

Supporting Material - Revised

Heteropolytopic phosphanylarylthiolato ligands: Formation of *cis* isomers of nickel(II), palladium(II) and platinum(II) complexes with 1-P(Biph)-2-SHC₆H₄ (Biph = 1,1'-biphenyl-2,2'-diyl)

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* deceased in December 2009 – he will be missed

Table 1S. Total and relative calculated energies for phosphanylarylthiolato complexes **1-3**, of their isomers not observed experimentally and of the tetrahedral triplet structures.

| | symm. | Imag. freq. | $\langle S^2 \rangle$ | Total E (a.u.) | Rel. E (kJ mol ⁻¹) | Rel. E (kJ mol ⁻¹) |
|---|-----------------|-------------|-----------------------|----------------|--------------------------------|--------------------------------|
| <i>trans</i> -[Ni{(BiphPS)-κ ² S,P} ₂] | C ₂ | none | 0 | -3033.657306 | 0.0 | 0.0 |
| <i>cis</i> -[Ni{(BiphPS)-κ ² S,P} ₂] (1) | C _{2h} | 16i | 0 | -3033.648820 | 5.3 | 22.3 |
| [Ni{(BiphPS)-κ ² S,P} ₂] tetrahedral | C ₂ | none | 2.02 | -3033.620864 | 22.9 | 95.7 |
| <i>trans</i> -[Pd{((BiphPS)-κ ² S,P) ₂ }] | C ₂ | none | 0 | -2991.085080 | 0.0 | 0.0 |
| <i>cis</i> -[Pd{((BiphPS)-κ ² S,P) ₂] (2) | C _{2h} | 13i | 0 | -2991.073531 | 7.2 | 30.3 |
| [Pd{((BiphPS)-κ ² S,P) ₂] tetrahedral | C ₂ | none | 2.01 | -2991.019921 | 40.9 | 171.1 |
| <i>trans</i> -[Pt{((BiphPS)-κ ² S,P) ₂ }] | C ₂ | none | 0 | -2983.495215 | 0.0 | 0.0 |
| <i>cis</i> -[Pt{((BiphPS)-κ ² S,P) ₂] (3) | C _{2h} | 11i | 0 | -2983.481048 | 8.9 | 37.2 |
| [Pt{((BiphPS)-κ ² S,P) ₂] tetrahedral | C ₂ | none | 2.01 | -2983.413477 | 51.3 | 214.6 |

Cartesian coordinates of the optimized geometries:

cis-[Ni{(BiphPS)- κ^2 S,P}₂]

| | | | |
|----|-------------|-------------|-------------|
| Ni | 0.00000000 | 0.00000000 | 1.76892400 |
| S | 0.13516400 | 1.52990800 | 3.38342600 |
| P | 0.00000000 | 1.62485700 | 0.32404400 |
| S | -0.13516400 | -1.52990800 | 3.38342600 |
| P | 0.00000000 | -1.62485700 | 0.32404400 |
| C | 0.41366300 | 3.06829700 | 2.56313000 |
| C | 0.39193700 | 3.17265100 | 1.16558800 |
| C | -1.57822400 | 1.84903300 | -0.55101800 |
| C | 0.90383600 | 1.60872100 | -1.25167700 |
| C | -0.41366300 | -3.06829700 | 2.56313000 |
| C | -0.39193700 | -3.17265100 | 1.16558800 |
| C | -0.90383600 | -1.60872100 | -1.25167700 |
| C | 1.57822400 | -1.84903300 | -0.55101800 |
| C | 0.65493100 | 4.23579200 | 3.30385300 |
| C | 0.60032200 | 4.39000700 | 0.51584100 |
| C | -2.84477500 | 1.95331200 | 0.00679600 |
| C | -1.38370200 | 1.88422100 | -1.94233600 |
| C | 0.02263600 | 1.74041700 | -2.33977700 |
| C | 2.27324300 | 1.48101200 | -1.44532700 |
| C | -0.65493100 | -4.23579200 | 3.30385300 |
| C | -0.60032200 | -4.39000700 | 0.51584100 |
| C | -2.27324300 | -1.48101200 | -1.44532700 |
| C | -0.02263600 | -1.74041700 | -2.33977700 |
| C | 1.38370200 | -1.88422100 | -1.94233600 |
| C | 2.84477500 | -1.95331200 | 0.00679600 |
| C | 0.86951800 | 5.44289600 | 2.65619300 |
| C | 0.84512900 | 5.53326500 | 1.26178600 |
| C | -3.93923600 | 2.11073800 | -0.84151400 |
| C | -2.48576300 | 2.03484500 | -2.78060700 |
| C | 0.53268600 | 1.71535400 | -3.63624900 |
| C | 2.77307500 | 1.47043000 | -2.74451200 |
| C | -0.86951800 | -5.44289600 | 2.65619300 |
| C | -0.84512900 | -5.53326500 | 1.26178600 |
| C | -2.77307500 | -1.47043000 | -2.74451200 |
| C | -0.53268600 | -1.71535400 | -3.63624900 |
| C | 2.48576300 | -2.03484500 | -2.78060700 |
| C | 3.93923600 | -2.11073800 | -0.84151400 |
| C | -3.75551700 | 2.15173500 | -2.22403000 |
| C | 1.90313000 | 1.57747300 | -3.83005400 |
| C | -1.90313000 | -1.57747300 | -3.83005400 |
| C | 3.75551700 | -2.15173500 | -2.22403000 |
| H | 0.67838700 | 4.17976400 | 4.39010800 |
| H | 0.57115900 | 4.43231100 | -0.57313200 |
| H | -2.96973500 | 1.91080700 | 1.08850800 |
| H | 2.93994300 | 1.37287600 | -0.59063100 |
| H | -0.67838700 | -4.17976400 | 4.39010800 |
| H | -0.57115900 | -4.43231100 | -0.57313200 |
| H | -2.93994300 | -1.37287600 | -0.59063100 |
| H | 2.96973500 | -1.91080700 | 1.08850800 |
| H | 1.06381900 | 6.33499700 | 3.24846800 |
| H | 1.01580800 | 6.48673000 | 0.76879600 |
| H | -4.93925100 | 2.20300500 | -0.42472400 |
| H | -2.35794000 | 2.05485700 | -3.86197000 |
| H | -0.13632800 | 1.79859200 | -4.49152300 |
| H | 3.84175700 | 1.36040600 | -2.91254700 |
| H | -1.06381900 | -6.33499700 | 3.24846800 |
| H | -1.01580800 | -6.48673000 | 0.76879600 |
| H | -3.84175700 | -1.36040600 | -2.91254700 |
| H | 0.13632800 | -1.79859200 | -4.49152300 |
| H | 2.35794000 | -2.05485700 | -3.86197000 |
| H | 4.93925100 | -2.20300500 | -0.42472400 |
| H | -4.61745000 | 2.27294100 | -2.87636600 |
| H | 2.30214100 | 1.55807000 | -4.84193300 |
| H | -2.30214100 | -1.55807000 | -4.84193300 |
| H | 4.61745000 | -2.27294100 | -2.87636600 |

trans-[Ni{(BiphPS)- κ^2 S,P}₂]

| | | | |
|----|-------------|-------------|-------------|
| Ni | 0.00000000 | 0.00000000 | 0.00000000 |
| S | -2.17729500 | 0.42103000 | 0.00000000 |
| P | -0.43833700 | -2.13798500 | 0.00000000 |
| S | 2.17729500 | -0.42103000 | 0.00000000 |
| P | 0.43833700 | 2.13798500 | 0.00000000 |
| C | -2.96429500 | -1.16373300 | 0.00000000 |
| C | -2.23226700 | -2.35879700 | 0.00000000 |
| C | 0.28095000 | -3.18565100 | 1.29494000 |
| C | 0.28095000 | -3.18565100 | -1.29494000 |
| C | 2.96429500 | 1.16373300 | 0.00000000 |
| C | 2.23226700 | 2.35879700 | 0.00000000 |
| C | -0.28095000 | 3.18565100 | -1.29494000 |
| C | -0.28095000 | 3.18565100 | 1.29494000 |
| C | -4.36438100 | -1.24615500 | 0.00000000 |
| C | -2.86802000 | -3.60228500 | 0.00000000 |
| C | 0.17410400 | -3.02540600 | 2.66871400 |
| C | 1.04741800 | -4.22243900 | 0.73476700 |
| C | 1.04741800 | -4.22243900 | -0.73476700 |
| C | 0.17410400 | -3.02540600 | -2.66871400 |
| C | 4.36438100 | 1.24615500 | 0.00000000 |
| C | 2.86802000 | 3.60228500 | 0.00000000 |
| C | -0.17410400 | 3.02540600 | -2.66871400 |
| C | -1.04741800 | 4.22243900 | -0.73476700 |
| C | -1.04741800 | 4.22243900 | 0.73476700 |
| C | -0.17410400 | 3.02540600 | 2.66871400 |
| C | -4.99168000 | -2.48281900 | 0.00000000 |
| C | -4.25318400 | -3.66895300 | 0.00000000 |
| C | 0.82941500 | -3.92616800 | 3.50401800 |
| C | 1.70537000 | -5.11288600 | 1.58030600 |
| C | 1.70537000 | -5.11288600 | -1.58030600 |
| C | 0.82941500 | -3.92616800 | -3.50401800 |
| C | 4.99168000 | 2.48281900 | 0.00000000 |
| C | 4.25318400 | 3.66895300 | 0.00000000 |
| C | -0.82941500 | 3.92616800 | -3.50401800 |
| C | -1.70537000 | 5.11288600 | -1.58030600 |
| C | -1.70537000 | 5.11288600 | 1.58030600 |
| C | -0.82941500 | 3.92616800 | 3.50401800 |
| C | 1.58976200 | -4.96004100 | 2.95821800 |
| C | 1.58976200 | -4.96004100 | -2.95821800 |
| C | -1.58976200 | 4.96004100 | -2.95821800 |
| C | -1.58976200 | 4.96004100 | 2.95821800 |
| H | -4.95016100 | -0.32930800 | 0.00000000 |
| H | -2.26640700 | -4.51152100 | 0.00000000 |
| H | -0.41170400 | -2.20393000 | 3.07931900 |
| H | -0.41170400 | -2.20393000 | -3.07931900 |
| H | 4.95016100 | 0.32930800 | 0.00000000 |
| H | 2.26640700 | 4.51152100 | 0.00000000 |
| H | 0.41170400 | 2.20393000 | -3.07931900 |
| H | 0.41170400 | 2.20393000 | 3.07931900 |
| H | -6.07898800 | -2.52717700 | 0.00000000 |
| H | -4.75751900 | -4.63175400 | 0.00000000 |
| H | 0.75472900 | -3.81986400 | 4.58335900 |
| H | 2.30826200 | -5.92076600 | 1.16915800 |
| H | 2.30826200 | -5.92076600 | -1.16915800 |
| H | 0.75472900 | -3.81986400 | -4.58335900 |
| H | 6.07898800 | 2.52717700 | 0.00000000 |
| H | 4.75751900 | 4.63175400 | 0.00000000 |
| H | -0.75472900 | 3.81986400 | -4.58335900 |
| H | -2.30826200 | 5.92076600 | -1.16915800 |
| H | -2.30826200 | 5.92076600 | 1.16915800 |
| H | -0.75472900 | 3.81986400 | 4.58335900 |
| H | 2.10393300 | -5.65457400 | 3.61863400 |
| H | 2.10393300 | -5.65457400 | -3.61863400 |
| H | -2.10393300 | 5.65457400 | -3.61863400 |
| H | -2.10393300 | 5.65457400 | 3.61863400 |

[Ni{(BiphPS)- κ^2S,P }]₂ tetrahedral

| | | | |
|----|-------------|-------------|-------------|
| Ni | 0.00000000 | 0.00000000 | 1.65397400 |
| S | 0.11888200 | 2.24142200 | 2.01555100 |
| P | -1.70009000 | 0.43191300 | 0.22535800 |
| S | -0.11888200 | -2.24142200 | 2.01555100 |
| P | 1.70009000 | -0.43191300 | 0.22535800 |
| C | -0.41124500 | 2.82476800 | 0.42635500 |
| C | -1.24609900 | 2.06338200 | -0.41840400 |
| C | -3.33235300 | 0.54196400 | 1.00741500 |
| C | -2.35961100 | -0.58932900 | -1.11700700 |
| C | 0.41124500 | -2.82476800 | 0.42635500 |
| C | 1.24609900 | -2.06338200 | -0.41840400 |
| C | 2.35961100 | 0.58932900 | -1.11700700 |
| C | 3.33235300 | -0.54196400 | 1.00741500 |
| C | 0.00000000 | 4.08656100 | -0.02450800 |
| C | -1.65013900 | 2.54920200 | -1.66349500 |
| C | -3.67524300 | 1.21871700 | 2.17022400 |
| C | -4.27752400 | -0.21306400 | 0.29015300 |
| C | -3.72649600 | -0.85817300 | -0.90761100 |
| C | -1.67798600 | -1.14740000 | -2.19234500 |
| C | 0.00000000 | -4.08656100 | -0.02450800 |
| C | 1.65013900 | -2.54920200 | -1.66349500 |
| C | 1.67798600 | 1.14740000 | -2.19234500 |
| C | 3.72649600 | 0.85817300 | -0.90761100 |
| C | 4.27752400 | 0.21306400 | 0.29015300 |
| C | 3.67524300 | -1.21871700 | 2.17022400 |
| C | -0.40008900 | 4.56120800 | -1.26564100 |
| C | -1.22344900 | 3.79829500 | -2.09464400 |
| C | -4.99154900 | 1.15108300 | 2.61956000 |
| C | -5.58816000 | -0.28033400 | 0.75710300 |
| C | -4.40451400 | -1.67998600 | -1.80577500 |
| C | -2.36840100 | -1.96026400 | -3.08659800 |
| C | 0.40008900 | -4.56120800 | -1.26564100 |
| C | 1.22344900 | -3.79829500 | -2.09464400 |
| C | 2.36840100 | 1.96026400 | -3.08659800 |
| C | 4.40451400 | 1.67998600 | -1.80577500 |
| C | 5.58816000 | 0.28033400 | 0.75710300 |
| C | 4.99154900 | -1.15108300 | 2.61956000 |
| C | -5.93682200 | 0.40401700 | 1.91694300 |
| C | -3.72408300 | -2.22109600 | -2.89113800 |
| C | 3.72408300 | 2.22109600 | -2.89113800 |
| C | 5.93682200 | -0.40401700 | 1.91694300 |
| H | 0.64984900 | 4.68410400 | 0.61120900 |
| H | -2.29379200 | 1.93555200 | -2.29379300 |
| H | -2.91840100 | 1.78555100 | 2.71148000 |
| H | -0.60909600 | -0.97628200 | -2.32426700 |
| H | -0.64984900 | -4.68410400 | 0.61120900 |
| H | 2.29379200 | -1.93555200 | -2.29379300 |
| H | 0.60909600 | 0.97628200 | -2.32426700 |
| H | 2.91840100 | -1.78555100 | 2.71148000 |
| H | -0.05833800 | 5.53978600 | -1.59696900 |
| H | -1.53355000 | 4.17871400 | -3.06478900 |
| H | -5.28198300 | 1.67816100 | 3.52504300 |
| H | -6.33602700 | -0.86200100 | 0.22072900 |
| H | -5.46031100 | -1.90055800 | -1.65855600 |
| H | -1.84427800 | -2.40324200 | -3.92995500 |
| H | 0.05833800 | -5.53978600 | -1.59696900 |
| H | 1.53355000 | -4.17871400 | -3.06478900 |
| H | 1.84427800 | 2.40324200 | -3.92995500 |
| H | 5.46031100 | 1.90055800 | -1.65855600 |
| H | 6.33602700 | 0.86200100 | 0.22072900 |
| H | 5.28198300 | -1.67816100 | 3.52504300 |
| H | -6.96018400 | 0.35302200 | 2.28159900 |
| H | -4.25496900 | -2.86330700 | -3.59008900 |
| H | 4.25496900 | 2.86330700 | -3.59008900 |
| H | 6.96018400 | -0.35302200 | 2.28159900 |

***cis*-[Pd{((BiphPS)- κ^2 S,P)}_2]**

| | | | |
|----|-------------|-------------|-------------|
| Pd | 0.00000000 | 0.00000000 | 1.74315300 |
| S | 0.11452300 | 1.69252200 | 3.41159500 |
| P | 0.00000000 | 1.72560500 | 0.22561400 |
| S | -0.11452300 | -1.69252200 | 3.41159500 |
| P | 0.00000000 | -1.72560500 | 0.22561400 |
| C | 0.32777700 | 3.19478900 | 2.50745200 |
| C | 0.31214100 | 3.27203700 | 1.10482600 |
| C | -1.50864400 | 1.91305400 | -0.76602400 |
| C | 1.01507200 | 1.65824900 | -1.27623000 |
| C | -0.32777700 | -3.19478900 | 2.50745200 |
| C | -0.31214100 | -3.27203700 | 1.10482600 |
| C | -1.01507200 | -1.65824900 | -1.27623000 |
| C | 1.50864400 | -1.91305400 | -0.76602400 |
| C | 0.51634500 | 4.39270900 | 3.21951500 |
| C | 0.47710700 | 4.48906800 | 0.43594200 |
| C | -2.80832500 | 2.05514800 | -0.30102300 |
| C | -1.22005400 | 1.87122700 | -2.14044700 |
| C | 0.21290100 | 1.71818400 | -2.43057300 |
| C | 2.39418000 | 1.51775300 | -1.36026700 |
| C | -0.51634500 | -4.39270900 | 3.21951500 |
| C | -0.47710700 | -4.48906800 | 0.43594200 |
| C | -2.39418000 | -1.51775300 | -1.36026700 |
| C | -0.21290100 | -1.71818400 | -2.43057300 |
| C | 1.22005400 | -1.87122700 | -2.14044700 |
| C | 2.80832500 | -2.05514800 | -0.30102300 |
| C | 0.68490800 | 5.59467100 | 2.55248100 |
| C | 0.66811800 | 5.65658600 | 1.15605900 |
| C | -3.84306600 | 2.16817000 | -1.22654700 |
| C | -2.26386000 | 1.97937500 | -3.05686000 |
| C | 0.81739300 | 1.62571500 | -3.68345700 |
| C | 2.98761200 | 1.44154200 | -2.61654400 |
| C | -0.68490800 | -5.59467100 | 2.55248100 |
| C | -0.66811800 | -5.65658600 | 1.15605900 |
| C | -2.98761200 | -1.44154200 | -2.61654400 |
| C | -0.81739300 | -1.62571500 | -3.68345700 |
| C | 2.26386000 | -1.97937500 | -3.05686000 |
| C | 3.84306600 | -2.16817000 | -1.22654700 |
| C | -3.56737900 | 2.13016100 | -2.59329100 |
| C | 2.19962300 | 1.48997500 | -3.76697600 |
| C | -2.19962300 | -1.48997500 | -3.76697600 |
| C | 3.56737900 | -2.13016100 | -2.59329100 |
| H | 0.53332500 | 4.35991800 | 4.30696400 |
| H | 0.45538700 | 4.50991800 | -0.65394400 |
| H | -3.00601500 | 2.07691800 | 0.77041700 |
| H | 2.99567800 | 1.46380700 | -0.45359300 |
| H | -0.53332500 | -4.35991800 | 4.30696400 |
| H | -0.45538700 | -4.50991800 | -0.65394400 |
| H | -2.99567800 | -1.46380700 | -0.45359300 |
| H | 3.00601500 | -2.07691800 | 0.77041700 |
| H | 0.83504800 | 6.50495200 | 3.12969400 |
| H | 0.80308800 | 6.60538100 | 0.64359400 |
| H | -4.86769000 | 2.28818600 | -0.88318500 |
| H | -2.06463100 | 1.94132400 | -4.12700500 |
| H | 0.21339000 | 1.65480200 | -4.58922400 |
| H | 4.06567300 | 1.32825500 | -2.70165800 |
| H | -0.83504800 | -6.50495200 | 3.12969400 |
| H | -0.80308800 | -6.60538100 | 0.64359400 |
| H | -4.06567300 | -1.32825500 | -2.70165800 |
| H | -0.21339000 | -1.65480200 | -4.58922400 |
| H | 2.06463100 | -1.94132400 | -4.12700500 |
| H | 4.86769000 | -2.28818600 | -0.88318500 |
| H | -4.38242300 | 2.21816100 | -3.30833600 |
| H | 2.67249500 | 1.41816300 | -4.74419700 |
| H | -2.67249500 | -1.41816300 | -4.74419700 |
| H | 4.38242300 | -2.21816100 | -3.30833600 |

trans-[Pd{((BiphPS)-κ²S,P)₂}]

| | | | |
|----|-------------|-------------|-------------|
| Pd | 0.00000000 | 0.00000000 | 0.00000000 |
| S | -2.36095800 | 0.26159000 | 0.00000000 |
| P | -0.39683800 | -2.27893200 | 0.00000000 |
| S | 2.36095800 | -0.26159000 | 0.00000000 |
| P | 0.39683800 | 2.27893200 | 0.00000000 |
| C | -2.99560000 | -1.38927100 | 0.00000000 |
| C | -2.18802000 | -2.53750800 | 0.00000000 |
| C | 0.34954800 | -3.30557600 | 1.29492100 |
| C | 0.34954800 | -3.30557600 | -1.29492100 |
| C | 2.99560000 | 1.38927100 | 0.00000000 |
| C | 2.18802000 | 2.53750800 | 0.00000000 |
| C | -0.34954800 | 3.30557600 | -1.29492100 |
| C | -0.34954800 | 3.30557600 | 1.29492100 |
| C | -4.38922000 | -1.57417500 | 0.00000000 |
| C | -2.74510100 | -3.82053500 | 0.00000000 |
| C | 0.22933200 | -3.15591700 | 2.66914500 |
| C | 1.15015500 | -4.31634500 | 0.73458700 |
| C | 1.15015500 | -4.31634500 | -0.73458700 |
| C | 0.22933200 | -3.15591700 | -2.66914500 |
| C | 4.38922000 | 1.57417500 | 0.00000000 |
| C | 2.74510100 | 3.82053500 | 0.00000000 |
| C | -0.22933200 | 3.15591700 | -2.66914500 |
| C | -1.15015500 | 4.31634500 | -0.73458700 |
| C | -1.15015500 | 4.31634500 | 0.73458700 |
| C | -0.22933200 | 3.15591700 | 2.66914500 |
| C | -4.93471000 | -2.84722600 | 0.00000000 |
| C | -4.12035100 | -3.98310900 | 0.00000000 |
| C | 0.90707900 | -4.04032000 | 3.50376100 |
| C | 1.83108000 | -5.18963500 | 1.57986700 |
| C | 1.83108000 | -5.18963500 | -1.57986700 |
| C | 0.90707900 | -4.04032000 | -3.50376100 |
| C | 4.93471000 | 2.84722600 | 0.00000000 |
| C | 4.12035100 | 3.98310900 | 0.00000000 |
| C | -0.90707900 | 4.04032000 | -3.50376100 |
| C | -1.83108000 | 5.18963500 | -1.57986700 |
| C | -1.83108000 | 5.18963500 | 1.57986700 |
| C | -0.90707900 | 4.04032000 | 3.50376100 |
| C | 1.70264400 | -5.04724000 | 2.95771800 |
| C | 1.70264400 | -5.04724000 | -2.95771800 |
| C | -1.70264400 | 5.04724000 | -2.95771800 |
| C | -1.70264400 | 5.04724000 | 2.95771800 |
| H | -5.03528200 | -0.69856200 | 0.00000000 |
| H | -2.08589600 | -4.68912700 | 0.00000000 |
| H | -0.38585800 | -2.35659000 | 3.08011900 |
| H | -0.38585800 | -2.35659000 | -3.08011900 |
| H | 5.03528200 | 0.69856200 | 0.00000000 |
| H | 2.08589600 | 4.68912700 | 0.00000000 |
| H | 0.38585800 | 2.35659000 | -3.08011900 |
| H | 0.38585800 | 2.35659000 | 3.08011900 |
| H | -6.01710400 | -2.96022800 | 0.00000000 |
| H | -4.55869500 | -4.97754100 | 0.00000000 |
| H | 0.82169200 | -3.94249500 | 4.58308200 |
| H | 2.46012300 | -5.97717300 | 1.16855100 |
| H | 2.46012300 | -5.97717300 | -1.16855100 |
| H | 0.82169200 | -3.94249500 | -4.58308200 |
| H | 6.01710400 | 2.96022800 | 0.00000000 |
| H | 4.55869500 | 4.97754100 | 0.00000000 |
| H | -0.82169200 | 3.94249500 | -4.58308200 |
| H | -2.46012300 | 5.97717300 | -1.16855100 |
| H | -2.46012300 | 5.97717300 | 1.16855100 |
| H | -0.82169200 | 3.94249500 | 4.58308200 |
| H | 2.23388900 | -5.72894800 | 3.61791100 |
| H | 2.23388900 | -5.72894800 | -3.61791100 |
| H | -2.23388900 | 5.72894800 | -3.61791100 |
| H | -2.23388900 | 5.72894800 | 3.61791100 |

[Pd{((BiphPS)- κ^2 S,P)}₂] triplet

| | | | |
|----|-------------|-------------|-------------|
| Pd | 0.00000000 | 0.00000000 | 1.64590100 |
| S | 0.45679500 | 2.39515600 | 1.77672800 |
| P | -1.69500200 | 0.74096500 | 0.14582900 |
| S | -0.45679500 | -2.39515600 | 1.77672800 |
| P | 1.69500200 | -0.74096500 | 0.14582900 |
| C | 0.00000000 | 2.89228300 | 0.14459500 |
| C | -0.94747000 | 2.19300200 | -0.63517500 |
| C | -3.24544500 | 1.22589300 | 0.94552200 |
| C | -2.57638000 | -0.23702100 | -1.09169700 |
| C | 0.00000000 | -2.89228300 | 0.14459500 |
| C | 0.94747000 | -2.19300200 | -0.63517500 |
| C | 2.57638000 | 0.23702100 | -1.09169700 |
| C | 3.24544500 | -1.22589300 | 0.94552200 |
| C | 0.59046900 | 4.03525700 | -0.41822500 |
| C | -1.27103400 | 2.61328900 | -1.92883700 |
| C | -3.41597400 | 2.05383400 | 2.04798200 |
| C | -4.33903000 | 0.59774200 | 0.32083400 |
| C | -3.96068500 | -0.23706400 | -0.82542200 |
| C | -2.04339600 | -0.99652400 | -2.12743700 |
| C | -0.59046900 | -4.03525700 | -0.41822500 |
| C | 1.27103400 | -2.61328900 | -1.92883700 |
| C | 2.04339600 | 0.99652400 | -2.12743700 |
| C | 3.96068500 | 0.23706400 | -0.82542200 |
| C | 4.33903000 | -0.59774200 | 0.32083400 |
| C | 3.41597400 | -2.05383400 | 2.04798200 |
| C | 0.26678700 | 4.44516000 | -1.70252100 |
| C | -0.66066400 | 3.73681900 | -2.46946000 |
| C | -4.70453400 | 2.27169200 | 2.52749600 |
| C | -5.62109900 | 0.81551000 | 0.82042700 |
| C | -4.80675400 | -0.99474400 | -1.63194500 |
| C | -2.90187400 | -1.74044600 | -2.93133700 |
| C | -0.26678700 | -4.44516000 | -1.70252100 |
| C | 0.66066400 | -3.73681900 | -2.46946000 |
| C | 2.90187400 | 1.74044600 | -2.93133700 |
| C | 4.80675400 | 0.99474400 | -1.63194500 |
| C | 5.62109900 | -0.81551000 | 0.82042700 |
| C | 4.70453400 | -2.27169200 | 2.52749600 |
| C | -5.79564600 | 1.65202600 | 1.91809200 |
| C | -4.27408000 | -1.73560500 | -2.68220100 |
| C | 4.27408000 | 1.73560500 | -2.68220100 |
| C | 5.79564600 | -1.65202600 | 1.91809200 |
| H | 1.32424300 | 4.58519100 | 0.16712400 |
| H | -2.00348300 | 2.05149600 | -2.50772800 |
| H | -2.54913400 | 2.51485600 | 2.52060200 |
| H | -0.96576800 | -1.03337900 | -2.29340600 |
| H | -1.32424300 | -4.58519100 | 0.16712400 |
| H | 2.00348300 | -2.05149600 | -2.50772800 |
| H | 0.96576800 | 1.03337900 | -2.29340600 |
| H | 2.54913400 | -2.51485600 | 2.52060200 |
| H | 0.75008600 | 5.32735200 | -2.11775000 |
| H | -0.91064900 | 4.06469400 | -3.47539400 |
| H | -4.86014300 | 2.92100700 | 3.38541800 |
| H | -6.48225900 | 0.33794900 | 0.35612900 |
| H | -5.87878500 | -1.00966000 | -1.44352700 |
| H | -2.49717000 | -2.33809200 | -3.74477200 |
| H | -0.75008600 | -5.32735200 | -2.11775000 |
| H | 0.91064900 | -4.06469400 | -3.47539400 |
| H | 2.49717000 | 2.33809200 | -3.74477200 |
| H | 5.87878500 | 1.00966000 | -1.44352700 |
| H | 6.48225900 | -0.33794900 | 0.35612900 |
| H | 4.86014300 | -2.92100700 | 3.38541800 |
| H | -6.79663000 | 1.82144300 | 2.30822000 |
| H | -4.93638800 | -2.32750300 | -3.30986200 |
| H | 4.93638800 | 2.32750300 | -3.30986200 |
| H | 6.79663000 | -1.82144300 | 2.30822000 |

cis-[Pt{((BiphPS)- κ^2 S,P)}₂]

| | | | |
|----|-------------|-------------|-------------|
| Pt | 0.00000000 | 0.00000000 | 1.58961100 |
| S | 0.13001300 | 1.68478500 | 3.27392600 |
| P | 0.00000000 | 1.71359300 | 0.08190500 |
| S | -0.13001300 | -1.68478500 | 3.27392600 |
| P | 0.00000000 | -1.71359300 | 0.08190500 |
| C | 0.35186200 | 3.18358800 | 2.36331600 |
| C | 0.32528400 | 3.25658900 | 0.96096100 |
| C | -1.50127800 | 1.92701000 | -0.91783700 |
| C | 1.02105100 | 1.63312100 | -1.41588400 |
| C | -0.35186200 | -3.18358800 | 2.36331600 |
| C | -0.32528400 | -3.25658900 | 0.96096100 |
| C | -1.02105100 | -1.63312100 | -1.41588400 |
| C | 1.50127800 | -1.92701000 | -0.91783700 |
| C | 0.55993700 | 4.37861000 | 3.07296700 |
| C | 0.49757100 | 4.47164300 | 0.29046600 |
| C | -2.80062400 | 2.08642100 | -0.45856000 |
| C | -1.20554800 | 1.89216400 | -2.29040200 |
| C | 0.22710400 | 1.71684500 | -2.57369600 |
| C | 2.39751800 | 1.46922800 | -1.49158100 |
| C | -0.55993700 | -4.37861000 | 3.07296700 |
| C | -0.49757100 | -4.47164300 | 0.29046600 |
| C | -2.39751800 | -1.46922800 | -1.49158100 |
| C | -0.22710400 | -1.71684500 | -2.57369600 |
| C | 1.20554800 | -1.89216400 | -2.29040200 |
| C | 2.80062400 | -2.08642100 | -0.45856000 |
| C | 0.73655200 | 5.57812600 | 2.40351800 |
| C | 0.70790300 | 5.63787900 | 1.00734900 |
| C | -3.82833700 | 2.22318500 | -1.38877000 |
| C | -2.24199200 | 2.02314300 | -3.21195000 |
| C | 0.83692400 | 1.62113400 | -3.82356400 |
| C | 2.99758000 | 1.39202500 | -2.74490900 |
| C | -0.73655200 | -5.57812600 | 2.40351800 |
| C | -0.70790300 | -5.63787900 | 1.00734900 |
| C | -2.99758000 | -1.39202500 | -2.74490900 |
| C | -0.83692400 | -1.62113400 | -3.82356400 |
| C | 2.24199200 | -2.02314300 | -3.21195000 |
| C | 3.82833700 | -2.22318500 | -1.38877000 |
| C | -3.54561000 | 2.19125500 | -2.75419400 |
| C | 2.21732300 | 1.46214800 | -3.89943000 |
| C | -2.21732300 | -1.46214800 | -3.89943000 |
| C | 3.54561000 | -2.19125500 | -2.75419400 |
| H | 0.58582600 | 4.34614700 | 4.16032500 |
| H | 0.46735100 | 4.49241900 | -0.79922700 |
| H | -3.00313200 | 2.09996200 | 0.61203300 |
| H | 2.98899200 | 1.39040200 | -0.58005300 |
| H | -0.58582600 | -4.34614700 | 4.16032500 |
| H | -0.46735100 | -4.49241900 | -0.79922700 |
| H | -2.98899200 | -1.39040200 | -0.58005300 |
| H | 3.00313200 | -2.09996200 | 0.61203300 |
| H | 0.90252600 | 6.48723900 | 2.97814700 |
| H | 0.84933500 | 6.58426500 | 0.49218000 |
| H | -4.85298700 | 2.35637100 | -1.05033300 |
| H | -2.03741700 | 1.98786100 | -4.28115600 |
| H | 0.23892800 | 1.66444400 | -4.73278100 |
| H | 4.07404300 | 1.26147600 | -2.82480300 |
| H | -0.90252600 | -6.48723900 | 2.97814700 |
| H | -0.84933500 | -6.58426500 | 0.49218000 |
| H | -4.07404300 | -1.26147600 | -2.82480300 |
| H | -0.23892800 | -1.66444400 | -4.73278100 |
| H | 2.03741700 | -1.98786100 | -4.28115600 |
| H | 4.85298700 | -2.35637100 | -1.05033300 |
| H | -4.35511100 | 2.29732200 | -3.47308800 |
| H | 2.69478700 | 1.38831300 | -4.87428900 |
| H | -2.69478700 | -1.38831300 | -4.87428900 |
| H | 4.35511100 | -2.29732200 | -3.47308800 |

trans-[Pt{((BiphPS)- κ^2 S,P)}₂]

| | | | |
|----|-------------|-------------|-------------|
| Pt | 0.00000000 | 0.00000000 | 0.00000000 |
| S | -2.36719000 | 0.26416000 | 0.00000000 |
| P | -0.38855100 | -2.27141100 | 0.00000000 |
| S | 2.36719000 | -0.26416000 | 0.00000000 |
| P | 0.38855100 | 2.27141100 | 0.00000000 |
| C | -2.99277000 | -1.38986900 | 0.00000000 |
| C | -2.17779500 | -2.53300700 | 0.00000000 |
| C | 0.35797400 | -3.29763900 | 1.29560800 |
| C | 0.35797400 | -3.29763900 | -1.29560800 |
| C | 2.99277000 | 1.38986900 | 0.00000000 |
| C | 2.17779500 | 2.53300700 | 0.00000000 |
| C | -0.35797400 | 3.29763900 | -1.29560800 |
| C | -0.35797400 | 3.29763900 | 1.29560800 |
| C | -4.38508900 | -1.58137800 | 0.00000000 |
| C | -2.72947400 | -3.81851300 | 0.00000000 |
| C | 0.24374700 | -3.14238200 | 2.66937400 |
| C | 1.14167200 | -4.32084800 | 0.73493900 |
| C | 1.14167200 | -4.32084800 | -0.73493900 |
| C | 0.24374700 | -3.14238200 | -2.66937400 |
| C | 4.38508900 | 1.58137800 | 0.00000000 |
| C | 2.72947400 | 3.81851300 | 0.00000000 |
| C | -0.24374700 | 3.14238200 | -2.66937400 |
| C | -1.14167200 | 4.32084800 | -0.73493900 |
| C | -1.14167200 | 4.32084800 | 0.73493900 |
| C | -0.24374700 | 3.14238200 | 2.66937400 |
| C | -4.92429400 | -2.85684700 | 0.00000000 |
| C | -4.10360900 | -3.98843800 | 0.00000000 |
| C | 0.91212000 | -4.03398300 | 3.50416300 |
| C | 1.81202200 | -5.20232900 | 1.57997100 |
| C | 1.81202200 | -5.20232900 | -1.57997100 |
| C | 0.91212000 | -4.03398300 | -3.50416300 |
| C | 4.92429400 | 2.85684700 | 0.00000000 |
| C | 4.10360900 | 3.98843800 | 0.00000000 |
| C | -0.91212000 | 4.03398300 | -3.50416300 |
| C | -1.81202200 | 5.20232900 | -1.57997100 |
| C | -1.81202200 | 5.20232900 | 1.57997100 |
| C | -0.91212000 | 4.03398300 | 3.50416300 |
| C | 1.69019000 | -5.05427400 | 2.95797500 |
| C | 1.69019000 | -5.05427400 | -2.95797500 |
| C | -1.69019000 | 5.05427400 | -2.95797500 |
| C | -1.69019000 | 5.05427400 | 2.95797500 |
| H | -5.03529700 | -0.70872300 | 0.00000000 |
| H | -2.06688700 | -4.68452900 | 0.00000000 |
| H | -0.35754000 | -2.33201800 | 3.07903000 |
| H | -0.35754000 | -2.33201800 | -3.07903000 |
| H | 5.03529700 | 0.70872300 | 0.00000000 |
| H | 2.06688700 | 4.68452900 | 0.00000000 |
| H | 0.35754000 | 2.33201800 | -3.07903000 |
| H | 0.35754000 | 2.33201800 | 3.07903000 |
| H | -6.00606900 | -2.97543300 | 0.00000000 |
| H | -4.53657600 | -4.98519800 | 0.00000000 |
| H | 0.83275600 | -3.93159400 | 4.58350700 |
| H | 2.42825700 | -5.99999400 | 1.16880100 |
| H | 2.42825700 | -5.99999400 | -1.16880100 |
| H | 0.83275600 | -3.93159400 | -4.58350700 |
| H | 6.00606900 | 2.97543300 | 0.00000000 |
| H | 4.53657600 | 4.98519800 | 0.00000000 |
| H | -0.83275600 | 3.93159400 | -4.58350700 |
| H | -2.42825700 | 5.99999400 | -1.16880100 |
| H | -2.42825700 | 5.99999400 | 1.16880100 |
| H | -0.83275600 | 3.93159400 | 4.58350700 |
| H | 2.21333100 | -5.74222300 | 3.61819500 |
| H | 2.21333100 | -5.74222300 | -3.61819500 |
| H | -2.21333100 | 5.74222300 | -3.61819500 |
| H | -2.21333100 | 5.74222300 | 3.61819500 |

[Pt{((BiphPS)- κ^2S,P)}₂ triplet

| | | | |
|----|-------------|-------------|-------------|
| Pt | 0.00000000 | 0.00000000 | 1.50567800 |
| S | 2.35552400 | 0.49083900 | 1.71769700 |
| P | 0.00000000 | 1.82970800 | 0.02523200 |
| S | -2.35552400 | -0.49083900 | 1.71769700 |
| P | 0.00000000 | -1.82970800 | 0.02523200 |
| C | 2.67767800 | 1.23096100 | 0.14052100 |
| C | 1.67890300 | 1.84236700 | -0.64656000 |
| C | -0.37154100 | 3.44454300 | 0.75037400 |
| C | -1.22060900 | 2.07649500 | -1.28436500 |
| C | -2.67767800 | -1.23096100 | 0.14052100 |
| C | -1.67890300 | -1.84236700 | -0.64656000 |
| C | 1.22060900 | -2.07649500 | -1.28436500 |
| C | 0.37154100 | -3.44454300 | 0.75037400 |
| C | 3.98644800 | 1.21356700 | -0.36476600 |
| C | 1.98359900 | 2.40887600 | -1.88781900 |
| C | 0.22226600 | 4.04197000 | 1.85503800 |
| C | -1.42432900 | 4.06717400 | 0.05451800 |
| C | -1.91943900 | 3.28390700 | -1.08287100 |
| C | -1.58771900 | 1.20076900 | -2.30070500 |
| C | -3.98644800 | -1.21356700 | -0.36476600 |
| C | -1.98359900 | -2.40887600 | -1.88781900 |
| C | 1.58771900 | -1.20076900 | -2.30070500 |
| C | 1.91943900 | -3.28390700 | -1.08287100 |
| C | 1.42432900 | -4.06717400 | 0.05451800 |
| C | -0.22226600 | -4.04197000 | 1.85503800 |
| C | 4.27946400 | 1.76684600 | -1.60204800 |
| C | 3.28228400 | 2.36652800 | -2.37424900 |
| C | -0.23366000 | 5.29148000 | 2.26470900 |
| C | -1.87778000 | 5.31232000 | 0.48367900 |
| C | -2.97628400 | 3.60861000 | -1.93058200 |
| C | -2.64240600 | 1.53809200 | -3.14240100 |
| C | -4.27946400 | -1.76684600 | -1.60204800 |
| C | -3.28228400 | -2.36652800 | -2.37424900 |
| C | 2.64240600 | -1.53809200 | -3.14240100 |
| C | 2.97628400 | -3.60861000 | -1.93058200 |
| C | 1.87778000 | -5.31232000 | 0.48367900 |
| C | 0.23366000 | -5.29148000 | 2.26470900 |
| C | -1.27809400 | 5.91744800 | 1.58325600 |
| C | -3.32949100 | 2.73742300 | -2.95572900 |
| C | 3.32949100 | -2.73742300 | -2.95572900 |
| C | 1.27809400 | -5.91744800 | 1.58325600 |
| H | 4.76738600 | 0.73748900 | 0.22453000 |
| H | 1.19005000 | 2.87544000 | -2.47153600 |
| H | 1.02615000 | 3.53289400 | 2.38526900 |
| H | -1.07494400 | 0.24791600 | -2.42755700 |
| H | -4.76738600 | -0.73748900 | 0.22453000 |
| H | -1.19005000 | -2.87544000 | -2.47153600 |
| H | 1.07494400 | -0.24791600 | -2.42755700 |
| H | -1.02615000 | -3.53289400 | 2.38526900 |
| H | 5.30061900 | 1.72486400 | -1.97565400 |
| H | 3.51931500 | 2.79962200 | -3.34279500 |
| H | 0.22207800 | 5.77904900 | 3.12297700 |
| H | -2.69191500 | 5.81205000 | -0.03877000 |
| H | -3.52772400 | 4.53638100 | -1.78905700 |
| H | -2.93817800 | 0.85653200 | -3.93628200 |
| H | -5.30061900 | -1.72486400 | -1.97565400 |
| H | -3.51931500 | -2.79962200 | -3.34279500 |
| H | 2.93817800 | -0.85653200 | -3.93628200 |
| H | 3.52772400 | -4.53638100 | -1.78905700 |
| H | 2.69191500 | -5.81205000 | -0.03877000 |
| H | -0.22207800 | -5.77904900 | 3.12297700 |
| H | -1.63038900 | 6.89049800 | 1.91773300 |
| H | -4.15885700 | 2.99103800 | -3.61191900 |
| H | 4.15885700 | -2.99103800 | -3.61191900 |
| H | 1.63038900 | -6.89049800 | 1.91773300 |