.14134 |
| H | 5.28729 | 0.99900 | 3.18351 |
| H | 5.70279 | 1.29419 | 1.46760 |
| H | 5.48966 | -0.38546 | 2.07490 |
| H | 3.05573 | -1.28715 | 2.65891 |
| H | 1.72210 | -0.07862 | 2.70678 |
| H | 3.09588 | 0.03879 | 3.85541 |
| C | 3.08317 | 2.15988 | 2.18361 |
| H | 1.99971 | 2.28137 | 1.96464 |
| H | 3.65086 | 2.95431 | 1.65926 |
| H | 3.21894 | 2.33140 | 3.27546 |
| C | 4.08572 | -1.29151 | -0.56583 |
| C | 4.01058 | -2.36890 | 0.54036 |
| H | 4.45404 | -3.30744 | 0.13801 |
| H | 2.96270 | -2.59865 | 0.82804 |
| H | 4.59034 | -2.10331 | 1.44728 |
| C | 5.56434 | -1.00846 | -0.90814 |
| H | 6.13049 | -0.56722 | -0.06376 |
| H | 5.67600 | -0.34656 | -1.79076 |
| H | 6.05440 | -1.97543 | -1.16628 |
| C | 3.37343 | -1.88157 | -1.80729 |
| H | 3.41701 | -1.22894 | -2.69793 |
| H | 2.31318 | -2.12534 | -1.59673 |
| H | 3.88403 | -2.83401 | -2.07721 |
| H | 4.94900 | 2.92164 | 0.09222 |
| H | 5.70918 | 1.69502 | -0.98025 |
| C | 3.39642 | 1.31794 | -2.61175 |
| H | 3.44063 | 2.21374 | -3.27157 |
| H | 4.23503 | 0.65716 | -2.90926 |
| H | 2.43414 | 0.80046 | -2.81776 |
| C | 2.81967 | -0.21693 | 2.80703 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 14.53 | 0.05751 | YES YES |
| 8 | a | 16.09 | 0.30470 | YES YES |
| 9 | a | 22.36 | 0.10946 | YES YES |
| 10 | a | 23.53 | 0.05255 | YES YES |
| 11 | a | 40.07 | 1.84542 | YES YES |
| 12 | a | 42.53 | 1.60108 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 13 | a | 48.76 | 0.21770 | YES | YES |
| 14 | a | 51.54 | 0.27052 | YES | YES |
| 15 | a | 56.93 | 0.58064 | YES | YES |
| 16 | a | 59.69 | 6.83413 | YES | YES |
| 17 | a | 64.41 | 12.94037 | YES | YES |
| 18 | a | 75.30 | 3.52564 | YES | YES |
| 19 | a | 79.19 | 50.75650 | YES | YES |
| 20 | a | 84.80 | 3.79246 | YES | YES |
| 21 | a | 96.33 | 0.24863 | YES | YES |
| 22 | a | 99.33 | 0.21237 | YES | YES |
| 23 | a | 101.12 | 10.48168 | YES | YES |
| 24 | a | 110.60 | 26.32649 | YES | YES |
| 25 | a | 120.89 | 0.28130 | YES | YES |
| 26 | a | 126.75 | 0.20136 | YES | YES |
| 27 | a | 130.22 | 0.62904 | YES | YES |
| 28 | a | 169.45 | 0.12635 | YES | YES |
| 29 | a | 186.07 | 0.98397 | YES | YES |
| 30 | a | 190.65 | 0.24054 | YES | YES |
| 31 | a | 195.18 | 1.03127 | YES | YES |
| 32 | a | 197.50 | 2.16851 | YES | YES |
| 33 | a | 202.56 | 1.04701 | YES | YES |
| 34 | a | 204.56 | 0.71344 | YES | YES |
| 35 | a | 209.96 | 0.65247 | YES | YES |
| 36 | a | 212.67 | 0.35926 | YES | YES |
| 37 | a | 223.37 | 14.63232 | YES | YES |
| 38 | a | 236.22 | 5.08841 | YES | YES |
| 39 | a | 238.52 | 0.61282 | YES | YES |
| 40 | a | 241.13 | 0.16744 | YES | YES |
| 41 | a | 249.35 | 1.57257 | YES | YES |
| 42 | a | 256.11 | 0.90689 | YES | YES |
| 43 | a | 256.92 | 0.34352 | YES | YES |
| 44 | a | 259.71 | 0.08091 | YES | YES |
| 45 | a | 262.90 | 0.41841 | YES | YES |
| 46 | a | 265.50 | 0.75888 | YES | YES |
| 47 | a | 277.94 | 0.61046 | YES | YES |
| 48 | a | 287.19 | 0.72795 | YES | YES |
| 49 | a | 289.89 | 0.34367 | YES | YES |
| 50 | a | 305.33 | 1.22120 | YES | YES |

**[PhSe(PPh3).PtBu3]+_iso1**

bp86-d3 energy (au): -4483.1449579760

Zero point energy (au): 0.7159353
Entropy (kJ mol^-1): 1.07382
Chemical potential (kJ mol^-1): 1676.99

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.05013 | 0.38567 | 0.02494 |
| Se | 0.52689 | 0.24054 | 0.00617 |
| C | 0.27717 | -1.68906 | -0.01451 |
| C | -0.09419 | -2.31500 | -1.22318 |
| H | -0.19107 | -1.72238 | -2.14617 |
| C | -0.35793 | -3.69499 | -1.24126 |
| H | -0.65490 | -4.17865 | -2.18585 |
| C | -0.24046 | -4.45329 | -0.06220 |
| H | -0.44059 | -5.53673 | -0.08130 |
| C | 0.12216 | -3.82502 | 1.14134 |
| H | 0.19699 | -4.41015 | 2.07211 |
| C | 0.36934 | -2.44127 | 1.17169 |
| H | 0.61496 | -1.94947 | 2.12332 |
| C | -2.93473 | -0.57858 | 1.29276 |
| C | -2.92434 | -1.99075 | 1.19002 |
| H | -2.44157 | -2.48413 | 0.33069 |
| C | -3.54205 | -2.76819 | 2.17994 |
| H | -3.53401 | -3.86652 | 2.09066 |
| C | -4.16171 | -2.15053 | 3.28164 |
| H | -4.64462 | -2.76471 | 4.05897 |
| C | -4.16864 | -0.74880 | 3.38799 |
| H | -4.66088 | -0.26137 | 4.24517 |
| C | -3.55849 | 0.03998 | 2.39878 |
| H | -3.57698 | 1.13836 | 2.48456 |
| C | -2.35827 | 2.15855 | 0.32538 |
| C | -3.26085 | 2.90538 | -0.46244 |
| H | -3.82239 | 2.41572 | -1.27451 |
| C | -3.44032 | 4.27522 | -0.20935 |
| H | -4.14605 | 4.85543 | -0.82559 |
| C | -2.72719 | 4.90373 | 0.82689 |
| H | -2.87318 | 5.97852 | 1.02251 |
| C | -1.82678 | 4.16248 | 1.61351 |
| H | -1.26753 | 4.65412 | 2.42605 |
| C | -1.63418 | 2.79511 | 1.36162 |
| H | -0.92274 | 2.21639 | 1.97523 |
| C | -2.77070 | -0.02616 | -1.60056 |
| C | -4.00654 | -0.69498 | -1.73561 |
| H | -4.57835 | -0.99141 | -0.84160 |
| C | -4.50971 | -0.98016 | -3.01626 |
| H | -5.47522 | -1.50180 | -3.11755 |
| C | -3.79056 | -0.59765 | -4.16180 |
| H | -4.18956 | -0.82364 | -5.16394 |
| C | -2.56077 | 0.07374 | -4.02939 |
| H | -1.99624 | 0.37622 | -4.92643 |
| C | -2.04730 | 0.35482 | -2.75451 |

| | | | |
|---|---|---|---|
| H | -1.07671 | 0.86907 | -2.64965 |
| P | 3.13226 | 0.27985 | 0.00000 |
| C | 3.48230 | 1.83924 | -1.10411 |
| C | 4.87619 | 2.45594 | -0.85671 |
| H | 5.03385 | 3.28029 | -1.58925 |
| C | 2.39401 | 2.91699 | -0.85558 |
| H | 2.62735 | 3.79401 | -1.50129 |
| H | 2.35002 | 3.28587 | 0.18505 |
| H | 1.38188 | 2.56332 | -1.14709 |
| C | 3.63941 | 0.63738 | 1.83844 |
| C | 5.16025 | 0.53476 | 2.08549 |
| H | 5.37053 | 0.83137 | 3.13862 |
| H | 5.74985 | 1.20660 | 1.43013 |
| H | 5.54180 | -0.49942 | 1.96084 |
| H | 3.11037 | -1.41941 | 2.54908 |
| H | 1.79124 | -0.20315 | 2.69561 |
| H | 3.19551 | -0.15795 | 3.81146 |
| C | 3.15018 | 2.04689 | 2.24581 |
| H | 2.06342 | 2.18347 | 2.05388 |
| H | 3.71175 | 2.86388 | 1.75002 |
| H | 3.30807 | 2.16425 | 3.34197 |
| C | 4.07626 | -1.27136 | -0.68897 |
| C | 4.02135 | -2.40059 | 0.36561 |
| H | 4.45059 | -3.32055 | -0.09136 |
| H | 2.97924 | -2.63955 | 0.66704 |
| H | 4.62342 | -2.18110 | 1.27022 |
| C | 5.54800 | -0.97630 | -1.05056 |
| H | 6.13427 | -0.57540 | -0.19960 |
| H | 5.64258 | -0.27458 | -1.90403 |
| H | 6.02923 | -1.93131 | -1.36381 |
| C | 3.33378 | -1.79856 | -1.94093 |
| H | 3.35542 | -1.10250 | -2.79924 |
| H | 2.27905 | -2.05327 | -1.71656 |
| H | 3.83714 | -2.73583 | -2.27042 |
| H | 4.96931 | 2.90177 | 0.15458 |
| H | 5.70145 | 1.72995 | -0.99560 |
| C | 3.35462 | 1.43677 | -2.59121 |
| H | 3.38971 | 2.36340 | -3.20719 |
| H | 4.18397 | 0.78821 | -2.93773 |
| H | 2.38601 | 0.93351 | -2.80266 |
| C | 2.88945 | -0.35623 | 2.75893 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 14.51 | 0.18890 | YES YES |
| 8 | a | 19.01 | 0.08736 | YES YES |
| 9 | a | 22.12 | 0.01913 | YES YES |
| 10 | a | 23.81 | 0.03401 | YES YES |
| 11 | a | 39.76 | 1.69714 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 43.07 | 0.72429 | YES | YES |
| 13 | a | 49.17 | 0.21573 | YES | YES |
| 14 | a | 52.51 | 0.40483 | YES | YES |
| 15 | a | 57.00 | 0.30357 | YES | YES |
| 16 | a | 59.65 | 3.04814 | YES | YES |
| 17 | a | 64.29 | 14.55168 | YES | YES |
| 18 | a | 76.01 | 7.01226 | YES | YES |
| 19 | a | 80.13 | 44.84862 | YES | YES |
| 20 | a | 84.69 | 7.43313 | YES | YES |
| 21 | a | 97.45 | 0.31551 | YES | YES |
| 22 | a | 100.82 | 0.90663 | YES | YES |
| 23 | a | 101.70 | 10.21644 | YES | YES |
| 24 | a | 111.39 | 27.81139 | YES | YES |
| 25 | a | 122.52 | 0.53719 | YES | YES |
| 26 | a | 129.37 | 0.45343 | YES | YES |
| 27 | a | 130.44 | 0.18611 | YES | YES |
| 28 | a | 172.26 | 0.08249 | YES | YES |
| 29 | a | 186.26 | 1.01767 | YES | YES |
| 30 | a | 194.06 | 0.48233 | YES | YES |
| 31 | a | 196.40 | 1.44044 | YES | YES |
| 32 | a | 198.08 | 1.42628 | YES | YES |
| 33 | a | 203.54 | 0.72158 | YES | YES |
| 34 | a | 207.65 | 0.67918 | YES | YES |
| 35 | a | 211.04 | 0.84578 | YES | YES |
| 36 | a | 220.49 | 0.80103 | YES | YES |
| 37 | a | 223.69 | 14.19091 | YES | YES |
| 38 | a | 235.81 | 4.66947 | YES | YES |
| 39 | a | 237.88 | 2.70666 | YES | YES |
| 40 | a | 238.42 | 0.19335 | YES | YES |
| 41 | a | 249.08 | 0.87318 | YES | YES |
| 42 | a | 256.03 | 0.99504 | YES | YES |
| 43 | a | 258.39 | 0.27667 | YES | YES |
| 44 | a | 258.93 | 0.42761 | YES | YES |
| 45 | a | 263.90 | 0.03628 | YES | YES |
| 46 | a | 265.25 | 0.74886 | YES | YES |
| 47 | a | 278.03 | 0.64266 | YES | YES |
| 48 | a | 287.37 | 0.68078 | YES | YES |
| 49 | a | 290.14 | 0.23826 | YES | YES |
| 50 | a | 305.41 | 1.28756 | YES | YES |

**[PhSe(PtBu3)]+**

bp86-d3 energy (au): -3447.3362016530

Zero point energy (au): 0.4484289
Entropy (kJ mol^-1): 0.68672
Chemical potential (kJ mol^-1): 1042.13

XYZ coordinates:

52

| | | | |
|---|---|---|---|
| P | 1.13004 | 0.10147 | -0.10517 |
| C | -4.81655 | 0.51798 | -0.47879 |
| H | -5.82068 | 0.83784 | -0.80018 |
| C | 1.67337 | 1.57515 | 1.03778 |
| C | -2.78224 | 0.93026 | 0.80157 |
| H | -2.21303 | 1.56146 | 1.49723 |
| C | 2.35997 | 1.01973 | 2.30587 |
| H | 2.53406 | 1.87417 | 2.99726 |
| H | 3.34875 | 0.56171 | 2.10598 |
| H | 1.71683 | 0.29269 | 2.84685 |
| C | -4.06039 | 1.33441 | 0.38072 |
| H | -4.47228 | 2.29025 | 0.74251 |
| C | 2.14945 | -2.28621 | -1.30532 |
| H | 2.86915 | -3.13230 | -1.23622 |
| H | 2.25830 | -1.85412 | -2.31991 |
| H | 1.12997 | -2.71191 | -1.19149 |
| C | -2.25357 | -0.28921 | 0.33459 |
| C | 2.49226 | -1.28635 | -0.17838 |
| C | -3.01622 | -1.12361 | -0.51038 |
| H | -2.61589 | -2.09288 | -0.84747 |
| C | -0.27829 | 1.97101 | -1.74627 |
| H | -0.63807 | 2.23017 | -2.76708 |
| H | 0.28317 | 2.85002 | -1.37198 |
| H | -1.17689 | 1.80894 | -1.11583 |
| C | 3.88469 | -0.66707 | -0.43629 |
| H | 4.60769 | -1.50278 | -0.57050 |
| H | 4.24990 | -0.06130 | 0.41723 |
| H | 3.92775 | -0.05036 | -1.35547 |
| C | -0.25883 | -0.37953 | -2.57630 |
| H | -1.21689 | -0.56033 | -2.05377 |
| H | 0.26088 | -1.34409 | -2.71555 |
| H | -0.50718 | 0.00744 | -3.58988 |
| C | 0.42421 | 2.34843 | 1.51663 |
| H | 0.77381 | 3.21433 | 2.12210 |
| H | -0.20614 | 1.71731 | 2.17720 |
| H | -0.20169 | 2.75189 | 0.69930 |
| C | 2.63550 | 2.53148 | 0.29752 |
| H | 2.13880 | 3.08504 | -0.52456 |
| H | 3.53526 | 2.02513 | -0.10551 |
| H | 2.99022 | 3.29135 | 1.02934 |
| C | 0.59255 | 0.69982 | -1.87009 |
| C | 2.51913 | -2.09210 | 1.14544 |
| H | 1.58183 | -2.66540 | 1.30956 |
| H | 2.73062 | -1.48566 | 2.04426 |
| H | 3.33691 | -2.84254 | 1.05932 |

| | | | |
|---|---|---|---|
| C | 1.84374 | 1.00795 | -2.72494 |
| H | 1.49090 | 1.44010 | -3.68826 |
| H | 2.42438 | 0.09763 | -2.97605 |
| H | 2.52433 | 1.75156 | -2.26595 |
| C | -4.29869 | -0.71433 | -0.91316 |
| H | -4.89552 | -1.36782 | -1.56976 |
| Se | -0.56556 | -1.00343 | 0.98490 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 37.10 | 0.22039 | YES YES |
| 8 | a | 55.74 | 0.25609 | YES YES |
| 9 | a | 74.73 | 0.24968 | YES YES |
| 10 | a | 92.18 | 0.24566 | YES YES |
| 11 | a | 96.15 | 0.29907 | YES YES |
| 12 | a | 115.02 | 0.17546 | YES YES |
| 13 | a | 124.84 | 0.11192 | YES YES |
| 14 | a | 129.93 | 0.14944 | YES YES |
| 15 | a | 160.15 | 0.44793 | YES YES |
| 16 | a | 169.07 | 0.12673 | YES YES |
| 17 | a | 196.63 | 0.41706 | YES YES |
| 18 | a | 198.84 | 1.05364 | YES YES |
| 19 | a | 202.25 | 0.95272 | YES YES |
| 20 | a | 208.08 | 0.72376 | YES YES |
| 21 | a | 210.28 | 0.34971 | YES YES |
| 22 | a | 226.40 | 0.11909 | YES YES |
| 23 | a | 232.15 | 0.35772 | YES YES |
| 24 | a | 237.70 | 0.39068 | YES YES |
| 25 | a | 244.08 | 0.42183 | YES YES |
| 26 | a | 256.22 | 0.40457 | YES YES |
| 27 | a | 257.80 | 0.10006 | YES YES |
| 28 | a | 264.93 | 0.25973 | YES YES |
| 29 | a | 280.63 | 0.21286 | YES YES |
| 30 | a | 283.78 | 0.07534 | YES YES |
| 31 | a | 288.88 | 0.28309 | YES YES |
| 32 | a | 297.40 | 0.07679 | YES YES |
| 33 | a | 303.14 | 1.56584 | YES YES |
| 34 | a | 332.93 | 0.45836 | YES YES |
| 35 | a | 348.35 | 0.52299 | YES YES |
| 36 | a | 354.59 | 0.55820 | YES YES |
| 37 | a | 369.17 | 1.24517 | YES YES |
| 38 | a | 376.65 | 0.09925 | YES YES |
| 39 | a | 380.74 | 0.17650 | YES YES |
| 40 | a | 405.42 | 0.68901 | YES YES |
| 41 | a | 406.10 | 0.31961 | YES YES |
| 42 | a | 408.31 | 0.37545 | YES YES |
| 43 | a | 411.72 | 0.61020 | YES YES |
| 44 | a | 458.42 | 10.47858 | YES YES |
| 45 | a | 460.76 | 8.75900 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 46 | a | 473.58 | 6.38361 | YES | YES |
| 47 | a | 496.65 | 26.77595 | YES | YES |
| 48 | a | 535.21 | 11.13578 | YES | YES |
| 49 | a | 565.15 | 3.51503 | YES | YES |
| 50 | a | 569.66 | 0.96611 | YES | YES |

**[PhS(PPh3)]+**

bp86-d3 energy (au): -1665.2026239570

Zero point energy (au): 0.3585327
Entropy (kJ mol^-1): 0.68915
Chemical potential (kJ mol^-1): 798.64

XYZ coordinates:

46

| | | | |
|---|---|---|---|
| P | 0.24249 | 0.58302 | 0.04101 |
| S | 2.11264 | -0.42410 | 0.16243 |
| C | 1.50583 | -2.11679 | 0.04701 |
| C | 1.22490 | -2.68302 | -1.21358 |
| H | 1.39010 | -2.10122 | -2.13349 |
| C | 0.72291 | -3.99294 | -1.27840 |
| H | 0.49793 | -4.44173 | -2.25925 |
| C | 0.51879 | -4.73189 | -0.09807 |
| H | 0.13120 | -5.76180 | -0.15599 |
| C | 0.81817 | -4.16487 | 1.15338 |
| H | 0.66501 | -4.74575 | 2.07698 |
| C | 1.30851 | -2.85144 | 1.23351 |
| H | 1.52671 | -2.39156 | 2.20977 |
| C | -0.95440 | -0.15515 | 1.17873 |
| C | -1.53758 | -1.40400 | 0.85268 |
| H | -1.30436 | -1.90340 | -0.10163 |
| C | -2.42187 | -2.00842 | 1.75729 |
| H | -2.87598 | -2.97957 | 1.50425 |
| C | -2.72391 | -1.37961 | 2.97839 |
| H | -3.42121 | -1.85846 | 3.68472 |
| C | -2.14369 | -0.13926 | 3.30010 |
| H | -2.38693 | 0.35566 | 4.25383 |
| C | -1.25610 | 0.47795 | 2.40590 |
| H | -0.81225 | 1.45387 | 2.65948 |
| C | 0.62370 | 2.29484 | 0.48823 |
| C | 0.07330 | 3.35186 | -0.27105 |
| H | -0.55751 | 3.14192 | -1.14968 |
| C | 0.34308 | 4.67817 | 0.10052 |
| H | -0.08144 | 5.50569 | -0.48983 |
| C | 1.15523 | 4.94890 | 1.21604 |
| H | 1.36618 | 5.99236 | 1.50053 |
| C | 1.70620 | 3.89414 | 1.96702 |
| H | 2.34790 | 4.10846 | 2.83644 |
| C | 1.44506 | 2.56324 | 1.60916 |
| H | 1.88490 | 1.73895 | 2.19413 |
| C | -0.40671 | 0.50873 | -1.65012 |
| C | -1.80239 | 0.49383 | -1.87312 |
| H | -2.50709 | 0.46083 | -1.02704 |
| C | -2.28935 | 0.52500 | -3.18989 |
| H | -3.37642 | 0.50915 | -3.36854 |
| C | -1.39480 | 0.57309 | -4.27351 |
| H | -1.78297 | 0.59364 | -5.30463 |
| C | -0.00567 | 0.59555 | -4.04744 |
| H | 0.69369 | 0.63494 | -4.89776 |
| C | 0.49431 | 0.56406 | -2.73769 |

H 1.58171 0.57657 -2.55743

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|
| 1 | | 0.00 | 0.00000 | - | - |
| 2 | | 0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 22.19 | 0.06566 | YES | YES |
| 8 | a | 31.12 | 0.01335 | YES | YES |
| 9 | a | 42.45 | 0.16126 | YES | YES |
| 10 | a | 46.58 | 0.06843 | YES | YES |
| 11 | a | 49.72 | 0.08357 | YES | YES |
| 12 | a | 58.00 | 0.14987 | YES | YES |
| 13 | a | 64.53 | 0.08094 | YES | YES |
| 14 | a | 73.09 | 0.20524 | YES | YES |
| 15 | a | 88.15 | 0.12172 | YES | YES |
| 16 | a | 103.88 | 0.49614 | YES | YES |
| 17 | a | 117.83 | 0.70494 | YES | YES |
| 18 | a | 187.81 | 1.61225 | YES | YES |
| 19 | a | 201.85 | 1.44981 | YES | YES |
| 20 | a | 213.01 | 1.79037 | YES | YES |
| 21 | a | 220.34 | 0.05476 | YES | YES |
| 22 | a | 241.87 | 0.71209 | YES | YES |
| 23 | a | 257.67 | 0.40197 | YES | YES |
| 24 | a | 268.20 | 0.61230 | YES | YES |
| 25 | a | 286.20 | 1.78473 | YES | YES |
| 26 | a | 317.69 | 2.81672 | YES | YES |
| 27 | a | 393.06 | 0.18354 | YES | YES |
| 28 | a | 393.96 | 0.02564 | YES | YES |
| 29 | a | 400.27 | 0.94402 | YES | YES |
| 30 | a | 403.66 | 0.03557 | YES | YES |
| 31 | a | 405.99 | 2.48077 | YES | YES |
| 32 | a | 437.51 | 6.65760 | YES | YES |
| 33 | a | 440.35 | 4.39988 | YES | YES |
| 34 | a | 450.42 | 6.83502 | YES | YES |
| 35 | a | 481.13 | 14.01029 | YES | YES |
| 36 | a | 497.26 | 55.81321 | YES | YES |
| 37 | a | 514.10 | 82.39456 | YES | YES |
| 38 | a | 547.59 | 60.70290 | YES | YES |
| 39 | a | 604.09 | 0.01115 | YES | YES |
| 40 | a | 605.10 | 0.52506 | YES | YES |
| 41 | a | 605.62 | 0.23716 | YES | YES |
| 42 | a | 606.72 | 0.46902 | YES | YES |
| 43 | a | 679.52 | 7.46182 | YES | YES |
| 44 | a | 688.21 | 1.40409 | YES | YES |
| 45 | a | 691.49 | 11.23322 | YES | YES |
| 46 | a | 692.63 | 53.92074 | YES | YES |
| 47 | a | 694.15 | 26.98044 | YES | YES |
| 48 | a | 697.69 | 12.64124 | YES | YES |
| 49 | a | 714.20 | 27.58473 | YES | YES |
| 50 | a | 715.17 | 32.94511 | YES | YES |

**[PhS(PPh3).PPh3]+**

bp86-d3 energy (au): -2701.0038358300

Zero point energy (au): 0.6254154
Entropy (kJ mol^-1): 1.09049
Chemical potential (kJ mol^-1): 1428.62

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.71849 | 0.61946 | 3.77926 |
| H | -5.76888 | 0.76673 | 4.07883 |
| C | 2.87683 | 2.35776 | 3.63580 |
| H | 3.96901 | 2.33819 | 3.48980 |
| S | -0.39058 | 0.02653 | -0.12731 |
| P | -0.30678 | 0.04571 | 2.47048 |
| C | 0.88345 | 3.42084 | 4.54438 |
| H | 0.41106 | 4.23454 | 5.11846 |
| C | -4.17859 | 1.37037 | 2.71971 |
| H | -4.80358 | 2.10539 | 2.18689 |
| C | -2.03571 | 0.24095 | 3.01726 |
| C | 2.08803 | 1.33606 | 3.08830 |
| H | 2.56659 | 0.52246 | 2.51842 |
| C | 1.11616 | -4.11292 | 3.96338 |
| H | 1.44661 | -5.10913 | 4.29959 |
| C | 0.68430 | 1.34705 | 3.27715 |
| C | 3.47116 | 1.38493 | -0.22577 |
| H | 3.98608 | 2.34755 | -0.37563 |
| C | -2.84307 | 1.17816 | 2.33205 |
| H | -2.42231 | 1.75855 | 1.49332 |
| C | 0.27600 | -1.56476 | 3.10465 |
| C | 0.26924 | -3.99237 | 2.84591 |
| H | -0.06555 | -4.89300 | 2.30575 |
| C | 0.08490 | 2.39792 | 4.00627 |
| H | -1.00608 | 2.41325 | 4.16145 |
| C | 2.27708 | 3.40362 | 4.36141 |
| H | 2.89927 | 4.20703 | 4.78818 |
| C | -2.58150 | -0.51355 | 4.07910 |
| H | -1.95812 | -1.25020 | 4.61181 |
| C | 1.12162 | -1.68931 | 4.22793 |
| H | 1.45208 | -0.79214 | 4.77568 |
| C | -0.14523 | -2.72427 | 2.41264 |
| H | -0.79620 | -2.62743 | 1.52730 |
| C | 2.14958 | -1.07223 | 0.16470 |
| H | 1.62611 | -2.03020 | 0.30423 |
| C | -3.92097 | -0.32199 | 4.45451 |
| H | -4.34482 | -0.91100 | 5.28411 |
| C | 1.53967 | -2.96251 | 4.65095 |
| H | 2.19852 | -3.05502 | 5.52974 |
| C | 3.55115 | -1.00954 | 0.22132 |
| H | 4.12883 | -1.92803 | 0.41289 |
| C | 2.06753 | 1.33679 | -0.26036 |
| H | 1.48187 | 2.25276 | -0.43047 |
| C | 4.21306 | 0.21535 | 0.01926 |
| H | 5.31369 | 0.25924 | 0.05599 |

| | | | |
|---|---|---|---|
| C | 1.40954 | 0.10458 | -0.07182 |
| C | -4.73945 | -1.05397 | -3.53973 |
| H | -5.78404 | -1.30185 | -3.78879 |
| C | 3.02686 | -2.06111 | -3.57965 |
| H | 4.11454 | -1.89440 | -3.52238 |
| P | -0.35657 | -0.03185 | -2.46434 |
| C | 1.13155 | -3.46153 | -4.19834 |
| H | 0.73187 | -4.39144 | -4.63401 |
| C | -4.08203 | -1.74505 | -2.50593 |
| H | -4.60925 | -2.53237 | -1.94352 |
| C | -2.07649 | -0.41870 | -2.90530 |
| C | 2.15193 | -1.07761 | -3.09747 |
| H | 2.55789 | -0.14929 | -2.66325 |
| C | 0.61640 | 4.14656 | -4.20553 |
| H | 0.83580 | 5.14734 | -4.61149 |
| C | 0.75266 | -1.28358 | -3.17331 |
| C | -2.75352 | -1.42865 | -2.18206 |
| H | -2.24160 | -1.96506 | -1.36614 |
| C | 0.06410 | 1.59296 | -3.16712 |
| C | -0.12767 | 4.01791 | -3.01788 |
| H | -0.49234 | 4.91578 | -2.49309 |
| C | 0.24459 | -2.48170 | -3.72384 |
| H | -0.84283 | -2.64619 | -3.79267 |
| C | 2.52019 | -3.25418 | -4.12704 |
| H | 3.21221 | -4.02508 | -4.50302 |
| C | -2.73862 | 0.27706 | -3.94083 |
| H | -2.21529 | 1.06940 | -4.50006 |
| C | 0.80518 | 1.72180 | -4.36231 |
| H | 1.16558 | 0.82680 | -4.89426 |
| C | -0.40251 | 2.74588 | -2.49480 |
| H | -0.97341 | 2.64229 | -1.55707 |
| C | -4.06884 | -0.04459 | -4.25367 |
| H | -4.58521 | 0.49767 | -5.06201 |
| C | 1.07992 | 3.00059 | -4.87489 |
| H | 1.65871 | 3.10008 | -5.80733 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 11.71 | 0.21045 | YES YES |
| 8 | a | 13.00 | 8.66956 | YES YES |
| 9 | a | 18.15 | 10.35528 | YES YES |
| 10 | a | 26.75 | 7.74266 | YES YES |
| 11 | a | 28.31 | 0.50355 | YES YES |
| 12 | a | 30.86 | 3.64463 | YES YES |
| 13 | a | 32.00 | 27.08949 | YES YES |
| 14 | a | 38.23 | 0.04784 | YES YES |
| 15 | a | 42.79 | 16.49858 | YES YES |
| 16 | a | 45.86 | 0.07016 | YES YES |
| 17 | a | 49.15 | 2.90867 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 18 | a | 50.33 | 8.30642 | YES | YES |
| 19 | a | 54.21 | 2.58702 | YES | YES |
| 20 | a | 57.78 | 1.47180 | YES | YES |
| 21 | a | 60.03 | 0.03597 | YES | YES |
| 22 | a | 62.58 | 55.30686 | YES | YES |
| 23 | a | 74.04 | 1.37743 | YES | YES |
| 24 | a | 78.47 | 37.44591 | YES | YES |
| 25 | a | 80.16 | 18.80348 | YES | YES |
| 26 | a | 93.84 | 49.82913 | YES | YES |
| 27 | a | 97.58 | 0.08996 | YES | YES |
| 28 | a | 120.17 | 2.73324 | YES | YES |
| 29 | a | 134.49 | 50.58788 | YES | YES |
| 30 | a | 143.80 | 0.89577 | YES | YES |
| 31 | a | 182.23 | 1.97841 | YES | YES |
| 32 | a | 186.73 | 1.00007 | YES | YES |
| 33 | a | 193.15 | 1.48712 | YES | YES |
| 34 | a | 198.34 | 2.43543 | YES | YES |
| 35 | a | 204.22 | 2.60378 | YES | YES |
| 36 | a | 210.18 | 3.77843 | YES | YES |
| 37 | a | 235.00 | 54.05797 | YES | YES |
| 38 | a | 238.66 | 1.17082 | YES | YES |
| 39 | a | 239.32 | 0.21173 | YES | YES |
| 40 | a | 253.48 | 1.38052 | YES | YES |
| 41 | a | 256.29 | 4.42552 | YES | YES |
| 42 | a | 265.40 | 0.81542 | YES | YES |
| 43 | a | 266.35 | 0.53460 | YES | YES |
| 44 | a | 300.66 | 7.42217 | YES | YES |
| 45 | a | 391.76 | 1.04254 | YES | YES |
| 46 | a | 393.17 | 0.30215 | YES | YES |
| 47 | a | 394.67 | 0.39932 | YES | YES |
| 48 | a | 394.99 | 0.98549 | YES | YES |
| 49 | a | 395.35 | 0.28036 | YES | YES |
| 50 | a | 398.41 | 5.24020 | YES | YES |

**[PhS(PtBu3).PPh3]+**

bp86-d3 energy (au): -2479.7007241250

Zero point energy (au): 0.7168914
Entropy (kJ mol^-1): 1.06541
Chemical potential (kJ mol^-1): 1681.15

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -1.97819 | 0.20015 | 0.50655 |
| S | 0.93595 | -0.01080 | 0.51307 |
| C | 0.58300 | -1.76621 | 0.27169 |
| C | 0.27543 | -2.29030 | -0.99915 |
| H | 0.31135 | -1.65401 | -1.89470 |
| C | -0.13704 | -3.62883 | -1.11598 |
| H | -0.38471 | -4.03002 | -2.11158 |
| C | -0.25818 | -4.43793 | 0.02569 |
| H | -0.58636 | -5.48528 | -0.07189 |
| C | 0.01938 | -3.90218 | 1.29735 |
| H | -0.09906 | -4.52299 | 2.19994 |
| C | 0.43211 | -2.56734 | 1.42391 |
| H | 0.60901 | -2.13214 | 2.42006 |
| C | -3.46699 | -0.64525 | 1.17481 |
| C | -3.36623 | -2.03878 | 1.39660 |
| H | -2.42172 | -2.56474 | 1.17248 |
| C | -4.46433 | -2.75474 | 1.89982 |
| H | -4.38172 | -3.84188 | 2.06282 |
| C | -5.66055 | -2.08303 | 2.20840 |
| H | -6.51931 | -2.64292 | 2.61335 |
| C | -5.75794 | -0.69467 | 2.00708 |
| H | -6.69374 | -0.16582 | 2.25184 |
| C | -4.66816 | 0.02516 | 1.48962 |
| H | -4.75348 | 1.11249 | 1.33003 |
| C | -2.26124 | 1.99961 | 0.74897 |
| C | -3.01734 | 2.80311 | -0.13395 |
| H | -3.48029 | 2.35258 | -1.02731 |
| C | -3.17701 | 4.17508 | 0.12176 |
| H | -3.76954 | 4.79484 | -0.57116 |
| C | -2.58962 | 4.75669 | 1.26010 |
| H | -2.71843 | 5.83348 | 1.45753 |
| C | -1.84057 | 3.96306 | 2.14657 |
| H | -1.38302 | 4.41423 | 3.04231 |
| C | -1.67303 | 2.59196 | 1.88962 |
| H | -1.08561 | 1.96802 | 2.58505 |
| C | -2.08073 | -0.04231 | -1.31693 |
| C | -2.75572 | -1.14234 | -1.88974 |
| H | -3.37629 | -1.79859 | -1.25864 |
| C | -2.63832 | -1.41256 | -3.26390 |
| H | -3.17536 | -2.27297 | -3.69597 |
| C | -1.85098 | -0.58885 | -4.08682 |
| H | -1.76478 | -0.80060 | -5.16503 |
| C | -1.19081 | 0.52104 | -3.52810 |
| H | -0.58588 | 1.18505 | -4.16778 |
| C | -1.29960 | 0.78923 | -2.15479 |

| | | | |
|---|---|---|---|
| H | -0.77583 | 1.66049 | -1.72737 |
| P | 3.05601 | 0.32890 | 0.06126 |
| C | 3.47077 | -0.07097 | -1.78940 |
| C | 4.73810 | 0.67370 | -2.26707 |
| H | 4.94675 | 0.35171 | -3.31246 |
| C | 2.27494 | 0.32494 | -2.68770 |
| H | 2.42682 | -0.13723 | -3.68846 |
| H | 2.19076 | 1.41547 | -2.84520 |
| H | 1.30271 | -0.03169 | -2.29746 |
| C | 3.05702 | 2.24793 | 0.38461 |
| C | 4.49984 | 2.77383 | 0.55641 |
| H | 4.45473 | 3.88486 | 0.60876 |
| H | 5.16585 | 2.51419 | -0.29048 |
| H | 4.97083 | 2.42607 | 1.49791 |
| H | 2.53414 | 2.06825 | 2.56121 |
| H | 1.13760 | 2.43786 | 1.48937 |
| H | 2.36163 | 3.69088 | 1.83427 |
| C | 2.38405 | 2.97508 | -0.80344 |
| H | 1.37051 | 2.57681 | -1.02124 |
| H | 2.99334 | 2.95242 | -1.72831 |
| H | 2.26390 | 4.04446 | -0.51990 |
| C | 4.22086 | -0.60775 | 1.29278 |
| C | 3.99188 | -0.04120 | 2.71124 |
| H | 4.55458 | -0.67781 | 3.43012 |
| H | 2.91996 | -0.07925 | 3.00095 |
| H | 4.36676 | 0.99436 | 2.83502 |
| C | 5.70647 | -0.46393 | 0.89407 |
| H | 6.04066 | 0.58768 | 0.79642 |
| H | 5.94454 | -1.00210 | -0.04615 |
| H | 6.32227 | -0.93027 | 1.69616 |
| C | 3.85089 | -2.10875 | 1.34404 |
| H | 3.95557 | -2.63442 | 0.37849 |
| H | 2.82134 | -2.27256 | 1.71263 |
| H | 4.54514 | -2.60009 | 2.06252 |
| H | 4.60461 | 1.77417 | -2.29151 |
| H | 5.63850 | 0.43873 | -1.66575 |
| C | 3.69279 | -1.59508 | -1.93162 |
| H | 3.80311 | -1.82532 | -3.01473 |
| H | 4.62207 | -1.94098 | -1.43582 |
| H | 2.83456 | -2.18872 | -1.55216 |
| C | 2.22433 | 2.60249 | 1.64486 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 7.52 | 0.03061 | YES YES |
| 8 | a | 21.20 | 0.39450 | YES YES |
| 9 | a | 24.11 | 0.03215 | YES YES |
| 10 | a | 30.37 | 1.72877 | YES YES |
| 11 | a | 42.70 | 0.11738 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 43.88 | 1.57672 | YES | YES |
| 13 | a | 50.20 | 0.22534 | YES | YES |
| 14 | a | 53.02 | 0.42411 | YES | YES |
| 15 | a | 54.07 | 1.07991 | YES | YES |
| 16 | a | 62.89 | 0.06616 | YES | YES |
| 17 | a | 66.17 | 1.16532 | YES | YES |
| 18 | a | 72.16 | 1.14437 | YES | YES |
| 19 | a | 83.68 | 0.75470 | YES | YES |
| 20 | a | 89.12 | 1.14240 | YES | YES |
| 21 | a | 95.74 | 9.75236 | YES | YES |
| 22 | a | 107.92 | 1.16322 | YES | YES |
| 23 | a | 111.45 | 0.64719 | YES | YES |
| 24 | a | 128.88 | 0.17124 | YES | YES |
| 25 | a | 131.83 | 0.94460 | YES | YES |
| 26 | a | 140.41 | 2.44510 | YES | YES |
| 27 | a | 143.82 | 0.54087 | YES | YES |
| 28 | a | 169.87 | 11.07762 | YES | YES |
| 29 | a | 178.33 | 13.45314 | YES | YES |
| 30 | a | 184.91 | 0.19633 | YES | YES |
| 31 | a | 192.02 | 2.72208 | YES | YES |
| 32 | a | 193.25 | 2.31891 | YES | YES |
| 33 | a | 205.63 | 2.33740 | YES | YES |
| 34 | a | 209.02 | 0.24246 | YES | YES |
| 35 | a | 211.91 | 0.88728 | YES | YES |
| 36 | a | 217.98 | 0.35361 | YES | YES |
| 37 | a | 234.17 | 0.36871 | YES | YES |
| 38 | a | 237.46 | 4.20043 | YES | YES |
| 39 | a | 239.57 | 1.32203 | YES | YES |
| 40 | a | 245.49 | 1.31435 | YES | YES |
| 41 | a | 247.02 | 1.08931 | YES | YES |
| 42 | a | 256.06 | 2.34671 | YES | YES |
| 43 | a | 259.48 | 5.83795 | YES | YES |
| 44 | a | 267.31 | 0.45389 | YES | YES |
| 45 | a | 269.67 | 16.26427 | YES | YES |
| 46 | a | 282.70 | 0.11862 | YES | YES |
| 47 | a | 284.38 | 17.24354 | YES | YES |
| 48 | a | 289.56 | 5.09931 | YES | YES |
| 49 | a | 294.82 | 16.16556 | YES | YES |
| 50 | a | 307.80 | 2.15273 | YES | YES |

**[PhS(PPh3).PtBu3]+_try4**

bp86-d3 energy (au): -2479.6999708390

Zero point energy (au): 0.7167281
Entropy (kJ mol^-1): 1.06330
Chemical potential (kJ mol^-1): 1681.27

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -1.92174 | 0.38667 | 0.02564 |
| S | 0.39147 | 0.17414 | -0.03847 |
| C | 0.25894 | -1.61861 | -0.09212 |
| C | -0.01373 | -2.26362 | -1.31576 |
| H | -0.11739 | -1.66970 | -2.23702 |
| C | -0.15106 | -3.66132 | -1.34827 |
| H | -0.36617 | -4.16581 | -2.30405 |
| C | -0.00115 | -4.41376 | -0.16895 |
| H | -0.09910 | -5.51092 | -0.20006 |
| C | 0.27209 | -3.76644 | 1.04912 |
| H | 0.38137 | -4.35250 | 1.97580 |
| C | 0.39141 | -2.36765 | 1.09372 |
| H | 0.57616 | -1.85168 | 2.04819 |
| C | -2.77086 | -0.62570 | 1.27093 |
| C | -2.84904 | -2.02530 | 1.06720 |
| H | -2.44939 | -2.47904 | 0.14552 |
| C | -3.43971 | -2.83902 | 2.04385 |
| H | -3.50091 | -3.92668 | 1.87882 |
| C | -3.94407 | -2.27180 | 3.22851 |
| H | -4.40505 | -2.91578 | 3.99488 |
| C | -3.86312 | -0.88331 | 3.43378 |
| H | -4.26500 | -0.43578 | 4.35711 |
| C | -3.27876 | -0.05671 | 2.46061 |
| H | -3.22916 | 1.03183 | 2.62393 |
| C | -2.11060 | 2.14928 | 0.42856 |
| C | -2.97749 | 2.98358 | -0.30990 |
| H | -3.57478 | 2.56889 | -1.13807 |
| C | -3.07380 | 4.34673 | 0.01351 |
| H | -3.75185 | 4.99643 | -0.56301 |
| C | -2.30998 | 4.88048 | 1.06647 |
| H | -2.38805 | 5.95138 | 1.31460 |
| C | -1.44544 | 4.05056 | 1.80299 |
| H | -0.84581 | 4.46814 | 2.62793 |
| C | -1.33889 | 2.68765 | 1.48607 |
| H | -0.65816 | 2.04013 | 2.06308 |
| C | -2.67464 | 0.08071 | -1.60166 |
| C | -3.94654 | -0.51774 | -1.73836 |
| H | -4.51539 | -0.82727 | -0.84700 |
| C | -4.48792 | -0.71472 | -3.01959 |
| H | -5.48030 | -1.18210 | -3.12464 |
| C | -3.77134 | -0.31409 | -4.16072 |
| H | -4.20079 | -0.47110 | -5.16342 |
| C | -2.50622 | 0.28748 | -4.02461 |
| H | -1.94455 | 0.60316 | -4.91865 |
| C | -1.95356 | 0.48179 | -2.75032 |
| H | -0.95685 | 0.94143 | -2.64201 |

| | | | |
|---|---|---|---|
| P | 3.05716 | 0.20138 | -0.03277 |
| C | 3.47713 | 1.34259 | -1.54946 |
| C | 4.80349 | 2.11959 | -1.40695 |
| H | 5.00037 | 2.67346 | -2.35409 |
| C | 2.31967 | 2.35125 | -1.77314 |
| H | 2.56414 | 2.96420 | -2.67032 |
| H | 2.16635 | 3.05502 | -0.93406 |
| H | 1.35695 | 1.83381 | -1.96922 |
| C | 3.35177 | 1.16859 | 1.62436 |
| C | 4.83606 | 1.30030 | 2.02784 |
| H | 4.90435 | 1.92055 | 2.95104 |
| H | 5.44837 | 1.79805 | 1.24897 |
| H | 5.30144 | 0.32128 | 2.26236 |
| H | 2.92800 | -0.57497 | 2.96197 |
| H | 1.48180 | 0.39256 | 2.51209 |
| H | 2.67836 | 1.03487 | 3.69121 |
| C | 2.73751 | 2.58374 | 1.50564 |
| H | 1.67338 | 2.55815 | 1.18521 |
| H | 3.30268 | 3.24344 | 0.81768 |
| H | 2.76805 | 3.06291 | 2.51081 |
| C | 4.17290 | -1.39695 | -0.07427 |
| C | 4.09687 | -2.11128 | 1.29457 |
| H | 4.61670 | -3.09189 | 1.20286 |
| H | 3.04888 | -2.32405 | 1.59340 |
| H | 4.60316 | -1.55419 | 2.10806 |
| C | 5.65207 | -1.11381 | -0.41376 |
| H | 6.12523 | -0.39515 | 0.28536 |
| H | 5.78649 | -0.73584 | -1.44767 |
| H | 6.22156 | -2.06905 | -0.34382 |
| C | 3.57966 | -2.38578 | -1.10844 |
| H | 3.58380 | -2.00420 | -2.14619 |
| H | 2.54177 | -2.67681 | -0.85066 |
| H | 4.19890 | -3.31154 | -1.09919 |
| H | 4.76199 | 2.87613 | -0.59596 |
| H | 5.67402 | 1.46004 | -1.22238 |
| C | 3.52547 | 0.46501 | -2.82171 |
| H | 3.59520 | 1.13378 | -3.70970 |
| H | 4.40770 | -0.20569 | -2.85593 |
| H | 2.60387 | -0.14695 | -2.93786 |
| C | 2.56549 | 0.44850 | 2.75064 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 12.46 | 0.06388 | YES YES |
| 8 | a | 17.28 | 1.18768 | YES YES |
| 9 | a | 23.37 | 0.34490 | YES YES |
| 10 | a | 26.09 | 0.86876 | YES YES |
| 11 | a | 42.39 | 0.55633 | YES YES |
| 12 | a | 46.64 | 0.29436 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 13 | a | 50.82 | 0.28956 | YES | YES |
| 14 | a | 55.16 | 1.87158 | YES | YES |
| 15 | a | 60.29 | 2.27829 | YES | YES |
| 16 | a | 61.42 | 8.39357 | YES | YES |
| 17 | a | 67.48 | 44.40369 | YES | YES |
| 18 | a | 73.64 | 45.90538 | YES | YES |
| 19 | a | 78.41 | 0.05598 | YES | YES |
| 20 | a | 86.76 | 0.01968 | YES | YES |
| 21 | a | 98.48 | 4.17279 | YES | YES |
| 22 | a | 100.11 | 2.10148 | YES | YES |
| 23 | a | 107.40 | 4.52644 | YES | YES |
| 24 | a | 118.27 | 2.07838 | YES | YES |
| 25 | a | 127.09 | 0.10820 | YES | YES |
| 26 | a | 137.36 | 106.81882 | YES | YES |
| 27 | a | 153.04 | 0.84784 | YES | YES |
| 28 | a | 180.23 | 1.64232 | YES | YES |
| 29 | a | 188.12 | 1.25069 | YES | YES |
| 30 | a | 188.37 | 0.00704 | YES | YES |
| 31 | a | 190.02 | 0.21871 | YES | YES |
| 32 | a | 200.09 | 1.60093 | YES | YES |
| 33 | a | 204.37 | 1.95647 | YES | YES |
| 34 | a | 208.82 | 2.49752 | YES | YES |
| 35 | a | 209.96 | 1.11566 | YES | YES |
| 36 | a | 211.64 | 1.93011 | YES | YES |
| 37 | a | 238.29 | 7.41593 | YES | YES |
| 38 | a | 240.98 | 43.03673 | YES | YES |
| 39 | a | 246.07 | 0.24999 | YES | YES |
| 40 | a | 248.32 | 4.95860 | YES | YES |
| 41 | a | 251.61 | 3.30961 | YES | YES |
| 42 | a | 255.76 | 0.59761 | YES | YES |
| 43 | a | 258.21 | 5.26432 | YES | YES |
| 44 | a | 262.55 | 0.13550 | YES | YES |
| 45 | a | 266.30 | 0.64852 | YES | YES |
| 46 | a | 276.94 | 1.23438 | YES | YES |
| 47 | a | 287.57 | 0.04717 | YES | YES |
| 48 | a | 288.64 | 0.13686 | YES | YES |
| 49 | a | 299.62 | 3.00009 | YES | YES |
| 50 | a | 302.76 | 6.22915 | YES | YES |

**[PhS(PtBu3)]+**

bp86-d3 energy (au): -1443.8975144210

Zero point energy (au): 0.4494198
Entropy (kJ mol^-1): 0.67887
Chemical potential (kJ mol^-1): 1046.08

XYZ coordinates:

52

| | | | |
|---|---|---|---|
| P | -0.98935 | -0.00649 | 0.01267 |
| C | 2.20779 | -0.67149 | 0.09442 |
| C | 4.28847 | -0.01147 | 1.17207 |
| H | 4.88057 | 0.13814 | 2.08914 |
| C | 4.85105 | 0.26105 | -0.08741 |
| H | 5.88639 | 0.63064 | -0.16022 |
| C | 4.09975 | 0.04134 | -1.25534 |
| H | 4.54682 | 0.22682 | -2.24518 |
| C | 2.78181 | -0.43761 | -1.17129 |
| H | 2.21680 | -0.64380 | -2.09194 |
| C | -0.81322 | 1.46401 | 1.25984 |
| C | -1.85258 | 2.56557 | 0.94845 |
| H | -1.78271 | 3.33073 | 1.75442 |
| C | 0.60873 | 2.07157 | 1.20222 |
| H | 0.62869 | 2.92626 | 1.91509 |
| H | 0.89452 | 2.46814 | 0.21229 |
| H | 1.38614 | 1.35501 | 1.52501 |
| C | -1.03883 | 0.58876 | -1.83302 |
| C | -2.44374 | 1.12439 | -2.19627 |
| H | -2.39245 | 1.52911 | -3.23187 |
| H | -2.78256 | 1.95105 | -1.54032 |
| H | -3.21922 | 0.33188 | -2.20022 |
| H | -1.42714 | -1.38963 | -2.79222 |
| H | 0.30521 | -1.03764 | -2.52970 |
| H | -0.61058 | -0.17341 | -3.80951 |
| C | 0.00102 | 1.71472 | -2.03802 |
| H | 1.02394 | 1.41826 | -1.72805 |
| H | -0.27586 | 2.65414 | -1.51986 |
| H | 0.03837 | 1.94674 | -3.12541 |
| C | -2.49318 | -1.17142 | 0.44408 |
| C | -2.75610 | -2.13923 | -0.73353 |
| H | -3.53481 | -2.86219 | -0.40431 |
| H | -1.85639 | -2.72968 | -1.00748 |
| H | -3.15201 | -1.63169 | -1.63532 |
| C | -3.75950 | -0.32650 | 0.71282 |
| H | -4.02190 | 0.35463 | -0.12082 |
| H | -3.68959 | 0.26266 | 1.64969 |
| H | -4.61254 | -1.03007 | 0.83974 |
| C | -2.18425 | -2.04364 | 1.68816 |
| H | -1.93937 | -1.46488 | 2.59688 |
| H | -1.36849 | -2.77200 | 1.50417 |
| H | -3.10299 | -2.63120 | 1.91024 |
| S | 0.58427 | -1.43134 | 0.28855 |
| C | 2.96856 | -0.47969 | 1.26867 |
| H | 2.52831 | -0.70343 | 2.25357 |

| | | | |
|---|---|---|---|
| H | -1.64448 | 3.08861 | -0.00684 |
| H | -2.89819 | 2.20121 | 0.93561 |
| C | -1.01995 | 0.92671 | 2.69310 |
| H | -0.78370 | 1.75095 | 3.40239 |
| H | -2.06380 | 0.61560 | 2.89782 |
| H | -0.33373 | 0.08409 | 2.92268 |
| C | -0.67373 | -0.58096 | -2.77627 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 29.35 | 0.14896 | YES YES |
| 8 | a | 59.29 | 0.06529 | YES YES |
| 9 | a | 66.58 | 0.09494 | YES YES |
| 10 | a | 86.09 | 0.46722 | YES YES |
| 11 | a | 97.60 | 0.14851 | YES YES |
| 12 | a | 125.10 | 0.26660 | YES YES |
| 13 | a | 129.61 | 0.16945 | YES YES |
| 14 | a | 132.58 | 0.73201 | YES YES |
| 15 | a | 160.32 | 0.05950 | YES YES |
| 16 | a | 176.64 | 0.52081 | YES YES |
| 17 | a | 183.33 | 0.25060 | YES YES |
| 18 | a | 191.65 | 0.10477 | YES YES |
| 19 | a | 205.50 | 1.15075 | YES YES |
| 20 | a | 212.82 | 1.20909 | YES YES |
| 21 | a | 213.82 | 0.73879 | YES YES |
| 22 | a | 241.21 | 0.48217 | YES YES |
| 23 | a | 242.11 | 1.12368 | YES YES |
| 24 | a | 254.22 | 0.36426 | YES YES |
| 25 | a | 257.98 | 0.41016 | YES YES |
| 26 | a | 261.86 | 0.03358 | YES YES |
| 27 | a | 270.98 | 0.39870 | YES YES |
| 28 | a | 279.83 | 0.50126 | YES YES |
| 29 | a | 288.93 | 0.21399 | YES YES |
| 30 | a | 292.22 | 0.48217 | YES YES |
| 31 | a | 308.47 | 0.10564 | YES YES |
| 32 | a | 323.17 | 0.17866 | YES YES |
| 33 | a | 335.20 | 0.23545 | YES YES |
| 34 | a | 344.15 | 0.51056 | YES YES |
| 35 | a | 348.55 | 0.66404 | YES YES |
| 36 | a | 369.77 | 1.13841 | YES YES |
| 37 | a | 377.75 | 0.36378 | YES YES |
| 38 | a | 387.05 | 0.60985 | YES YES |
| 39 | a | 399.00 | 0.74688 | YES YES |
| 40 | a | 405.34 | 1.81245 | YES YES |
| 41 | a | 408.79 | 0.96764 | YES YES |
| 42 | a | 414.86 | 0.06703 | YES YES |
| 43 | a | 420.19 | 2.65538 | YES YES |
| 44 | a | 459.91 | 11.59598 | YES YES |
| 45 | a | 463.59 | 8.94133 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 46 | a | 488.39 | 8.37350 | YES | YES |
| 47 | a | 513.54 | 9.11553 | YES | YES |
| 48 | a | 547.11 | 16.48070 | YES | YES |
| 49 | a | 572.49 | 4.84325 | YES | YES |
| 50 | a | 579.18 | 8.80090 | YES | YES |

**TS [PhS(PPh3)2]+**

bp86-d3 energy (au): -2701.0038127390

Zero point energy (au): 0.6253348
Entropy (kJ mol^-1): 1.06380
Chemical potential (kJ mol^-1): 1434.06

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.71984 | 0.66605 | 3.43775 |
| H | -5.76862 | 0.82214 | 3.73887 |
| C | 2.87827 | 2.35166 | 3.33284 |
| H | 3.97027 | 2.33563 | 3.18494 |
| S | -0.38729 | 0.04069 | -0.38712 |
| P | -0.31247 | 0.06130 | 2.13890 |
| C | 0.88578 | 3.39529 | 4.26736 |
| H | 0.41379 | 4.19643 | 4.85945 |
| C | -4.17503 | 1.41272 | 2.37759 |
| H | -4.79503 | 2.15246 | 1.84569 |
| C | -2.04226 | 0.26574 | 2.67192 |
| C | 2.08990 | 1.34042 | 2.76563 |
| H | 2.56856 | 0.53844 | 2.17985 |
| C | 1.05914 | -4.13228 | 3.57199 |
| H | 1.37619 | -5.13702 | 3.89440 |
| C | 0.68618 | 1.34881 | 2.95653 |
| C | 3.47646 | 1.38419 | -0.56582 |
| H | 3.99261 | 2.34454 | -0.72840 |
| C | -2.84106 | 1.21151 | 1.98890 |
| H | -2.41574 | 1.79082 | 1.15199 |
| C | 0.25255 | -1.56363 | 2.74857 |
| C | 0.17982 | -3.98862 | 2.48258 |
| H | -0.19362 | -4.87927 | 1.95115 |
| C | 0.08682 | 2.38417 | 3.70863 |
| H | -1.00394 | 2.39636 | 3.86579 |
| C | 2.27914 | 3.38213 | 4.08116 |
| H | 2.90178 | 4.17690 | 4.52300 |
| C | -2.59249 | -0.48520 | 3.73435 |
| H | -1.97422 | -1.22708 | 4.26555 |
| C | 1.12948 | -1.71059 | 3.84425 |
| H | 1.49667 | -0.82341 | 4.38469 |
| C | -0.21886 | -2.71048 | 2.06659 |
| H | -0.89694 | -2.59575 | 1.20386 |
| C | 2.15264 | -1.06763 | -0.14481 |
| H | 1.62822 | -2.02366 | 0.00427 |
| C | -3.92964 | -0.28204 | 4.11233 |
| H | -4.35708 | -0.86710 | 4.94295 |
| C | 1.53061 | -2.99458 | 4.24945 |
| H | 2.21371 | -3.10510 | 5.10662 |
| C | 3.55607 | -1.01007 | -0.11576 |
| H | 4.13420 | -1.93078 | 0.06429 |
| C | 2.07151 | 1.34070 | -0.57508 |
| H | 1.48516 | 2.25712 | -0.74124 |
| C | 4.21878 | 0.21255 | -0.33052 |
| H | 5.32050 | 0.25259 | -0.31275 |

| | | | |
|---|---|---|---|
| C | 1.41253 | 0.11158 | -0.36694 |
| C | -4.71132 | -1.10387 | -3.89196 |
| H | -5.75149 | -1.36281 | -4.14611 |
| C | 3.05683 | -2.04451 | -3.89956 |
| H | 4.14312 | -1.86814 | -3.84026 |
| P | -0.34366 | -0.03896 | -2.78992 |
| C | 1.17430 | -3.46048 | -4.52204 |
| H | 0.78316 | -4.39397 | -4.95823 |
| C | -4.05810 | -1.77498 | -2.84308 |
| H | -4.58435 | -2.55777 | -2.27348 |
| C | -2.05841 | -0.44096 | -3.24559 |
| C | 2.17218 | -1.06955 | -3.41802 |
| H | 2.56976 | -0.13898 | -2.98084 |
| C | 0.60287 | 4.13694 | -4.55697 |
| H | 0.81485 | 5.13726 | -4.96815 |
| C | 0.77439 | -1.28530 | -3.49821 |
| C | -2.73518 | -1.44379 | -2.51299 |
| H | -2.22655 | -1.96369 | -1.68420 |
| C | 0.06588 | 1.58341 | -3.50768 |
| C | -0.15669 | 4.00765 | -3.37930 |
| H | -0.54047 | 4.90469 | -2.86718 |
| C | 0.27800 | -2.48778 | -4.04990 |
| H | -0.80800 | -2.66137 | -4.12069 |
| C | 2.56126 | -3.24146 | -4.44896 |
| H | 3.26025 | -4.00620 | -4.82432 |
| C | -2.71691 | 0.23516 | -4.29540 |
| H | -2.19441 | 1.02348 | -4.86105 |
| C | 0.82344 | 1.71350 | -4.69204 |
| H | 1.20212 | 0.81910 | -5.21170 |
| C | -0.42223 | 2.73594 | -2.85045 |
| H | -1.00493 | 2.63232 | -1.92001 |
| C | -4.04180 | -0.10007 | -4.61418 |
| H | -4.55459 | 0.42716 | -5.43441 |
| C | 1.09081 | 2.99176 | -5.20991 |
| H | 1.68216 | 3.09155 | -6.13439 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | a | -36.09 | 0.00000 | YES YES |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | | 0.00 | 0.00000 | - - |
| 8 | a | 12.36 | 0.00200 | YES YES |
| 9 | a | 15.94 | 1.76672 | YES YES |
| 10 | a | 22.22 | 1.09731 | YES YES |
| 11 | a | 27.12 | 4.14742 | YES YES |
| 12 | a | 29.41 | 0.00875 | YES YES |
| 13 | a | 31.18 | 0.39858 | YES YES |
| 14 | a | 38.04 | 2.64403 | YES YES |
| 15 | a | 41.20 | 0.09706 | YES YES |
| 16 | a | 45.22 | 4.12322 | YES YES |
| 17 | a | 47.80 | 0.11624 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 18 | a | 50.04 | 0.50135 | YES | YES |
| 19 | a | 54.16 | 4.90790 | YES | YES |
| 20 | a | 56.41 | 24.78094 | YES | YES |
| 21 | a | 57.51 | 0.03609 | YES | YES |
| 22 | a | 60.05 | 1.15056 | YES | YES |
| 23 | a | 75.63 | 22.48699 | YES | YES |
| 24 | a | 76.77 | 5.51923 | YES | YES |
| 25 | a | 82.03 | 2.40786 | YES | YES |
| 26 | a | 93.08 | 22.78435 | YES | YES |
| 27 | a | 100.57 | 0.17172 | YES | YES |
| 28 | a | 118.45 | 2.36660 | YES | YES |
| 29 | a | 126.79 | 5.34730 | YES | YES |
| 30 | a | 145.35 | 1.11709 | YES | YES |
| 31 | a | 184.17 | 2.02096 | YES | YES |
| 32 | a | 185.60 | 1.14848 | YES | YES |
| 33 | a | 196.12 | 0.96321 | YES | YES |
| 34 | a | 197.92 | 3.92722 | YES | YES |
| 35 | a | 203.98 | 1.68985 | YES | YES |
| 36 | a | 210.23 | 3.91590 | YES | YES |
| 37 | a | 236.49 | 42.40653 | YES | YES |
| 38 | a | 238.97 | 0.67031 | YES | YES |
| 39 | a | 239.41 | 1.31485 | YES | YES |
| 40 | a | 254.23 | 0.15677 | YES | YES |
| 41 | a | 256.08 | 6.44924 | YES | YES |
| 42 | a | 265.55 | 0.70424 | YES | YES |
| 43 | a | 266.71 | 0.40693 | YES | YES |
| 44 | a | 302.05 | 6.54072 | YES | YES |
| 45 | a | 392.19 | 1.49954 | YES | YES |
| 46 | a | 393.20 | 0.48400 | YES | YES |
| 47 | a | 394.13 | 0.99258 | YES | YES |
| 48 | a | 394.35 | 0.56191 | YES | YES |
| 49 | a | 395.50 | 1.09565 | YES | YES |
| 50 | a | 396.72 | 1.31307 | YES | YES |

**TS [PhS(PPh3)(PtBu3)]+**

bp86-d3 energy (au): -2479.6997558530

Zero point energy (au): 0.7166162
Entropy (kJ mol^-1): 1.06836
Chemical potential (kJ mol^-1): 1679.79

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.15560 | 0.20525 | 0.03142 |
| S | 0.24253 | 0.02625 | -0.01367 |
| C | 0.11215 | -1.76841 | 0.00575 |
| C | -0.19969 | -2.45316 | -1.18751 |
| H | -0.31631 | -1.88963 | -2.12623 |
| C | -0.36584 | -3.84763 | -1.16624 |
| H | -0.61352 | -4.38130 | -2.09804 |
| C | -0.20770 | -4.56015 | 0.03676 |
| H | -0.33209 | -5.65511 | 0.04904 |
| C | 0.10269 | -3.87436 | 1.22426 |
| H | 0.21451 | -4.42795 | 2.17060 |
| C | 0.25216 | -2.47739 | 1.21495 |
| H | 0.46248 | -1.93304 | 2.14761 |
| C | -3.06478 | -0.75408 | 1.27895 |
| C | -3.07749 | -2.16527 | 1.15770 |
| H | -2.58729 | -2.65656 | 0.30138 |
| C | -3.72243 | -2.94285 | 2.12966 |
| H | -3.73371 | -4.03998 | 2.02747 |
| C | -4.34481 | -2.32707 | 3.23116 |
| H | -4.84750 | -2.94216 | 3.99514 |
| C | -4.32731 | -0.92687 | 3.35615 |
| H | -4.82072 | -0.44179 | 4.21402 |
| C | -3.69089 | -0.13698 | 2.38499 |
| H | -3.69156 | 0.96041 | 2.48389 |
| C | -2.31680 | 1.98145 | 0.39240 |
| C | -3.06577 | 2.85047 | -0.42924 |
| H | -3.61875 | 2.45376 | -1.29577 |
| C | -3.10085 | 4.22477 | -0.14057 |
| H | -3.68667 | 4.90147 | -0.78331 |
| C | -2.39518 | 4.73589 | 0.96275 |
| H | -2.42622 | 5.81504 | 1.18422 |
| C | -1.64923 | 3.87136 | 1.78489 |
| H | -1.09680 | 4.26994 | 2.65138 |
| C | -1.60169 | 2.49837 | 1.49991 |
| H | -1.01177 | 1.82305 | 2.14197 |
| C | -2.88408 | -0.11774 | -1.60488 |
| C | -4.13805 | -0.74708 | -1.76365 |
| H | -4.71698 | -1.06295 | -0.88110 |
| C | -4.64916 | -0.96558 | -3.05394 |
| H | -5.62892 | -1.45488 | -3.17550 |
| C | -3.92011 | -0.55634 | -4.18424 |
| H | -4.32709 | -0.72814 | -5.19403 |
| C | -2.67100 | 0.07300 | -4.02754 |
| H | -2.09883 | 0.39542 | -4.91263 |
| C | -2.14832 | 0.28657 | -2.74372 |

| | | | |
|---|---|---|---|
| H | -1.16381 | 0.76819 | -2.61961 |
| P | 2.77779 | 0.21091 | -0.02648 |
| C | 3.06342 | 1.43790 | -1.50396 |
| C | 4.36540 | 2.25922 | -1.38204 |
| H | 4.49483 | 2.86261 | -2.31009 |
| C | 1.86235 | 2.41255 | -1.62645 |
| H | 2.05009 | 3.07730 | -2.49983 |
| H | 1.71944 | 3.06858 | -0.74807 |
| H | 0.91042 | 1.87345 | -1.81398 |
| C | 3.07901 | 1.11640 | 1.66220 |
| C | 4.57289 | 1.28673 | 2.01395 |
| H | 4.65233 | 1.87679 | 2.95551 |
| H | 5.13627 | 1.83547 | 1.23236 |
| H | 5.08265 | 0.31878 | 2.19613 |
| H | 2.73907 | -0.71234 | 2.90701 |
| H | 1.26665 | 0.27184 | 2.59700 |
| H | 2.52209 | 0.84798 | 3.74783 |
| C | 2.41042 | 2.51122 | 1.62822 |
| H | 1.33931 | 2.46072 | 1.33654 |
| H | 2.93282 | 3.22531 | 0.96098 |
| H | 2.45248 | 2.93983 | 2.65555 |
| C | 3.95005 | -1.33686 | -0.18482 |
| C | 3.95274 | -2.11309 | 1.15215 |
| H | 4.51507 | -3.06220 | 0.99925 |
| H | 2.92614 | -2.39072 | 1.47199 |
| H | 4.45863 | -1.56932 | 1.97463 |
| C | 5.40024 | -0.96658 | -0.56278 |
| H | 5.86651 | -0.25628 | 0.14947 |
| H | 5.47742 | -0.54133 | -1.58405 |
| H | 6.01442 | -1.89615 | -0.55309 |
| C | 3.36463 | -2.30187 | -1.24467 |
| H | 3.32210 | -1.87528 | -2.26401 |
| H | 2.34904 | -2.64847 | -0.96857 |
| H | 4.02194 | -3.19940 | -1.29435 |
| H | 4.33261 | 2.97571 | -0.53536 |
| H | 5.26920 | 1.62895 | -1.26946 |
| C | 3.08548 | 0.61815 | -2.81439 |
| H | 3.08341 | 1.32695 | -3.67346 |
| H | 3.99207 | -0.01084 | -2.91854 |
| H | 2.18468 | -0.02698 | -2.91302 |
| C | 2.36100 | 0.31921 | 2.78067 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 14.67 | 9.54740 | YES YES |
| 8 | a | 16.81 | 26.97966 | YES YES |
| 9 | a | 21.13 | 0.02649 | YES YES |
| 10 | a | 26.72 | 9.52686 | YES YES |
| 11 | a | 38.26 | 64.02273 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 45.73 | 73.37596 | YES | YES |
| 13 | a | 48.83 | 5.94534 | YES | YES |
| 14 | a | 51.25 | 4.81896 | YES | YES |
| 15 | a | 56.86 | 3.00080 | YES | YES |
| 16 | a | 62.38 | 1.03149 | YES | YES |
| 17 | a | 63.80 | 0.29190 | YES | YES |
| 18 | a | 72.47 | 11.45846 | YES | YES |
| 19 | a | 78.22 | 0.02974 | YES | YES |
| 20 | a | 86.10 | 0.03122 | YES | YES |
| 21 | a | 91.41 | 1.90672 | YES | YES |
| 22 | a | 99.95 | 1.57095 | YES | YES |
| 23 | a | 105.96 | 11.44110 | YES | YES |
| 24 | a | 117.79 | 23.02596 | YES | YES |
| 25 | a | 121.58 | 7.18783 | YES | YES |
| 26 | a | 127.49 | 1.49972 | YES | YES |
| 27 | a | 155.15 | 1.54051 | YES | YES |
| 28 | a | 174.07 | 2.33930 | YES | YES |
| 29 | a | 182.74 | 0.13061 | YES | YES |
| 30 | a | 187.28 | 1.10693 | YES | YES |
| 31 | a | 195.05 | 0.61581 | YES | YES |
| 32 | a | 199.83 | 0.77557 | YES | YES |
| 33 | a | 201.35 | 2.20342 | YES | YES |
| 34 | a | 203.94 | 2.29637 | YES | YES |
| 35 | a | 209.96 | 0.99306 | YES | YES |
| 36 | a | 211.48 | 1.36014 | YES | YES |
| 37 | a | 236.17 | 12.96442 | YES | YES |
| 38 | a | 237.55 | 5.49890 | YES | YES |
| 39 | a | 238.63 | 24.41792 | YES | YES |
| 40 | a | 244.83 | 9.57443 | YES | YES |
| 41 | a | 255.07 | 0.39832 | YES | YES |
| 42 | a | 258.36 | 0.94732 | YES | YES |
| 43 | a | 259.42 | 1.41498 | YES | YES |
| 44 | a | 261.89 | 0.26289 | YES | YES |
| 45 | a | 263.97 | 0.55048 | YES | YES |
| 46 | a | 274.79 | 0.57682 | YES | YES |
| 47 | a | 282.95 | 0.11438 | YES | YES |
| 48 | a | 289.71 | 1.10105 | YES | YES |
| 49 | a | 300.02 | 11.08640 | YES | YES |
| 50 | a | 304.85 | 0.86105 | YES | YES |

**TS [PhSe(PPh3)2]+**

bp86-d3 energy (au): -4704.4492843920

Zero point energy (au): 0.6246426
Entropy (kJ mol^-1): 1.09860
Chemical potential (kJ mol^-1): 1425.03

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.70687 | 0.75361 | 4.02354 |
| H | -5.73957 | 0.93881 | 4.36100 |
| C | 2.95059 | 2.20243 | 3.55897 |
| H | 4.03908 | 2.11070 | 3.41389 |
| Se | -0.52496 | 0.00056 | -0.00095 |
| P | -0.37199 | 0.00670 | 2.56250 |
| C | 1.02492 | 3.43428 | 4.39790 |
| H | 0.60166 | 4.30836 | 4.91886 |
| C | -4.16693 | 1.51087 | 2.96854 |
| H | -4.77341 | 2.28928 | 2.47780 |
| C | -2.07110 | 0.27778 | 3.16375 |
| C | 2.10382 | 1.19202 | 3.08137 |
| H | 2.53465 | 0.31607 | 2.56957 |
| C | 0.97687 | -4.14194 | 4.13687 |
| H | 1.28748 | -5.13500 | 4.50020 |
| C | 0.70413 | 1.29762 | 3.26849 |
| C | 3.51735 | 1.20019 | -0.24018 |
| H | 4.06322 | 2.13922 | -0.42609 |
| C | -2.85454 | 1.27164 | 2.53177 |
| H | -2.43523 | 1.86099 | 1.69851 |
| C | 0.19133 | -1.60484 | 3.20668 |
| C | 0.15693 | -4.03465 | 2.99837 |
| H | -0.17714 | -4.94189 | 2.46918 |
| C | 0.16756 | 2.42576 | 3.92799 |
| H | -0.91952 | 2.51386 | 4.08525 |
| C | 2.41435 | 3.32595 | 4.21438 |
| H | 3.08325 | 4.11856 | 4.58715 |
| C | -2.61612 | -0.48336 | 4.22095 |
| H | -2.01216 | -1.26398 | 4.71143 |
| C | 1.00845 | -1.71433 | 4.35277 |
| H | 1.33877 | -0.81021 | 4.88890 |
| C | -0.23246 | -2.77107 | 2.52950 |
| H | -0.86242 | -2.68497 | 1.62813 |
| C | 2.11503 | -1.19743 | 0.23417 |
| H | 1.56534 | -2.13541 | 0.40594 |
| C | -3.93272 | -0.24224 | 4.64539 |
| H | -4.35686 | -0.83668 | 5.47081 |
| C | 1.39984 | -2.98338 | 4.81126 |
| H | 2.03792 | -3.06594 | 5.70609 |
| C | 3.52024 | -1.18785 | 0.24591 |
| H | 4.06837 | -2.12536 | 0.43281 |
| C | 2.11210 | 1.20587 | -0.23086 |
| H | 1.56010 | 2.14233 | -0.40359 |
| C | 4.22148 | 0.00713 | 0.00343 |
| H | 5.32360 | 0.00865 | 0.00431 |
| C | 1.41582 | 0.00323 | 0.00097 |

| | | | |
|---|---|---|---|
| C | -4.69655 | -0.77024 | -4.03146 |
| H | -5.72804 | -0.95930 | -4.37048 |
| C | 2.96536 | -2.19224 | -3.55070 |
| H | 4.05329 | -2.09612 | -3.40422 |
| P | -0.36683 | -0.00688 | -2.56355 |
| C | 1.04555 | -3.43327 | -4.38949 |
| H | 0.62629 | -4.31017 | -4.90894 |
| C | -4.15558 | -1.52509 | -2.97525 |
| H | -4.76017 | -2.30519 | -2.48488 |
| C | -2.06382 | -0.28467 | -3.16778 |
| C | 2.11412 | -1.18388 | -3.07668 |
| H | 2.54090 | -0.30521 | -2.56609 |
| C | 0.97175 | 4.14355 | -4.14194 |
| H | 1.27982 | 5.13700 | -4.50636 |
| C | 0.71509 | -1.29519 | -3.26550 |
| C | -2.84467 | -1.28115 | -2.53668 |
| H | -2.42443 | -1.86886 | -1.70273 |
| C | 0.19251 | 1.60550 | -3.20910 |
| C | 0.15211 | 4.03543 | -3.00332 |
| H | -0.18399 | 4.94238 | -2.47492 |
| C | 0.18375 | -2.42681 | -3.92330 |
| H | -0.90274 | -2.51920 | -4.08224 |
| C | 2.43428 | -3.31934 | -4.20417 |
| H | 3.10669 | -4.11032 | -4.57405 |
| C | -2.60984 | 0.47395 | -4.22628 |
| H | -2.00784 | 1.25642 | -4.71625 |
| C | 1.00926 | 1.71582 | -4.35541 |
| H | 1.34169 | 0.81192 | -4.89066 |
| C | -0.23429 | 2.77138 | -2.53321 |
| H | -0.86430 | 2.68462 | -1.63192 |
| C | -3.92493 | 0.22798 | -4.65266 |
| H | -4.34983 | 0.82045 | -5.47910 |
| C | 1.39758 | 2.98535 | -4.81517 |
| H | 2.03556 | 3.06855 | -5.71001 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 9.80 | 0.00190 | YES YES |
| 8 | a | 11.77 | 0.12689 | YES YES |
| 9 | a | 19.52 | 0.00849 | YES YES |
| 10 | a | 27.24 | 0.04257 | YES YES |
| 11 | a | 28.86 | 0.00010 | YES YES |
| 12 | a | 30.48 | 0.03476 | YES YES |
| 13 | a | 38.03 | 0.01914 | YES YES |
| 14 | a | 40.48 | 0.08149 | YES YES |
| 15 | a | 41.54 | 2.53796 | YES YES |
| 16 | a | 46.29 | 0.04527 | YES YES |
| 17 | a | 47.97 | 3.01276 | YES YES |
| 18 | a | 50.16 | 2.72662 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 19 | a | 53.64 | 0.60586 | YES | YES |
| 20 | a | 58.22 | 0.02995 | YES | YES |
| 21 | a | 59.58 | 0.00625 | YES | YES |
| 22 | a | 64.76 | 16.70906 | YES | YES |
| 23 | a | 74.78 | 0.00699 | YES | YES |
| 24 | a | 80.22 | 0.01885 | YES | YES |
| 25 | a | 85.38 | 37.62862 | YES | YES |
| 26 | a | 95.13 | 0.01312 | YES | YES |
| 27 | a | 100.91 | 88.17640 | YES | YES |
| 28 | a | 104.83 | 0.08815 | YES | YES |
| 29 | a | 115.93 | 1.16746 | YES | YES |
| 30 | a | 125.08 | 0.02112 | YES | YES |
| 31 | a | 184.25 | 2.54960 | YES | YES |
| 32 | a | 185.06 | 0.48245 | YES | YES |
| 33 | a | 194.68 | 0.07694 | YES | YES |
| 34 | a | 195.81 | 4.83483 | YES | YES |
| 35 | a | 204.53 | 1.20545 | YES | YES |
| 36 | a | 205.96 | 3.29412 | YES | YES |
| 37 | a | 220.78 | 12.21506 | YES | YES |
| 38 | a | 238.08 | 7.44069 | YES | YES |
| 39 | a | 238.98 | 0.35554 | YES | YES |
| 40 | a | 239.98 | 0.04183 | YES | YES |
| 41 | a | 253.59 | 0.01048 | YES | YES |
| 42 | a | 254.25 | 1.68898 | YES | YES |
| 43 | a | 265.97 | 0.98640 | YES | YES |
| 44 | a | 266.73 | 0.14350 | YES | YES |
| 45 | a | 306.93 | 0.01774 | YES | YES |
| 46 | a | 393.36 | 0.04426 | YES | YES |
| 47 | a | 393.58 | 0.09574 | YES | YES |
| 48 | a | 394.33 | 1.03264 | YES | YES |
| 49 | a | 394.85 | 0.21426 | YES | YES |
| 50 | a | 395.98 | 0.37077 | YES | YES |

**TS [PhSe(PPh3)(PtBu3)]+**

bp86-d3 energy (au): -4483.1449057450

Zero point energy (au): 0.7161509
Entropy (kJ mol^-1): 1.07491
Chemical potential (kJ mol^-1): 1677.11

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.05303 | 0.39302 | 0.03638 |
| Se | 0.53382 | 0.24348 | 0.04356 |
| C | 0.27331 | -1.68561 | 0.00159 |
| C | -0.10127 | -2.29777 | -1.21331 |
| H | -0.20110 | -1.69575 | -2.12977 |
| C | -0.37202 | -3.67619 | -1.24556 |
| H | -0.67187 | -4.14802 | -2.19520 |
| C | -0.26013 | -4.44719 | -0.07430 |
| H | -0.46620 | -5.52927 | -0.10450 |
| C | 0.10289 | -3.83246 | 1.13613 |
| H | 0.17236 | -4.42674 | 2.06152 |
| C | 0.35724 | -2.45038 | 1.18042 |
| H | 0.60063 | -1.96962 | 2.13792 |
| C | -2.96592 | -0.56707 | 1.28731 |
| C | -2.94642 | -1.97999 | 1.19598 |
| H | -2.44167 | -2.47776 | 0.35209 |
| C | -3.58491 | -2.75273 | 2.17645 |
| H | -3.56981 | -3.85170 | 2.09601 |
| C | -4.23493 | -2.12957 | 3.25739 |
| H | -4.73399 | -2.74004 | 4.02742 |
| C | -4.25068 | -0.72711 | 3.35268 |
| H | -4.76579 | -0.23543 | 4.19385 |
| C | -3.61957 | 0.05688 | 2.37286 |
| H | -3.64462 | 1.15581 | 2.44957 |
| C | -2.37253 | 2.16620 | 0.32475 |
| C | -3.27976 | 2.90206 | -0.46825 |
| H | -3.83463 | 2.40424 | -1.27996 |
| C | -3.47261 | 4.27099 | -0.22059 |
| H | -4.18229 | 4.84245 | -0.84047 |
| C | -2.76789 | 4.90970 | 0.81525 |
| H | -2.92332 | 5.98408 | 1.00585 |
| C | -1.86327 | 4.17944 | 1.60722 |
| H | -1.31163 | 4.67881 | 2.42024 |
| C | -1.65756 | 2.81288 | 1.36078 |
| H | -0.94327 | 2.24263 | 1.97893 |
| C | -2.73790 | -0.02152 | -1.60430 |
| C | -3.95180 | -0.72288 | -1.76781 |
| H | -4.53315 | -1.04008 | -0.88727 |
| C | -4.42131 | -1.01460 | -3.05986 |
| H | -5.37028 | -1.56132 | -3.18305 |
| C | -3.69037 | -0.60671 | -4.18891 |
| H | -4.06315 | -0.83772 | -5.19996 |
| C | -2.48266 | 0.09802 | -4.02834 |
| H | -1.90880 | 0.42103 | -4.91221 |
| C | -2.00303 | 0.38619 | -2.74206 |

| | | | |
|---|---|---|---|
| H | -1.04953 | 0.92704 | -2.61574 |
| P | 3.13101 | 0.28124 | 0.01290 |
| C | 3.45706 | 1.90462 | -1.00298 |
| C | 4.86343 | 2.49466 | -0.76161 |
| H | 5.00487 | 3.36333 | -1.44464 |
| C | 2.38564 | 2.97113 | -0.65170 |
| H | 2.60430 | 3.88524 | -1.24932 |
| H | 2.37882 | 3.27476 | 0.41057 |
| H | 1.36111 | 2.64375 | -0.93084 |
| C | 3.69446 | 0.52188 | 1.85319 |
| C | 5.22003 | 0.38426 | 2.04774 |
| H | 5.46418 | 0.61218 | 3.11055 |
| H | 5.80011 | 1.08879 | 1.41841 |
| H | 5.58275 | -0.64467 | 1.84763 |
| H | 3.14133 | -1.56676 | 2.44285 |
| H | 1.85954 | -0.33401 | 2.71861 |
| H | 3.30156 | -0.39561 | 3.78345 |
| C | 3.23857 | 1.90943 | 2.36084 |
| H | 2.14803 | 2.06809 | 2.21417 |
| H | 3.79442 | 2.74928 | 1.89796 |
| H | 3.43345 | 1.95733 | 3.45639 |
| C | 4.04083 | -1.23005 | -0.79731 |
| C | 3.99672 | -2.42450 | 0.18387 |
| H | 4.40393 | -3.31764 | -0.34151 |
| H | 2.95892 | -2.67118 | 0.49485 |
| H | 4.62190 | -2.27066 | 1.08609 |
| C | 5.50642 | -0.92633 | -1.17727 |
| H | 6.11959 | -0.58629 | -0.31890 |
| H | 5.58656 | -0.17201 | -1.98654 |
| H | 5.96875 | -1.86365 | -1.56346 |
| C | 3.26421 | -1.66820 | -2.06235 |
| H | 3.27332 | -0.91889 | -2.87507 |
| H | 2.21261 | -1.92716 | -1.82971 |
| H | 3.75002 | -2.58692 | -2.46218 |
| H | 4.99331 | 2.87394 | 0.27248 |
| H | 5.67697 | 1.77307 | -0.97274 |
| C | 3.28022 | 1.59797 | -2.50784 |
| H | 3.30134 | 2.56154 | -3.06449 |
| H | 4.09526 | 0.97019 | -2.92046 |
| H | 2.30297 | 1.11206 | -2.71975 |
| C | 2.95491 | -0.51579 | 2.73193 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 12.28 | 0.20466 | YES YES |
| 8 | a | 15.94 | 0.02268 | YES YES |
| 9 | a | 22.13 | 0.04644 | YES YES |
| 10 | a | 24.01 | 0.05804 | YES YES |
| 11 | a | 39.85 | 1.81795 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 42.42 | 0.31488 | YES | YES |
| 13 | a | 48.92 | 0.16649 | YES | YES |
| 14 | a | 53.92 | 0.78329 | YES | YES |
| 15 | a | 56.22 | 0.33038 | YES | YES |
| 16 | a | 60.87 | 2.73518 | YES | YES |
| 17 | a | 63.69 | 13.36530 | YES | YES |
| 18 | a | 76.47 | 5.45993 | YES | YES |
| 19 | a | 81.16 | 34.45298 | YES | YES |
| 20 | a | 86.31 | 21.37884 | YES | YES |
| 21 | a | 99.96 | 13.21943 | YES | YES |
| 22 | a | 103.47 | 1.12509 | YES | YES |
| 23 | a | 104.50 | 0.77461 | YES | YES |
| 24 | a | 111.13 | 22.27491 | YES | YES |
| 25 | a | 122.59 | 0.74007 | YES | YES |
| 26 | a | 128.10 | 0.65648 | YES | YES |
| 27 | a | 134.08 | 0.60476 | YES | YES |
| 28 | a | 176.98 | 0.28441 | YES | YES |
| 29 | a | 186.06 | 1.08141 | YES | YES |
| 30 | a | 194.35 | 0.65652 | YES | YES |
| 31 | a | 196.82 | 1.54920 | YES | YES |
| 32 | a | 199.90 | 0.85684 | YES | YES |
| 33 | a | 200.82 | 0.81541 | YES | YES |
| 34 | a | 205.71 | 0.67167 | YES | YES |
| 35 | a | 210.79 | 1.16460 | YES | YES |
| 36 | a | 218.97 | 0.49229 | YES | YES |
| 37 | a | 224.62 | 15.90173 | YES | YES |
| 38 | a | 235.86 | 4.64958 | YES | YES |
| 39 | a | 238.41 | 0.53795 | YES | YES |
| 40 | a | 241.88 | 1.11099 | YES | YES |
| 41 | a | 248.70 | 0.42728 | YES | YES |
| 42 | a | 254.72 | 0.28870 | YES | YES |
| 43 | a | 256.04 | 0.93647 | YES | YES |
| 44 | a | 258.34 | 0.56370 | YES | YES |
| 45 | a | 264.78 | 0.43677 | YES | YES |
| 46 | a | 266.46 | 0.37999 | YES | YES |
| 47 | a | 278.06 | 0.94098 | YES | YES |
| 48 | a | 285.50 | 0.30362 | YES | YES |
| 49 | a | 288.26 | 0.36456 | YES | YES |
| 50 | a | 300.73 | 1.12528 | YES | YES |

## BP86-D3/def2-TZVPP level optimisations

**$PPh_3$**

bp86-d3_def2-tzvpp energy (au): -1036.6639706350

Zero point energy (au): 0.2658278
Entropy (kJ mol^-1): 0.55878
Chemical potential (kJ mol^-1): 576.65

XYZ coordinates:

34

| | | | |
|---|---|---|---|
| P | 0.00345 | -1.25939 | -0.00475 |
| C | 1.16677 | -0.43197 | 1.16378 |
| C | -0.11502 | -0.98809 | -2.76943 |
| H | -0.74188 | -1.87940 | -2.70051 |
| C | 1.24566 | 0.70395 | -1.70462 |
| H | 1.67629 | 1.14774 | -0.80685 |
| C | 0.42819 | -0.43204 | -1.59793 |
| C | 3.39304 | -0.42647 | 2.14902 |
| H | 4.38104 | -0.87836 | 2.24273 |
| C | 1.50877 | 1.27203 | -2.95405 |
| H | 2.14809 | 2.15299 | -3.02220 |
| C | 0.85471 | 0.71785 | 1.90598 |
| H | -0.13186 | 1.17207 | 1.81125 |
| C | 0.95229 | 0.72023 | -4.11072 |
| H | 1.15833 | 1.16587 | -5.08415 |
| C | 2.44407 | -1.00186 | 1.30277 |
| H | 2.69389 | -1.90385 | 0.74045 |
| C | 1.80074 | 1.28547 | 2.76341 |
| H | 1.54394 | 2.17790 | 3.33545 |
| C | 3.07195 | 0.71838 | 2.88466 |
| H | 3.80870 | 1.16332 | 3.55392 |
| C | 0.13572 | -0.41090 | -4.01510 |
| H | -0.29875 | -0.85027 | -4.91363 |
| C | -2.13944 | 0.64473 | -0.28118 |
| H | -1.61495 | 1.04887 | -1.14710 |
| C | -1.59008 | -0.43577 | 0.42611 |
| C | -2.28636 | -0.94059 | 1.53879 |
| H | -1.87554 | -1.78866 | 2.09040 |
| C | -3.35357 | 1.20983 | 0.11983 |
| H | -3.76943 | 2.04778 | -0.44093 |
| C | -4.02924 | 0.71105 | 1.23606 |
| H | -4.97467 | 1.15510 | 1.54848 |
| C | -3.49000 | -0.36569 | 1.94760 |
| H | -4.01295 | -0.76428 | 2.81752 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 28.28 | 0.32442 | YES YES |
| 8 | a | 32.03 | 0.34528 | YES YES |
| 9 | a | 47.83 | 0.01536 | YES YES |
| 10 | a | 52.20 | 0.09672 | YES YES |
| 11 | a | 53.28 | 0.05906 | YES YES |
| 12 | a | 64.24 | 0.37231 | YES YES |
| 13 | a | 177.87 | 0.25643 | YES YES |
| 14 | a | 193.97 | 1.13167 | YES YES |
| 15 | a | 196.57 | 1.14462 | YES YES |
| 16 | a | 240.72 | 0.83264 | YES YES |
| 17 | a | 251.41 | 0.40088 | YES YES |
| 18 | a | 253.59 | 0.44026 | YES YES |
| 19 | a | 389.20 | 1.28089 | YES YES |
| 20 | a | 389.92 | 1.47820 | YES YES |
| 21 | a | 393.40 | 0.13850 | YES YES |
| 22 | a | 397.27 | 0.28675 | YES YES |
| 23 | a | 417.13 | 5.17343 | YES YES |
| 24 | a | 419.75 | 6.04148 | YES YES |
| 25 | a | 488.47 | 24.64764 | YES YES |
| 26 | a | 491.68 | 25.65993 | YES YES |
| 27 | a | 501.44 | 16.30215 | YES YES |
| 28 | a | 611.93 | 0.18146 | YES YES |
| 29 | a | 612.33 | 0.20631 | YES YES |
| 30 | a | 612.68 | 0.06433 | YES YES |
| 31 | a | 673.55 | 1.17894 | YES YES |
| 32 | a | 686.83 | 0.43275 | YES YES |
| 33 | a | 687.69 | 0.45543 | YES YES |
| 34 | a | 692.91 | 36.57445 | YES YES |
| 35 | a | 693.19 | 35.13637 | YES YES |
| 36 | a | 694.15 | 29.92496 | YES YES |
| 37 | a | 738.30 | 27.96569 | YES YES |
| 38 | a | 738.96 | 22.31890 | YES YES |
| 39 | a | 739.55 | 25.84029 | YES YES |
| 40 | a | 835.91 | 0.07200 | YES YES |
| 41 | a | 836.88 | 0.10637 | YES YES |
| 42 | a | 839.83 | 0.20341 | YES YES |
| 43 | a | 904.60 | 1.07637 | YES YES |
| 44 | a | 905.46 | 0.79626 | YES YES |
| 45 | a | 908.05 | 0.41986 | YES YES |
| 46 | a | 956.40 | 0.00653 | YES YES |
| 47 | a | 956.78 | 0.11902 | YES YES |
| 48 | a | 958.62 | 0.13514 | YES YES |
| 49 | a | 971.48 | 0.01770 | YES YES |
| 50 | a | 971.92 | 0.01536 | YES YES |

**$P(^tBu)_3$**

bp86-d3_def2-tzvpp energy (au): -815.1643359689

Zero point energy (au): 0.3571682
Entropy (kJ mol^-1): 0.54042
Chemical potential (kJ mol^-1): 827.61

XYZ coordinates:

40

| | | | |
|---|---|---|---|
| P | 0.70323 | 0.00039 | -0.00038 |
| C | -0.01696 | 1.69470 | -0.61119 |
| C | -1.49417 | 1.72726 | -1.03735 |
| H | -1.76984 | 2.75523 | -1.32687 |
| C | 0.86701 | 2.15083 | -1.79648 |
| H | 0.60176 | 3.18715 | -2.06177 |
| H | 0.73524 | 1.54251 | -2.69549 |
| H | 1.93197 | 2.13204 | -1.52753 |
| C | -0.01672 | -1.37605 | -1.16255 |
| C | -1.49291 | -1.76414 | -0.97555 |
| H | -1.76709 | -2.53073 | -1.71947 |
| H | -2.16953 | -0.91336 | -1.11487 |
| H | -1.68840 | -2.19344 | 0.01395 |
| H | 0.74288 | -3.10235 | 0.01193 |
| H | 1.93420 | -2.38392 | -1.08763 |
| H | 0.60365 | -3.37879 | -1.72780 |
| C | 0.19374 | -0.94934 | -2.62933 |
| H | 1.23051 | -0.63965 | -2.82030 |
| H | -0.47565 | -0.13898 | -2.93789 |
| H | -0.01920 | -1.81175 | -3.28097 |
| C | -0.01887 | -0.31784 | 1.77237 |
| C | 0.19144 | -1.80179 | 2.13677 |
| H | -0.02414 | -1.93540 | 3.20906 |
| H | 1.22901 | -2.11986 | 1.96625 |
| H | -0.47583 | -2.47523 | 1.58789 |
| C | -1.49553 | 0.03805 | 2.01433 |
| H | -2.17117 | -0.50636 | 1.34529 |
| H | -1.69120 | 1.11008 | 1.89490 |
| H | -1.76991 | -0.22571 | 3.04934 |
| C | 0.86759 | 0.47753 | 2.76033 |
| H | 0.74265 | 1.56109 | 2.68080 |
| H | 1.93136 | 0.24683 | 2.61215 |
| H | 0.59846 | 0.19340 | 3.79080 |
| H | -1.69078 | 1.08681 | -1.90498 |
| H | -2.16892 | 1.42019 | -0.23024 |
| C | 0.19651 | 2.75085 | 0.49213 |
| H | -0.01964 | 3.74694 | 0.07371 |
| H | -0.46951 | 2.61147 | 1.35092 |
| H | 1.23454 | 2.76196 | 0.85165 |
| C | 0.87030 | -2.62875 | -0.96567 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 92.53 | 0.01627 | YES YES |
| 8 | a | 97.96 | 0.01382 | YES YES |
| 9 | a | 128.99 | 0.00118 | YES YES |
| 10 | a | 171.55 | 0.07846 | YES YES |
| 11 | a | 182.35 | 0.03587 | YES YES |
| 12 | a | 183.30 | 0.00634 | YES YES |
| 13 | a | 199.81 | 0.03290 | YES YES |
| 14 | a | 202.69 | 0.00348 | YES YES |
| 15 | a | 208.41 | 0.03285 | YES YES |
| 16 | a | 231.65 | 0.13097 | YES YES |
| 17 | a | 241.25 | 0.04557 | YES YES |
| 18 | a | 244.02 | 0.13850 | YES YES |
| 19 | a | 256.63 | 0.25812 | YES YES |
| 20 | a | 258.16 | 0.24053 | YES YES |
| 21 | a | 265.85 | 0.00543 | YES YES |
| 22 | a | 272.73 | 0.00504 | YES YES |
| 23 | a | 279.26 | 0.01648 | YES YES |
| 24 | a | 288.89 | 0.00145 | YES YES |
| 25 | a | 320.12 | 0.06846 | YES YES |
| 26 | a | 327.93 | 0.24446 | YES YES |
| 27 | a | 336.30 | 0.23137 | YES YES |
| 28 | a | 349.67 | 0.00729 | YES YES |
| 29 | a | 363.41 | 0.29787 | YES YES |
| 30 | a | 365.44 | 0.30351 | YES YES |
| 31 | a | 397.32 | 0.44636 | YES YES |
| 32 | a | 398.88 | 0.28725 | YES YES |
| 33 | a | 401.92 | 0.17004 | YES YES |
| 34 | a | 448.17 | 3.65293 | YES YES |
| 35 | a | 450.77 | 3.71831 | YES YES |
| 36 | a | 472.05 | 1.01593 | YES YES |
| 37 | a | 529.53 | 0.31072 | YES YES |
| 38 | a | 557.99 | 5.95101 | YES YES |
| 39 | a | 559.33 | 6.03573 | YES YES |
| 40 | a | 787.36 | 9.34079 | YES YES |
| 41 | a | 788.58 | 7.51422 | YES YES |
| 42 | a | 791.33 | 4.60246 | YES YES |
| 43 | a | 903.91 | 0.85428 | YES YES |
| 44 | a | 905.10 | 1.99040 | YES YES |
| 45 | a | 906.86 | 1.49548 | YES YES |
| 46 | a | 911.21 | 0.26771 | YES YES |
| 47 | a | 913.69 | 1.02224 | YES YES |
| 48 | a | 915.22 | 1.19177 | YES YES |
| 49 | a | 922.15 | 0.08711 | YES YES |
| 50 | a | 928.57 | 0.71637 | YES YES |

**$[GaCl_4]^-$**

bp86-d3_def2-tzvpp energy (au): -3766.5388836840

Zero point energy (au): 0.0045852
Entropy (kJ mol^-1): 0.36433
Chemical potential (kJ mol^-1): -73.78

XYZ coordinates:

5

| | | | |
|---|---|---|---|
| Ga | 0.00000 | 0.00000 | 0.00000 |
| Cl | -1.28247 | -1.28247 | -1.28247 |
| Cl | 1.28247 | 1.28247 | -1.28247 |
| Cl | 1.28247 | -1.28247 | 1.28247 |
| Cl | -1.28247 | 1.28247 | 1.28247 |

Vibrational Spectrum:

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | e | 98.16 | 0.00000 | NO YES |
| 8 | e | 98.16 | 0.00000 | NO YES |
| 9 | t2 | 140.22 | 8.85721 | YES YES |
| 10 | t2 | 140.22 | 8.85721 | YES YES |
| 11 | t2 | 140.22 | 8.85721 | YES YES |
| 12 | a1 | 319.28 | 0.00000 | NO YES |
| 13 | t2 | 358.82 | 91.28713 | YES YES |
| 14 | t2 | 358.82 | 91.28713 | YES YES |
| 15 | t2 | 358.82 | 91.28713 | YES YES |

**[PhS]+**

bp86-d3_def2-tzvpp energy (au): -629.6624710265

Zero point energy (au): 0.0880504
Entropy (kJ mol^-1): 0.32874
Chemical potential (kJ mol^-1): 151.34

XYZ coordinates:

12

| | | | |
|---|---|---|---|
| C | -2.26181 | -0.00004 | -0.00139 |
| H | -3.35356 | -0.00010 | -0.00301 |
| C | -0.20703 | 1.25773 | 0.00126 |
| H | 0.36152 | 2.18757 | 0.00211 |
| C | -1.58065 | 1.24276 | -0.00035 |
| H | -2.15007 | 2.17125 | -0.00090 |
| C | 0.53135 | 0.00004 | 0.00149 |
| C | -0.20696 | -1.25770 | 0.00122 |
| H | 0.36168 | -2.18749 | 0.00202 |
| C | -1.58057 | -1.24282 | -0.00036 |
| H | -2.14995 | -2.17133 | -0.00091 |
| S | 2.18663 | 0.00008 | 0.00068 |

Vibrational Spectrum:

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 100.18 | 0.00211 | YES YES |
| 8 | a | 290.93 | 0.00137 | YES YES |
| 9 | a | 302.89 | 0.00000 | YES YES |
| 10 | a | 357.88 | 0.30587 | YES YES |
| 11 | a | 428.06 | 0.20155 | YES YES |
| 12 | a | 565.83 | 2.41127 | YES YES |
| 13 | a | 602.92 | 41.89345 | YES YES |
| 14 | a | 717.64 | 3.70454 | YES YES |
| 15 | a | 786.09 | 31.59819 | YES YES |
| 16 | a | 799.75 | 0.00000 | YES YES |
| 17 | a | 967.13 | 6.16503 | YES YES |
| 18 | a | 983.43 | 8.23508 | YES YES |
| 19 | a | 987.15 | 0.88116 | YES YES |
| 20 | a | 996.07 | 0.00001 | YES YES |
| 21 | a | 1018.22 | 1.83927 | YES YES |
| 22 | a | 1075.39 | 3.34157 | YES YES |
| 23 | a | 1122.63 | 21.69596 | YES YES |
| 24 | a | 1154.07 | 13.63161 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 25 | a | 1188.65 | 0.89158 | YES | YES |
| 26 | a | 1242.64 | 4.25495 | YES | YES |
| 27 | a | 1352.10 | 1.47093 | YES | YES |
| 28 | a | 1417.31 | 17.31537 | YES | YES |
| 29 | a | 1437.44 | 97.69182 | YES | YES |
| 30 | a | 1502.70 | 14.00518 | YES | YES |
| 31 | a | 1591.28 | 130.04811 | YES | YES |
| 32 | a | 3114.63 | 0.82861 | YES | YES |
| 33 | a | 3129.94 | 1.48883 | YES | YES |
| 34 | a | 3131.62 | 8.55309 | YES | YES |
| 35 | a | 3141.34 | 15.08453 | YES | YES |
| 36 | a | 3143.74 | 0.21805 | YES | YES |

**PhSCl.GaCl3_iso2**

bp86-d3_def2-tzvpp energy (au): -4396.3903114070

Zero point energy (au): 0.0946623
Entropy (kJ mol^-1): 0.54742
Chemical potential (kJ mol^-1): 127.41

XYZ coordinates:

17

| | | | |
|---|---|---|---|
| S | 0.29509 | 0.98241 | 1.82167 |
| C | -0.91818 | 0.00730 | 1.01746 |
| C | -0.87645 | -0.10110 | -0.38565 |
| H | -0.06048 | 0.36547 | -0.93417 |
| C | -1.86452 | -0.82791 | -1.04605 |
| H | -1.83609 | -0.91615 | -2.13136 |
| C | -2.86688 | -1.46848 | -0.31325 |
| H | -3.62558 | -2.05434 | -0.83208 |
| C | -2.90000 | -1.37412 | 1.08444 |
| H | -3.68220 | -1.88174 | 1.64785 |
| C | -1.93507 | -0.63026 | 1.75385 |
| H | -1.94551 | -0.54365 | 2.83958 |
| Ga | 2.24478 | -2.07114 | 0.77262 |
| Cl | 1.61807 | -0.48729 | 2.64669 |
| Cl | 3.92812 | -2.96628 | 1.78115 |
| Cl | 2.62751 | -0.68207 | -0.83820 |
| Cl | 0.44141 | -3.25365 | 0.63743 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 28.29 | 0.34861 | YES YES |
| 8 | a | 47.53 | 0.47937 | YES YES |
| 9 | a | 56.57 | 0.00090 | YES YES |
| 10 | a | 65.86 | 1.04879 | YES YES |
| 11 | a | 73.53 | 0.07715 | YES YES |
| 12 | a | 99.07 | 0.35324 | YES YES |
| 13 | a | 103.14 | 0.67925 | YES YES |
| 14 | a | 122.02 | 4.08102 | YES YES |
| 15 | a | 125.97 | 5.53411 | YES YES |
| 16 | a | 137.15 | 25.84846 | YES YES |
| 17 | a | 169.55 | 24.10540 | YES YES |
| 18 | a | 235.54 | 4.85213 | YES YES |
| 19 | a | 272.18 | 2.45470 | YES YES |
| 20 | a | 342.96 | 11.91649 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 21 | a | 377.84 | 38.35038 | YES | YES |
| 22 | a | 392.05 | 1.69466 | YES | YES |
| 23 | a | 406.83 | 6.35091 | YES | YES |
| 24 | a | 415.27 | 65.16579 | YES | YES |
| 25 | a | 420.80 | 82.25474 | YES | YES |
| 26 | a | 481.94 | 12.15404 | YES | YES |
| 27 | a | 604.48 | 0.02943 | YES | YES |
| 28 | a | 672.48 | 37.97673 | YES | YES |
| 29 | a | 705.16 | 1.87677 | YES | YES |
| 30 | a | 747.97 | 38.06638 | YES | YES |
| 31 | a | 825.25 | 1.82409 | YES | YES |
| 32 | a | 923.28 | 3.34902 | YES | YES |
| 33 | a | 962.70 | 0.64026 | YES | YES |
| 34 | a | 984.94 | 0.16609 | YES | YES |
| 35 | a | 991.99 | 2.02412 | YES | YES |
| 36 | a | 1017.85 | 0.09358 | YES | YES |
| 37 | a | 1063.12 | 33.56447 | YES | YES |
| 38 | a | 1074.93 | 6.34838 | YES | YES |
| 39 | a | 1156.24 | 0.35356 | YES | YES |
| 40 | a | 1169.40 | 2.83536 | YES | YES |
| 41 | a | 1290.76 | 1.00923 | YES | YES |
| 42 | a | 1340.40 | 5.64126 | YES | YES |
| 43 | a | 1431.50 | 13.93469 | YES | YES |
| 44 | a | 1455.96 | 0.82231 | YES | YES |
| 45 | a | 1560.58 | 0.80390 | YES | YES |
| 46 | a | 1573.53 | 22.13211 | YES | YES |
| 47 | a | 3106.94 | 0.36569 | YES | YES |
| 48 | a | 3118.03 | 3.73629 | YES | YES |
| 49 | a | 3125.87 | 5.41407 | YES | YES |
| 50 | a | 3132.82 | 5.73460 | YES | YES |

**[PhSe]+**

bp86-d3_def2-tzvpp energy (au): -2633.2606731340

Zero point energy (au): 0.0874825
Entropy (kJ mol^-1): 0.34047
Chemical potential (kJ mol^-1): 146.83

XYZ coordinates:

12

| | | | |
|---|---|---|---|
| C | -3.00003 | -0.00007 | -0.00016 |
| H | -4.09135 | -0.00013 | -0.00026 |
| C | -0.93951 | 1.25215 | 0.00019 |
| H | -0.37717 | 2.18549 | 0.00033 |
| C | -2.31599 | 1.23888 | 0.00001 |
| H | -2.88121 | 2.16987 | 0.00023 |
| C | -0.21266 | 0.00002 | 0.00014 |
| C | -0.93942 | -1.25216 | 0.00032 |
| H | -0.37705 | -2.18548 | 0.00026 |
| C | -2.31591 | -1.23897 | 0.00002 |
| H | -2.88106 | -2.17001 | -0.00008 |
| Se | 1.60034 | 0.00008 | -0.00053 |

Vibrational Spectrum:

| # mode | symmetry | wave number | IR intensity | selection rules | |
|---|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR | RAMAN |
| 1 | | 0.00 | 0.00000 | - | - |
| 2 | | 0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 92.88 | 0.00479 | YES | YES |
| 8 | a | 240.21 | 0.00060 | YES | YES |
| 9 | a | 311.62 | 0.00000 | YES | YES |
| 10 | a | 330.92 | 0.03551 | YES | YES |
| 11 | a | 364.08 | 0.04692 | YES | YES |
| 12 | a | 569.21 | 1.80632 | YES | YES |
| 13 | a | 608.16 | 41.37138 | YES | YES |
| 14 | a | 681.99 | 3.26909 | YES | YES |
| 15 | a | 773.80 | 33.59309 | YES | YES |
| 16 | a | 805.14 | 0.00001 | YES | YES |
| 17 | a | 971.39 | 14.38549 | YES | YES |
| 18 | a | 976.69 | 0.89729 | YES | YES |
| 19 | a | 988.92 | 6.17189 | YES | YES |
| 20 | a | 993.71 | 0.00010 | YES | YES |
| 21 | a | 1014.56 | 1.23401 | YES | YES |
| 22 | a | 1056.85 | 24.65728 | YES | YES |
| 23 | a | 1078.05 | 3.86789 | YES | YES |
| 24 | a | 1156.11 | 9.49275 | YES | YES |
| 25 | a | 1183.22 | 4.91222 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 26 | a | 1252.08 | 5.56957 | YES | YES |
| 27 | a | 1353.46 | 3.11711 | YES | YES |
| 28 | a | 1420.39 | 13.31610 | YES | YES |
| 29 | a | 1428.98 | 77.41372 | YES | YES |
| 30 | a | 1500.00 | 9.57197 | YES | YES |
| 31 | a | 1584.99 | 140.83584 | YES | YES |
| 32 | a | 3116.95 | 0.40110 | YES | YES |
| 33 | a | 3129.61 | 1.37081 | YES | YES |
| 34 | a | 3131.58 | 7.25232 | YES | YES |
| 35 | a | 3141.09 | 11.72519 | YES | YES |
| 36 | a | 3143.71 | 0.16757 | YES | YES |

**PhSeCl.GaCl3_iso2**

bp86-d3_def2-tzvpp energy (au): -6399.9905396430

Zero point energy (au): 0.0938354
Entropy (kJ mol^-1): 0.55997
Chemical potential (kJ mol^-1): 122.48

XYZ coordinates:

17

| | | | |
|---|---|---|---|
| Se | 0.35104 | 1.10861 | 1.86826 |
| C | -0.95789 | 0.03249 | 1.00292 |
| C | -0.90403 | -0.10396 | -0.39467 |
| H | -0.09180 | 0.35658 | -0.95393 |
| C | -1.87746 | -0.86287 | -1.04244 |
| H | -1.83995 | -0.97766 | -2.12508 |
| C | -2.87567 | -1.49954 | -0.30050 |
| H | -3.62282 | -2.10835 | -0.80960 |
| C | -2.91763 | -1.37287 | 1.09353 |
| H | -3.69494 | -1.87837 | 1.66575 |
| C | -1.96519 | -0.60019 | 1.75158 |
| H | -1.98561 | -0.49194 | 2.83512 |
| Ga | 2.26367 | -2.07338 | 0.76306 |
| Cl | 1.72899 | -0.51820 | 2.67168 |
| Cl | 3.96716 | -3.00954 | 1.70022 |
| Cl | 2.62493 | -0.67453 | -0.84688 |
| Cl | 0.44121 | -3.22928 | 0.64296 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 28.34 | 0.22112 | YES YES |
| 8 | a | 46.38 | 0.23431 | YES YES |
| 9 | a | 53.55 | 0.20080 | YES YES |
| 10 | a | 58.20 | 0.87532 | YES YES |
| 11 | a | 71.36 | 0.02647 | YES YES |
| 12 | a | 89.82 | 0.12134 | YES YES |
| 13 | a | 97.92 | 0.25507 | YES YES |
| 14 | a | 122.07 | 4.21270 | YES YES |
| 15 | a | 125.12 | 5.50554 | YES YES |
| 16 | a | 136.31 | 24.11961 | YES YES |
| 17 | a | 171.08 | 24.75813 | YES YES |
| 18 | a | 214.85 | 4.53918 | YES YES |
| 19 | a | 232.12 | 0.80803 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 20 | a | 298.16 | 31.41035 | YES | YES |
| 21 | a | 315.35 | 10.98643 | YES | YES |
| 22 | a | 346.81 | 5.80637 | YES | YES |
| 23 | a | 392.45 | 0.90013 | YES | YES |
| 24 | a | 413.64 | 60.26055 | YES | YES |
| 25 | a | 419.62 | 72.63105 | YES | YES |
| 26 | a | 454.25 | 7.89304 | YES | YES |
| 27 | a | 603.79 | 0.05322 | YES | YES |
| 28 | a | 672.59 | 1.46546 | YES | YES |
| 29 | a | 674.41 | 33.10119 | YES | YES |
| 30 | a | 739.10 | 41.92552 | YES | YES |
| 31 | a | 825.56 | 1.45026 | YES | YES |
| 32 | a | 919.48 | 2.76295 | YES | YES |
| 33 | a | 961.30 | 0.47277 | YES | YES |
| 34 | a | 983.63 | 0.26266 | YES | YES |
| 35 | a | 991.19 | 2.33203 | YES | YES |
| 36 | a | 1013.55 | 1.13735 | YES | YES |
| 37 | a | 1048.63 | 23.85653 | YES | YES |
| 38 | a | 1073.43 | 3.65970 | YES | YES |
| 39 | a | 1155.85 | 0.26258 | YES | YES |
| 40 | a | 1170.53 | 4.31827 | YES | YES |
| 41 | a | 1292.59 | 1.59288 | YES | YES |
| 42 | a | 1337.76 | 5.16478 | YES | YES |
| 43 | a | 1429.70 | 13.74799 | YES | YES |
| 44 | a | 1454.88 | 0.87019 | YES | YES |
| 45 | a | 1561.52 | 1.30591 | YES | YES |
| 46 | a | 1568.74 | 17.05232 | YES | YES |
| 47 | a | 3106.79 | 0.40197 | YES | YES |
| 48 | a | 3117.83 | 4.10211 | YES | YES |
| 49 | a | 3125.75 | 4.99700 | YES | YES |
| 50 | a | 3132.73 | 5.69652 | YES | YES |

**[PhSe(PPh3)]+**

bp86-d3_def2-tzvpp energy (au): -3670.0876135790

Zero point energy (au): 0.3570830
Entropy (kJ mol^-1): 0.71020
Chemical potential (kJ mol^-1): 790.16

XYZ coordinates:

46

| | | | |
|---|---|---|---|
| C | -1.03007 | 5.00723 | -1.15208 |
| H | -1.25861 | 6.03870 | -1.41848 |
| C | 2.76235 | -1.79097 | -1.67433 |
| H | 3.23091 | -2.74152 | -1.42265 |
| Se | -1.98726 | -0.46901 | -0.25782 |
| P | -0.04415 | 0.66391 | -0.03692 |
| C | 2.50109 | 0.09248 | -3.17852 |
| H | 2.77290 | 0.61254 | -4.09631 |
| C | -1.48431 | 3.96235 | -1.96337 |
| H | -2.06531 | 4.17661 | -2.85949 |
| C | -0.45032 | 2.36654 | -0.46601 |
| C | 1.82171 | -1.23923 | -0.80734 |
| H | 1.56234 | -1.75911 | 0.11452 |
| C | 1.48048 | 0.63580 | 4.29639 |
| H | 1.84100 | 0.64896 | 5.32450 |
| C | 1.21635 | -0.00965 | -1.13157 |
| C | -0.31594 | -4.21894 | -1.12887 |
| H | -0.09996 | -4.79689 | -2.02685 |
| C | -1.19968 | 2.64023 | -1.62578 |
| H | -1.55840 | 1.82718 | -2.25741 |
| C | 0.55672 | 0.58768 | 1.66363 |
| C | 0.10548 | 0.60306 | 4.04080 |
| H | -0.60528 | 0.59338 | 4.86624 |
| C | 1.55627 | 0.65574 | -2.32160 |
| H | 1.09878 | 1.61207 | -2.57162 |
| C | 3.10097 | -1.12885 | -2.85806 |
| H | 3.83938 | -1.56350 | -3.53121 |
| C | 0.00254 | 3.41551 | 0.35153 |
| H | 0.57359 | 3.20425 | 1.25493 |
| C | 1.93857 | 0.62855 | 1.91919 |
| H | 2.65280 | 0.64356 | 1.09697 |
| C | -0.36101 | 0.57947 | 2.72752 |
| H | -1.43207 | 0.54797 | 2.52678 |
| C | -0.88634 | -2.73679 | 1.18299 |
| H | -1.11232 | -2.15945 | 2.07795 |
| C | -0.29020 | 4.73392 | 0.00150 |
| H | 0.05782 | 5.54859 | 0.63531 |
| C | 2.39334 | 0.65108 | 3.23843 |
| H | 3.46393 | 0.67957 | 3.43791 |
| C | -0.27439 | -3.98816 | 1.28430 |
| H | -0.02822 | -4.38872 | 2.26720 |
| C | -0.91533 | -2.96268 | -1.24568 |
| H | -1.15218 | -2.55237 | -2.22606 |
| C | 0.01120 | -4.72656 | 0.13127 |
| H | 0.48301 | -5.70496 | 0.21691 |

C -1.19424 -2.23134 -0.08583

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|
| 1 | | 0.00 | 0.00000 | - | - |
| 2 | | 0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 14.43 | 0.07798 | YES | YES |
| 8 | a | 30.25 | 0.02390 | YES | YES |
| 9 | a | 38.49 | 0.14963 | YES | YES |
| 10 | a | 45.31 | 0.07136 | YES | YES |
| 11 | a | 47.69 | 0.17102 | YES | YES |
| 12 | a | 55.29 | 0.16034 | YES | YES |
| 13 | a | 60.10 | 0.10101 | YES | YES |
| 14 | a | 67.06 | 0.09922 | YES | YES |
| 15 | a | 82.80 | 0.11003 | YES | YES |
| 16 | a | 89.21 | 0.37226 | YES | YES |
| 17 | a | 98.08 | 0.38281 | YES | YES |
| 18 | a | 182.02 | 1.59622 | YES | YES |
| 19 | a | 188.89 | 1.27550 | YES | YES |
| 20 | a | 206.15 | 1.45794 | YES | YES |
| 21 | a | 213.32 | 0.14108 | YES | YES |
| 22 | a | 228.91 | 1.18393 | YES | YES |
| 23 | a | 240.35 | 0.63311 | YES | YES |
| 24 | a | 243.57 | 0.81700 | YES | YES |
| 25 | a | 255.32 | 0.39825 | YES | YES |
| 26 | a | 267.06 | 0.24853 | YES | YES |
| 27 | a | 296.91 | 0.57433 | YES | YES |
| 28 | a | 387.95 | 0.07777 | YES | YES |
| 29 | a | 389.07 | 0.02121 | YES | YES |
| 30 | a | 396.27 | 0.06921 | YES | YES |
| 31 | a | 397.91 | 0.32905 | YES | YES |
| 32 | a | 417.84 | 6.79991 | YES | YES |
| 33 | a | 434.39 | 7.67561 | YES | YES |
| 34 | a | 442.54 | 6.54467 | YES | YES |
| 35 | a | 461.91 | 6.54367 | YES | YES |
| 36 | a | 491.17 | 51.50704 | YES | YES |
| 37 | a | 505.76 | 75.20848 | YES | YES |
| 38 | a | 520.32 | 75.74747 | YES | YES |
| 39 | a | 604.88 | 0.00486 | YES | YES |
| 40 | a | 605.84 | 0.43456 | YES | YES |
| 41 | a | 608.27 | 0.06254 | YES | YES |
| 42 | a | 609.00 | 0.12940 | YES | YES |
| 43 | a | 660.94 | 2.42094 | YES | YES |
| 44 | a | 679.22 | 3.96503 | YES | YES |
| 45 | a | 685.54 | 0.22423 | YES | YES |
| 46 | a | 686.30 | 64.73354 | YES | YES |
| 47 | a | 687.38 | 21.92729 | YES | YES |
| 48 | a | 689.92 | 8.37274 | YES | YES |
| 49 | a | 712.55 | 25.87330 | YES | YES |
| 50 | a | 713.90 | 31.17941 | YES | YES |

**[PhSe(PPh3).PPh3]+**

bp86-d3_def2-tzvpp energy (au): -4706.7874280170

Zero point energy (au): 0.6237177
Entropy (kJ mol^-1): 1.11976
Chemical potential (kJ mol^-1): 1417.06

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.72713 | 0.67722 | 3.88253 |
| H | -5.76080 | 0.84166 | 4.18587 |
| C | 2.87383 | 2.26859 | 3.59809 |
| H | 3.95245 | 2.21217 | 3.45422 |
| Se | -0.47590 | 0.00481 | -0.00313 |
| P | -0.36292 | 0.01159 | 2.55666 |
| C | 0.92563 | 3.41866 | 4.45892 |
| H | 0.48282 | 4.25849 | 4.99386 |
| C | -4.16287 | 1.46199 | 2.87230 |
| H | -4.75359 | 2.23864 | 2.38726 |
| C | -2.07256 | 0.25188 | 3.10636 |
| C | 2.06094 | 1.25207 | 3.10071 |
| H | 2.50986 | 0.41001 | 2.57367 |
| C | 1.01085 | -4.09378 | 4.14837 |
| H | 1.32795 | -5.07106 | 4.51151 |
| C | 0.66625 | 1.31196 | 3.28717 |
| C | 3.55392 | 1.19055 | -0.25194 |
| H | 4.09504 | 2.11404 | -0.45610 |
| C | -2.84211 | 1.24775 | 2.47753 |
| H | -2.40435 | 1.85625 | 1.68487 |
| C | 0.20465 | -1.58187 | 3.21250 |
| C | 0.19144 | -4.00004 | 3.01851 |
| H | -0.13262 | -4.90260 | 2.50080 |
| C | 0.10251 | 2.40286 | 3.96889 |
| H | -0.97436 | 2.45442 | 4.12636 |
| C | 2.30900 | 3.35493 | 4.27435 |
| H | 2.94775 | 4.14881 | 4.66068 |
| C | -2.64347 | -0.53542 | 4.11903 |
| H | -2.05469 | -1.31340 | 4.60445 |
| C | 1.02061 | -1.67969 | 4.35030 |
| H | 1.33975 | -0.77964 | 4.87467 |
| C | -0.20702 | -2.74993 | 2.54713 |
| H | -0.83373 | -2.67478 | 1.65749 |
| C | 2.15714 | -1.18030 | 0.27012 |
| H | 1.61131 | -2.10251 | 0.46064 |
| C | -3.96838 | -0.32020 | 4.50161 |
| H | -4.40849 | -0.93272 | 5.28813 |
| C | 1.42277 | -2.93505 | 4.81145 |
| H | 2.05678 | -3.00630 | 5.69494 |
| C | 3.55399 | -1.17098 | 0.28780 |
| H | 4.09520 | -2.09298 | 0.49824 |
| C | 2.15688 | 1.19594 | -0.25071 |
| H | 1.61076 | 2.11665 | -0.44772 |
| C | 4.25221 | 0.01079 | 0.02226 |
| H | 5.34189 | 0.01239 | 0.02907 |

| | | | |
|---|---|---|---|
| C | 1.46395 | 0.00693 | 0.00604 |
| C | -4.68674 | -0.70807 | -3.92524 |
| H | -5.71566 | -0.87968 | -4.24039 |
| C | 2.91729 | -2.25783 | -3.55225 |
| H | 3.99544 | -2.18828 | -3.41062 |
| P | -0.34130 | -0.01245 | -2.55360 |
| C | 0.97945 | -3.44367 | -4.38766 |
| H | 0.54424 | -4.29837 | -4.90497 |
| C | -4.13518 | -1.47524 | -2.89477 |
| H | -4.73120 | -2.24510 | -2.40542 |
| C | -2.04409 | -0.26476 | -3.11914 |
| C | 2.09522 | -1.23915 | -3.07472 |
| H | 2.53637 | -0.38273 | -2.56438 |
| C | 1.03135 | 4.08270 | -4.17156 |
| H | 1.34769 | 5.05763 | -4.54155 |
| C | 0.70108 | -1.31576 | -3.25930 |
| C | -2.82031 | -1.25226 | -2.48532 |
| H | -2.39247 | -1.84749 | -1.67735 |
| C | 0.22728 | 1.57701 | -3.21794 |
| C | 0.21228 | 3.99633 | -3.04092 |
| H | -0.11215 | 4.90225 | -2.52939 |
| C | 0.14717 | -2.42573 | -3.91805 |
| H | -0.92925 | -2.49048 | -4.07397 |
| C | 2.36230 | -3.36300 | -4.20576 |
| H | 3.00830 | -4.15843 | -4.57650 |
| C | -2.60254 | 0.50546 | -4.15183 |
| H | -2.00873 | 1.27720 | -4.64116 |
| C | 1.04276 | 1.66734 | -4.35686 |
| H | 1.36253 | 0.76379 | -4.87490 |
| C | -0.18537 | 2.74927 | -2.56075 |
| H | -0.81193 | 2.67977 | -1.67052 |
| C | -3.92145 | 0.28116 | -4.54944 |
| H | -4.35181 | 0.88031 | -5.35149 |
| C | 1.44388 | 2.91972 | -4.82684 |
| H | 2.07764 | 2.98529 | -5.71096 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 5.88 | 0.00286 | YES YES |
| 8 | a | 7.75 | 0.13103 | YES YES |
| 9 | a | 18.24 | 0.00455 | YES YES |
| 10 | a | 23.00 | 0.00701 | YES YES |
| 11 | a | 23.18 | 0.09220 | YES YES |
| 12 | a | 26.33 | 0.03969 | YES YES |
| 13 | a | 35.97 | 0.07380 | YES YES |
| 14 | a | 38.67 | 0.03970 | YES YES |
| 15 | a | 40.48 | 2.74725 | YES YES |
| 16 | a | 43.28 | 0.04774 | YES YES |
| 17 | a | 45.54 | 6.24987 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 18 | a | 48.74 | 0.74447 | YES | YES |
| 19 | a | 52.27 | 0.14524 | YES | YES |
| 20 | a | 56.56 | 0.02899 | YES | YES |
| 21 | a | 58.98 | 0.02477 | YES | YES |
| 22 | a | 60.22 | 21.36435 | YES | YES |
| 23 | a | 73.69 | 0.37858 | YES | YES |
| 24 | a | 73.96 | 0.01283 | YES | YES |
| 25 | a | 80.73 | 24.37585 | YES | YES |
| 26 | a | 87.96 | 0.00673 | YES | YES |
| 27 | a | 93.62 | 89.40082 | YES | YES |
| 28 | a | 103.41 | 0.08126 | YES | YES |
| 29 | a | 115.29 | 0.83777 | YES | YES |
| 30 | a | 124.49 | 0.04887 | YES | YES |
| 31 | a | 182.22 | 2.97204 | YES | YES |
| 32 | a | 183.18 | 0.43642 | YES | YES |
| 33 | a | 192.82 | 0.25353 | YES | YES |
| 34 | a | 194.74 | 4.36579 | YES | YES |
| 35 | a | 202.19 | 0.99984 | YES | YES |
| 36 | a | 203.74 | 3.05765 | YES | YES |
| 37 | a | 216.54 | 11.99671 | YES | YES |
| 38 | a | 236.25 | 7.62052 | YES | YES |
| 39 | a | 237.84 | 0.34273 | YES | YES |
| 40 | a | 238.37 | 0.41145 | YES | YES |
| 41 | a | 252.46 | 0.10658 | YES | YES |
| 42 | a | 253.17 | 1.59229 | YES | YES |
| 43 | a | 263.96 | 0.94950 | YES | YES |
| 44 | a | 264.83 | 0.19526 | YES | YES |
| 45 | a | 304.72 | 0.02490 | YES | YES |
| 46 | a | 387.89 | 0.00330 | YES | YES |
| 47 | a | 388.52 | 0.14396 | YES | YES |
| 48 | a | 388.88 | 0.19709 | YES | YES |
| 49 | a | 389.26 | 1.02459 | YES | YES |
| 50 | a | 390.45 | 0.33747 | YES | YES |

**[PhSe(PtBu3).PPh3]+**

bp86-d3_def2-tzvpp energy (au): -4485.2910788000

Zero point energy (au): 0.7160305
Entropy (kJ mol^-1): 1.08565
Chemical potential (kJ mol^-1): 1674.77

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.05919 | 0.38462 | -0.03737 |
| Se | 0.52559 | 0.23680 | 0.04992 |
| C | 0.27582 | -1.69269 | 0.13388 |
| C | -0.06718 | -2.38342 | -1.03648 |
| H | -0.14991 | -1.84967 | -1.98211 |
| C | -0.33003 | -3.75409 | -0.98108 |
| H | -0.60305 | -4.28576 | -1.89223 |
| C | -0.24262 | -4.43805 | 0.23525 |
| H | -0.44146 | -5.50865 | 0.27449 |
| C | 0.08829 | -3.74411 | 1.40147 |
| H | 0.13823 | -4.26716 | 2.35613 |
| C | 0.33521 | -2.36925 | 1.35648 |
| H | 0.55191 | -1.82775 | 2.27333 |
| C | -3.00721 | -0.46146 | 1.25347 |
| C | -2.98099 | -1.86907 | 1.28965 |
| H | -2.44679 | -2.42853 | 0.52149 |
| C | -3.64838 | -2.55223 | 2.30441 |
| H | -3.62976 | -3.64173 | 2.32098 |
| C | -4.33433 | -1.84426 | 3.29679 |
| H | -4.85270 | -2.38142 | 4.09062 |
| C | -4.35744 | -0.44752 | 3.26722 |
| H | -4.89734 | 0.10719 | 4.03428 |
| C | -3.69802 | 0.24632 | 2.25070 |
| H | -3.72863 | 1.33532 | 2.22846 |
| C | -2.37004 | 2.16670 | 0.09755 |
| C | -3.25489 | 2.83694 | -0.76180 |
| H | -3.79267 | 2.28322 | -1.53109 |
| C | -3.44313 | 4.21394 | -0.63067 |
| H | -4.13180 | 4.72992 | -1.29926 |
| C | -2.75580 | 4.92789 | 0.35505 |
| H | -2.90725 | 6.00247 | 0.45424 |
| C | -1.87343 | 4.26471 | 1.21329 |
| H | -1.33779 | 4.81969 | 1.98317 |
| C | -1.67383 | 2.89008 | 1.08337 |
| H | -0.98250 | 2.37375 | 1.75112 |
| C | -2.69804 | -0.15318 | -1.64880 |
| C | -3.88223 | -0.89262 | -1.78999 |
| H | -4.47159 | -1.15526 | -0.91228 |
| C | -4.30770 | -1.29013 | -3.05974 |
| H | -5.22836 | -1.86394 | -3.16342 |
| C | -3.56326 | -0.94858 | -4.19145 |
| H | -3.89985 | -1.26013 | -5.17993 |
| C | -2.38593 | -0.20475 | -4.05560 |
| H | -1.80517 | 0.06636 | -4.93705 |
| C | -1.94982 | 0.18647 | -2.79076 |

| | | | |
|---|---|---|---|
| H | -1.02413 | 0.75377 | -2.68247 |
| P | 3.10867 | 0.29871 | 0.06136 |
| C | 3.42880 | 1.89448 | -0.96547 |
| C | 4.82917 | 2.49393 | -0.73607 |
| H | 4.95535 | 3.34956 | -1.41690 |
| C | 2.36086 | 2.96388 | -0.63152 |
| H | 2.57750 | 3.85323 | -1.24190 |
| H | 2.35958 | 3.28095 | 0.41306 |
| H | 1.34793 | 2.63459 | -0.89684 |
| C | 3.67563 | 0.56536 | 1.87801 |
| C | 5.19758 | 0.43547 | 2.07439 |
| H | 5.43304 | 0.66943 | 3.12375 |
| H | 5.76716 | 1.12985 | 1.44768 |
| H | 5.55941 | -0.58062 | 1.88352 |
| H | 3.12524 | -1.49846 | 2.50279 |
| H | 1.86506 | -0.27274 | 2.76862 |
| H | 3.29937 | -0.31835 | 3.80911 |
| C | 3.22094 | 1.95426 | 2.36990 |
| H | 2.14265 | 2.10528 | 2.22812 |
| H | 3.76469 | 2.77889 | 1.89853 |
| H | 3.42014 | 2.01075 | 3.45030 |
| C | 4.01986 | -1.20160 | -0.72318 |
| C | 3.97508 | -2.38542 | 0.26476 |
| H | 4.39232 | -3.26590 | -0.24551 |
| H | 2.94870 | -2.63511 | 0.56241 |
| H | 4.57924 | -2.21848 | 1.16238 |
| C | 5.48360 | -0.90700 | -1.10106 |
| H | 6.08987 | -0.57776 | -0.25133 |
| H | 5.56547 | -0.15915 | -1.89752 |
| H | 5.93167 | -1.83620 | -1.48528 |
| C | 3.25715 | -1.65526 | -1.98641 |
| H | 3.29897 | -0.93422 | -2.80511 |
| H | 2.20877 | -1.88026 | -1.76941 |
| H | 3.72493 | -2.58401 | -2.34568 |
| H | 4.96170 | 2.87268 | 0.28300 |
| H | 5.63587 | 1.78480 | -0.94798 |
| C | 3.25813 | 1.57419 | -2.46388 |
| H | 3.27764 | 2.52355 | -3.01901 |
| H | 4.06740 | 0.95297 | -2.86090 |
| H | 2.29609 | 1.08781 | -2.67193 |
| C | 2.94635 | -0.45597 | 2.77631 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 11.32 | 0.09564 | YES YES |
| 8 | a | 16.40 | 0.04808 | YES YES |
| 9 | a | 23.14 | 0.34415 | YES YES |
| 10 | a | 25.03 | 0.14258 | YES YES |
| 11 | a | 38.88 | 3.79306 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 43.06 | 0.86337 | YES | YES |
| 13 | a | 48.72 | 0.11583 | YES | YES |
| 14 | a | 51.83 | 1.68161 | YES | YES |
| 15 | a | 55.66 | 2.90898 | YES | YES |
| 16 | a | 58.52 | 15.08528 | YES | YES |
| 17 | a | 62.47 | 13.45723 | YES | YES |
| 18 | a | 74.29 | 38.65931 | YES | YES |
| 19 | a | 75.74 | 7.81731 | YES | YES |
| 20 | a | 82.81 | 7.20340 | YES | YES |
| 21 | a | 95.65 | 0.04491 | YES | YES |
| 22 | a | 97.24 | 10.47810 | YES | YES |
| 23 | a | 101.41 | 0.50756 | YES | YES |
| 24 | a | 108.95 | 13.83704 | YES | YES |
| 25 | a | 119.52 | 0.87410 | YES | YES |
| 26 | a | 126.24 | 0.33029 | YES | YES |
| 27 | a | 129.60 | 0.27033 | YES | YES |
| 28 | a | 166.00 | 0.07684 | YES | YES |
| 29 | a | 183.46 | 1.24840 | YES | YES |
| 30 | a | 189.93 | 0.30960 | YES | YES |
| 31 | a | 194.61 | 1.60993 | YES | YES |
| 32 | a | 196.98 | 1.81869 | YES | YES |
| 33 | a | 197.23 | 0.33167 | YES | YES |
| 34 | a | 202.65 | 0.79475 | YES | YES |
| 35 | a | 205.23 | 0.99582 | YES | YES |
| 36 | a | 211.55 | 0.38625 | YES | YES |
| 37 | a | 221.57 | 16.14691 | YES | YES |
| 38 | a | 226.90 | 0.20270 | YES | YES |
| 39 | a | 234.80 | 4.09854 | YES | YES |
| 40 | a | 237.74 | 0.64877 | YES | YES |
| 41 | a | 241.18 | 0.28331 | YES | YES |
| 42 | a | 251.12 | 0.18108 | YES | YES |
| 43 | a | 254.37 | 1.11001 | YES | YES |
| 44 | a | 254.54 | 0.41301 | YES | YES |
| 45 | a | 257.55 | 0.40045 | YES | YES |
| 46 | a | 263.67 | 0.63480 | YES | YES |
| 47 | a | 272.18 | 0.55035 | YES | YES |
| 48 | a | 275.81 | 0.04960 | YES | YES |
| 49 | a | 279.55 | 0.04045 | YES | YES |
| 50 | a | 289.22 | 1.19756 | YES | YES |

**[PhSe(PPh3).PtBu3]+_iso1**

bp86-d3_def2-tzvpp energy (au): -4485.2910762470

Zero point energy (au): 0.7160289
Entropy (kJ mol^-1): 1.08484
Chemical potential (kJ mol^-1): 1674.97

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.04946 | 0.38089 | 0.01359 |
| Se | 0.52874 | 0.22577 | 0.02473 |
| C | 0.28095 | -1.70495 | 0.03151 |
| C | -0.08681 | -2.34336 | -1.16081 |
| H | -0.18443 | -1.76852 | -2.08060 |
| C | -0.35077 | -3.71496 | -1.15998 |
| H | -0.64287 | -4.20638 | -2.08768 |
| C | -0.23859 | -4.45152 | 0.02322 |
| H | -0.43874 | -5.52260 | 0.01988 |
| C | 0.12052 | -3.81011 | 1.21092 |
| H | 0.19220 | -4.37515 | 2.13993 |
| C | 0.36858 | -2.43465 | 1.22128 |
| H | 0.61063 | -1.93505 | 2.15564 |
| C | -2.94927 | -0.53670 | 1.28980 |
| C | -2.93898 | -1.94383 | 1.23399 |
| H | -2.44799 | -2.45719 | 0.40703 |
| C | -3.56631 | -2.68514 | 2.23329 |
| H | -3.56032 | -3.77354 | 2.17859 |
| C | -4.19593 | -2.03676 | 3.30085 |
| H | -4.68304 | -2.61945 | 4.08229 |
| C | -4.20319 | -0.64087 | 3.36231 |
| H | -4.69975 | -0.13208 | 4.18823 |
| C | -3.58380 | 0.11132 | 2.36221 |
| H | -3.60280 | 1.19970 | 2.41144 |
| C | -2.34755 | 2.15296 | 0.25946 |
| C | -3.24515 | 2.87628 | -0.54159 |
| H | -3.80258 | 2.37058 | -1.32972 |
| C | -3.42103 | 4.24463 | -0.32829 |
| H | -4.11961 | 4.80190 | -0.95194 |
| C | -2.70879 | 4.89716 | 0.68195 |
| H | -2.85081 | 5.96514 | 0.84551 |
| C | -1.81349 | 4.18095 | 1.48230 |
| H | -1.25846 | 4.68796 | 2.27132 |
| C | -1.62577 | 2.81499 | 1.26994 |
| H | -0.92386 | 2.25766 | 1.89215 |
| C | -2.74900 | -0.06760 | -1.59963 |
| C | -3.95937 | -0.76485 | -1.73529 |
| H | -4.52744 | -1.05230 | -0.85131 |
| C | -4.43760 | -1.08796 | -3.00725 |
| H | -5.37821 | -1.62918 | -3.10698 |
| C | -3.71966 | -0.71402 | -4.14595 |
| H | -4.09729 | -0.96779 | -5.13613 |
| C | -2.51607 | -0.01273 | -4.01505 |
| H | -1.95565 | 0.28273 | -4.90182 |
| C | -2.02761 | 0.30448 | -2.74848 |

| | | | |
|---|---|---|---|
| H | -1.08209 | 0.83897 | -2.64441 |
| P | 3.11869 | 0.28238 | 0.01660 |
| C | 3.44346 | 1.87936 | -1.00737 |
| C | 4.84009 | 2.48362 | -0.76798 |
| H | 4.96918 | 3.33839 | -1.44939 |
| C | 2.37047 | 2.94652 | -0.68277 |
| H | 2.59015 | 3.83597 | -1.29195 |
| H | 2.35981 | 3.26459 | 0.36152 |
| H | 1.36095 | 2.61376 | -0.95609 |
| C | 3.67057 | 0.54998 | 1.83787 |
| C | 5.19188 | 0.43155 | 2.04616 |
| H | 5.41756 | 0.66510 | 3.09779 |
| H | 5.76083 | 1.13159 | 1.42522 |
| H | 5.56338 | -0.58117 | 1.85585 |
| H | 3.14254 | -1.51844 | 2.46429 |
| H | 1.85878 | -0.31139 | 2.70690 |
| H | 3.27935 | -0.33060 | 3.76751 |
| C | 3.20222 | 1.93552 | 2.32674 |
| H | 2.12444 | 2.08057 | 2.17465 |
| H | 3.74513 | 2.76356 | 1.86024 |
| H | 3.39127 | 1.99319 | 3.40890 |
| C | 4.04256 | -1.21445 | -0.76083 |
| C | 4.00474 | -2.39663 | 0.22910 |
| H | 4.42911 | -3.27494 | -0.27913 |
| H | 2.97971 | -2.65341 | 0.52498 |
| H | 4.60621 | -2.22401 | 1.12742 |
| C | 5.50550 | -0.91071 | -1.13458 |
| H | 6.10576 | -0.57412 | -0.28330 |
| H | 5.58564 | -0.16514 | -1.93330 |
| H | 5.96190 | -1.83806 | -1.51347 |
| C | 3.28507 | -1.67679 | -2.02415 |
| H | 3.31406 | -0.95335 | -2.84141 |
| H | 2.24041 | -1.91841 | -1.80573 |
| H | 3.76659 | -2.59733 | -2.38652 |
| H | 4.96250 | 2.86494 | 0.25148 |
| H | 5.65100 | 1.77691 | -0.97155 |
| C | 3.28364 | 1.55718 | -2.50659 |
| H | 3.30675 | 2.50576 | -3.06296 |
| H | 4.09523 | 0.93521 | -2.89762 |
| H | 2.32281 | 1.07069 | -2.72039 |
| C | 2.94277 | -0.47782 | 2.73052 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 11.71 | 0.20916 | YES YES |
| 8 | a | 16.11 | 0.03764 | YES YES |
| 9 | a | 23.26 | 0.16084 | YES YES |
| 10 | a | 24.96 | 0.00448 | YES YES |
| 11 | a | 39.13 | 3.36636 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 43.53 | 1.03435 | YES | YES |
| 13 | a | 48.91 | 0.17615 | YES | YES |
| 14 | a | 51.58 | 0.76720 | YES | YES |
| 15 | a | 56.42 | 4.28632 | YES | YES |
| 16 | a | 58.80 | 16.21078 | YES | YES |
| 17 | a | 62.46 | 14.22494 | YES | YES |
| 18 | a | 74.23 | 35.63279 | YES | YES |
| 19 | a | 76.24 | 9.28973 | YES | YES |
| 20 | a | 82.54 | 5.55539 | YES | YES |
| 21 | a | 96.51 | 5.46165 | YES | YES |
| 22 | a | 97.55 | 3.91164 | YES | YES |
| 23 | a | 101.58 | 0.84170 | YES | YES |
| 24 | a | 109.26 | 16.54026 | YES | YES |
| 25 | a | 119.85 | 0.37742 | YES | YES |
| 26 | a | 127.19 | 0.72038 | YES | YES |
| 27 | a | 128.82 | 0.18074 | YES | YES |
| 28 | a | 168.78 | 0.09354 | YES | YES |
| 29 | a | 183.58 | 1.26053 | YES | YES |
| 30 | a | 190.06 | 0.28902 | YES | YES |
| 31 | a | 194.52 | 1.51952 | YES | YES |
| 32 | a | 196.40 | 1.81385 | YES | YES |
| 33 | a | 197.28 | 0.40334 | YES | YES |
| 34 | a | 203.10 | 0.73076 | YES | YES |
| 35 | a | 205.85 | 1.12837 | YES | YES |
| 36 | a | 211.05 | 0.35232 | YES | YES |
| 37 | a | 220.50 | 16.00348 | YES | YES |
| 38 | a | 228.31 | 0.18541 | YES | YES |
| 39 | a | 234.98 | 4.13688 | YES | YES |
| 40 | a | 237.70 | 0.72903 | YES | YES |
| 41 | a | 240.94 | 0.35787 | YES | YES |
| 42 | a | 252.50 | 0.13170 | YES | YES |
| 43 | a | 254.11 | 0.85523 | YES | YES |
| 44 | a | 254.48 | 0.52175 | YES | YES |
| 45 | a | 257.59 | 0.40446 | YES | YES |
| 46 | a | 263.81 | 0.63111 | YES | YES |
| 47 | a | 272.42 | 0.54556 | YES | YES |
| 48 | a | 276.58 | 0.04577 | YES | YES |
| 49 | a | 279.32 | 0.03455 | YES | YES |
| 50 | a | 289.48 | 1.19756 | YES | YES |

**[PhSe(PtBu3)]+**

bp86-d3_def2-tzvpp energy (au): -3448.5928732650

Zero point energy (au): 0.4487617
Entropy (kJ mol^-1): 0.69574
Chemical potential (kJ mol^-1): 1041.12

XYZ coordinates:

52

| | | | |
|---|---|---|---|
| P | 1.12513 | 0.09488 | -0.10856 |
| C | -4.80324 | 0.53486 | -0.45117 |
| H | -5.79758 | 0.85761 | -0.75755 |
| C | 1.65803 | 1.55709 | 1.01884 |
| C | -2.77309 | 0.92076 | 0.81646 |
| H | -2.20393 | 1.53155 | 1.51165 |
| C | 2.34203 | 1.01309 | 2.28862 |
| H | 2.51214 | 1.86522 | 2.96214 |
| H | 3.31761 | 0.55757 | 2.09397 |
| H | 1.70581 | 0.29854 | 2.82660 |
| C | -4.04568 | 1.33125 | 0.41210 |
| H | -4.44938 | 2.27108 | 0.78754 |
| C | 2.15414 | -2.27260 | -1.30216 |
| H | 2.87959 | -3.09565 | -1.23063 |
| H | 2.25492 | -1.84214 | -2.30338 |
| H | 1.15318 | -2.70699 | -1.19047 |
| C | -2.25401 | -0.28318 | 0.32777 |
| C | 2.48075 | -1.27059 | -0.17774 |
| C | -3.01579 | -1.09761 | -0.52110 |
| H | -2.62040 | -2.05005 | -0.87207 |
| C | -0.26956 | 1.95385 | -1.74658 |
| H | -0.60676 | 2.20798 | -2.76177 |
| H | 0.27727 | 2.82151 | -1.36434 |
| H | -1.16592 | 1.79030 | -1.13761 |
| C | 3.86996 | -0.65168 | -0.43155 |
| H | 4.58545 | -1.47933 | -0.54260 |
| H | 4.21895 | -0.03716 | 0.40470 |
| H | 3.91757 | -0.05718 | -1.34898 |
| C | -0.23810 | -0.38744 | -2.57393 |
| H | -1.18733 | -0.57078 | -2.06480 |
| H | 0.28013 | -1.33812 | -2.70950 |
| H | -0.47461 | 0.00233 | -3.57462 |
| C | 0.41395 | 2.33279 | 1.49459 |
| H | 0.76530 | 3.18814 | 2.08903 |
| H | -0.20733 | 1.71155 | 2.15021 |
| H | -0.20491 | 2.72730 | 0.68541 |
| C | 2.61849 | 2.51476 | 0.28574 |
| H | 2.13172 | 3.05250 | -0.53440 |
| H | 3.51396 | 2.01759 | -0.10133 |
| H | 2.95397 | 3.26959 | 1.01127 |
| C | 0.60320 | 0.68766 | -1.85787 |
| C | 2.51358 | -2.07625 | 1.14115 |
| H | 1.58689 | -2.63950 | 1.30708 |
| H | 2.72672 | -1.47580 | 2.02720 |
| H | 3.32076 | -2.81717 | 1.04651 |

| | | | |
|---|---|---|---|
| C | 1.85226 | 1.00023 | -2.70758 |
| H | 1.50058 | 1.41466 | -3.66353 |
| H | 2.43592 | 0.10417 | -2.94285 |
| H | 2.51427 | 1.74508 | -2.25579 |
| C | -4.29283 | -0.68314 | -0.90676 |
| H | -4.88729 | -1.31796 | -1.56308 |
| Se | -0.56261 | -1.01176 | 0.95834 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 27.31 | 0.16901 | YES YES |
| 8 | a | 54.54 | 0.24576 | YES YES |
| 9 | a | 69.56 | 0.24631 | YES YES |
| 10 | a | 83.62 | 0.08479 | YES YES |
| 11 | a | 95.42 | 0.37731 | YES YES |
| 12 | a | 113.72 | 0.23995 | YES YES |
| 13 | a | 126.21 | 0.24456 | YES YES |
| 14 | a | 129.02 | 0.06744 | YES YES |
| 15 | a | 157.62 | 0.43018 | YES YES |
| 16 | a | 164.97 | 0.09569 | YES YES |
| 17 | a | 191.63 | 0.29988 | YES YES |
| 18 | a | 196.23 | 1.11102 | YES YES |
| 19 | a | 197.44 | 0.88169 | YES YES |
| 20 | a | 205.90 | 0.57519 | YES YES |
| 21 | a | 207.91 | 0.23675 | YES YES |
| 22 | a | 218.45 | 0.16223 | YES YES |
| 23 | a | 223.04 | 0.46479 | YES YES |
| 24 | a | 228.25 | 0.32132 | YES YES |
| 25 | a | 233.33 | 0.27486 | YES YES |
| 26 | a | 253.66 | 0.46381 | YES YES |
| 27 | a | 255.88 | 0.02371 | YES YES |
| 28 | a | 260.61 | 0.10954 | YES YES |
| 29 | a | 274.27 | 0.35780 | YES YES |
| 30 | a | 279.59 | 0.10275 | YES YES |
| 31 | a | 281.49 | 0.05672 | YES YES |
| 32 | a | 286.29 | 0.09256 | YES YES |
| 33 | a | 299.65 | 1.39295 | YES YES |
| 34 | a | 321.13 | 0.29371 | YES YES |
| 35 | a | 336.15 | 0.35438 | YES YES |
| 36 | a | 343.89 | 0.53795 | YES YES |
| 37 | a | 363.39 | 0.97683 | YES YES |
| 38 | a | 372.26 | 0.18191 | YES YES |
| 39 | a | 376.33 | 0.25871 | YES YES |
| 40 | a | 398.84 | 0.51073 | YES YES |
| 41 | a | 401.44 | 0.28197 | YES YES |
| 42 | a | 402.82 | 0.66514 | YES YES |
| 43 | a | 407.59 | 1.00864 | YES YES |
| 44 | a | 453.80 | 10.37741 | YES YES |
| 45 | a | 455.37 | 8.61739 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 46 | a | 468.11 | 5.97040 | YES | YES |
| 47 | a | 491.57 | 27.26655 | YES | YES |
| 48 | a | 532.56 | 18.56318 | YES | YES |
| 49 | a | 565.85 | 6.04265 | YES | YES |
| 50 | a | 571.69 | 2.31465 | YES | YES |

**[PhS(PPh3)]+**

bp86-d3_def2-tzvpp energy (au): -1666.4966123460

Zero point energy (au): 0.3581723
Entropy (kJ mol^-1): 0.69606
Chemical potential (kJ mol^-1): 795.94

XYZ coordinates:

46

| | | | |
|---|---|---|---|
| P | 0.23717 | 0.57326 | 0.04585 |
| S | 2.08180 | -0.42862 | 0.17019 |
| C | 1.49991 | -2.11993 | 0.04588 |
| C | 1.22258 | -2.67887 | -1.20938 |
| H | 1.36719 | -2.09151 | -2.11454 |
| C | 0.75282 | -3.99127 | -1.28169 |
| H | 0.53333 | -4.43175 | -2.25370 |
| C | 0.57560 | -4.73989 | -0.11341 |
| H | 0.21494 | -5.76609 | -0.17642 |
| C | 0.87015 | -4.18028 | 1.13301 |
| H | 0.73951 | -4.76587 | 2.04234 |
| C | 1.32845 | -2.86467 | 1.22016 |
| H | 1.54243 | -2.41325 | 2.18767 |
| C | -0.96405 | -0.14677 | 1.17463 |
| C | -1.54800 | -1.38925 | 0.85998 |
| H | -1.30742 | -1.89364 | -0.07557 |
| C | -2.44039 | -1.97471 | 1.75543 |
| H | -2.89276 | -2.93520 | 1.51202 |
| C | -2.75174 | -1.33300 | 2.95794 |
| H | -3.45254 | -1.79401 | 3.65342 |
| C | -2.17289 | -0.09929 | 3.26931 |
| H | -2.42317 | 0.40370 | 4.20261 |
| C | -1.27663 | 0.49782 | 2.38342 |
| H | -0.83472 | 1.46348 | 2.62601 |
| C | 0.62552 | 2.27425 | 0.48866 |
| C | 0.08819 | 3.32726 | -0.27078 |
| H | -0.53180 | 3.11922 | -1.14211 |
| C | 0.36048 | 4.64548 | 0.09534 |
| H | -0.05280 | 5.46378 | -0.49296 |
| C | 1.16404 | 4.91429 | 1.20685 |
| H | 1.37629 | 5.94594 | 1.48588 |
| C | 1.70238 | 3.86555 | 1.95956 |
| H | 2.33324 | 4.07694 | 2.82200 |
| C | 1.43741 | 2.54323 | 1.60657 |
| H | 1.86081 | 1.72691 | 2.19178 |
| C | -0.41504 | 0.50959 | -1.63366 |
| C | -1.80330 | 0.49360 | -1.85202 |
| H | -2.49496 | 0.45658 | -1.01143 |
| C | -2.29384 | 0.52700 | -3.15825 |
| H | -3.36951 | 0.51090 | -3.32986 |
| C | -1.40960 | 0.57944 | -4.23902 |
| H | -1.79768 | 0.60118 | -5.25695 |
| C | -0.02791 | 0.60424 | -4.02005 |
| H | 0.65984 | 0.64805 | -4.86366 |
| C | 0.47416 | 0.57045 | -2.72042 |

H 1.55030 0.58518 -2.54724

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 16.62 | 0.05952 | YES YES |
| 8 | a | 28.72 | 0.01867 | YES YES |
| 9 | a | 40.43 | 0.10157 | YES YES |
| 10 | a | 43.85 | 0.06002 | YES YES |
| 11 | a | 48.58 | 0.11053 | YES YES |
| 12 | a | 55.67 | 0.08976 | YES YES |
| 13 | a | 61.50 | 0.07185 | YES YES |
| 14 | a | 69.35 | 0.14880 | YES YES |
| 15 | a | 83.94 | 0.12844 | YES YES |
| 16 | a | 102.14 | 0.36043 | YES YES |
| 17 | a | 115.84 | 0.64628 | YES YES |
| 18 | a | 184.06 | 1.39555 | YES YES |
| 19 | a | 199.04 | 1.30274 | YES YES |
| 20 | a | 212.31 | 1.60002 | YES YES |
| 21 | a | 218.06 | 0.02338 | YES YES |
| 22 | a | 241.06 | 0.79453 | YES YES |
| 23 | a | 256.34 | 0.40448 | YES YES |
| 24 | a | 265.01 | 0.54651 | YES YES |
| 25 | a | 284.86 | 1.49269 | YES YES |
| 26 | a | 318.49 | 2.78963 | YES YES |
| 27 | a | 387.93 | 0.11600 | YES YES |
| 28 | a | 389.00 | 0.03359 | YES YES |
| 29 | a | 396.39 | 0.63569 | YES YES |
| 30 | a | 397.99 | 0.14853 | YES YES |
| 31 | a | 404.20 | 3.55272 | YES YES |
| 32 | a | 435.16 | 7.02832 | YES YES |
| 33 | a | 439.40 | 4.42208 | YES YES |
| 34 | a | 447.92 | 5.20153 | YES YES |
| 35 | a | 478.43 | 15.23696 | YES YES |
| 36 | a | 495.90 | 56.73522 | YES YES |
| 37 | a | 513.16 | 80.57710 | YES YES |
| 38 | a | 551.90 | 66.93492 | YES YES |
| 39 | a | 606.25 | 0.01315 | YES YES |
| 40 | a | 606.71 | 0.50934 | YES YES |
| 41 | a | 608.09 | 0.09553 | YES YES |
| 42 | a | 609.23 | 0.60964 | YES YES |
| 43 | a | 680.47 | 5.62657 | YES YES |
| 44 | a | 683.87 | 20.90405 | YES YES |
| 45 | a | 686.92 | 43.44317 | YES YES |
| 46 | a | 687.98 | 10.10750 | YES YES |
| 47 | a | 688.69 | 23.35973 | YES YES |
| 48 | a | 691.43 | 9.88646 | YES YES |
| 49 | a | 714.72 | 31.71987 | YES YES |
| 50 | a | 715.75 | 33.06996 | YES YES |

**[PhS(PPh3).PPh3]+**

bp86-d3_def2-tzvpp energy (au): -2703.1871371190

Zero point energy (au): 0.6250430
Entropy (kJ mol^-1): 1.09116
Chemical potential (kJ mol^-1): 1427.48

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.70934 | 0.58915 | 3.66711 |
| H | -5.75600 | 0.72017 | 3.94099 |
| C | 2.80911 | 2.42290 | 3.74504 |
| H | 3.88523 | 2.46321 | 3.57675 |
| S | -0.33964 | 0.07293 | -0.20171 |
| P | -0.28338 | 0.09064 | 2.45720 |
| C | 0.81143 | 3.30617 | 4.78727 |
| H | 0.32671 | 4.03528 | 5.43634 |
| C | -4.15204 | 1.36488 | 2.64625 |
| H | -4.76219 | 2.10066 | 2.12268 |
| C | -2.01843 | 0.25076 | 2.96780 |
| C | 2.05193 | 1.42987 | 3.12622 |
| H | 2.54069 | 0.70220 | 2.47749 |
| C | 1.13280 | -4.09206 | 3.81659 |
| H | 1.46375 | -5.08748 | 4.11179 |
| C | 0.66256 | 1.36023 | 3.34650 |
| C | 3.50208 | 1.42452 | -0.26400 |
| H | 4.01458 | 2.37077 | -0.43455 |
| C | -2.81361 | 1.19236 | 2.29092 |
| H | -2.37966 | 1.79130 | 1.48865 |
| C | 0.28349 | -1.52865 | 3.05936 |
| C | 0.21335 | -3.94058 | 2.77253 |
| H | -0.17482 | -4.81723 | 2.25401 |
| C | 0.04640 | 2.30816 | 4.17940 |
| H | -1.02777 | 2.26227 | 4.35760 |
| C | 2.19079 | 3.36554 | 4.57351 |
| H | 2.78425 | 4.14395 | 5.05247 |
| C | -2.58381 | -0.52699 | 3.99105 |
| H | -1.97399 | -1.26254 | 4.51550 |
| C | 1.20074 | -1.68685 | 4.10895 |
| H | 1.58190 | -0.81363 | 4.63734 |
| C | -0.20405 | -2.66682 | 2.39018 |
| H | -0.91201 | -2.54830 | 1.56826 |
| C | 2.17933 | -1.00291 | 0.18226 |
| H | 1.65788 | -1.94363 | 0.34949 |
| C | -3.92577 | -0.35660 | 4.33533 |
| H | -4.35971 | -0.96113 | 5.13162 |
| C | 1.62334 | -2.96561 | 4.48121 |
| H | 2.33389 | -3.08032 | 5.29968 |
| C | 3.57069 | -0.93797 | 0.26744 |
| H | 4.13701 | -1.83770 | 0.50567 |
| C | 2.10796 | 1.37362 | -0.33059 |
| H | 1.53259 | 2.27194 | -0.54636 |
| C | 4.23351 | 0.27194 | 0.03755 |
| H | 5.32059 | 0.31735 | 0.09784 |

| | | | |
|---|---|---|---|
| C | 1.44835 | 0.15635 | -0.11395 |
| C | -4.72081 | -1.01743 | -3.42873 |
| H | -5.75953 | -1.25596 | -3.65589 |
| C | 2.98431 | -2.11851 | -3.56536 |
| H | 4.06323 | -1.97244 | -3.52469 |
| P | -0.33465 | -0.02637 | -2.45254 |
| C | 1.06842 | -3.48489 | -4.13916 |
| H | 0.65194 | -4.40284 | -4.55278 |
| C | -4.05806 | -1.69678 | -2.40224 |
| H | -4.57733 | -2.46353 | -1.82819 |
| C | -2.05752 | -0.40211 | -2.84632 |
| C | 2.13812 | -1.11940 | -3.08957 |
| H | 2.55955 | -0.20298 | -2.67669 |
| C | 0.64211 | 4.07211 | -4.30768 |
| H | 0.86262 | 5.04846 | -4.73838 |
| C | 0.74215 | -1.29979 | -3.14436 |
| C | -2.72965 | -1.39175 | -2.10575 |
| H | -2.21453 | -1.91958 | -1.30300 |
| C | 0.08506 | 1.56683 | -3.19896 |
| C | -0.11189 | 3.98158 | -3.13252 |
| H | -0.48081 | 4.88492 | -2.64764 |
| C | 0.21026 | -2.48889 | -3.67062 |
| H | -0.86838 | -2.63220 | -3.72446 |
| C | 2.45274 | -3.30253 | -4.08703 |
| H | 3.11873 | -4.08195 | -4.45630 |
| C | -2.72630 | 0.28076 | -3.87517 |
| H | -2.21098 | 1.05325 | -4.44529 |
| C | 0.83402 | 1.65873 | -4.38294 |
| H | 1.19613 | 0.75743 | -4.87579 |
| C | -0.38888 | 2.73461 | -2.57517 |
| H | -0.96558 | 2.66161 | -1.65253 |
| C | -4.05563 | -0.03089 | -4.16240 |
| H | -4.57293 | 0.49937 | -4.96133 |
| C | 1.11181 | 2.91292 | -4.93034 |
| H | 1.69441 | 2.98217 | -5.84850 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 10.94 | 0.18803 | YES YES |
| 8 | a | 11.83 | 1.52879 | YES YES |
| 9 | a | 18.13 | 3.50095 | YES YES |
| 10 | a | 24.39 | 0.59173 | YES YES |
| 11 | a | 28.08 | 0.33366 | YES YES |
| 12 | a | 30.27 | 2.68462 | YES YES |
| 13 | a | 31.78 | 8.04655 | YES YES |
| 14 | a | 40.35 | 0.09653 | YES YES |
| 15 | a | 45.02 | 0.65380 | YES YES |
| 16 | a | 48.10 | 0.06645 | YES YES |
| 17 | a | 50.01 | 0.65391 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 18 | a | 51.02 | 0.41816 | YES | YES |
| 19 | a | 53.69 | 0.42384 | YES | YES |
| 20 | a | 58.41 | 1.90242 | YES | YES |
| 21 | a | 59.69 | 0.58092 | YES | YES |
| 22 | a | 65.92 | 25.46259 | YES | YES |
| 23 | a | 73.40 | 0.75903 | YES | YES |
| 24 | a | 76.09 | 10.18533 | YES | YES |
| 25 | a | 81.88 | 29.02501 | YES | YES |
| 26 | a | 88.65 | 40.75452 | YES | YES |
| 27 | a | 96.50 | 3.08106 | YES | YES |
| 28 | a | 120.84 | 0.73067 | YES | YES |
| 29 | a | 142.59 | 3.98847 | YES | YES |
| 30 | a | 156.43 | 91.30610 | YES | YES |
| 31 | a | 181.18 | 3.89546 | YES | YES |
| 32 | a | 186.97 | 0.68352 | YES | YES |
| 33 | a | 192.10 | 1.47058 | YES | YES |
| 34 | a | 196.95 | 1.31987 | YES | YES |
| 35 | a | 205.66 | 2.50685 | YES | YES |
| 36 | a | 212.16 | 3.85236 | YES | YES |
| 37 | a | 236.58 | 22.03871 | YES | YES |
| 38 | a | 239.26 | 10.01616 | YES | YES |
| 39 | a | 240.38 | 30.46198 | YES | YES |
| 40 | a | 253.06 | 2.38470 | YES | YES |
| 41 | a | 256.38 | 6.55629 | YES | YES |
| 42 | a | 262.36 | 0.59631 | YES | YES |
| 43 | a | 265.86 | 1.28603 | YES | YES |
| 44 | a | 301.57 | 9.76260 | YES | YES |
| 45 | a | 386.74 | 0.59295 | YES | YES |
| 46 | a | 389.22 | 0.16321 | YES | YES |
| 47 | a | 389.40 | 0.52405 | YES | YES |
| 48 | a | 390.24 | 0.22134 | YES | YES |
| 49 | a | 391.11 | 0.36851 | YES | YES |
| 50 | a | 397.14 | 0.69547 | YES | YES |

**[PhS(PtBu3).PPh3]+**

bp86-d3_def2-tzvpp energy (au): -2481.6919528460

Zero point energy (au): 0.7171672
Entropy (kJ mol^-1): 1.06784
Chemical potential (kJ mol^-1): 1681.61

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.00156 | 0.18128 | 0.55231 |
| S | 0.99101 | -0.04459 | 0.51344 |
| C | 0.62923 | -1.78214 | 0.22511 |
| C | 0.32023 | -2.26572 | -1.05174 |
| H | 0.36302 | -1.61226 | -1.91933 |
| C | -0.10359 | -3.58796 | -1.20460 |
| H | -0.35079 | -3.95507 | -2.19995 |
| C | -0.23764 | -4.42007 | -0.09176 |
| H | -0.57441 | -5.44871 | -0.21632 |
| C | 0.03912 | -3.92397 | 1.18670 |
| H | -0.08933 | -4.55897 | 2.06273 |
| C | 0.46555 | -2.60638 | 1.34819 |
| H | 0.64230 | -2.20406 | 2.34488 |
| C | -3.50338 | -0.64762 | 1.18671 |
| C | -3.41377 | -2.03206 | 1.41931 |
| H | -2.47321 | -2.55291 | 1.22825 |
| C | -4.52054 | -2.74051 | 1.88994 |
| H | -4.44565 | -3.81480 | 2.05896 |
| C | -5.71749 | -2.06982 | 2.15734 |
| H | -6.57877 | -2.62006 | 2.53558 |
| C | -5.80594 | -0.69065 | 1.94724 |
| H | -6.73663 | -0.16480 | 2.16054 |
| C | -4.70672 | 0.02005 | 1.46042 |
| H | -4.78489 | 1.09483 | 1.29636 |
| C | -2.27222 | 1.97264 | 0.80264 |
| C | -3.02024 | 2.78498 | -0.06626 |
| H | -3.48015 | 2.34920 | -0.95341 |
| C | -3.17268 | 4.14689 | 0.20039 |
| H | -3.75684 | 4.76870 | -0.47817 |
| C | -2.58565 | 4.71159 | 1.33736 |
| H | -2.70931 | 5.77462 | 1.54360 |
| C | -1.84320 | 3.91098 | 2.20972 |
| H | -1.38845 | 4.34654 | 3.09952 |
| C | -1.68296 | 2.55017 | 1.94010 |
| H | -1.10220 | 1.92305 | 2.61951 |
| C | -2.09311 | -0.03825 | -1.26485 |
| C | -2.77120 | -1.11798 | -1.85270 |
| H | -3.39737 | -1.76543 | -1.23924 |
| C | -2.64746 | -1.37470 | -3.22016 |
| H | -3.18512 | -2.21512 | -3.65957 |
| C | -1.84931 | -0.55734 | -4.02456 |
| H | -1.75849 | -0.75685 | -5.09200 |
| C | -1.18430 | 0.53236 | -3.45258 |
| H | -0.57613 | 1.18967 | -4.07476 |
| C | -1.29961 | 0.78599 | -2.08568 |

| | | | |
|---|---|---|---|
| H | -0.77746 | 1.63842 | -1.64955 |
| P | 3.05819 | 0.32652 | 0.05887 |
| C | 3.49760 | -0.10440 | -1.76026 |
| C | 4.76941 | 0.62494 | -2.23828 |
| H | 4.96908 | 0.29714 | -3.26927 |
| C | 2.32631 | 0.28089 | -2.69140 |
| H | 2.44427 | -0.27364 | -3.63248 |
| H | 2.32020 | 1.34473 | -2.94008 |
| H | 1.34418 | 0.03356 | -2.28015 |
| C | 3.03944 | 2.23150 | 0.33233 |
| C | 4.47202 | 2.77696 | 0.49647 |
| H | 4.40853 | 3.87408 | 0.53577 |
| H | 5.13123 | 2.51925 | -0.33880 |
| H | 4.94374 | 2.44897 | 1.42856 |
| H | 2.52805 | 2.12701 | 2.49911 |
| H | 1.13440 | 2.42334 | 1.43716 |
| H | 2.31997 | 3.69943 | 1.71929 |
| C | 2.37091 | 2.92325 | -0.87333 |
| H | 1.37830 | 2.51136 | -1.09031 |
| H | 2.98292 | 2.88539 | -1.77966 |
| H | 2.23932 | 3.98350 | -0.61504 |
| C | 4.21645 | -0.55510 | 1.30491 |
| C | 4.00650 | 0.05163 | 2.70613 |
| H | 4.57248 | -0.56139 | 3.42211 |
| H | 2.95207 | 0.02235 | 3.00853 |
| H | 4.37885 | 1.07708 | 2.79393 |
| C | 5.69880 | -0.43244 | 0.90138 |
| H | 6.03099 | 0.60224 | 0.77063 |
| H | 5.93009 | -0.99420 | -0.01013 |
| H | 6.30233 | -0.87025 | 1.70998 |
| C | 3.84057 | -2.04769 | 1.41313 |
| H | 3.87691 | -2.59143 | 0.46725 |
| H | 2.84628 | -2.18273 | 1.84556 |
| H | 4.56480 | -2.51938 | 2.09319 |
| H | 4.64496 | 1.71261 | -2.26736 |
| H | 5.65680 | 0.38831 | -1.64334 |
| C | 3.72469 | -1.62650 | -1.87415 |
| H | 3.87416 | -1.86123 | -2.93756 |
| H | 4.62236 | -1.95985 | -1.34353 |
| H | 2.86412 | -2.20909 | -1.52589 |
| C | 2.20474 | 2.61498 | 1.57764 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 9.18 | 0.01269 | YES YES |
| 8 | a | 21.12 | 0.10082 | YES YES |
| 9 | a | 23.17 | 0.04007 | YES YES |
| 10 | a | 31.22 | 1.50263 | YES YES |
| 11 | a | 40.60 | 1.39992 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 43.61 | 0.13349 | YES | YES |
| 13 | a | 48.45 | 0.08819 | YES | YES |
| 14 | a | 51.84 | 1.41971 | YES | YES |
| 15 | a | 54.79 | 0.32352 | YES | YES |
| 16 | a | 61.78 | 0.10756 | YES | YES |
| 17 | a | 65.45 | 1.16931 | YES | YES |
| 18 | a | 70.41 | 0.47360 | YES | YES |
| 19 | a | 81.08 | 2.61379 | YES | YES |
| 20 | a | 86.78 | 0.52125 | YES | YES |
| 21 | a | 93.16 | 4.79574 | YES | YES |
| 22 | a | 103.15 | 0.26072 | YES | YES |
| 23 | a | 113.93 | 0.77553 | YES | YES |
| 24 | a | 132.17 | 0.31853 | YES | YES |
| 25 | a | 136.08 | 0.36600 | YES | YES |
| 26 | a | 145.08 | 1.12803 | YES | YES |
| 27 | a | 151.67 | 2.93897 | YES | YES |
| 28 | a | 176.94 | 2.89140 | YES | YES |
| 29 | a | 181.96 | 2.77673 | YES | YES |
| 30 | a | 183.44 | 1.84336 | YES | YES |
| 31 | a | 191.15 | 3.74328 | YES | YES |
| 32 | a | 196.07 | 0.10355 | YES | YES |
| 33 | a | 204.93 | 0.81777 | YES | YES |
| 34 | a | 206.25 | 0.92553 | YES | YES |
| 35 | a | 211.44 | 0.68377 | YES | YES |
| 36 | a | 217.74 | 0.53559 | YES | YES |
| 37 | a | 226.85 | 0.40365 | YES | YES |
| 38 | a | 236.24 | 0.92258 | YES | YES |
| 39 | a | 237.98 | 3.59798 | YES | YES |
| 40 | a | 243.00 | 1.02436 | YES | YES |
| 41 | a | 244.68 | 3.02861 | YES | YES |
| 42 | a | 251.99 | 1.85758 | YES | YES |
| 43 | a | 258.31 | 0.02071 | YES | YES |
| 44 | a | 265.76 | 0.52491 | YES | YES |
| 45 | a | 268.69 | 4.01591 | YES | YES |
| 46 | a | 276.79 | 2.71600 | YES | YES |
| 47 | a | 280.33 | 5.66241 | YES | YES |
| 48 | a | 283.33 | 0.09378 | YES | YES |
| 49 | a | 291.90 | 2.39930 | YES | YES |
| 50 | a | 296.15 | 22.36439 | YES | YES |

**[PhS(PPh3).PtBu3]+_try4**

bp86-d3_def2-tzvpp energy (au): -2481.6911023530

Zero point energy (au): 0.7170464
Entropy (kJ mol^-1): 1.07641
Chemical potential (kJ mol^-1): 1678.56

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -1.94140 | 0.39557 | 0.02507 |
| S | 0.26722 | 0.18006 | -0.04092 |
| C | 0.19825 | -1.60537 | -0.12682 |
| C | -0.05226 | -2.24123 | -1.34995 |
| H | -0.19306 | -1.64679 | -2.25119 |
| C | -0.11961 | -3.63528 | -1.40177 |
| H | -0.31562 | -4.13066 | -2.35227 |
| C | 0.07717 | -4.39143 | -0.24218 |
| H | 0.03437 | -5.47915 | -0.28826 |
| C | 0.33186 | -3.75315 | 0.97514 |
| H | 0.48355 | -4.34002 | 1.88049 |
| C | 0.38321 | -2.35983 | 1.03852 |
| H | 0.55915 | -1.85322 | 1.98613 |
| C | -2.77016 | -0.61988 | 1.26501 |
| C | -2.86549 | -2.00964 | 1.05579 |
| H | -2.48736 | -2.45540 | 0.13578 |
| C | -3.44444 | -2.81809 | 2.03126 |
| H | -3.51858 | -3.89202 | 1.86370 |
| C | -3.92187 | -2.25567 | 3.21965 |
| H | -4.37178 | -2.89248 | 3.98085 |
| C | -3.82596 | -0.87767 | 3.43030 |
| H | -4.20496 | -0.43666 | 4.35171 |
| C | -3.25219 | -0.05656 | 2.45858 |
| H | -3.19035 | 1.01847 | 2.62425 |
| C | -2.12408 | 2.14639 | 0.43334 |
| C | -3.01496 | 2.96370 | -0.28015 |
| H | -3.61422 | 2.54565 | -1.08858 |
| C | -3.12620 | 4.31611 | 0.04579 |
| H | -3.81848 | 4.94869 | -0.50881 |
| C | -2.35260 | 4.85676 | 1.07660 |
| H | -2.44113 | 5.91392 | 1.32547 |
| C | -1.46461 | 4.04482 | 1.78880 |
| H | -0.86114 | 4.46571 | 2.59241 |
| C | -1.34560 | 2.69216 | 1.47126 |
| H | -0.65175 | 2.06132 | 2.02714 |
| C | -2.70171 | 0.09662 | -1.58772 |
| C | -3.96919 | -0.49545 | -1.71005 |
| H | -4.51893 | -0.80579 | -0.82230 |
| C | -4.52561 | -0.68339 | -2.97678 |
| H | -5.50854 | -1.14415 | -3.06973 |
| C | -3.82855 | -0.27921 | -4.11822 |
| H | -4.26675 | -0.42898 | -5.10455 |
| C | -2.56920 | 0.31844 | -3.99731 |
| H | -2.02635 | 0.63618 | -4.88704 |
| C | -2.00268 | 0.50488 | -2.73775 |

| | | | |
|---|---|---|---|
| H | -1.01639 | 0.96005 | -2.64159 |
| P | 3.05463 | 0.18411 | -0.03375 |
| C | 3.51560 | 1.29905 | -1.53822 |
| C | 4.83089 | 2.08444 | -1.38938 |
| H | 5.02774 | 2.62995 | -2.32590 |
| C | 2.36077 | 2.29597 | -1.79817 |
| H | 2.61707 | 2.89156 | -2.68742 |
| H | 2.18694 | 2.99729 | -0.97834 |
| H | 1.41881 | 1.77361 | -2.00584 |
| C | 3.35016 | 1.16598 | 1.59703 |
| C | 4.82344 | 1.30893 | 2.01966 |
| H | 4.87375 | 1.92252 | 2.93267 |
| H | 5.43368 | 1.80393 | 1.25651 |
| H | 5.28674 | 0.34457 | 2.25544 |
| H | 2.92409 | -0.53915 | 2.95781 |
| H | 1.49124 | 0.39745 | 2.48414 |
| H | 2.65809 | 1.06559 | 3.64446 |
| C | 2.73782 | 2.57613 | 1.46209 |
| H | 1.68810 | 2.54532 | 1.14091 |
| H | 3.29645 | 3.21878 | 0.77429 |
| H | 2.76557 | 3.05887 | 2.45082 |
| C | 4.17787 | -1.38809 | -0.04039 |
| C | 4.08717 | -2.09095 | 1.32906 |
| H | 4.60343 | -3.05947 | 1.24973 |
| H | 3.04856 | -2.29813 | 1.61483 |
| H | 4.57581 | -1.53167 | 2.13351 |
| C | 5.65980 | -1.12123 | -0.36055 |
| H | 6.12268 | -0.41535 | 0.33761 |
| H | 5.80783 | -0.74498 | -1.37864 |
| H | 6.21233 | -2.07070 | -0.28580 |
| C | 3.60106 | -2.38841 | -1.06777 |
| H | 3.63236 | -2.02680 | -2.09835 |
| H | 2.56616 | -2.65912 | -0.83091 |
| H | 4.20361 | -3.30844 | -1.02677 |
| H | 4.77963 | 2.83210 | -0.58926 |
| H | 5.69214 | 1.43662 | -1.19835 |
| C | 3.59397 | 0.41764 | -2.80132 |
| H | 3.68214 | 1.07614 | -3.67860 |
| H | 4.46582 | -0.24502 | -2.80948 |
| H | 2.68736 | -0.18915 | -2.93300 |
| C | 2.55950 | 0.46507 | 2.72714 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 5.38 | 0.00731 | YES YES |
| 8 | a | 14.63 | 0.20132 | YES YES |
| 9 | a | 20.04 | 0.49924 | YES YES |
| 10 | a | 23.39 | 0.14959 | YES YES |
| 11 | a | 40.98 | 1.95006 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 45.18 | 0.93777 | YES | YES |
| 13 | a | 47.96 | 0.06684 | YES | YES |
| 14 | a | 51.30 | 0.18912 | YES | YES |
| 15 | a | 57.26 | 0.31576 | YES | YES |
| 16 | a | 64.38 | 1.12545 | YES | YES |
| 17 | a | 67.63 | 6.33880 | YES | YES |
| 18 | a | 71.38 | 22.65807 | YES | YES |
| 19 | a | 74.23 | 9.10143 | YES | YES |
| 20 | a | 82.64 | 1.63716 | YES | YES |
| 21 | a | 94.18 | 1.16981 | YES | YES |
| 22 | a | 105.58 | 2.37099 | YES | YES |
| 23 | a | 109.70 | 0.35558 | YES | YES |
| 24 | a | 117.38 | 0.07257 | YES | YES |
| 25 | a | 135.88 | 0.12179 | YES | YES |
| 26 | a | 147.78 | 1.85043 | YES | YES |
| 27 | a | 170.24 | 81.03072 | YES | YES |
| 28 | a | 184.39 | 4.20253 | YES | YES |
| 29 | a | 187.02 | 0.41870 | YES | YES |
| 30 | a | 189.00 | 0.52802 | YES | YES |
| 31 | a | 194.81 | 2.14942 | YES | YES |
| 32 | a | 204.30 | 1.22757 | YES | YES |
| 33 | a | 206.37 | 1.16462 | YES | YES |
| 34 | a | 207.36 | 1.05014 | YES | YES |
| 35 | a | 210.18 | 4.35576 | YES | YES |
| 36 | a | 212.82 | 1.18363 | YES | YES |
| 37 | a | 238.49 | 6.05680 | YES | YES |
| 38 | a | 240.33 | 15.57181 | YES | YES |
| 39 | a | 241.21 | 26.31193 | YES | YES |
| 40 | a | 246.09 | 27.24991 | YES | YES |
| 41 | a | 252.25 | 0.69992 | YES | YES |
| 42 | a | 256.80 | 4.88732 | YES | YES |
| 43 | a | 256.85 | 1.09396 | YES | YES |
| 44 | a | 262.69 | 0.17470 | YES | YES |
| 45 | a | 265.74 | 1.77103 | YES | YES |
| 46 | a | 273.49 | 0.27264 | YES | YES |
| 47 | a | 282.23 | 0.02725 | YES | YES |
| 48 | a | 284.42 | 0.30934 | YES | YES |
| 49 | a | 291.68 | 0.73973 | YES | YES |
| 50 | a | 302.09 | 11.79111 | YES | YES |

**[PhS(PtBu3)]+**

bp86-d3_def2-tzvpp energy (au): -1444.9992513780

Zero point energy (au): 0.4496041
Entropy (kJ mol^-1): 0.69066
Chemical potential (kJ mol^-1): 1043.99

XYZ coordinates:

52

| | | | |
|---|---|---|---|
| P | -0.97754 | -0.01123 | 0.01835 |
| C | 2.20282 | -0.66012 | 0.09773 |
| C | 4.28725 | -0.02726 | 1.15075 |
| H | 4.88391 | 0.10765 | 2.05222 |
| C | 4.83357 | 0.25193 | -0.10490 |
| H | 5.85868 | 0.61157 | -0.18534 |
| C | 4.07126 | 0.05109 | -1.25884 |
| H | 4.50201 | 0.24329 | -2.24094 |
| C | 2.75972 | -0.41836 | -1.16412 |
| H | 2.18801 | -0.60992 | -2.06900 |
| C | -0.82107 | 1.45030 | 1.24756 |
| C | -1.85123 | 2.55284 | 0.92878 |
| H | -1.77646 | 3.31152 | 1.72170 |
| C | 0.59794 | 2.05670 | 1.20734 |
| H | 0.60081 | 2.90974 | 1.90130 |
| H | 0.89839 | 2.43331 | 0.22841 |
| H | 1.35677 | 1.35087 | 1.55260 |
| C | -1.03120 | 0.58287 | -1.80737 |
| C | -2.43099 | 1.11943 | -2.17390 |
| H | -2.37574 | 1.50827 | -3.20089 |
| H | -2.76120 | 1.94298 | -1.53271 |
| H | -3.19917 | 0.33890 | -2.16834 |
| H | -1.42753 | -1.36697 | -2.78465 |
| H | 0.28750 | -1.04169 | -2.51781 |
| H | -0.60300 | -0.15998 | -3.77349 |
| C | 0.00257 | 1.70829 | -2.01774 |
| H | 1.01597 | 1.41602 | -1.72184 |
| H | -0.26754 | 2.63280 | -1.49806 |
| H | 0.02645 | 1.93801 | -3.09219 |
| C | -2.46920 | -1.16179 | 0.43911 |
| C | -2.73471 | -2.13073 | -0.73185 |
| H | -3.50881 | -2.83754 | -0.40204 |
| H | -1.84796 | -2.71812 | -0.99956 |
| H | -3.11960 | -1.62884 | -1.62499 |
| C | -3.73562 | -0.32096 | 0.69989 |
| H | -3.99658 | 0.34277 | -0.13040 |
| H | -3.66647 | 0.27112 | 1.61864 |
| H | -4.57312 | -1.02076 | 0.83246 |
| C | -2.17816 | -2.03118 | 1.68458 |
| H | -1.93748 | -1.45704 | 2.58120 |
| H | -1.37761 | -2.75796 | 1.51042 |
| H | -3.09440 | -2.60131 | 1.89520 |
| S | 0.58461 | -1.40903 | 0.30662 |
| C | 2.97284 | -0.48323 | 1.25758 |
| H | 2.54476 | -0.70734 | 2.23419 |

| | | | |
|---|---|---|---|
| H | -1.64228 | 3.06086 | -0.01867 |
| H | -2.88527 | 2.19569 | 0.91709 |
| C | -1.04268 | 0.92870 | 2.68047 |
| H | -0.82009 | 1.75421 | 3.37138 |
| H | -2.07490 | 0.61838 | 2.87184 |
| H | -0.36457 | 0.10175 | 2.92491 |
| C | -0.67338 | -0.57717 | -2.75929 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 21.53 | 0.09735 | YES YES |
| 8 | a | 54.85 | 0.01945 | YES YES |
| 9 | a | 58.84 | 0.14637 | YES YES |
| 10 | a | 75.13 | 0.30232 | YES YES |
| 11 | a | 89.51 | 0.19200 | YES YES |
| 12 | a | 120.10 | 0.36760 | YES YES |
| 13 | a | 126.63 | 0.15274 | YES YES |
| 14 | a | 129.13 | 0.61882 | YES YES |
| 15 | a | 154.35 | 0.12521 | YES YES |
| 16 | a | 167.11 | 0.04330 | YES YES |
| 17 | a | 174.01 | 0.17680 | YES YES |
| 18 | a | 187.39 | 0.39347 | YES YES |
| 19 | a | 204.79 | 0.76791 | YES YES |
| 20 | a | 209.55 | 0.48077 | YES YES |
| 21 | a | 210.13 | 1.60838 | YES YES |
| 22 | a | 226.18 | 0.66412 | YES YES |
| 23 | a | 237.10 | 0.98945 | YES YES |
| 24 | a | 248.80 | 0.40998 | YES YES |
| 25 | a | 251.71 | 0.15404 | YES YES |
| 26 | a | 258.38 | 0.04659 | YES YES |
| 27 | a | 270.02 | 0.36436 | YES YES |
| 28 | a | 276.58 | 0.24098 | YES YES |
| 29 | a | 280.90 | 0.28662 | YES YES |
| 30 | a | 285.47 | 0.34630 | YES YES |
| 31 | a | 302.63 | 0.06701 | YES YES |
| 32 | a | 316.89 | 0.16190 | YES YES |
| 33 | a | 326.90 | 0.29350 | YES YES |
| 34 | a | 331.82 | 0.18217 | YES YES |
| 35 | a | 340.21 | 0.41493 | YES YES |
| 36 | a | 362.97 | 0.97815 | YES YES |
| 37 | a | 372.21 | 0.50183 | YES YES |
| 38 | a | 379.58 | 0.47184 | YES YES |
| 39 | a | 394.03 | 0.79159 | YES YES |
| 40 | a | 399.06 | 1.58683 | YES YES |
| 41 | a | 404.03 | 0.97618 | YES YES |
| 42 | a | 408.08 | 0.52826 | YES YES |
| 43 | a | 417.18 | 3.85572 | YES YES |
| 44 | a | 453.21 | 11.33154 | YES YES |
| 45 | a | 456.87 | 9.10968 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 46 | a | 483.90 | 8.29296 | YES | YES |
| 47 | a | 507.61 | 7.50584 | YES | YES |
| 48 | a | 547.58 | 23.13008 | YES | YES |
| 49 | a | 572.89 | 7.07769 | YES | YES |
| 50 | a | 582.48 | 14.05892 | YES | YES |

**TS [PhS(PPh3)2]+**

bp86-d3_def2-tzvpp energy (au): -2703.1869807660

Zero point energy (au): 0.6243858
Entropy (kJ mol^-1): 1.08627
Chemical potential (kJ mol^-1): 1425.62

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.74033 | 0.64697 | 3.28823 |
| H | -5.78765 | 0.79659 | 3.54975 |
| C | 2.81639 | 2.37872 | 3.36005 |
| H | 3.89778 | 2.37529 | 3.22552 |
| S | -0.38729 | 0.04069 | -0.38712 |
| P | -0.31247 | 0.06130 | 2.13890 |
| C | 0.81453 | 3.39525 | 4.26449 |
| H | 0.33227 | 4.18396 | 4.84160 |
| C | -4.15675 | 1.41470 | 2.27605 |
| H | -4.74665 | 2.16278 | 1.74696 |
| C | -2.04869 | 0.26110 | 2.62119 |
| C | 2.04981 | 1.36359 | 2.79151 |
| H | 2.53672 | 0.57651 | 2.21480 |
| C | 1.03916 | -4.09825 | 3.60946 |
| H | 1.35301 | -5.08946 | 3.93565 |
| C | 0.65227 | 1.35259 | 2.96717 |
| C | 3.44286 | 1.41153 | -0.56901 |
| H | 3.94324 | 2.36300 | -0.74637 |
| C | -2.81749 | 1.21961 | 1.93647 |
| H | -2.36360 | 1.81367 | 1.14219 |
| C | 0.23645 | -1.54810 | 2.77121 |
| C | 0.16189 | -3.96280 | 2.52786 |
| H | -0.21009 | -4.84706 | 2.01052 |
| C | 0.03854 | 2.37753 | 3.70601 |
| H | -1.04143 | 2.37590 | 3.85133 |
| C | 2.20123 | 3.39849 | 4.09390 |
| H | 2.80291 | 4.19346 | 4.53382 |
| C | -2.64002 | -0.50924 | 3.63559 |
| H | -2.05135 | -1.25789 | 4.16550 |
| C | 1.11105 | -1.68879 | 3.85935 |
| H | 1.47623 | -0.80745 | 4.38556 |
| C | -0.23342 | -2.69496 | 2.10500 |
| H | -0.90634 | -2.58779 | 1.25315 |
| C | 2.15141 | -1.02970 | -0.10878 |
| H | 1.64233 | -1.97710 | 0.05957 |
| C | -3.98252 | -0.31428 | 3.96389 |
| H | -4.43711 | -0.91235 | 4.75333 |
| C | 1.51071 | -2.96226 | 4.27177 |
| H | 2.18859 | -3.06538 | 5.11886 |
| C | 3.54486 | -0.95736 | -0.07336 |
| H | 4.12508 | -1.85726 | 0.12821 |
| C | 2.04779 | 1.35254 | -0.58512 |
| H | 1.45947 | 2.24953 | -0.76920 |
| C | 4.19159 | 0.25984 | -0.30920 |
| H | 5.27987 | 0.31113 | -0.28836 |

| | | | |
|---|---|---|---|
| C | 1.40229 | 0.12874 | -0.36061 |
| C | -4.76234 | -1.06311 | -3.69014 |
| H | -5.80000 | -1.31099 | -3.91219 |
| C | 2.95728 | -2.05854 | -3.88417 |
| H | 4.03420 | -1.89823 | -3.84336 |
| P | -0.38300 | -0.02981 | -2.71796 |
| C | 1.05935 | -3.44200 | -4.47378 |
| H | 0.65436 | -4.35954 | -4.89969 |
| C | -4.08873 | -1.73524 | -2.66597 |
| H | -4.59872 | -2.50595 | -2.08884 |
| C | -2.10109 | -0.42240 | -3.11994 |
| C | 2.09822 | -1.07910 | -3.39096 |
| H | 2.50821 | -0.16393 | -2.96335 |
| C | 0.54136 | 4.12552 | -4.47943 |
| H | 0.75219 | 5.11562 | -4.88279 |
| C | 0.70451 | -1.27561 | -3.44609 |
| C | -2.76199 | -1.41670 | -2.37558 |
| H | -2.23819 | -1.93805 | -1.57415 |
| C | 0.00933 | 1.58307 | -3.44032 |
| C | -0.21862 | 3.99397 | -3.31206 |
| H | -0.60159 | 4.87962 | -2.80559 |
| C | 0.18875 | -2.46451 | -3.98882 |
| H | -0.88817 | -2.62170 | -4.04213 |
| C | 2.44120 | -3.24196 | -4.42257 |
| H | 3.11687 | -4.00651 | -4.80508 |
| C | -2.78130 | 0.25242 | -4.14661 |
| H | -2.27430 | 1.02783 | -4.72026 |
| C | 0.76419 | 1.71712 | -4.61646 |
| H | 1.14084 | 0.83380 | -5.13081 |
| C | -0.48200 | 2.72897 | -2.78958 |
| H | -1.06221 | 2.62448 | -1.87211 |
| C | -4.10903 | -0.07138 | -4.42786 |
| H | -4.63441 | 0.45225 | -5.22589 |
| C | 1.02951 | 2.98885 | -5.12888 |
| H | 1.61655 | 3.08986 | -6.04135 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | a | -34.26 | 0.00000 | YES YES |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | | 0.00 | 0.00000 | - - |
| 8 | a | 5.02 | 0.00117 | YES YES |
| 9 | a | 11.44 | 1.94227 | YES YES |
| 10 | a | 19.96 | 3.06978 | YES YES |
| 11 | a | 21.84 | 3.48264 | YES YES |
| 12 | a | 24.22 | 1.83295 | YES YES |
| 13 | a | 28.46 | 0.40988 | YES YES |
| 14 | a | 37.62 | 5.26687 | YES YES |
| 15 | a | 40.03 | 2.84156 | YES YES |
| 16 | a | 43.15 | 0.05027 | YES YES |
| 17 | a | 45.42 | 3.12490 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 18 | a | 48.29 | 1.95090 | YES | YES |
| 19 | a | 53.10 | 21.60261 | YES | YES |
| 20 | a | 53.20 | 0.44155 | YES | YES |
| 21 | a | 56.72 | 0.23670 | YES | YES |
| 22 | a | 58.80 | 0.18238 | YES | YES |
| 23 | a | 71.87 | 2.93063 | YES | YES |
| 24 | a | 72.20 | 9.01989 | YES | YES |
| 25 | a | 76.51 | 3.42430 | YES | YES |
| 26 | a | 86.95 | 15.05784 | YES | YES |
| 27 | a | 90.84 | 0.00597 | YES | YES |
| 28 | a | 121.97 | 0.93956 | YES | YES |
| 29 | a | 130.88 | 18.65695 | YES | YES |
| 30 | a | 145.04 | 0.72793 | YES | YES |
| 31 | a | 180.95 | 2.49918 | YES | YES |
| 32 | a | 183.82 | 1.38591 | YES | YES |
| 33 | a | 191.85 | 0.87297 | YES | YES |
| 34 | a | 195.84 | 2.89697 | YES | YES |
| 35 | a | 202.69 | 1.71442 | YES | YES |
| 36 | a | 208.70 | 2.60371 | YES | YES |
| 37 | a | 232.45 | 47.12021 | YES | YES |
| 38 | a | 237.50 | 0.28224 | YES | YES |
| 39 | a | 238.14 | 0.19343 | YES | YES |
| 40 | a | 252.39 | 0.20879 | YES | YES |
| 41 | a | 253.76 | 4.81938 | YES | YES |
| 42 | a | 262.67 | 0.67672 | YES | YES |
| 43 | a | 264.20 | 0.47511 | YES | YES |
| 44 | a | 301.62 | 8.33489 | YES | YES |
| 45 | a | 384.84 | 1.08401 | YES | YES |
| 46 | a | 386.91 | 0.19537 | YES | YES |
| 47 | a | 388.56 | 0.41034 | YES | YES |
| 48 | a | 390.22 | 0.81809 | YES | YES |
| 49 | a | 390.38 | 0.21550 | YES | YES |
| 50 | a | 393.39 | 4.04042 | YES | YES |

**TS [PhS(PPh3)(PtBu3)]+**

bp86-d3_def2-tzvpp energy (au): -2481.6904001350

Zero point energy (au): 0.7168680
Entropy (kJ mol^-1): 1.05530
Chemical potential (kJ mol^-1): 1682.58

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.09674 | 0.17592 | 0.02075 |
| S | 0.24253 | 0.02625 | -0.01367 |
| C | 0.16343 | -1.76054 | -0.04991 |
| C | -0.13388 | -2.41867 | -1.25206 |
| H | -0.28448 | -1.83999 | -2.16194 |
| C | -0.23802 | -3.81070 | -1.27274 |
| H | -0.47376 | -4.31979 | -2.20682 |
| C | -0.02820 | -4.54803 | -0.10294 |
| H | -0.09888 | -5.63506 | -0.12444 |
| C | 0.26986 | -3.89034 | 1.09365 |
| H | 0.42485 | -4.46134 | 2.00866 |
| C | 0.35396 | -2.49674 | 1.12619 |
| H | 0.55475 | -1.97700 | 2.06133 |
| C | -2.97948 | -0.77674 | 1.27716 |
| C | -2.97414 | -2.18202 | 1.17801 |
| H | -2.48449 | -2.67205 | 0.33599 |
| C | -3.60119 | -2.94939 | 2.15730 |
| H | -3.59873 | -4.03567 | 2.07241 |
| C | -4.22554 | -2.32953 | 3.24485 |
| H | -4.71197 | -2.93317 | 4.01061 |
| C | -4.22867 | -0.93612 | 3.34797 |
| H | -4.72180 | -0.45063 | 4.18967 |
| C | -3.60963 | -0.15694 | 2.36903 |
| H | -3.62661 | 0.92949 | 2.44886 |
| C | -2.27916 | 1.94383 | 0.35935 |
| C | -3.04693 | 2.78271 | -0.46293 |
| H | -3.59370 | 2.36730 | -1.30903 |
| C | -3.10507 | 4.15206 | -0.19704 |
| H | -3.70261 | 4.80018 | -0.83747 |
| C | -2.40222 | 4.68993 | 0.88448 |
| H | -2.44967 | 5.75968 | 1.08644 |
| C | -1.63876 | 3.85701 | 1.70847 |
| H | -1.09269 | 4.27375 | 2.55441 |
| C | -1.57114 | 2.48886 | 1.44747 |
| H | -0.97358 | 1.84031 | 2.08918 |
| C | -2.83229 | -0.17285 | -1.59558 |
| C | -4.06474 | -0.83111 | -1.73158 |
| H | -4.61836 | -1.14576 | -0.84760 |
| C | -4.58215 | -1.07937 | -3.00471 |
| H | -5.53946 | -1.58988 | -3.10631 |
| C | -3.88081 | -0.67076 | -4.14188 |
| H | -4.28913 | -0.86659 | -5.13294 |
| C | -2.65457 | -0.00993 | -4.00936 |
| H | -2.10715 | 0.31073 | -4.89540 |
| C | -2.12696 | 0.23480 | -2.74271 |

| | | | |
|---|---|---|---|
| H | -1.16544 | 0.73876 | -2.63750 |
| P | 2.77779 | 0.21091 | -0.02648 |
| C | 3.06508 | 1.42631 | -1.49351 |
| C | 4.35557 | 2.25834 | -1.37455 |
| H | 4.47260 | 2.85557 | -2.29219 |
| C | 1.86559 | 2.39487 | -1.63235 |
| H | 2.07385 | 3.06373 | -2.48048 |
| H | 1.69703 | 3.02656 | -0.75693 |
| H | 0.93462 | 1.86021 | -1.85262 |
| C | 3.08573 | 1.12069 | 1.63995 |
| C | 4.57345 | 1.31798 | 1.98582 |
| H | 4.64122 | 1.89162 | 2.92276 |
| H | 5.11385 | 1.88067 | 1.21724 |
| H | 5.09769 | 0.37059 | 2.15093 |
| H | 2.80152 | -0.68375 | 2.90549 |
| H | 1.31507 | 0.24064 | 2.59438 |
| H | 2.54236 | 0.86478 | 3.71458 |
| C | 2.40212 | 2.50387 | 1.61091 |
| H | 1.33976 | 2.44057 | 1.34288 |
| H | 2.89671 | 3.20872 | 0.93496 |
| H | 2.46034 | 2.93187 | 2.62315 |
| C | 3.97648 | -1.29903 | -0.18006 |
| C | 4.01396 | -2.07022 | 1.15449 |
| H | 4.58839 | -2.99484 | 0.99231 |
| H | 3.01156 | -2.36615 | 1.48600 |
| H | 4.51224 | -1.52015 | 1.95899 |
| C | 5.41490 | -0.91101 | -0.56937 |
| H | 5.86953 | -0.20154 | 0.13029 |
| H | 5.47784 | -0.49166 | -1.57911 |
| H | 6.03182 | -1.82276 | -0.56087 |
| C | 3.41115 | -2.28652 | -1.22495 |
| H | 3.30122 | -1.86017 | -2.22491 |
| H | 2.44304 | -2.69167 | -0.91451 |
| H | 4.11285 | -3.13012 | -1.30612 |
| H | 4.31752 | 2.96361 | -0.53650 |
| H | 5.25422 | 1.64395 | -1.26627 |
| C | 3.09989 | 0.61076 | -2.80155 |
| H | 3.10155 | 1.31470 | -3.64718 |
| H | 3.99665 | -0.00971 | -2.89734 |
| H | 2.21220 | -0.02846 | -2.90590 |
| C | 2.39520 | 0.32163 | 2.76887 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | a | -26.71 | 0.00000 | YES YES |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | | 0.00 | 0.00000 | - - |
| 8 | a | 9.32 | 4.00591 | YES YES |
| 9 | a | 14.52 | 4.04686 | YES YES |
| 10 | a | 20.44 | 5.81923 | YES YES |
| 11 | a | 28.11 | 18.03090 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 41.37 | 0.86026 | YES | YES |
| 13 | a | 46.21 | 0.52806 | YES | YES |
| 14 | a | 50.28 | 0.16625 | YES | YES |
| 15 | a | 54.34 | 0.01777 | YES | YES |
| 16 | a | 60.57 | 2.04106 | YES | YES |
| 17 | a | 62.77 | 0.01600 | YES | YES |
| 18 | a | 71.29 | 4.06592 | YES | YES |
| 19 | a | 78.62 | 0.05053 | YES | YES |
| 20 | a | 83.23 | 0.09134 | YES | YES |
| 21 | a | 89.96 | 1.21132 | YES | YES |
| 22 | a | 94.95 | 1.53383 | YES | YES |
| 23 | a | 109.67 | 8.19360 | YES | YES |
| 24 | a | 120.23 | 15.68526 | YES | YES |
| 25 | a | 123.65 | 13.89729 | YES | YES |
| 26 | a | 131.80 | 1.06922 | YES | YES |
| 27 | a | 154.67 | 0.92193 | YES | YES |
| 28 | a | 177.32 | 0.02696 | YES | YES |
| 29 | a | 185.62 | 1.74058 | YES | YES |
| 30 | a | 189.46 | 0.05031 | YES | YES |
| 31 | a | 194.50 | 0.55624 | YES | YES |
| 32 | a | 196.31 | 0.09479 | YES | YES |
| 33 | a | 203.67 | 2.70187 | YES | YES |
| 34 | a | 205.40 | 2.73256 | YES | YES |
| 35 | a | 208.23 | 1.31960 | YES | YES |
| 36 | a | 210.75 | 0.40456 | YES | YES |
| 37 | a | 229.08 | 7.25543 | YES | YES |
| 38 | a | 236.27 | 27.83322 | YES | YES |
| 39 | a | 237.50 | 8.62022 | YES | YES |
| 40 | a | 244.33 | 1.78255 | YES | YES |
| 41 | a | 252.22 | 0.55867 | YES | YES |
| 42 | a | 257.71 | 1.96360 | YES | YES |
| 43 | a | 259.40 | 0.10342 | YES | YES |
| 44 | a | 261.95 | 0.51512 | YES | YES |
| 45 | a | 263.85 | 0.42112 | YES | YES |
| 46 | a | 270.40 | 0.23664 | YES | YES |
| 47 | a | 283.13 | 0.78780 | YES | YES |
| 48 | a | 285.36 | 0.62073 | YES | YES |
| 49 | a | 297.65 | 2.37273 | YES | YES |
| 50 | a | 300.13 | 4.23570 | YES | YES |

**TS [PhSe(PPh3)2]+**

bp86-d3_def2-tzvpp energy (au): -4706.7874395860

Zero point energy (au): 0.6237693
Entropy (kJ mol^-1): 1.11698
Chemical potential (kJ mol^-1): 1417.98

XYZ coordinates:

80

| | | | |
|---|---|---|---|
| C | -4.71792 | 0.65681 | 3.87488 |
| H | -5.75261 | 0.81636 | 4.17731 |
| C | 2.87063 | 2.29910 | 3.58815 |
| H | 3.94863 | 2.25665 | 3.43521 |
| Se | -0.46658 | 0.00183 | -0.00065 |
| P | -0.34892 | 0.01324 | 2.55426 |
| C | 0.91637 | 3.41755 | 4.47649 |
| H | 0.46824 | 4.24666 | 5.02356 |
| C | -4.15561 | 1.44616 | 2.86715 |
| H | -4.74893 | 2.22133 | 2.38296 |
| C | -2.06052 | 0.24458 | 3.10156 |
| C | 2.06555 | 1.27834 | 3.08669 |
| H | 2.52007 | 0.44664 | 2.54820 |
| C | 1.04723 | -4.08537 | 4.14303 |
| H | 1.36985 | -5.06126 | 4.50503 |
| C | 0.67176 | 1.32023 | 3.28489 |
| C | 3.56123 | 1.18676 | -0.28223 |
| H | 4.10081 | 2.10814 | -0.49959 |
| C | -2.83341 | 1.23855 | 2.47384 |
| H | -2.39701 | 1.85100 | 1.68350 |
| C | 0.22632 | -1.57709 | 3.21034 |
| C | 0.20834 | -3.99606 | 3.02709 |
| H | -0.12516 | -4.90065 | 2.51902 |
| C | 0.10105 | 2.39741 | 3.98249 |
| H | -0.97504 | 2.43486 | 4.14895 |
| C | 2.29880 | 3.37172 | 4.28020 |
| H | 2.93146 | 4.16898 | 4.66957 |
| C | -2.62936 | -0.54727 | 4.11187 |
| H | -2.03782 | -1.32354 | 4.59667 |
| C | 1.06187 | -1.67035 | 4.33411 |
| H | 1.39043 | -0.76829 | 4.84910 |
| C | -0.19734 | -2.74787 | 2.55708 |
| H | -0.83907 | -2.67623 | 1.67791 |
| C | 2.16835 | -1.17890 | 0.27299 |
| H | 1.62397 | -2.09919 | 0.47660 |
| C | -3.95579 | -0.33865 | 4.49293 |
| H | -4.39431 | -0.95474 | 5.27756 |
| C | 1.47133 | -2.92402 | 4.79360 |
| H | 2.12055 | -2.99175 | 5.66628 |
| C | 3.56532 | -1.16890 | 0.28267 |
| H | 4.10810 | -2.08837 | 0.50014 |
| C | 2.16423 | 1.19185 | -0.27277 |
| H | 1.61668 | 2.11023 | -0.47646 |
| C | 4.26159 | 0.01014 | 0.00022 |
| H | 5.35128 | 0.01203 | 0.00021 |

| | | | |
|---|---|---|---|
| C | 1.47322 | 0.00523 | -0.00005 |
| C | -4.70893 | -0.67348 | -3.88551 |
| H | -5.74241 | -0.83694 | -4.19000 |
| C | 2.88521 | -2.28823 | -3.57738 |
| H | 3.96314 | -2.23903 | -3.42592 |
| P | -0.34534 | -0.01249 | -2.55576 |
| C | 0.93584 | -3.42371 | -4.45477 |
| H | 0.49146 | -4.25935 | -4.99492 |
| C | -4.14769 | -1.45624 | -2.87207 |
| H | -4.74067 | -2.23017 | -2.38547 |
| C | -2.05475 | -0.25095 | -3.10668 |
| C | 2.07536 | -1.26780 | -3.08294 |
| H | 2.52613 | -0.42981 | -2.55106 |
| C | 1.04302 | 4.08624 | -4.15096 |
| H | 1.36402 | 5.06217 | -4.51427 |
| C | 0.68160 | -1.31841 | -3.27931 |
| C | -2.82705 | -1.24362 | -2.47618 |
| H | -2.39147 | -1.85110 | -1.68160 |
| C | 0.22662 | 1.57784 | -3.21460 |
| C | 0.20415 | 3.99705 | -3.03500 |
| H | -0.13091 | 4.90177 | -2.52821 |
| C | 0.11578 | -2.40400 | -3.96782 |
| H | -0.96028 | -2.44844 | -4.13276 |
| C | 2.31825 | -3.36916 | -4.26046 |
| H | 2.95464 | -4.16607 | -4.64440 |
| C | -2.62257 | 0.53439 | -4.12264 |
| H | -2.03155 | 1.30973 | -4.60959 |
| C | 1.06188 | 1.67099 | -4.33862 |
| H | 1.39221 | 0.76878 | -4.85225 |
| C | -0.19938 | 2.74882 | -2.56326 |
| H | -0.84111 | 2.67733 | -1.68407 |
| C | -3.94732 | 0.32053 | -4.50658 |
| H | -4.38502 | 0.93143 | -5.29571 |
| C | 1.46911 | 2.92472 | -4.79993 |
| H | 2.11815 | 2.99238 | -5.67274 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 6.80 | 0.00140 | YES YES |
| 8 | a | 8.38 | 0.14397 | YES YES |
| 9 | a | 18.37 | 0.00489 | YES YES |
| 10 | a | 22.86 | 0.17980 | YES YES |
| 11 | a | 24.12 | 0.00580 | YES YES |
| 12 | a | 26.35 | 0.03386 | YES YES |
| 13 | a | 36.21 | 0.05980 | YES YES |
| 14 | a | 38.57 | 0.04642 | YES YES |
| 15 | a | 40.49 | 2.69294 | YES YES |
| 16 | a | 44.12 | 0.04001 | YES YES |
| 17 | a | 45.47 | 5.94857 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 18 | a | 49.35 | 1.07067 | YES | YES |
| 19 | a | 52.27 | 0.13267 | YES | YES |
| 20 | a | 56.68 | 0.03063 | YES | YES |
| 21 | a | 58.94 | 0.06732 | YES | YES |
| 22 | a | 59.86 | 21.01239 | YES | YES |
| 23 | a | 73.99 | 0.71143 | YES | YES |
| 24 | a | 74.42 | 0.02286 | YES | YES |
| 25 | a | 80.98 | 21.18293 | YES | YES |
| 26 | a | 88.41 | 0.02124 | YES | YES |
| 27 | a | 93.87 | 92.67092 | YES | YES |
| 28 | a | 104.18 | 0.08326 | YES | YES |
| 29 | a | 115.15 | 0.85976 | YES | YES |
| 30 | a | 124.58 | 0.00863 | YES | YES |
| 31 | a | 182.24 | 3.07461 | YES | YES |
| 32 | a | 183.28 | 0.41482 | YES | YES |
| 33 | a | 193.42 | 0.30174 | YES | YES |
| 34 | a | 195.16 | 4.33762 | YES | YES |
| 35 | a | 202.13 | 0.96938 | YES | YES |
| 36 | a | 203.98 | 2.91840 | YES | YES |
| 37 | a | 216.83 | 11.86863 | YES | YES |
| 38 | a | 236.31 | 8.13653 | YES | YES |
| 39 | a | 237.65 | 0.33825 | YES | YES |
| 40 | a | 238.23 | 0.11816 | YES | YES |
| 41 | a | 252.97 | 0.04650 | YES | YES |
| 42 | a | 253.66 | 1.75207 | YES | YES |
| 43 | a | 263.67 | 0.94740 | YES | YES |
| 44 | a | 264.52 | 0.19541 | YES | YES |
| 45 | a | 304.69 | 0.02299 | YES | YES |
| 46 | a | 388.07 | 0.00468 | YES | YES |
| 47 | a | 388.30 | 0.01998 | YES | YES |
| 48 | a | 388.94 | 0.34892 | YES | YES |
| 49 | a | 389.23 | 1.15322 | YES | YES |
| 50 | a | 390.33 | 0.26921 | YES | YES |

**TS [PhSe(PPh3)(PtBu3)]+**

bp86-d3_def2-tzvpp energy (au): -4485.2910933010

Zero point energy (au): 0.7161251
Entropy (kJ mol^-1): 1.08308
Chemical potential (kJ mol^-1): 1675.68

XYZ coordinates:

86

| | | | |
|---|---|---|---|
| P | -2.05415 | 0.37740 | 0.02778 |
| Se | 0.52828 | 0.22294 | 0.05258 |
| C | 0.28132 | -1.70832 | 0.03135 |
| C | -0.08680 | -2.33105 | -1.16914 |
| H | -0.18903 | -1.74384 | -2.08056 |
| C | -0.34850 | -3.70295 | -1.18687 |
| H | -0.64094 | -4.18189 | -2.12095 |
| C | -0.23475 | -4.45546 | -0.01396 |
| H | -0.43285 | -5.52675 | -0.03190 |
| C | 0.12203 | -3.82936 | 1.18263 |
| H | 0.19324 | -4.40649 | 2.10420 |
| C | 0.36810 | -2.45387 | 1.21138 |
| H | 0.60592 | -1.96583 | 2.15279 |
| C | -2.97782 | -0.54580 | 1.28301 |
| C | -2.95318 | -1.95292 | 1.23054 |
| H | -2.43441 | -2.46345 | 0.41896 |
| C | -3.60292 | -2.69791 | 2.21270 |
| H | -3.58563 | -3.78633 | 2.16083 |
| C | -4.26976 | -2.05307 | 3.25966 |
| H | -4.77457 | -2.63861 | 4.02761 |
| C | -4.29143 | -0.65722 | 3.31777 |
| H | -4.81662 | -0.15133 | 4.12758 |
| C | -3.64943 | 0.09857 | 2.33478 |
| H | -3.67928 | 1.18680 | 2.38099 |
| C | -2.35061 | 2.14869 | 0.28193 |
| C | -3.23020 | 2.88273 | -0.52918 |
| H | -3.77635 | 2.38596 | -1.33074 |
| C | -3.40264 | 4.25041 | -0.30867 |
| H | -4.08710 | 4.81610 | -0.94035 |
| C | -2.70518 | 4.89145 | 0.71905 |
| H | -2.84459 | 5.95889 | 0.88825 |
| C | -1.82814 | 4.16440 | 1.52982 |
| H | -1.28475 | 4.66237 | 2.33257 |
| C | -1.64362 | 2.79919 | 1.31016 |
| H | -0.95583 | 2.23330 | 1.94035 |
| C | -2.73141 | -0.05638 | -1.59921 |
| C | -3.92923 | -0.77003 | -1.75767 |
| H | -4.50307 | -1.07714 | -0.88410 |
| C | -4.38787 | -1.08468 | -3.03901 |
| H | -5.31910 | -1.63848 | -3.15621 |
| C | -3.66277 | -0.68606 | -4.16466 |
| H | -4.02522 | -0.93307 | -5.16219 |
| C | -2.47160 | 0.03175 | -4.01105 |
| H | -1.90575 | 0.34689 | -4.88753 |
| C | -2.00265 | 0.34060 | -2.73517 |

| | | | |
|---|---|---|---|
| H | -1.06666 | 0.88800 | -2.61381 |
| P | 3.11337 | 0.28672 | 0.02248 |
| C | 3.41695 | 1.92766 | -0.93630 |
| C | 4.81910 | 2.52003 | -0.69939 |
| H | 4.93434 | 3.40528 | -1.34329 |
| C | 2.35187 | 2.97884 | -0.54104 |
| H | 2.55900 | 3.89482 | -1.11418 |
| H | 2.36387 | 3.24927 | 0.51650 |
| H | 1.33616 | 2.65917 | -0.80733 |
| C | 3.70401 | 0.47338 | 1.84154 |
| C | 5.22890 | 0.34146 | 2.01183 |
| H | 5.47754 | 0.52840 | 3.06757 |
| H | 5.78731 | 1.06621 | 1.40996 |
| H | 5.59215 | -0.66321 | 1.76997 |
| H | 3.17344 | -1.61893 | 2.38233 |
| H | 1.90826 | -0.41448 | 2.71474 |
| H | 3.35452 | -0.49543 | 3.73654 |
| C | 3.25075 | 1.83697 | 2.40098 |
| H | 2.17036 | 1.99030 | 2.27878 |
| H | 3.78613 | 2.68386 | 1.96045 |
| H | 3.46284 | 1.84579 | 3.48036 |
| C | 4.01765 | -1.17450 | -0.84011 |
| C | 3.99246 | -2.40054 | 0.09555 |
| H | 4.40379 | -3.25628 | -0.45966 |
| H | 2.97179 | -2.66676 | 0.39834 |
| H | 4.61074 | -2.27096 | 0.98970 |
| C | 5.47453 | -0.85769 | -1.22660 |
| H | 6.09183 | -0.56180 | -0.37251 |
| H | 5.54191 | -0.07665 | -1.99194 |
| H | 5.92052 | -1.76789 | -1.65603 |
| C | 3.23684 | -1.57613 | -2.10986 |
| H | 3.25634 | -0.81694 | -2.89422 |
| H | 2.19486 | -1.82248 | -1.88498 |
| H | 3.70723 | -2.48182 | -2.52093 |
| H | 4.96432 | 2.85374 | 0.33363 |
| H | 5.62445 | 1.82324 | -0.95316 |
| C | 3.22624 | 1.67371 | -2.44496 |
| H | 3.23768 | 2.64667 | -2.95787 |
| H | 4.03014 | 1.07139 | -2.88016 |
| H | 2.26153 | 1.19612 | -2.66112 |
| C | 2.99076 | -0.59054 | 2.70266 |

Vibrational Spectrum (first 50 lines):

| # mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|
| # | | cm**(-1) | km/mol | IR RAMAN |
| 1 | | 0.00 | 0.00000 | - - |
| 2 | | 0.00 | 0.00000 | - - |
| 3 | | 0.00 | 0.00000 | - - |
| 4 | | 0.00 | 0.00000 | - - |
| 5 | | 0.00 | 0.00000 | - - |
| 6 | | 0.00 | 0.00000 | - - |
| 7 | a | 12.77 | 0.22862 | YES YES |
| 8 | a | 17.56 | 0.01628 | YES YES |
| 9 | a | 23.12 | 0.21246 | YES YES |
| 10 | a | 25.29 | 0.04940 | YES YES |
| 11 | a | 38.86 | 3.44993 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 12 | a | 43.32 | 0.99128 | YES | YES |
| 13 | a | 49.14 | 0.13523 | YES | YES |
| 14 | a | 51.79 | 1.14285 | YES | YES |
| 15 | a | 56.05 | 3.40172 | YES | YES |
| 16 | a | 58.41 | 15.16789 | YES | YES |
| 17 | a | 62.63 | 12.73542 | YES | YES |
| 18 | a | 74.60 | 38.03646 | YES | YES |
| 19 | a | 75.77 | 7.82661 | YES | YES |
| 20 | a | 82.28 | 7.71881 | YES | YES |
| 21 | a | 95.98 | 4.70397 | YES | YES |
| 22 | a | 96.85 | 6.08149 | YES | YES |
| 23 | a | 101.19 | 0.43045 | YES | YES |
| 24 | a | 109.12 | 15.13092 | YES | YES |
| 25 | a | 119.81 | 0.69045 | YES | YES |
| 26 | a | 127.13 | 0.39734 | YES | YES |
| 27 | a | 129.35 | 0.27312 | YES | YES |
| 28 | a | 168.23 | 0.08527 | YES | YES |
| 29 | a | 183.59 | 1.27666 | YES | YES |
| 30 | a | 190.86 | 0.33805 | YES | YES |
| 31 | a | 194.64 | 1.54493 | YES | YES |
| 32 | a | 197.15 | 1.45328 | YES | YES |
| 33 | a | 198.87 | 0.78720 | YES | YES |
| 34 | a | 203.58 | 0.65771 | YES | YES |
| 35 | a | 205.98 | 1.03552 | YES | YES |
| 36 | a | 213.51 | 0.31509 | YES | YES |
| 37 | a | 221.12 | 16.20360 | YES | YES |
| 38 | a | 230.09 | 0.19483 | YES | YES |
| 39 | a | 235.06 | 4.19109 | YES | YES |
| 40 | a | 237.64 | 0.60445 | YES | YES |
| 41 | a | 240.23 | 0.28904 | YES | YES |
| 42 | a | 251.57 | 0.17797 | YES | YES |
| 43 | a | 254.79 | 0.85947 | YES | YES |
| 44 | a | 255.10 | 0.74505 | YES | YES |
| 45 | a | 258.74 | 0.22333 | YES | YES |
| 46 | a | 263.50 | 0.64780 | YES | YES |
| 47 | a | 271.99 | 0.45760 | YES | YES |
| 48 | a | 276.88 | 0.06061 | YES | YES |
| 49 | a | 280.16 | 0.04109 | YES | YES |
| 50 | a | 288.83 | 1.27723 | YES | YES |

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